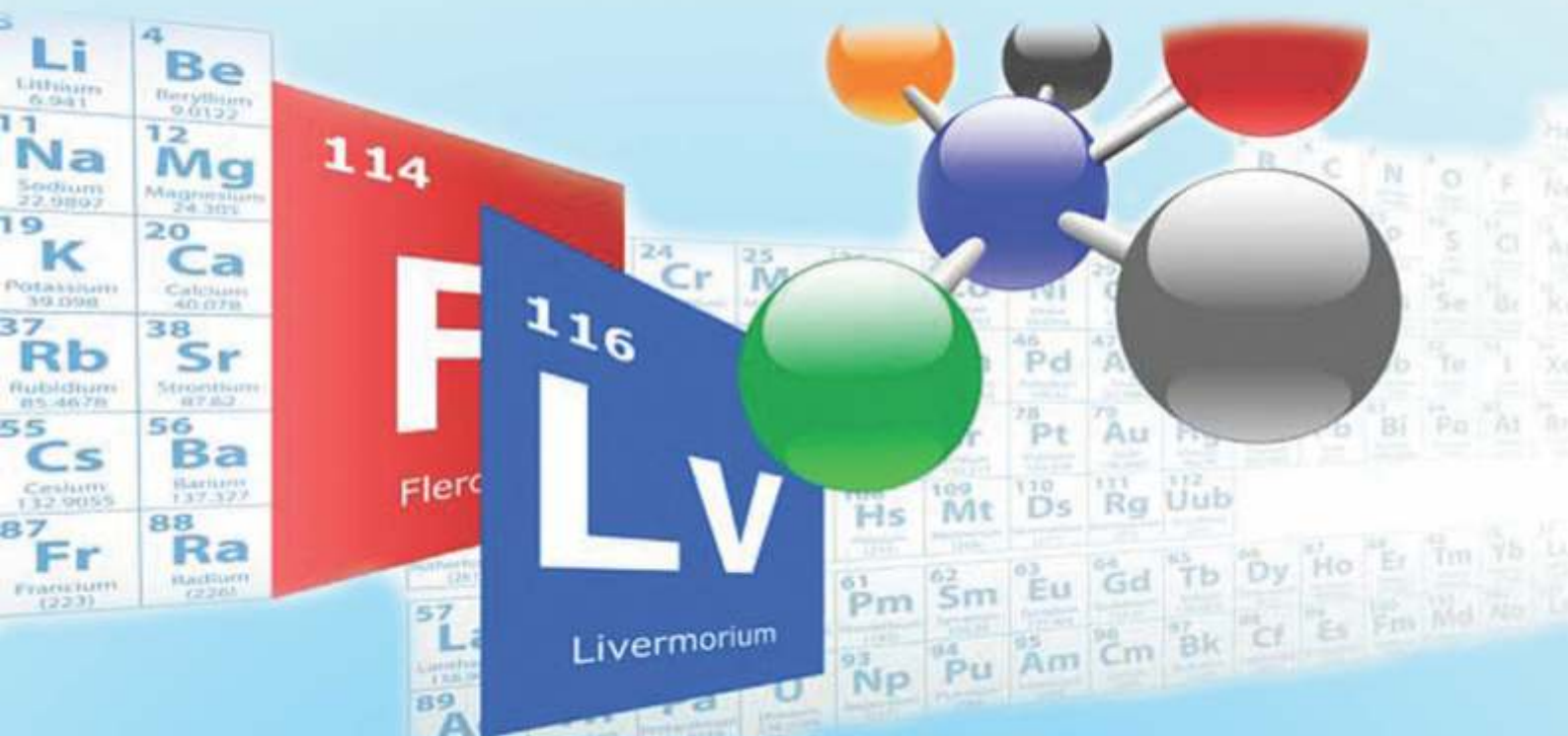


CHEMISTRY

IN SRI LANKA



SEPTEMBER 2012 VOLUME 29 - NO. 3

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



41ST ANNUAL SESSIONS OF THE INSTITUTE OF CHEMISTRY CEYLON



Prof. Tina Overton, Chief Guest lighting the oil lamp.



Prof. S Sotheeswaran delivering the Presidential Address.



Ms. P K V Ranji receives her Kandiah Award for Basic Chemistry certificate



Prof. W S Fernando receives his Distinguished Services Award Medal



winners of the all Island interschool chemistry quiz competition 2011/2012



Cocktail Reception at Adamantane House to welcome all the delegates for the International Conference on Chemical Sciences (ICCS) 2012



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. 29 No. 3

September 2012

	Pages
Council 2012/2013	02
Outline of our Institute	02
Chemistry in Sri Lanka	02
Committees 2012/13	03
Message from the President	04
Guest Editorial	05
International Conference on Chemical Sciences and the 41 st Annual Sessions of the Institute of Chemistry Ceylon	06
Workshop on "The Use of Chemistry for Industrial Revival in Sri Lanka" - Keynote Address <i>Chemistry and Chemical Industry for the Wellbeing of the Society</i>	11
Guest Articles	
<i>A New Delivery Agent for Cancer Therapeutics</i>	16
<i>Chemistry of Natural and Photoswitchable Cyclic Enediynes</i>	17
<i>The Concept of Metal-Drug Synergism in the Search for Novel Chloroquine Derived Antimalarial Drugs</i>	20
International Conference on Chemical Sciences - Chemical Education - Keynote Address <i>Implication of Some Research Findings for Teaching and Learning Chemistry: Language, visualisation and the 'reality'</i>	26
Kandiah Award for Basic Chemistry - 2012 <i>Bioactivity Directed Chemical Investigation of Fungal Extracts: Citriquinones A and B from Penicillium citrinum and Butyrolactone I and (+)-Geodin from Aspergillus terreus</i>	34
Student Corner	
Post Graduate Research in Sri Lanka (a student perspective)	39
Publications of the Institute of Chemistry Ceylon	43
RSC News	44

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Role of Chemistry for Sustainable Agriculture

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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

- directly become **Licentiate**
- 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

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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 2013.

- 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.

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Cover Page

The International Union of Pure and Applied Chemistry (IUPAC) officially approved new names for elements 114 and 116, the latest heavy elements to be added to the periodic table. More information on the elements are on page 4.

Message from the President



It is an honour and a great pleasure to serve as the President of the Institute of Chemistry in the current year 2012/13. Although I live far away from Colombo, it is with your support and full cooperation that I have taken up the position of President of the Institute. During this year, the Institute is growing academically with the largest intake of students to date, as well as physically with the commencement of the construction of the second phase of buildings at Rajagiriya. In addition to the Graduateship programme, the Institute conducts a well established Diploma programme for laboratory technicians. The Institute of Chemistry conducts several other activities to disseminate knowledge in chemistry among school children and teachers. The all island interschool chemistry quiz, seminars, workshops and site visits to chemical industries are examples of some of the other academic activities

conducted by the Institute.

Sri Lanka is predominantly an agricultural country. It is now self sufficient in rice. Rice is our staple food followed by coconut. As with coconut, tea and rubber, rice and its products will be exported in large quantities in the near future. Sri Lanka requires increase crop production and value added product development. This requires substantial knowledge of chemistry and the role of chemists is therefore important. This year's theme is devoted to this aspect of increase crop production and value addition. There will be several seminars on this topic. Chemists can play an efficient and effective role in the economic development of the country through scientific studies in agriculture and plantation crops and product development. In the rubber sector instead of exporting latex, Sri Lanka is now exporting finished products such as good quality tyres. Similarly, value added tea products are exported. Research is underway to produce value added products from coconut. Virgin coconut oil and golden coconut honey are good examples. In the same way, instead of exporting raw rice, value added rice products have to be exported. Therefore, much research needs to be undertaken on value added product development with rice as a raw material.

The broad objective of the Institute can only be achieved by active participation of all concerned. I earnestly request all members to participate in the activities of the Institute to make this year a successful one.

Dr. S. Mohanadas

Bsc (Hons), Ph.D (Adelaide), C.Chem. , F.I.Chem. C

Discovery of two new elements with atomic numbers 114 and 116 Livermorium and Flerovium join the periodic table of elements

The International Union of Pure and Applied Chemistry confirmed the discovery of two elements with atomic numbers 114 and 116 and officially approved the new names of the elements on 31st May 2012. The discoverers proposed the name Flerovium with the symbol **Fl** for the element 114, and Livermorium with the symbol **Lv** for the element 116.

Both elements are man made. They have been first synthesized at the Joint Institute of Nuclear Research in Dubna, Russia in 1998 and 2000. The discoveries were confirmed with further work at Lawrence Livermore National Laboratory in California.

The names honour the laboratories of their creation. Flerovium was chosen for Flerov Laboratory of Nuclear Research in Dubna, Russia, a facility where many super heavy elements have been produced. The laboratory is named after a renowned physicist Georgiy N Flerov. He is the founder of the Joint Institute of Nuclear Research.

Livermorium is chosen to honour Lawrence Livermore Laboratory in California and has been involved in the discovery of six elements with atomic numbers 113,114,115,116,117 and 118. Another element, Lawrencium – element 103 - is already named after the laboratory's founder, Ernest O Lawrence.

The elements, 114 and 116 were created by smashing calcium ions (with 20 protons each) into a curium target (96 protons), combining to form element 116, Livermorium. This element decayed almost immediately into Flerovium with 114 protons. The scientists also created element 114 separately by replacing curium with a plutonium target (94 protons).

Herbal Healthcare Industry

Dr. A.L. Jayewardene

President Elect, Institute of Chemistry Ceylon

“Herbs are staging a comeback and herbal healthcare renaissance is happening as we speak”. It is well accepted today that research efforts in relation to therapies of traditional pharmacopoeias need to be intensified. There are many diseases for which there are no satisfactory therapies although diagnostic procedures exist which can ensure early detection. There is also the more mundane and less altruistic outlook that we are looking at a billion dollar industry. The World Health Organisation (WHO) has always promoted the use of phytotherapy in healthcare efforts, meaning, the use of traditional pharmacopoeias. This is also called phytopharmacy. Phytopharmaceuticals, those chemical entities derived from plants and including whole or partial plant extracts have been shown to be a major factor in the continuing search for new therapeutic agents, and in policies shaping modern disease control mechanisms. A specialized international journal committed to the sciences of Phototherapy and Phytopharmacology called Phytomedicine has recommended a new course of research in the field of Medicinal and Aromatic Plants (MAP) and the herbal products industry. The editorial of the Phytomedicine journal (Vol 16, No 1 of 2009) emphasized the need for standardization of herbal extracts used in pharmacological and clinical investigations among other suggestions. This is a departure from the past, as the western oriented mind-set was sometimes hostile to the concept of extracts as therapeutic agents. Pure chemical entities were deemed necessary as they submitted to easy dosage and quality control. Admittedly, modern analytical tools have made it possible to assess the quality of more complex therapeutic agents which contain several active principles in a single preparation. Most herbal preparations are such complex extracts and it is a challenge to analytical chemists to devise methods for quality control of such preparations to ensure safety, reproducibility, dosage management and adherence to quality standards which may be desired. There is a scientific challenge here to place in the market herbal preparations on par with any other as far as the consumer is concerned by ensuring quality as assessed by their adherence to established standards and specifications/ Editorial Link Natural Products Digest, Vol. 5, issue 1, of 2009. Some of the significant facts

concerning the phytopharmaceutical industry as given in the book of Medicinal Plants, published by the Kerala Agricultural University are;

1. Almost 75% of the world population relies on plants and their extracts for health care.
2. Estimates of annual production of raw material from medicinal and aromatic plants is US\$ 1500 million in 2010 and it is projected to US\$ 5 trillion by 2050.
3. In the US plant based drugs are 25% of total drugs used, while in India and China this contribution is around 80%.
4. While India is still exporting, quality raw materials from medicinal plants it is very likely that with today's rapid depletion of the habitat taking place India herself will stop exports of these valuable resources.

We in Sri Lanka depend a lot on raw materials from India and are liable to be left without many dried raw materials in a few years time. A solution to this looming catastrophe is to grow our own medicinal plant for raw materials, starting today.

An initiative designated, “Saving Plants that Save Lives and Livelihoods” is being promoted by three international organizations, namely, the International Union for the Conservation of Nature (IUCN), the World Wild Life Funds and TRAFFIC which is the Wild Life Trade Monitoring Network. This joint promotion was adopted at the Ninth Conference of Parties of the Convention of Biological Diversity. (See Therapy for Endangered Medicinal Plants, Link Natural Products Digest, Vol.5, Issue 1 of 2009).

As the requirements of herbal drugs around the world keep growing and the competition for the limited supply of raw material increases, it will become imperative for supplies to be grown locally. Our scientists will have a big responsibility to the herbal products industry in ensuring authentic, correctly identified plant materials are produced. Once they become available they also need quality assurance and proper standardization in order to supply to the international markets. I have no doubt that work by Sri Lankan scientists are even now being undertaken will help towards achieving these goals.

INTERNATIONAL CONFERENCE ON CHEMICAL SCIENCES AND THE 41ST ANNUAL SESSIONS OF THE INSTITUTE OF CHEMISTRY CEYLON

THEME: “ROLE OF CHEMISTRY RESEARCH IN NATIONAL DEVELOPMENT”

(Prepared by Dr Buddhie Lankage, Institute of Chemistry Ceylon, Rajagiriya, Sri Lanka)

A three-day 41st Annual Sessions of the Institute of Chemistry Ceylon and the International Conference on the “*Role of Chemistry Research in National Development*” was held at Waters Edge and Sri Lanka Foundation Institute (SLFI), Colombo, Sri Lanka from 20th to 22nd June 2012. A large number of participants, a total of 200, including guests, industrialists, Government officers, students and general public attended the inauguration ceremony held on 20 June. The participants of the international conference on chemical sciences and 41st annual sessions were from all the regions of Sri Lanka representing 38 different institutions of higher education. International participants were from India, Pakistan, Malaysia, Taiwan, Japan, Fiji Islands, Australia, Sudan, Egypt, Nigeria, UK, USA and Canada.

The international conference was sponsored by the international organizations namely, OPCW, Netherlands; IUPAC, USA and the Royal Society of Chemistry UK; National Science Foundation of Sri Lanka, local industries, institutions, past students and members of the Institute of Chemistry Ceylon. The Institute of Chemistry Ceylon greatly appreciates and acknowledges all the sponsors for their financial assistance which enabled us to have a successful International conference and 41st Annual Sessions.

Among the participants there were 46 young scientists who received grants through the IUPAC Programme to cover the cost of conference participation. The National Science Council of Sri Lanka (NSF) also supported the participation of 22 local participants.

The major aim of the conference was to discuss how the chemistry meets the global challenges such as clean air and safe water, healthy food, dependable medicine from plants/natural products and how chemical education imparted to achieve the UN millennium development goals. Consequently, the conference brought together chemists, environmentalists, food scientist, educationists and other scientists from different sectors on a common platform giving them a greater opportunity to exchange ideas, to discuss the role of chemistry research in national development and to foster research collaborations.

Day 1 – Wednesday, June 20th, 2012

The 41st Annual Sessions of the Institute and the International Conference on Chemical Sciences were ceremonially inaugurated at Waters Edge in Colombo on 20th June 2012 by lighting of the traditional oil lamp and playing the national anthem.

The Chief Guest was Prof. Tina Overton, Deputy Head of Department of Physical Sciences, University of Hull, UK and the Guest of Honour was Prof. John

Dyke, University of Southampton, UK.

Prof. Tina Overton kindly accepted our invitation to grace the inaugural ceremony as the Chief Guest and delivered a valuable speech on “*The Role of Chemistry Education Research in Developing Graduates for the 21st Century*” and stated the importance of chemistry in the national development. She mentioned that the chemistry curriculum has to deliver chemistry content but must adopt a pedagogy that delivers transferable skills development (such as team working, problem solving, information refinement, ability to identify and pull out the information from a complex problem and presentation skills) and to make graduates ready for the workplace with the knowledge, skills and attributes that will enable them to succeed in an increasingly competitive and challenging environment. One of her recent research programmes in the UK has identified that the graduates are deficient in the transferable skills and knowledge. The traditional chemistry education provides the students with only an extensive knowledge of chemistry, but they are not prepared to cater to the existing challenging needs. This is due to the cognitive learning practice in chemistry education and to overcome this problem, it is necessary to apply the Cognitive Load Theory (CLT).

Prof. Ramanee Wijesekara, University of Colombo, Sri Lanka, the Master of Ceremonies of the day, agreed with the Prof. Tina Overton's research findings in the UK context. She pointed out that it was very similar to the Sri Lankan chemistry education and it is one of the major current problems in sustainable development.

The Presidential address on “*The Role of Chemistry Research in National Development*” was delivered by Prof. S. Sotheeswaran, President, Institute of Chemistry Ceylon. He highlighted that Sri Lanka should have a hand in hand with high level of chemical education and chemistry research mainly at the postgraduate level in universities, research institutes and industries. In addition, the current political and economic climate in Sri Lanka was conducive to motivate young chemists participating in chemistry research and in national development. He elaborated on how chemistry has influenced in the day to day lives of Sri Lankans and its mutual benefits of national development *via* chemistry research i.e. food, nutrition, metal industries, dye, medicine, cosmetics, agriculture, traditional and non-traditional export crops etc.

One of the piercing facts that came out during the conference was the role of chemical education and chemistry research in national development. To encourage this, the Institute of Chemistry Ceylon gave away numerous awards and prizes at the ceremonial inauguration of the conference to the school students who performed well in the chemistry competitions held

Island-wide. Many other prizes and awards were also given to the students following the Graduateship in Chemistry courses at the College of Chemical Sciences of the Institute of Chemistry Ceylon. To promote research at the postgraduate level, an award by the name of Kandiah Memorial Research Award for basic chemistry was also given to a young researcher of the Open University of Sri Lanka for her work in the area of natural products.

The winner of the Kandiah Research Award for Basic Chemistry, Ms. P. K. V. Ranji, delivered her lecture on “*Bioactivity Directed Chemical Investigation of Fungal Extract : Citriquinones A & B from Penicillium citrinum and Butyrolactone I & (+)-Geodin from Aspergillus terreus*” based on her M.Sc. research work at the Open University of Sri Lanka. Prof S. Sotheeswaran presented her the award.

Novel findings of her research was the isolation of two novel bioactive compounds called “Citriquinones A & B” from the fungus *Penicillium citrinum* and *Aspergillus terreus*, which were isolated from a soil sample and rhizosphere of *Suveda* maritime plant, respectively. Preliminary studies showed that they had promising anticancer activity and this could merit further studies relating to the evaluation of the anticancer properties, which would be more beneficial when considering the anticancer drugs with lesser cytotoxicity. Furthermore this research is a collaboration between Sri Lanka and USA and was an example of exchanging resources among countries for the national development.

In recognition of the yeoman service rendered towards the activities of the Institute of Chemistry Ceylon, in an honorary capacity, a “Distinguished Service Award, 2012” was given to Emeritus Professor W. S. Fernando, formerly at the University of Sri Jayawardenepura, Sri Lanka.

Prizes and certificates were also awarded to the winners of the all Island interschool chemistry quiz competition 2011/2012 which were held in various parts of the country.

The closure of the grand inauguration ceremony was followed by the vote of thanks by Dr. S. Mohanadas, President elect, Institute of Chemistry Ceylon.

Simultaneously, Annual General Meeting (AGM) of the Institute of Chemistry Ceylon and the International conference registration took place at the Water's Edge.

Four plenary lectures were presented during the afternoon sessions on DAY 1 of the Conference. They are summarised below:

- “**Atmospheric Chemistry and Climate Change**” by Prof. John Dyke of University of Southampton, UK – In this talk, the chemistry of troposphere; its relevance to climate change; classical and photochemical smog, acid rain, ozone depletion and global warming were discussed in detail by considering the factors of greenhouse effect, radioactive gases and particles in the atmosphere, radioactive forcing and feedback mechanisms. He explained the evidence for projected changes in atmospheric concentrations

(i.e. long-lived gases and short-lived aerosols) and climate change with an example of the oxidation mechanisms of dimethyl sulfide.

- “**Global Food Trade and Laboratory Accreditation**” by Prof. Upali Samarajeewa of UNIDO based in Sri Lanka – This presentation highlighted the importance of the accredited laboratories for the food trade, their uses, maintenance according to the ISO standards and problems of implementing these at national level in developing countries.
- “**Harnessing Natural Products for National Development: Some Innovative Strategies**” by Prof. A. A. Leslie Gunathilaka of University of Arizona, USA – This lecture highlighted the importance of developing innovative strategies for a sustainable harvesting and utilisation of Natural Product (NP) resources (i.e. novel NPs from conventional resources, large scale production, their uses, potential agricultural and medicinal applications. Recent survey has shown that NPs (i.e. anticancer, anti-effective and all range of drugs) are widely used in the World's pharmaceutical market.
- “**An Outstanding Contribution to Tertiary Chemical Education (over four decades) by the Institute of Chemistry Ceylon**” by Prof. J. N. O. Fernando of Institute of Chemistry Ceylon – This talk was a detailed description of entry of the Institute of Chemistry Ceylon to formal Tertiary Chemical Education in 1973 commencing with the Laboratory Technician Certificate Course (LTCC) programme and later it upgraded to two year Diploma in Laboratory Technology Programme (DLTC) and the Graduateship in Chemistry Programme of the College of Chemical Sciences (CCS). The CCS is the educational arm of the institute which produces an average of over 75 special degree level Graduate Chemists annually. He also said that the Institute was the only place in Sri Lanka, which produces all-rounded chemistry technicians who were capable of being employed in any type of scientific laboratory. The CCS has become a very reliable, dependable and viable alternative path to obtain invaluable professional qualifications in the chemical sciences with maximum speed and at minimal cost over the past three decades for adults, the employed, late developers and school leavers who did not get a chance to enter the national universities to study in the area of science education. He highlighted the significant improvements, achievements and the future plans of the CCS and the Institute for chemical education and research that could cater to the specific interests and/or market demands locally and internationally.

A Cocktail reception was hosted by the College of Chemical Sciences (CCS) at the premises of Adamantane House, Institute of Chemistry Ceylon, Rajagiriya to welcome all the delegates for the International Conference on Chemical Sciences (ICCS) 2012.

Days 2 and 3 – Thursday and Friday, June 21st and 22nd, 2012

Programme for days 2 and 3 consisted of several parallel sessions of Invited and Keynote Lectures and Poster sessions in the areas of Natural Products, Environmental Chemistry, Food Science, New Technological Developments, Miscellaneous and Chemical Education topics. A Chemical Education Workshop was also conducted on Day 2.

Chemical Education

One of the major points discussed during the sessions was that the research in chemical education is given a low value and also under estimated around the world. Only very sluggish actions have been taken to overcome these problems. However, recent researches have shown that the chemical education and chemistry research should progress hand in hand in fostering national development.

Local keynote presentations highlighted that Sri Lanka chemical education has a significant problem in the teaching system in schools, universities and institutions i.e. from primary schools to tertiary education. This problem was mainly due to the poor teaching practices, difficulties in explaining the theories and examples, teachers without proper training and an incorrect understanding of the chemistry theories by the teachers/tutors/lecturers. Another frequently asked question was the reasons for the tuition tradition and no reliance of the school teaching, which was an ambiguous and unanswerable question for everyone.

Prof. John Dyke emphasised that the mathematical skill in chemistry plays a vital role in the development of student-centred learning and teaching programme and it will acquire the confidence to use mathematics throughout their chemistry courses. Due to the heavy work load and the allocation of limited periods, the students have limited time to understand the basic principle, concept or theory and for the problem solving. Also he stated that the grades are the “campus currency” virus that devalue the qualifications and there is a major need of developing transferable skills such as team work, recording and etc. by further referring to the Prof. Tina Overton's research findings at the University of Hull, UK.

The Chemical Education Workshop conducted on Day 2 was titled “Some non-standard ways of developing deep understandings and of assessing understandings of students of chemistry” and was lead by Professor Mei-Hung Chiu of National Taiwan Normal University, Taipei, Taiwan and Professor Bob Bucat of The University of Western Australia, Perth, Australia.

The workshop session was really interesting and fruitful because Prof Mei-Hung and Prof Bob Bucat explained their research findings and understandings in relation to the student psychology. Also this workshop provided the participants with a hands-on and close-up experience with the teaching and learning resources described in the lectures. In teaching, *language, gestures/wordings, visualisation and reality* are the significant facts or the rate determining step of the students to understand a theory/concept or principle.

For example,

Q: what is the shape of water? **A:** water takes the shape of the container

Q: what is the shape of the water molecule? **A:** “V” shaped

It was highlighted that the significant difference between the answers was due to the wording of the question. This was a good brain storming session to understand the student's psychology.

The objective of the workshop was:

- To update the methods of teaching and learning chemistry at the secondary and tertiary levels in Asia.
- To promote a learner-centred curriculum in the B.Sc. programme for chemistry.
- Development of new assessment tools.
- Design and implementation of hands on experience at all levels of chemistry education, using the micro-scale approach whenever feasible.
- Promotion partnerships among universities, industries and governments and also between each of these sectors.
- Creation of international and intra-national networks for real and virtual partnerships for sharing and monitoring innovative practices.
- To facilitate the adoption of innovative schemes in laboratory instructions towards reducing the cost and hazards associated with the laboratory courses.

These sessions were chaired by Prof. J. N. O. Fernando of CCS, Dr. G. Bandarage and Mr. M. R. M. Haniffa of the Open University of Sri Lanka.

Natural Products

Natural products sessions were one of the highly discussed, lively and interesting sessions of the conference which was fuelled by the local & international plenary and invited lectures.

- **“Molecular Approach towards the Treatment of Ulcers and MDR-Infections”** by Prof. M. Iqbal Choudhary of University of Karachi, Pakistan – In his talk, chemistry of enzyme inhibitors i.e. Urease and their role in human and animal health i.e. ulcers, related problems such as Multi Drug Resistance (MDR), underlying philosophy and novel discovery of lead molecules were discussed in detail.
- **“Synthesis of Alkaloids Using a Chiral Auxiliary Cleavable by Metathesis”** by Prof. Claude Spino of Université de Sherbrooke, Canada – This presentation discussed the key steps of introduction of the chiral C–N bond i.e. ring closer metathesis of alkene using Grubbs' 2nd generation catalyst and advances towards the synthesis of highly complex alkaloid daphniphylline.
- **“Oligomeric Proanthocyanidins from Tea leaves – Separation, Structures and Biological Properties”** by Prof. Savitri Kumar of the Institute of Fundamental Studies (IFS), Sri Lanka – In this talk, she discussed the importance of the oligomeric and polymeric proanthocyanidins

(PAs), their importance i.e. potent antioxidant properties-antiviral, antibacterial and antiherpetic activity in the fields of nutrition, health and medicine, their occurrence as an active compounds plants and plant-derived extracts.

In summary, the key note lectures highlighted that every country has its unique natural herbs and plants and that these have been used often in the traditional system of medicines. Furthermore we have to get hold of them to make use of prevention and curing of human & animal diseases, viruses and as well as natural cosmetic applications [e.g. *Osbeckia octandra* (Heen bovitiya)] i.e. vegetable and fruit extracts, plants and herbs. Also these are valuable resources and avenues for further research in natural products. Namely, *Xanthone glycosides* (*Mammea Odorata*), *Anthelmintic* compounds (*Solanum Indicum* (SI) Fruit), *Gmelina arborea* (Et-demata), *Spondias pinnata* (Emberella), *Kokoona zeylanica* (Kokun), *Syzygium caryophyllatum* (Heen-dan), *Alpinia calcarata* Rosc. (Zingiberaceae), *Oryza sativa* L. (Red rice/bran) and etc.

These sessions were chaired by Professors A. A. L. Gunatilaka, Iqbal M. Choudary, Claude Spino, Savitri Kumar, P. Paranagama of University of Kaleniya, Sri Lanka and Dr. V. Thadhani, University of Sri Jayawadanepura, Sri Lanka.

Environmental Chemistry

These sessions were chaired by Profs S. P. Deraniyagala and N. Priyantha, Drs S. Weliwegama and W.A. Wickramasinghe.

An arsenic contamination in the field of agriculture was a huge problem in Sri Lanka during the year 2011 and the discussions have lead to directions for new openings of chemistry research. The majority of the research findings related to the arsenic contaminations and were discussed during these sessions, i.e. chicken eggs and synthetic fertilizer.

Geology, hydro-geology, geomorphology, mineralogy, agriculture and anthropogenic activities have played cumulative role in the development of soil and water salinity. The pollution is by means of high concentrations of heavy metal, dyes and ions-nitrates, phosphates and sulphates in developing countries i.e. Sri Lanka, India and Sudan. Educating the farmers and creating awareness to adopt better farm management practices had been suggested to reduce the problem of soil degradation and water pollution.

Two major highlights of this session were the strong requirement of the treatment of industrial and agricultural waste which are most essential to minimise the massive environmental pollution happening around the world.

Mr. W. Sanjaya and Dr. S. Weliwagamage presented two effective, promising, natural and low-cost effluent treatment methods, which could be used in the treatment of effluents using the methods, his team has developed using Neem Leaves Powder (NLP) and paddy husk charcoal.

Food Science

These sessions were chaired by Prof. Navam Hettiarachchy of the University of Arkansas, USA

Professor Sukumal Wimalasena of the University of Kelaniya and Mr. E. G. Somapala of Institute of Chemistry Ceylon.

The main topics discussed in the session were Food processing industry, Food science for a healthy life, Nutritional benefits such as cardiovascular diseases, diabetes, hyperlipidemia, insulin resistance, antioxidant activity etc. of the fruits, vegetables, plants and herbs unique to the country of origin, i.e. Sri Lanka – palmyrah (palmyrah tuber flour), cereals (soy sauce), range of tea (flavonols and polyphenols), bee honey, avocado and cashew nut oils, green leafy porridge and pomegranate and India – *Colocasia esculenta*. In conclusion it was mentioned that raw fruits, vegetable and herbs exhibited high and effective nutrition values compared to cooked food.

Water pollution is a significant problem as discussed in the environmental section and it shows evidently how the natural cycle has been affected i.e. heavy metal content in sea food. Mr. B. K. K. K. Jinadasa reported qualitative and quantitative analysis of heavy metals and the matters arising from the heavy metal content in sea-food.

New Technological Developments

These sessions were chaired by Dr Channa de Silva of Western Carolina University, USA and Dr. R. Parthipan of CCS.

Biomedical imaging and therapeutic applications, Field of Nanotechnology such as Non-viral nano-carriers for gene delivery and liquid crystals, Value addition to Sri Lankan graphite and cement were the foremost and interesting areas discussed in this section.

Invited lecture on “**Lanthanide-Based Nanomaterials for Biomedical Imaging and Therapy**” by Dr. Channa de Silva discussed the recent developments in synthesis, bio-labelling and bio-imaging of lanthanide-based nano materials as novel nano-biotechnological improvements in nanoscience and therapeutic applications.

Mr. K. Abeygoonaratne of Holcim Lanka Ltd. presented the new technological developments in cement manufacturing and long term benefits including environmental impact of introducing blended cement in Sri Lanka.

Mr. L. D. C. Nayanajith of Industrial Technology Institute, Sri Lanka discussed the importance of value addition to the natural graphite in Sri Lanka. Highlights of his presentation were that Sri Lanka was exporting natural/raw graphite at a very low price and importing products made out of graphite material at a very high price. Some of these products - Graphene and graphite oxide (GO)- are very valuable products and have a huge demand in vast variety of practical applications i.e. electronics.

Miscellaneous Topics

Presentations in this section were listed under several topics and could not be categorized under the above mentioned sections. Areas discussed were organic and inorganic synthesis of heterocycles, complexes and mechanisms; applications of Metal-EDTA titration and characterisation, analytical and determination methods.

Dr. Rajendra Surasani of Dr. Reddy's Laboratories Ltd. in India presented very interesting results demonstrating a highly effective synthesis of N-substituted pyrroles in water as a green solvent catalysed by various resins as a heterogeneous reusable and eco-friendly catalyst. The process is operationally simple, environmental friendly and has excellent yield in short reaction time. Furthermore, catalyst can be recovered conventionally and reused efficiently.

Ms. D. A. S. Gamage from the University of Peradeniya, Sri Lanka demonstrated that paddy husk charcoal coated urea can be used as a slow releasing nitrogen fertilizer which reduces leaching losses of urea. It also helps to reduce the phosphate and potassium leaching, it increases the pH value of the soil to the desired level, contributes to the mitigation of atmospheric & water pollution and that it is eco-friendly and a low-cost fertilizer.

These sessions were chaired by Profs M. D. P. De Costa of University of Colombo, Sri Lanka, M. Thirumala Chary of JNT University College of Engineering, India and Vaidehi Ganesan of Indira Gandhi Centre for Atomic Research, India.

Poster Presentations

Poster presentations were displayed on Days two (21 June) and three (22nd June). There were 26 local and international poster participants. Examiners of the poster sessions were Prof. John Dyke (Guest of Honour) and Prof. Tina Overton (Chief Guest from UK) and Prof. Leslie Gunatilaka, Drs. Channa De Silva and Navam Hettiarachchy from the USA. The authors of the five best poster paper winners were namely: Ms. K. Nagahawatte, Ms. M. Ganesharajah, Mr. Angelo Perera, Mr C. H. Manoratne and Ms W. P. K M. Abeysekera. They were each awarded a cash prize of Rs 5,000. All of them are young scientists from Sri Lanka.

Prizes were sponsored by a past student of the CCS, Prof. Eugene de Silva, currently the Director, Virginia Research Institute, USA.

41st Annual and Conference Dinner

The 41st Annual Dinner was held on 22nd June at Water's Edge and was very well attended. Mr Tilak Karunaratne, a part-sponsor of the dinner, Chairman of the Multiform Chemicals Pvt. Ltd. graced the occasion as the Chief Guest and delivered a short valuable speech emphasizing the importance of chemistry in the national development.

Mr. N. M. S. Hettigedera, Hony Treasurer of the institute and Mr. A. M. Jayasekara, Additional Registrar CCS, organised a grand Cultural Show which was conducted by the Ministry of National Heritage for the guests, invitees and participants. Show consisted of very colourful traditional dances, namely, *Praja Narthanaya*, *Naga Gurulu*, *Yak Thum Padaya*, *Thelme*, *Jana Gayanaya*, *Pathuru Narthanaya*, *Salu Paaliya* and *Wes Dance* songs and music. All foreign and local participants, officials and members of the

institute enjoyed the cultural show very much.

Prof. S. Sotheeswaran, President of the institute, gave the concluding remarks, acknowledging and appreciating everyone's efforts and support for a fruitful international conference and also for the assistance rendered with regard to other activities of the institute during his tenure.

Dr. S. Mohanadas of the University Jaffna was ceremonially inducted as the new President by Prof. S. Sotheeswaran. While presenting the President's Medal, Prof. S. Sotheeswaran received the past president's medal from Dr. S. Mohanadas. Mrs Nirmala Pieris, a university batch mate of Dr. S. Mohanadas read the citation of his career and services. Dr Mohandas addressed the audience and promised to render his services to the institute and also for the national development.

Traditional Sri Lankan souvenirs were presented to the plenary, keynote and invited speakers. Profs S. Sotheeswaran and J. N. O. Fernando were presented with appreciation gifts for their valuable services rendered to the institute.

On 23rd June, twenty five Conference participants joined in a trip to Pinnawala Elephant Orphanage in the Central Province.

Summary

The culmination of the conference was the presentation of the output of the parallel group discussions, wherein the participants evaluated the applicability of the approaches or strategies presented in the lectures. The participants affirmed that visualisation, micro-scale laboratory experiments, low-cost instrumentation, integrated laboratory courses and research methodologies could be implemented in various courses in the B.Sc. Chemistry programs offered by the universities, colleges and institutions in the country.

They expressed an enthusiasm in carrying out the newly learned approaches at the conference and in adopting newly learned technologies to improve the teaching, learning and research in chemistry. Furthermore, creation of collaborations, real & virtual partnerships for sharing & monitoring the national development of chemical education and research such as:

- Assisting in the development of curricula.
- Helping to develop and implement teacher training and preparation programmes.
- Assisting in the establishment of partnerships among universities, industries and governments to reinforce chemistry research.
- Developing successful international conferences to gain expert advices on aspects of chemistry education and research and in
- Helping to identify and approach sources of funding.

were also the outcomes of the conference.

CHEMISTRY AND CHEMICAL INDUSTRY FOR THE WELLBEING OF THE SOCIETY

Professor M D P de Costa

Department of Chemistry, University of Colombo

Chemistry is a broad science because it connects with physics and other natural sciences such as geology and biology. It is also known as the central science. Chemistry deals with the concept of creation of molecules and the manipulation of atoms which leads to the changes in the composition and constitution of molecules at both microscopic and macroscopic scales.

Recognition of Chemistry by the United Nations underscores the pivotal role it played in contributing much to the benefits of mankind. The International Year of Chemistry (IYC) was celebrated worldwide with the support of the International Union of Pure and Applied Chemistry (IUPAC) and the United Nations Educational, Scientific and Cultural Organization (UNESCO). Years 2000 and 2005 gave the same recognition to the Mathematics and Physics, respectively to bring the awareness and appreciation of the importance of these major subjects' fundamental to the humanity's understanding of the world and the universe.

The Institute of Chemistry Ceylon as the professional body of chemists, took the leading role in organizing many events (i.e. CHEMEX 2011 Exhibition & Trade Fair, educational workshops, seminars, interschool chemistry quiz and debate competitions, newspaper articles, radio and television programmes) throughout the year to celebrate IYC 2011 in Sri Lanka in the fields of education, continuous professional development and dissemination of knowledge in chemistry among the general public which are useful in their day to day activities.

IYC 2011 activities brought a huge success to the Institute and the College and also a greater awareness of chemistry and life to the education sector and to the society. As a result, IYC activities continued in year 2012 too for the National development of Sri Lanka.

In science the major highlight of the 20th century was chemical, nuclear and electronic ages. The chemical age is the oldest and it will last forever till the end of the world. Although the impact of the chemical age has been less dramatic than the other two, its consequences have affected our lives more systematically and deeply.

Chemistry affects the living beings in our planet, protecting and preserving the health, ecology, culture and heritage. Chemistry meets the global challenges of world economy, environment (i.e. clean air and safe water), nutritious food, dependable medicine from plants, culture and influence scientific discoveries.

Chemistry and Society

Society consists of groups of people in various living conditions and different age levels. Everyone needs satisfactory standard of living, in other words satisfactory levels of food, clothing, shelter, healthcare, education and recreation.

Society as a whole has undergone tremendous hardships to achieve some of the basic needs in life. Life expectancy and the comfort factor were very poor before the chemical age. Chemists have developed many things for the betterment of life such as,

- Development of new materials and medicine for comfort and good health
- Improvement of food quality and safety
- Development of new methods for harvesting and storage are a few examples.

Chemist plays a major role in the production of many basic needs in the society, research and industry to make the process going on and to monitor the quality and purity.

For continuous national development we have to take steps to increase the public appreciation of chemistry in meeting world's needs, increase the interest of young people in chemistry, generate enthusiasm for the creative future of chemistry. The most important factor here is education. Without education (i.e. either formal, informal or both) we cannot have a satisfactory standard of living.

Chemistry Research and Education in National Development

In Sri Lanka, schools provide the basic education of chemical sciences starting from Ordinary level to Advance Level for the young students. Subsequently, universities, institutions (i.e. CCS) and international affiliated colleges (i.e. American College and Royal Institute, etc.) provide the tertiary education of teaching and training for bright young people in the basic and advanced chemical sciences. These tertiary education sectors in the chemical sciences field provide wide range of opportunities for the students who would like to get qualified in the science field such as biotechnology, agricultural chemistry, chemical engineering, chemical biology, food chemistry, polymer chemistry, nanotechnology etc. Universities and CCS play a vital role in the training of graduates and as partners with the industry in collaborative research and development to make them ready for the workplace with the knowledge, skills and attributes that will enable them to succeed in an increasingly competitive and challenging environment. Currently, there is a significant need of trained chemists for the industry and research institutions in Sri Lanka. The main sources of producing graduate chemists are from national universities and CCS. The CCS has been a great place to the employed and late developers to a preponderance of school leavers, who find this to be very reliable, dependable and viable alternative path to obtain invaluable professional qualifications in the chemical sciences. Also CCS is the only place that conducts a Diploma in laboratory Technology

Programme (DLTC) for producing Chemistry Technicians in Sri Lanka. In addition, the Institute of Chemistry Ceylon is the only professional body that issues membership (Licentiate, Associate, Chartered, and Fellow) to chemists which is recognized by the Royal Society of Chemistry UK.

In Sri Lanka most of the chemistry research has been done at the postgraduate and undergraduate levels in universities (i.e. Universities Colombo, Sri Jayawardenapura and Peradeniya – analytical, food chemistry & polymer chemistry, respectively), research institutes (i.e. ITI - natural products, SLINTECH – nanotechnology & NSF etc.) and in industries (i.e. Nestle & Unilever). Sri Lanka Institute of Nanotechnology (SLINTECH) is one of the outstanding semi government industrial research institute in Sri Lanka which possess excellent collaboration between the private sector and the government, including the facility of world class high technology and instrumentation. They produce excellent international research papers including patents and highly qualified, skilful, talented researchers (i.e. M.Sc. and PhD) to cater to the existing challenging needs for the national development in Sri Lanka.

However, there are more upliftments and methods need to be developed for the human wellbeing and to the wealth of the Nation and individuals. Therefore, it is necessary to develop industrial research to a higher level with the participation of the vividly skilled scientists and chemists to apply their knowledge and skills to enhance the industrial products and to develop new materials out of natural resources in Sri Lanka.

One of the major problems for the national development in Sri Lanka is the country's resources and brain drain to developed countries. As a developing country Sri Lanka has experienced considerable brain drain during the past few decades and has created a vacuum in the development and innovations in the Science and Technology field. A significant number of eminent scientists and technologists have moved out of the country due to many reasons. Sri Lanka needs to realign its efforts to build a strong network to pave the way for the efficient use of science and technology expatriates. Keeping pace with modern advanced technological trends based on local expertise and innovation would be the key to empower chemistry and science graduates to remain in Sri Lanka and as well as to attract young students in to the field of chemistry. In Sri Lanka we are talking about partnerships with the private and industrial sectors. Professionals from different disciplines in the field of chemistry can be absorbed to the national university system as senior lecturers. (grade two). This is very much important for the sustainability of the system and especially in research and development with regard to business education. Promoting and sustaining a globally engaged scientific research community in the country will pave the way to development in the long-term, not only encourage technology transfers but also attract foreign investments as well.

Chemistry & Industry

The possible chemical industries in Sri Lanka

depending on some of the natural recourses of the country are:

- Fertilizers: Urea, Tri Super Phosphate (TSP), Single Super Phosphate (SSP) – Eppawala rock phosphate.
- Value added Food: Coconut, Cocoa, Fruits, Spices – Cinnamon, Nutmeg etc.
- Building materials: Cement, Limestone, Coral
- Metals: Copper, Magnetite
- Cosmetics: Soap, Shampoo, Cream, Essential oils
- Pharmaceuticals: Only formulation is done in Sri Lanka
- Gases: Paranthan chemical industry, i.e. gases of Cl_2 , H_2 and NH_3

Sri Lankan economy has been dependent on agriculture, and fertilizers are one of the key materials for plantation industry. Therefore, the Eppawala rock phosphate is a channel to a massive source of industry in Sri Lanka. This is an interesting development in the fertiliser research and for the entire agriculture sector. Sri Lanka produced urea from naphtha (Urea process: reaction between CO_2 from naphtha and NH_3 from the Paranthan chemical industry) a by-product of petroleum purification during early 1970's. This Urea production plant was closed down due to many reasons.

Gases such as CO_2 , Cl_2 , H_2 and NH_3 are by products of chemical industry (i.e. Paranthan chemical industry and petroleum industry) and are important source of material for a further industrial usage such as production of urea, carbonated drinks and bleaching products.

Most of the products used in Sri Lankan are made out of raw materials from the environment. These natural sources are obtained from land, ocean, atmosphere and plants. Land consists of different types of rocks, minerals and soils. Soils are formed by weathering of rocks and minerals. Rocks and soils are very valuable resources for many industries in Sri Lanka.

- Following table is a summary of a few important resources and raw material found in the land of Sri Lanka.

Area	Resources
Kankasanturai	Limestone/ Coral
Jaffna	Limestone
Pulmudai	Mineral Sand/Coral, e.g. ilmenite – TiO , FeO
Talawa	Graphite
Seruwila	Copper / Magnetite
Elahara	Dolomite/Quartz/Feldspar
Marawila	Silica sand
Bogala	Graphite
Kochchikade	Clay
Ragala	Dolomite/Quartz
Ratnapura	Gems/Mica/Quartz
Meetiyyagoda	Kaolin/Coral/Quartz/Dolomite
Matale & Badulla	Feldspar
Eppawala	Rock Phosphate
Boralasgamuwa	Clay
Hambantota	Mineral sands/Dolomite/Quartz

- Sri Lanka is surrounded by the sea which is a major source of many resources such as Sea water - Salts: Sea water salinity is ~3.5% and it

consists of various types of salts that are essential resources for many industries i.e. domestic salt and other salts (MgCl_2 , MgSO_4 , CaSO_4 , K_2SO_4 etc.).

Coastal Sand: Ilmenite, rutile, zircon, garnet, monazite, silmenite.

Minerals: Valuable minerals from the sea i.e. Cu, Ni, Mn etc.

- Resource materials that are found in the troposphere are Nitrogen, Oxygen, Hydrogen and other gasses

Two major salt production plants are Hambantota and Kankasanthurai. Kankasanthurai was the largest plant and it was closed down due to the conflict problems in the country, at present respective authorities have taken action to reopen the plant.

Plants are a good source of raw materials for various industries, namely

Name of the plant	Material of the Plant material	Industry& Production
Jack, Teak, Nadun, Halmilla, Buruta	Mature trunks	Timber
Coconut	Husk of fruit	Fiber (coir)
Jute, Pineapple, Banana	Mature Leaves	Fiber
Rubber	Latex	Latex industry
Coconut, Palm	Oil	Soap, Food
Pine	Bark	Paper making industry
Turpentine	Stem/bark	Turpentine industry
Acasia (Kihiri)	Bark (exudates)	Gum, Filler , Glue
Mango, Pineapple, Citrus, Papaya	Fruit	Cordial and Food
Cinnamon	Leaves, Bark	Cinnamon oil

History of Industries in Sri Lanka

The enactment of the State Industrial Corporations Act of 1957 provided for the reconstitution of existing state enterprises as well as the establishment of new corporations to promote the development of large-scale and basic industries. The period 1958 to 1963 witnessed the first phase in the rapid growth of state industrial corporations. By 1963 fourteen such corporations were engaged in such fields as textiles, cement, sugar, paper, chemicals, edible oils and fats, ceramics, mineral sands, plywood and leather. By 1974 there were twenty-five state corporations, including such major undertakings as a steel mill and an oil refinery. Despite the 1977 policy shift in favour of the private sector, in early 1988 government-controlled enterprises continued to play a major role in industry. State-owned corporations accounted for nearly 60% of total industrial output. The most important public company was the Ceylon Petroleum Corporation, which accounted for about 55% of all public-sector production.

Failure of Industries in Sri Lanka

Public sector enterprises were associated with objectives that reflected both growth and welfare considerations for the economy. They became the chief instruments furthering state ownership and social control in the economy and they were expected to promote capital formation and long-term development. Most government owned large scale industries were in trouble due to

- management inefficiency
- technical deficiencies in planning
- overstaffing: chiefly as a major sources of employment
- defective pricing policies: providing goods services

to the public at relatively low prices

- poor chemical and hazardous waste management
- environment pollution and health problems at relevant areas

As a result, a number of the state industrial corporations have lost money. In 1987 the debts of state-owned corporations were Rs. 19 billion, of which Rs. 15 billion owed to foreign sources and Rs. 4 billion to the two state-owned banks.

National Milk Board was dissolved in 1986. It was established in 1953, but had never succeeded in developing the milk industry. In 1987 it was reported that consideration has been given to transfer to private control several state-run industrial enterprises. These included the four government textile mills, the State Distilleries Corporation, the National Paper Corporation, the Mineral Sands Corporation, Paranthan Chemicals, Sri Lanka Tyre and Union Motors.

A few other major reasons for the failure of Sri Lankan Industries were lack of security in the country because of the 30 years lengthy war, safety of the industries & their damage to the environment (chemical and hazardous waste management) and lack of knowledge of the public.

At present most of the chemical industries have closed down in Sri Lanka, such as

- Sulfuric acid plant
- Paranthan chemical Industry
- Kankasanthurai salt Industry
- Ceramics Industry
- Paper Industry
- Textile Industry
- Tyre Industry

Possible Future Chemical Industries in Sri Lanka

Identifying the feasible chemical industries in Sri Lanka is one of the major problems due to lack of technology, skilled personnel, lack of funding and other pertinent facilities, lack of knowledge of the public and meagre support from the government authorities etc. Role of a chemist is very significant in such situations and there are several factors that need to be considered, i.e.

- National needs
- Availability of raw materials and their maximum, effective and productive usage
- Technology
- Usage of side products, minimise the wastage and recycling
- Effluent treatment and environmental pollution

Chemistry & Industrial Research

Industrial research is the key for the development of the economy of a country. Therefore, the new products that were produced as a solution for the existing problematic products are found to initiate for a more comfortable life.

Most of the countries have productive and collaborative research for national development which Sri Lanka needs improvement on.

Without research in the field of chemistry and chemical engineering there would be fewer improvements in the quality of life. Unfortunately, the communication between universities and industries is very much poor in Sri Lanka. The rules and regulations of national universities and private sector industries have significantly affected the development of such collaborative research. Government dependent research institutions play a bigger role in industrial research. However, collaborations and sustainability from the universities are lacking due to various reasons.

At present, only university students carry out their industrial training with such research institutions and private sector industries. Most of the Industrial research and development is carried out on a small scale and may be due to the small market in Sri Lanka. However, our industries must target the world market and only quality products can reach that level i.e. Japan, Korea and Singapore.

Therefore, continuous research and development must be carried out by the Industries in Sri Lanka to achieve such high standards. Chemistry laboratories in universities and research institutes need adequate provision of instruments through local and national facilitation. They also need modern laboratories, equipped with modern safety standards, confirming 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. Universities can provide well-informed human resources. This will definitely enhance the effective use of higher education in Chemistry among the university students.

Chemists and scientists from universities and private sector should focus their attention on encouraging research that is industry-oriented to deliver innovative products and processes that will

definitely provide a competitive edge to the industry, enabling them to compete and harness opportunities in the global market. There should be a forum to create opportunities for scientists and entrepreneurs to discuss, deliberate and draw road-maps for research, alliances and industrial successes. Unfortunately this is lacking in Sri Lanka.

Industry and Chemical Engineers

Chemical engineers play a vital role in Industry. Unfortunately, the Departments of Chemical & Process Engineering of Universities of Moratuwa and Peradeniya are the only places that produce chemical & process engineers in Sri Lanka. However, majority of them leave the country to work in other affluent countries or some of them join careers in the business and management sectors. This is due to the unawareness of the chemical & process knowledge among the entrepreneurs and citizens of Sri Lanka.

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. Chemical engineers are trained to develop methods to scale up to industrial levels. It is an important indicator of how efficiently chemical feedstock and other reaction inputs can be utilized in a reaction step. Efficient use of chemical feed stocks inevitably increases the cost effectiveness of a reaction or synthetic pathway. 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 feed stocks 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 of 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, travelling 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. Chemists are expected to fulfil 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 i.e. genetically modified and nano-scale materials.

Hazardous chemicals are defined as those that produce severe health or environmental effects, observable within a short period of time. Unfortunately, to exacerbate the situation, developing countries do not have poison-control centres. This, together with the danger that those using chemicals may lack the knowledge, equipment and ability to use the products safely, creates a difficult situation. Many countries are faced with the hazardous problem of the disposal of used and unused chemicals which find their way to illegal dumps or are stored under unsafe conditions and have the potential to pollute the environment, soil or water in the vicinity.

Problems which can be identified as chemical hazard communication in industrial production sector in Sri Lanka

- Absence of a proper classification and definition of hazardous chemicals.
- Absence of a proper training system for chemical hazard communication in the industrial sector.

- Only accidents resulting in death or incapacitation are reported and these accidents are not classified into types (e.g. chemical related).
- There are no industrial associations dealing with chemical hazard communication.
- There is a lack of research work on chemical hazard communication in the industrial production sector, although there is work on laboratory safety.

Role of Chemist for the Better Future of Society:

Future chemists have a challenging role to 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 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.

Future of the Chemical Industries:

Safety and security are the most important factors to be considered in the development of the chemical industries in future. Chemistry education of the school students and the society should become the key factor to achieve the safety and security of the country and the public. A governing body should be established to supervise the safety and security in the chemical Industries and laboratories with high technology and instrumentation.

The aims and objective of the work shop was to increase the public awareness and the appreciation of chemistry in meeting world's needs, increase the interest of young people in chemistry and generate enthusiasm for the creative future of chemistry.

Graduate Chemists Welfare Fund

This fund has been established with effect from 1-1-2012. The principal benefits towards CCS Graduate Chemists would be,

- a) To provide partial assistance towards international travel of those proceeding abroad for PG degrees (once a life time)
- b) To provide partial assistance towards registration fees in respect of IChemC/CCS events such as International Conferences (Preference for those presenting papers)
- c) To provide assistance towards registration fees for IChemC/CCS training seminars etc.
- d) To provide partial assistance towards activities of the Alumni Association.

Note: Depending on the demand, Graduate Chemists who maintain positive content and participate in IChemC/Alumni activities will get preference for the above mentioned benefits.

A New Delivery Agent for Cancer Therapeutics

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With almost 13 million new cases and 7.6 million deaths each year, cancer is a leading cause of death worldwide. In Sri Lanka, the National Cancer Institute, Maharagama admitted a total of 1,11,377 patients during the three years 2006 – 2008. Of these, 10275 were new cases admitted for the first time in 2007 alone¹. All of them depend on cancer drugs (chemotherapy) or radiation therapy/surgery in combination with chemotherapy for recovery from this disease. Cancer drugs are toxic not only to cancer cells, but can also affect normal cells. Hence a growing demand for novel approaches for the effective and targeted delivery of therapeutics is necessary. Many delivery systems have been developed for the delivery of drugs, but the success of these systems has not been promising in clinical applications.

The most common examples of nanotechnology platforms for cancer therapy include polymeric nanoparticles, liposomes, dendrimers, and superparamagnetic nanoparticles². For an ideal delivery system, the carrier should be biocompatible, biodegradable, small in size (nano range), have prolonged circulation time, optimum loading capacity of drug and preferably specific targeting ability. Polymeric nanoparticles (ranging from chitosan, a natural biodegradable polymer to inorganic polymers based on silicon) are one of the most extensively investigated delivery agents. Some of these nano-sized therapeutic medicines are now in routine clinical administration. Successful applications have used both naturally occurring polymers, such as chitosan and albumin and synthetic polymers like poly(lactic acid) (PLA) and poly(lactic co-glycolic acid). Synthetic polymers in the form of polymer micelles (polymerosomes), block copolymers and polymer drug conjugates are in clinical trials with some already in the market. The covalent conjugation of synthetic polymers, particularly poly(ethyleneglycol) (PEG), to protein drugs increases their therapeutic index. The PEGylated enzyme L-asparaginase is marketed as Oncaspar for the treatment of acute lympho blastic leukemia. Albumin-entrapped paclitaxel³ is an example of a natural protein-drug complex in clinical use marketed under the name Abraxane for the treatment of metastatic breast cancer.

Lipid-based carriers have emerged as another widely investigated versatile carrier system for targeted delivery. Lipids in the form of liposomes, solid lipid nanoparticles (SLN) and nanostructured lipids (NSL) have been investigated extensively, and many lipid-based formulations are in clinical use. The first clinically approved liposomal drug formulation, DOXIL, is a treatment for breast cancer, advanced ovarian cancer, multiple myeloma and AIDS-related Kaposi's sarcoma⁴. Others now in use are Marqib-Vincristine sulphate liposome injection⁵; DuanoXome, a duanorubicin citrate liposome injection⁶; and DepoCyt, a liposomal cytarabine

formulation⁷. The use of lipid carriers for drug delivery has been extensively reviewed⁸. Chemical modifications to the lipid carrier through linking tumor-targeting agents (*e.g.* antibody fragments or small molecules) to the lipid enables tumor-targeting and reducing side effects due to toxicity to normal cells (see fig.1).

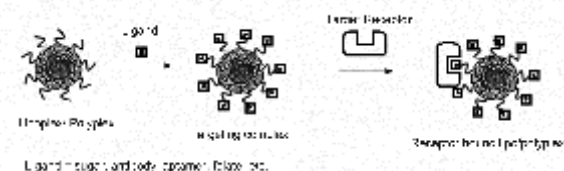


Fig. 1 Linking of a targeting ligand to a carrier (lipid or polymer) to bind to a specific receptor site on a cell. (Adopted from Jafari et al., 2012)⁹

A hitherto untested but promising platform for delivery of both nucleic acids and drugs for cancer therapy has emerged in the form of short peptides with the ability to carry drugs and nucleic acids efficiently. Reports on the ability of peptides to carry drugs or genes have emerged from several research laboratories^{10,11}. Peptides are able to self-assemble through non-covalent interactions such as ionic bond formation, hydrophobic interactions, hydrogen bonding and π -stacking¹² a feature exploited in complexing the drug/nucleic acid with the peptide. Fung et al.¹³ found that the hydrophobic anticancer drug Ellipticine is stabilized by a short peptide in an aqueous solution thereby increasing both the solubility of the drug and its efficacy.

Peptides rich in positively charged amino acids *e.g.* cationic peptides, protein-derived cell penetrating peptides (CPPs), designed amphiphilic peptides, cell targeting peptides (CTP), endosomolytic peptides and nuclear localization peptides have the ability to form complexes with negatively charged nucleic acids. The small size of the complex enables the peptides to condense NAs into compact nanoparticles. Depending on the nature of the peptide, functions such as targeting cells or tissue-specific receptors, penetrating the cell membrane or inducing endosomal escape is possible. A good example is the polypeptide reported by Lee et al., 2001, in which the polypeptide-based targeted gene delivery system consisted of (i) a cationic peptide for DNA condensation, (ii) a ligand peptide for epidermal growth factor receptor (EGFR) recognition, and (iii) an endosome-releasing peptide for endosomolysis¹⁴.

A suitable peptide for drug or nucleic acid complexation may be designed by exploring proteins with ability to penetrate a membrane. By selecting the relevant peptide sequences like Tat and Penetratin, from cell penetrating proteins, successful delivery of oligonucleotides, plasmid, and proteins have been possible. Penetratin is a 16-mer peptide, derived from

a membrane transduction protein. Its α -helical secondary structure interacts with the endosomal membrane and eventually causes membrane disruption and pore formation which helps to deliver its cargo.

Other methods for designing peptide carriers utilize the incorporation of both hydrophilic and hydrophobic moieties in the peptide. The hydrophilic domain can interact with hydrophilic drugs, genes, and the hydrophilic heads of the lipid bilayer; while, the hydrophobic domain is anchored in the hydrophobic core of the bilayer, mediating the translocation of peptide-cargo complex to the cytosol.

Use of peptide carriers for drug or gene delivery is still in its infancy. The success of any delivery system lies in several factors such as the stability, ability to release the cargo at the desired site and ability to protect the drug from the outside environment. In the case of peptides, action of proteolytic enzymes on the peptide, effects of salt concentration in the blood on destabilizing the complex and strength of the interaction between the peptide and cargo for effective release need to be established. Thus the fight against cancer is a continuing battle and a challenge unto scientists striving in the search for new discoveries.

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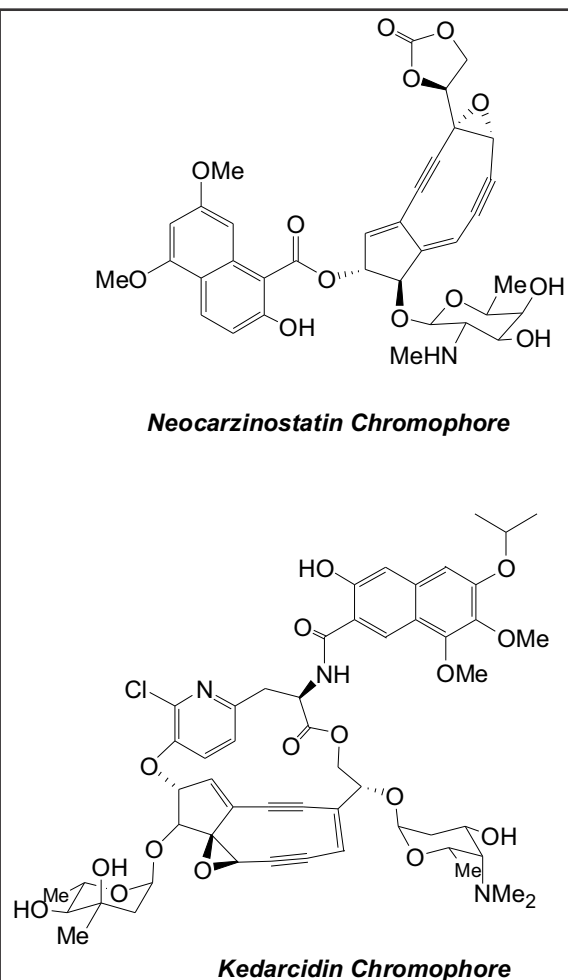
## Chemistry of Natural and Photoswitchable Cyclic Enediynes

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The cyclic enediynes, a relatively new class of antitumor antibiotics are strong DNA cleavage agents and exhibit remarkable antitumor activities both in vitro and in vivo. Naturally occurring enediyne antitumor antibiotics are divided into two groups according to the 9- or 10-membered ring core structure. The first enediyne antibiotic, neocarzinostatin (NCS) consisting of 1:1 mixture of an apoprotein and a chromophoric molecule (shown in

Figure 1.1), was isolated from *Streptomyces carzinostaticus* in 1965. However, the structure of the NCS chromophore was determined twenty years later. Following the disclosure of the unprecedented molecular structure of neocarzinostatin, two families of 10-membered ring enediynes were discovered in 1987, as represented by calicheamicin from *Micromonospora echinospora* and esperamicin-A<sub>1</sub> from *Actinomadura verrucospora*.



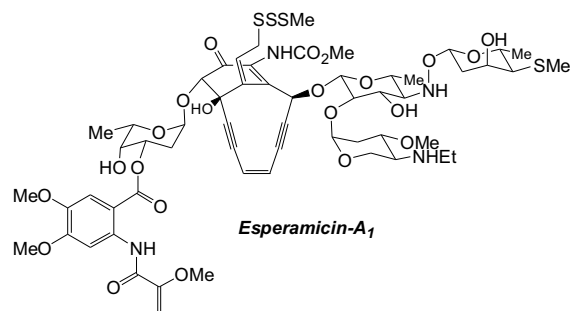
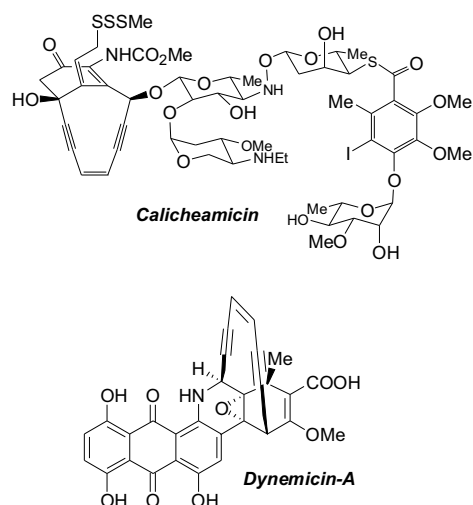
**Figure 1.1.** Naturally occurring 9-membered ring enediyne anticancer antibiotics.

Another unique subtype of antibiotics, featuring a hybrid of an anthraquinone moiety and a 10-membered ring enediyne core, was isolated in 1989 from the culture of *Micromonospora chersina* as illustrated by the structure of dynemicin-A (Figure 1.2). This shows a high potency against various tumor cell lines that significantly prolongs the life span of mice inoculated with P 388 leukemia and B 16 melanoma cells. In addition, dynemicin-A is unique among these cyclic enediynes as it contains both a cyclic enediyne ring and an anthraquinone chromophore. Because of its structural novelty, complexity and highly potent activity, the mechanistic and synthetic studies of dynemicin-A have been explored by many researchers including Schreiber, Myers and Danishefsky.

Natural enediyne antibiotics can be divided into three families: (1) the calicheamicin/esperamicin family, possessing a strained bicyclo[7.3.1]tridec-9-ene-2,6-diyne system, polysugar fragment and a methyl trisulfide moiety; (2) the dynemicin family, containing a distinctive structural feature of 1,5-diyne-3-ene unit embedded within a 10-membered ring in association with anthraquinone system; (3) the chromoprotein family, consisting of a nonpeptide chromophore such as neocarzinostatin, kedarcidin or C-1027 in complex with an apoprotein that acts as a

carrier. The related structural features found of this family are a severely strained bicyclo[7.3.0]dodecadienedi- yne core and the annulated epoxide ring. All members of the first two families have the enediyne unit incorporated into a 10-membered ring and do not need any additional stabilization factors. In contrast, all members of the third family possess a 9-membered ring enediyne core structure that requires a specific associated protein for chromophore stabilization.

Natural enediyne antibiotics possess an unusual (Z)-3-ene-1,5-diyne fragment (hence the name), which is responsible for their extreme cytotoxicity.<sup>12</sup> Upon binding to a double-stranded DNA molecule, this enediyne moiety is usually positioned within the minor groove of the host.

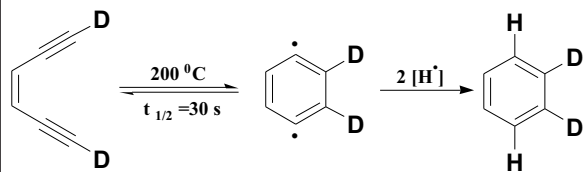


**Figure 1.2.** Naturally occurring 10-membered ring enediyne anticancer antibiotics.

Reductive or nucleophilic activation of the natural enediynes removes stereochemical blocking device and the (Z)-3-ene-1,5-diyne fragment undergoes Bergman<sup>13</sup> cyclization to produce a *p*-benzyne diradical,<sup>12</sup> which might exist in equilibrium with the enediyne precursor (*Scheme 1*). By its size; *p*-benzyne (ca. 3.8 Å) is perfectly suitable to perform a double hydrogen abstraction from carbohydrate backbones of opposite DNA strands (1'H to 1'H distance is about 5.78 Å).

Theoretical studies and experimental data suggest that this diradical has relatively low reactivity.<sup>14</sup> Initial hydrogen abstraction from one strand, however, converts *p*-benzyne into a 10-100 times more reactive

phenyl radical,<sup>14</sup> which immediately abstracts the second hydrogen from the opposite DNA strand. This process leads to an oxidative double-strand dDNA scission.<sup>12</sup> While natural enediynes are very powerful dDNA cleaving machines, the lack of antitumor selectivity results in a very high general toxicity, which hampers clinical applications of natural enediyne antibiotics.<sup>15</sup>

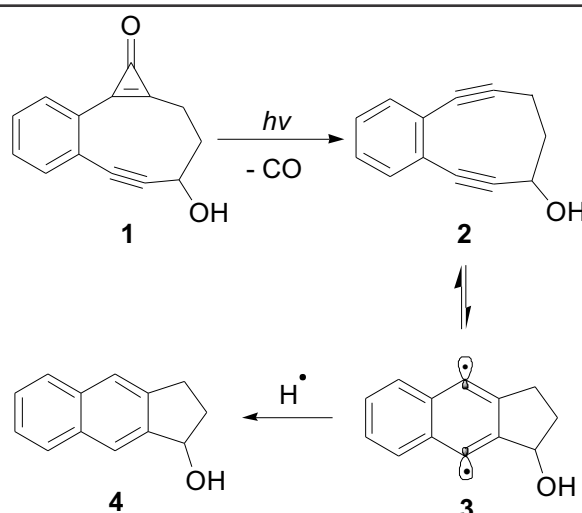


(Z)-3-ene-1,5-diyne *p*-benzyne diradical benzene  
**Scheme 1.** Bergman cyclization of the (Z)-3-ene-1,5-diyne fragment.

Photochemical triggering of the cycloaromatization reaction might help to alleviate this problem by allowing for the spatial and temporal control of enediyne reactivity.<sup>16</sup> The direct irradiation of acyclic and cyclic enediynes, as well as the natural enediyne antibiotic Dynemicin A, demonstrated that the Bergman cyclization can be induced photochemically, albeit with low efficiency. The quantum yield of the photochemical Bergman cyclization can be substantially improved by adjusting the electronic properties of substituents and/or using different modes of excitation energy transfer, for example MLCT.<sup>17</sup> In addition, several caged enediynes have been prepared which undergo conventional chemical activation after the photochemical uncaging step.

Popik's group explored an alternative strategy for the photo-triggering of the cycloaromatization reaction: the in situ generation of an activated enediyne system.<sup>18</sup> Ideally, a photoswitchable analogue of natural enediyne antibiotics should be stable in the dark but undergo rapid and reversible cyclization to *p*-benzyne after irradiation. They have recently shown that masking one of the triple bonds in 10-membered cyclic enediynes with cyclopropanone moiety produces thermally stable enediyne precursors. While photolysis of cyclopropanone precursors under single- or two-photon excitation<sup>19</sup> conditions results in efficient generation of corresponding enediynes, the cycloaromatization of the latter was not fast enough ( $\tau_{40^\circ\text{C}} > 16$  h) to achieve temporal and spatial resolution of *p*-benzyne generation in biological systems. To enhance the rate of Bergman cyclization of photoswitchable enediynes, they decided to design a nine-membered ring cyclopropanone-containing enediyne precursor (Scheme 2).

Highly strained nine-membered enediynes are predicted to undergo very facile cycloaromatization under ambient conditions. Irradiation of the thermally stable cyclopropanone precursor **1** produced the first known example<sup>20</sup> of a benzannulated nine-membered ring enediyne, 4,5-benzocyclonona-2,6-diynol (**2**). The enediyne **2** exists in a rapid equilibrium with a



**Scheme 2.** Photo-activation (decarbonylation) of the cyclopropanone containing enediyne precursor and Bergman cyclization.

corresponding *p*-benzyne analogue, 4,9-didehydrobenz[*f*]indanol (**3**), even at 25 °C ( $K_{\text{eq}} \approx 10^{-11}$ ). In the presence of hydrogen donors, **3** undergoes double hydrogen abstraction quantitatively producing benz[*f*]indanol (**4**). Kinetic data indicates that the latter process is a rate-limiting step for the Bergman cyclization of the enediyne **2**. While **2** is rapidly consumed in neat 2-propanol ( $\tau = 111$  min), the lifetime in aqueous solution is much longer,  $\tau_{\text{H}_2\text{O}} > 96$  h. In other words, if **2** is generated in a cellular environment, it will survive in active form until it encounters an appropriate hydrogen donor (DNA, thiol, protein, etc.). Enediyne **2** induces single and double strand cleavage of dDNA molecules, albeit with moderate efficiency. Cyclopropanone precursor **1**, on the other hand, does not produce DNA damage. Therefore, cyclopropanone **1** equipped with a DNA-binding moiety is a promising candidate for the development of an efficient in vivo photonuclease. Further development of this concept is focused on enhancing the two-photon absorptivity of photoswitchable enediynes and on conjugation of enediyne precursors with dDNA minor groove-binding or intercalating groups.

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The Concept of Metal-Drug Synergism in the Search for Novel Chloroquine Derived Antimalarial Drugs

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Malaria is widespread in many tropical and subtropical regions and it kills more people than any other communicable disease except for tuberculosis. According to the World Health Organization, 300-500 million people become infected and close to a million die of malaria each year, mostly children under 5 years of age. About 40% of the world's population is at risk of contracting malaria, particularly in the poorest countries.¹ It is believed that malaria originated in West and Central Africa and spread all across the globe to become the worst killer disease (Figure 1).

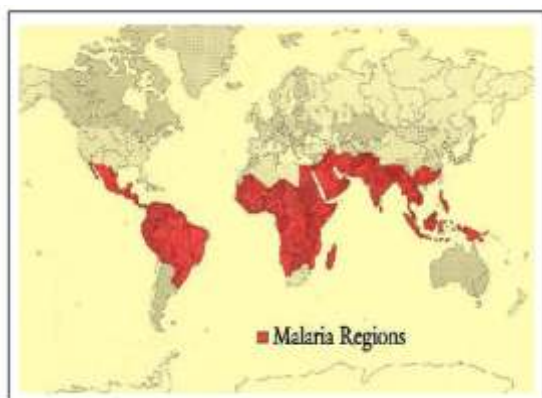


Figure 1. Distribution of malaria in the world²

The disease spreads to other areas through human migrations. Malaria seems to have been known in China for almost 5,000 years (men from ancient China, who traveled to areas with malaria, were advised to arrange for their wives to be remarried³). Today malaria is a major problem in areas of Africa, China, South East Asia, Central and South America.

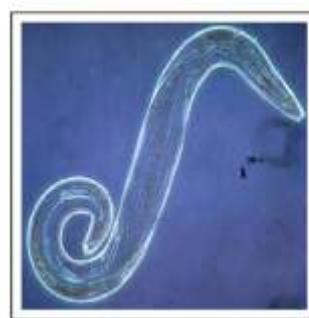


Figure 2. *Plasmodium falciparum*⁴

Antimalarial drugs are designed to prevent or cure malaria. Indians and South Americans have used the bark of Cinchona, a plant native to South America as a treatment for malaria long before any treatments were available in Europe. In 1639, Jesuit missionaries introduced the bark of this plant to Europe, where it became the main treatment for malaria fever.⁵ In 1820 the French chemists Pierre Joseph Pelletier and Joseph Bienaime Caventou identified quinine, an alkaloid,

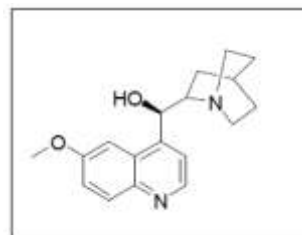


Figure 3. The structure of quinine

Until World War I, quinine was the only drug used to treat malaria for more than three centuries. It

is now only used for treating severe *falciparum* malaria because of undesirable side effects.⁷ Hence there was a continuous search for new antimalarials and so far chemotherapy of malaria has relied on chemically related drugs belonging to four classes of compounds: 4-aminoquinolines, 8-aminoquinolines, antifolate compounds and artemisinin and its derivatives Table 1).

Table 1. Four classes of antimalarials

| The class of compounds | Antimalarial drugs |
|---------------------------|--|
| 4- Aminoquinolines | Chloroquine
Quinine
Mefloquine
Amodiaquine
Halofantrin |
| 8- Aminoquinolines | Primaquine |
| Antifolates | Pyrimethamine
Proguanil
Chlorcycloguanil
Dapsone
Sulfadoxine |
| Artemisinin & Derivatives | Artemisinin
Artesunate
Artemether
Arteether
Dihydroartemisinin |

Even though several drugs have been used to treat malaria, chloroquine (CQ) remained the main treatment for malaria for 5 decades (Since the time of its introduction in the 1940s) until the spread of resistant organisms. However, CQ has saved more lives than any other drug in history and chloroquine remains the treatment of choice for *P. vivax*, *P. ovale*, *P. malariae* and uncomplicated *P. falciparum* malaria in those few geographical areas where this drug can still be relied on.

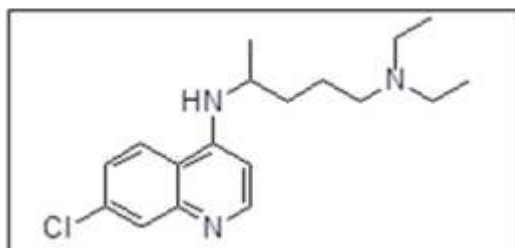


Figure 4. The structure of chloroquine (CQ)

The most important issue in the treatment of diseases like malaria today is the widespread emergence of resistance to commonly used organic drugs. There are two major approaches in drug design to overcome this problem. One of the approaches would be the synthesis of new drugs by modifying the molecular structure of existing compounds with known activity in order to overcome resistance, while maintaining the same target. The second approach would be developing new families of drugs based on

understanding of both pathogen biology and the chosen molecular target. One way of modifying the activity of organic drugs for which resistance has emerged is to incorporate a metal ion into the molecular structure of the organic drug. The concept of metal drug synergism^{8,9} is of great use in this type of drug design.

Metal Drug Synergism

Two beneficial effects result from the coordination of an organic drug to a metal ion (Figure 5). The first is the enhancement of the activity of the drug due to stabilization by complexation, which results in longer residence times in the organism, allowing the drug to reach its biological target more efficiently. The second effect is a decrease in the toxicity associated with metal ions, due to the fact that binding to the organic drug makes the metal less available for undesirable side reactions while in transit to the site of therapeutic action. The organic compound may serve as a carrier for the metal to the point of action, while the metal-containing fragment can in turn improve transport and delivery of the organic drug to its own target.

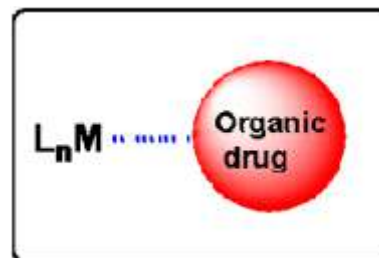


Figure 5. Metal-drug synergism arises by coordination of metal to an organic drug

In 1975, it was found that substituting the aromatic groups in the antibiotic penicillin and cephalosporine with ferrocenyl moieties produced compounds with enhanced antibacterial activity compared to the starting materials, especially to the strains of *Staphylococcus aureus* resistance to penicillin-type antibiotics (Figure 6).¹⁰

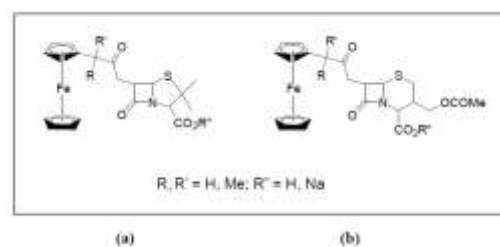


Figure 6. Organometallic complexes of known organic antiproliferation agents designed to overcome drug resistance; (a) ferrocenyl-penicillin derivatives, (b) ferrocenylcephalosporin derivatives¹⁰

Another example to show metal-drug synergism is ferrocifen (Figure 7); a treatment for breast cancer, a hormone related disease. Ferrocifen has improved antiestrogenic properties and increased cytotoxicity compared to the common organic drug tamoxifen. In ferrocifen, the phenyl group of tamoxifen is replaced by the iron containing ferrocenyl moiety

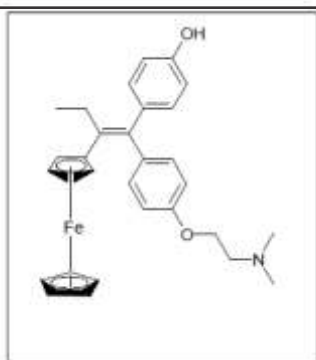


Figure 7. The structure of ferrocifen

The concept of metal – drug synergism has also been used in the design and synthesis of antiparasitic drugs especially against resistant strains. Dr. Sanchez-Delgado and his co-workers successfully applied the concept of metal-drug synergism by demonstrating that the activity of clotrimazole (CTZ) and ketoconazole (KTZ) against *T. cruzi*, the causative agent of 'Chagas' disease (American trypanosomiasis), is markedly enhanced by complexation to Ru (Figure 8), while the toxicity of the parent drugs is lowered.¹¹⁻¹⁵

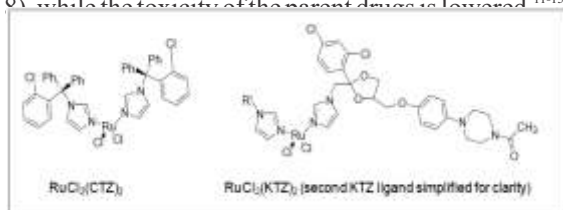


Figure 8. Two ruthenium complexes show improved activity over their organic drug

A support for the metal-based approach to antimalarial drugs comes from the work of Brocard and Biot.¹⁶ In this case iron is introduced into the structure of CQ in the form of a ferrocenyl moiety, through a covalent C-C link of one cyclopentadienyl ring to the side chain of CQ. This results in a stable, non-toxic, potent

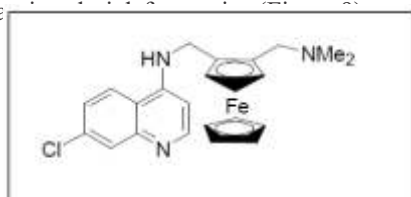


Figure 9. The structure of ferroquine

The *in vitro* activity of this compound is similar to that of chloroquine diphosphate against CQ-sensitive strains of *P. falciparum*, but it is about 30 times higher for resistant strains. They have clearly demonstrated that the presence of both CQ and Fe in the same molecule is related to the ability of the drug to overcome CQ-resistance¹⁷⁻²⁰ but ferrocene alone shows no antimalarial activity. This drug is now in phase II²¹ clinical trial.

Further, the work of Sanchez-Delgado and group has shown that the concept of metal-drug synergism can be adapted to produce novel metal-based antimalarials,

by attaching chloroquine to metal containing fragments.^{22,23} Some of the metals used in this study were Ru(II), Au(I) and Rh(I) (Figure 10) and in some cases a notable activity against resistant strains was

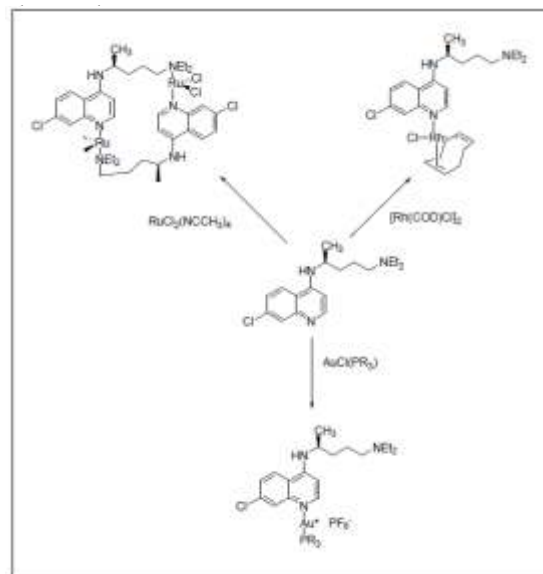


Figure 10. Examples of the syntheses and structures of metal-chloroquine complexes^{22,23}

As shown by the examples presented in Table 2, the complexes $[RuCl_2(CQ)_2]$ and $[Au(PPh_3)(CQ)]PF_6$ are more active than chloroquine diphosphate (CQDP; the standard form of the drug used in antimalarial treatment- Figure 11) against two moderately CQ-resistant strains of *P. falciparum* (FcB1 and FcB2).

Table 2. Effect of CQDP and two metal-chloroquine complexes on the *in vitro* growth of chloroquine-

| Compound | IC ₅₀ (nM) ^a | |
|-----------------------|------------------------------------|-------|
| | FcB1 | FcB2 |
| CQDP | 47.0 | 110.0 |
| $[RuCl_2(CQ)_2]$ | 11.0 | 47.0 |
| $[Au(PPh_3)(CQ)]PF_6$ | 5.1 | 23.0 |

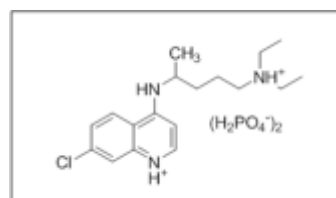


Figure 11. The structure of chloroquine diphosphate (CQDP)

Also, *in vivo* tests using the rodent malaria parasite, *P. berghei* showed the higher efficacy of $[RuCl_2(CQ)_2]$ and $[Au(CQ)(PPh_3)]PF_6$, as compared to metal free drug; chloroquine diphosphate (Figure 12).^{22,23}

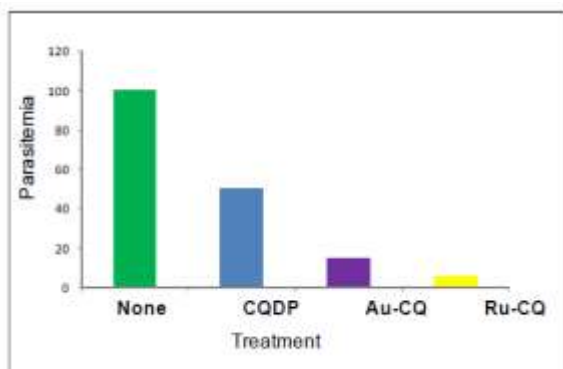


Figure 12. Effect of CQDP and metal-chloroquine complexes on *P.berghei* parasitemia in mice treated with 1 mg of CQ equivalents per Kg of body weight.^{22,23}

One limitation in the use of these complexes is their low solubility in water; more soluble compounds with improved antimalarial potential would be welcome and the new design of cationic π -arene-Ru-CQ envisaged and appears as a promising alternative for new treatments of malaria, especially for the resistant strains.²⁴

Synthesis of New Ru-Chloroquine Complexes

The well-known dimers $\text{Ru}(\eta^6\text{-arene})\text{Cl}_2$; (arene = *p*-cymene or benzene) are convenient precursors to new Ru(II) complexes containing CQ. The synthesis of the starting materials $[\text{Ru}(\eta^6\text{-p-cymene})\text{Cl}_2]_2$ and $[\text{Ru}(\eta^6\text{-benzene})\text{Cl}_2]_2$ was performed by dehydrogenation of α -phellandrene or 1,3-cyclohexadiene by ruthenium trichloride hydrate, respectively, according to the general method published by Bennett (Figure 13).²⁵

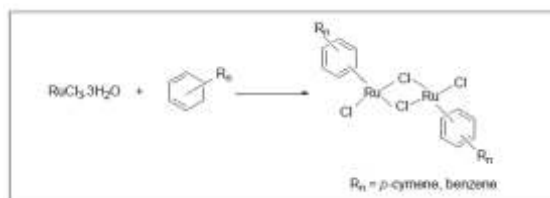


Figure 13. Preparation of starting materials²⁵

A series of complexes with the formulas $[\text{Ru}(\eta^6\text{-p-cymene})\text{Cl}_2(\text{CQ})]$ (**1**), $[\text{Ru}(\eta^6\text{-benzene})\text{Cl}_2(\text{CQ})]$ (**2**), $[\text{Ru}(\eta^6\text{-p-cymene})(\text{H}_2\text{O})_2(\text{CQ})][\text{BF}_4]_2$ (**3**) and $[\text{Ru}(\eta^6\text{-p-cymene})(\text{CQDP})][\text{BF}_4]_2$ (**4**) has successfully synthesized according to the set of reactions represented in Figure 14.²⁴

Upon reaction of the *p*-cymene dimer with chloroquine in acetone, the chloride bridge in $[\text{Ru}(\eta^6\text{-p-cymene})\text{Cl}_2]_2$ splits and the complete reaction affords the neutral dichloro species (**1**) in high yield. Conductivity measurements indicate that (**1**) remains neutral in chloroform solution (non-conducting) but it rapidly exchanges one chloride ligand by a solvent molecule in polar solvents forming the corresponding monocationic complex (**1'**). An analogous reaction of the benzene dimer in acetonitrile yields the corresponding product $\text{Ru}(\eta^6\text{-benzene})\text{Cl}_2(\text{CQ})$ (**2**), which also dissociates one chloride ligand rapidly in

water to form the corresponding monocationic derivative $[\text{Ru}(\eta^6\text{-benzene})\text{Cl}(\text{H}_2\text{O})(\text{CQ})]^+$ (**2'**). On the other hand, the dicationic complex $[\text{Ru}(\eta^6\text{-p-cymene})(\text{H}_2\text{O})_2(\text{CQ})][\text{BF}_4]_2$ (**3**) is best obtained in a one-pot procedure by treatment of $[\text{Ru}(\eta^6\text{-p-cymene})\text{Cl}_2]_2$ with 4 equiv of AgBF_4 at 55 °C, followed by reaction with CQ at the same temperature. The conductivity of a freshly prepared 1 mM solution of (**3**) in de-ionized water was 232 μScm^{-1} , a value within a range corresponds to a typical three ions in an aqueous solution, support the proposed dicationic complex.²⁴

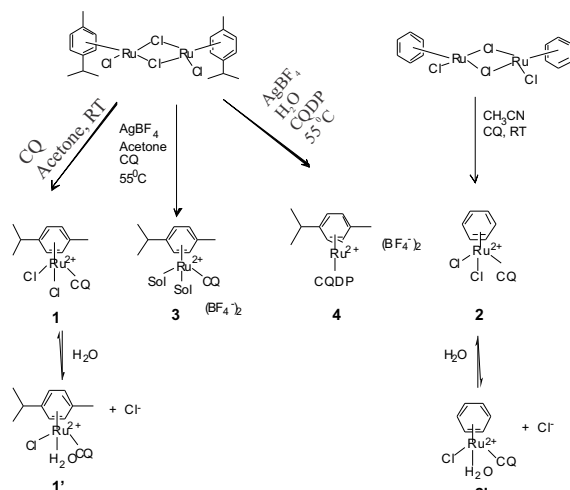


Figure 14. Synthesis of new Ru-chloroquine complexes²⁴

Another feature of interest in connection with biological properties is to compare complexes containing chloroquine base (CQ) with those containing chloroquine diphosphate (CQDP), which is the form in which this drug is administered. In structural terms, when the two nitrogen atoms are protonated, N-coordination of chloroquine to ruthenium is no longer possible and binding through the aromatic rings of the ligand will be favored. In order to obtain dicationic π -bonded “sandwich” compounds a different approach was developed. This involves the abstraction of the four chlorides in $[\text{Ru}(\text{p-cymene})\text{Cl}_2]_2$ by use of an 4 eq of AgBF_4 in the presence of 2 eq of CQDP in water. Upon chloride removal, the labile intermediate $[\text{Ru}(\text{p-cymene})(\text{H}_2\text{O})_3]^{2+}$ was stabilized by quickly replacing the coordinated water molecules by CQDP, which acts as a 6-electron donor, in a π – fashion (**4**). The conductivity of a freshly prepared 1 mM solution of $[\text{Ru-p-cymene-CQDP}]^{+2}(\text{BF}_4)_2$ in de-ionized water was 522 μScm^{-1} , a value within a range corresponds to a typical five ions in an aqueous solution, support the proposed dicationic sandwich complex.

The complexes were fully characterized including the mode of binding of Ru to CQ/CQDP in each complex by a combination of 1D and 2D NMR (^1H , ^{13}C , COSY, HSQC, HMBC, $T_1\rho\text{-H}$), FTIR, elemental analysis and DFT based computation of relative energies and IR simulations²⁴ and the structural assignments for new Ru-CQ complexes are depicted in Figure 15.

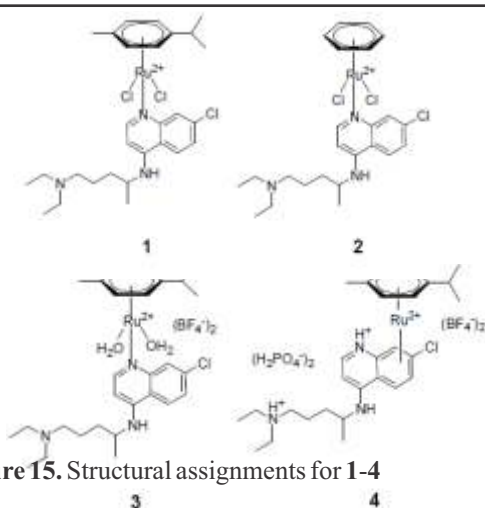


Figure 15. Structural assignments for 1-4

Antimalarial Activity of New Ru-Chloroquine Complexes

The activity of **1**, **2**, **3**, and **4** was evaluated *in vitro* against three CQ-resistant strains (W2, Dd2, and K1) of *P. falciparum* in collaboration with Prof. Joseph Schrevel of the National Museum of Natural History in Paris. The most relevant results are summarized in Table 3. Values in parentheses, represent the relative activity compared to CQDP for which an activity of 1.0 was assigned.

Table 3. Antimalarial activity of new Ru-CQ complexes against *P. falciparum*

| Compound | IC ₅₀ (nM) | | |
|----------|-----------------------|------------------|------------|
| | Dd2 | K1 | W2 |
| CQDP | 1184 ± 188 (1.0) | 1883 ± 165 (1.0) | 2155 (1.0) |
| 1 | 483 ± 110 (2.5) | 600 ± 87 (3.1) | 1667 (1.3) |
| 2 | 442 ± 30 (2.7) | 508 ± 84 (3.7) | 1619 (1.3) |
| 3 | 234 ± 41 (5.0) | 353 ± 61 (5.3) | 906 (2.4) |
| 4 | 557 ± 49 (2.1) | 529 ± 97 (3.6) | 2549 (0.8) |

against the malaria parasites. More importantly, in the case of the CQ-resistant parasites we note that the potency of all Ru-CQ complexes is consistently higher than that of CQDP, with the single exception of **4** which is of slightly lower activity than CQDP against the highly resistant W2 strain. The highest activities were observed for the dicationic N-bonded complex **3**, reaching values around 5 times better than CQDP for the Dd2 and K1 strains and 2.4 times better for the highly resistant W2.

It is therefore clear that the combination of Ru(II) and chloroquine in a single molecule enhances the activity against resistant strains of the parasite, demonstrating the validity of the concept of metal-drug synergism in the search for novel CQ derived antimalarial drugs capable of overcoming resistance.

Acknowledgment

I would like to express my sincere gratitude to Prof. Roberto Sanchez-Delgado and Dr. Alberto Martinez at the Department of Chemistry, Brooklyn College, City University of New York, USA for their support and guidance during my research work.

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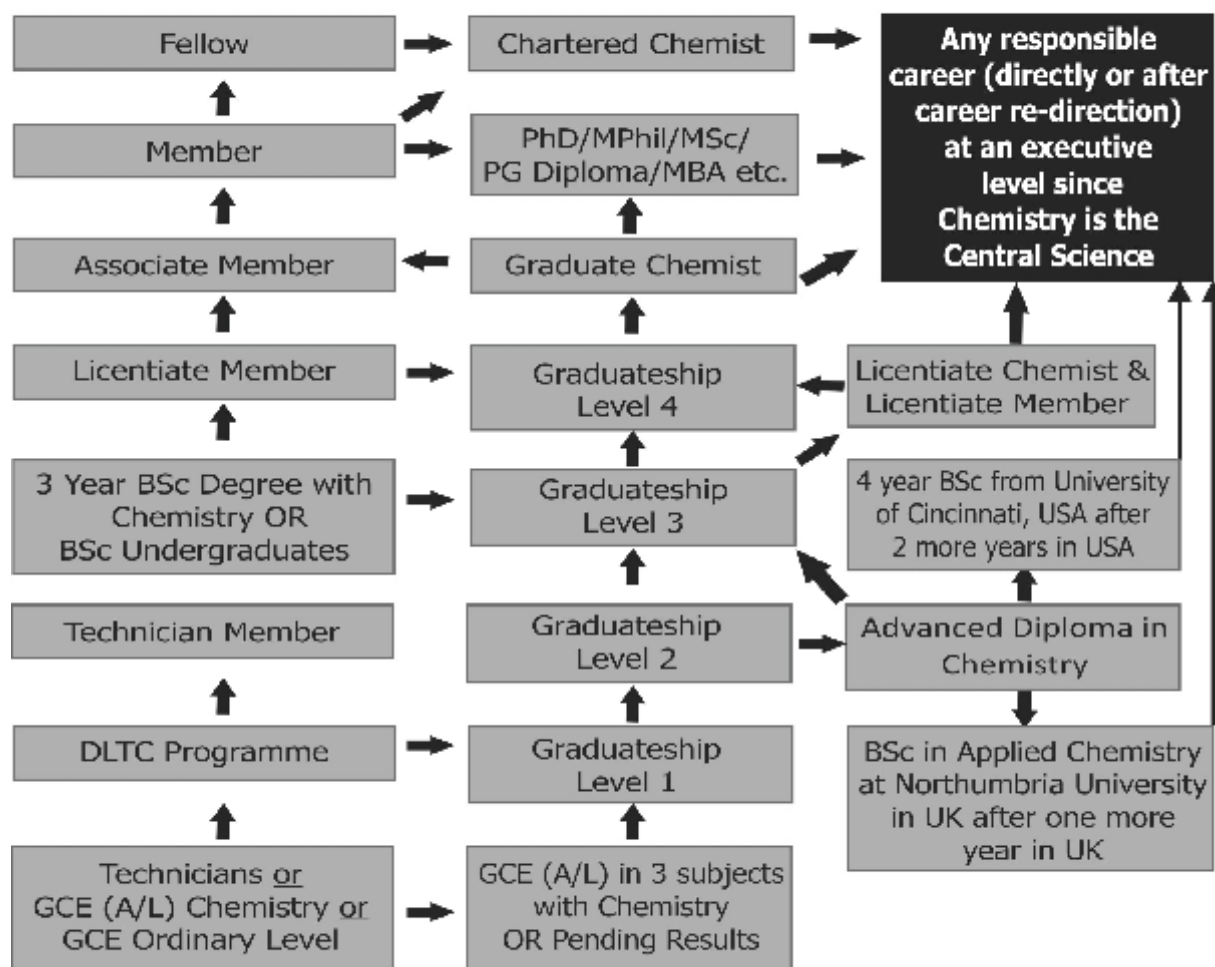
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Structure of the Graduateship Programme in Chemistry

The present structure of the Graduateship Programme in Chemistry has multiple entry and exit points as indicated below.



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- **Long life** Benefits: Rs. 10,000 (over 70)/ Rs. 15,000 (over 75)/Rs. 20,000 (over 80)
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Implication of Some Research Findings for Teaching and Learning Chemistry: Language, visualisation and the 'reality'

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Abstract

Research into what students learn, and how they respond to tasks, can tell us about the demands of learning chemistry. These findings can, in turn, tell us something about how we might design our teaching.

This presentation is based on the premise that visualization of systems at the molecular level is at the heart of meaningful understanding of chemistry - and that therefore the development of quality imagery should be an important component of the teaching learning process.

A focus of the presentation is the importance of the interdependence among (i) observable chemical phenomena, (ii) visualisation at the level of atoms, molecules and ions, and (iii) the language and symbolism used to communicate ideas - as well as an awareness by students of the distinction and interdependence among these 'levels' of chemical knowing.

Research shows that some chemistry students try to make sense by consideration of the symbolism that we present on the printed page or the computer screen, rather than of the 'reality' that the symbolism represents. This lack of appropriate visualisation of 'reality' can lead to serious misconceptions. It is also common for students to (i) visualize the molecular level, although the symbolism refers to the observational level, or (ii) to visualize single molecules when the appropriate mental imagery for sense-making is of vast numbers of molecules.

While the classical saying is that "a picture can paint a thousand words", it is also true that words can affect the mental image that one adopts. One does not have to look far to see published examples of how the language that we use in the classroom can be misleading. Sometimes we use rather loose language which is perhaps not a problem when experts talk with experts, but which is inappropriate when talking with novices.

A broader context of the talk is that teaching chemistry is demanding, and our abilities can be improved by research, just as is the case for practitioners in other disciplines. What do we need to know? Content knowledge (knowing chemistry) is a necessary, but insufficient condition for quality teaching. Pedagogical knowledge is also a necessary, but insufficient condition. Every teacher needs *pedagogical content knowledge*: specific knowledge, based on evidence, about how we might teach about specific concepts. In particular, there the issue of how we can enhance the likelihood that our students will automatically develop appropriate images when they see our representations (language, symbols, formulas, molecular structures, and chemical equations).

Introduction: Pedagogical content knowledge

Having knowledge about teaching chemistry is different from both (i) having knowledge about chemistry, and (ii) having knowledge about general teaching principles. In many countries, teacher education involves separately learning chemistry (for example, thermochemistry, stoichiometry, kinetic theory, and chemical bonding) and pedagogy (principles of teaching). But seldom do they address the challenges of teaching about thermochemistry, stoichiometry, kinetic theory, and chemical bonding, etc.

The content of this paper illustrates the notion of *pedagogical content knowledge* (PCK) - which might be simply described as particular knowledge about teaching particular content which can be used to improve the learning of that content. While *content knowledge* refers to one's understanding of the subject matter, and *pedagogical knowledge* refers to one's understanding of teaching and learning processes independent of subject matter, *pedagogical content knowledge* refers to knowledge about the teaching and learning of particular subject matter, taking into account the particular learning demands inherent in the subject matter.

The fundamental assumption of this paper is that for quality teaching:

- Possession of content knowledge is a necessary, but insufficient, condition.
- Possession of pedagogical knowledge is a necessary, but insufficient, condition.

The notion of pedagogical content knowledge is generally attributed to Lee Shulman. Commenting on content-free criteria that were commonly used for evaluation of teaching, Shulman (1986) asked "Where did the subject matter go? What happened to the content?"

Geddis (1993) supported the case for PCK concisely:

The outstanding teacher is not simply a 'teacher', but rather a 'history teacher', a 'chemistry teacher', or an 'English teacher'. While in some sense there are generic teaching skills, many of the pedagogical skills of the outstanding teacher are content-specific. Beginning teachers need to learn not just 'how to teach', but rather 'how to teach electricity', how to teach world history', or 'how to teach fractions'. (p. 675)

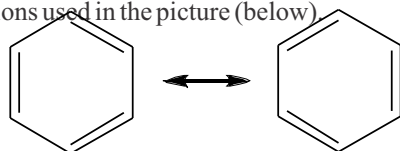
Or (I might add) 'how to teach stoichiometry', or 'how to teach chemical equilibrium', or 'how to teach thermochemistry'. Obviously the demands of

learning about thermochemistry' are different from the demands of learning about chemical equilibrium. Teachers need to be very aware of the different demands teaching and learning about different chemical ideas.

I can try to make this point by reference to teaching about benzene. Please forgive the fact that most of my examples come from the tertiary level of education, in which most of my research in chemistry education has been centred.

- We may want to teach about the substance benzene – which we can see, smell, feel, test its dissolving power of different substances, measure its density and refractive index, study some of its reactions, and even know that its composition corresponds with the formula C_6H_6 without any need to refer to its structural components (molecular, ionic, metallic, etc.).
- Or, we may want to teach that the substance benzene is composed of molecules, each of which has a hexagonal distribution of carbon atoms, each bound to the two adjacent ones on either side of it, and each bound to one H atom. So far, there has been no need to mention electrons.

We may want to teach about the distribution of electrons in each benzene molecule (in this case, only in bonds, with no lone pairs). But chemists' models of the distribution of electrons in benzene molecules are not simple, and involve the idea of *resonance*. Putting aside the challenge of "getting across" a good understanding of this concept, resonance in a benzene molecule is commonly represented by a picture which can only be correctly interpreted if one understands the conventions used in the picture (below)



It does not take much research into student understandings to realise that at any level of education, some students take this picture to imply that we are talking about two molecules (as implied by the wording in some textbooks, when, of course, we are referring to the electron distribution in just one molecule), and that (i) some think it means equilibrium between the two forms, (ii) some think there is a 'switching' between the two structures, and (iii) some think the two molecules are identical, as can be seen by turning either through 60° .

It is a challenge to teach what this diagram means in the understanding of the term *resonance*, especially because the diagram is intent on telling us what the electron distribution is not (rather than what it is)!

While it is often accepted that a picture is worth a thousand words, in this (and many other) cases, the words (and other forms of chemical language) associated with presentation of the picture are fundamentally important influences on the mental image that the student develops.

Each chemistry teacher has a unique knowledge of chemistry. None of us can hope to transmit to the students a duplicate of this knowledge. The teacher's

job is to re-package and re-present his/her knowledge in such a way that gives the students some hope of achieving sensible understandings. The re-packaging task will depend upon the nature of the subject matter. And so we teachers have to come to know the subject matter, not only for itself, but also in terms of its teachability and learnability. This task has been conceptualised (Shulman, 1986) as 'transformation of subject-matter knowledge into forms accessible to the students'. Geddis (1993) points out:

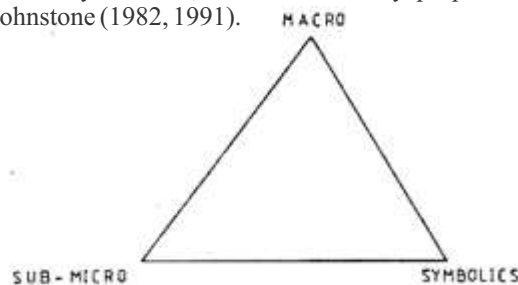
In order to be able to transform subject matter content knowledge into a form accessible to students, teachers need to know a multitude of particular things about the content that are relevant to its teachability. (p. 676)

Developing ways to do this is indeed the creation of new knowledge of a type that characterises the good teacher and is part of his/her professional skill. The requirement for teachers to invent this new knowledge should be recognised.

All teachers have some PCK developed through experience, but usually this is lost generationally (called *amnesia of the profession*) because there are limits to how much of their PCK is transferred to colleagues through informal ways of sharing. For chemical education scholarship to be regarded as a true discipline, PCK should be based on research evidence of what 'works', and documentation and publication of the findings. This is standard practice in other disciplines that allows practitioners to learn from the work of the people who practised before them.

Macroscopic, sub-microscopic and symbolic levels of operation – Johnstone

The idea that chemists switch between three levels of operation, and that this need to switch between levels is a key source of difficulty for chemistry students, was first formally proposed by Johnstone (1982, 1991).



Triangle of levels of chemical thought - taken from Johnstone (1991)

In this view, the *macro* level refers to substances, phenomena and bulk properties that we can observe, the *sub-microscopic* level is the engagement of our imagination in the process of modelling a reality in terms of interactions of atoms, ions and molecules, and the *symbolic* level refers to our use of a myriad of language forms (words, diagrams, symbols, formulas, chemical equations) to represent either observed phenomena or the visualised sub-microscopic world as we communicate with each other. Through this distinction, Johnstone has raised our consciousness of

the challenge presented by the kinetic molecular theory of matter which uses models of discrete, discontinuous matter at the sub-microscopic level to rationalise apparently continuous macro properties (density, enthalpy, solubility).

The need to operate at these distinct levels has now become accepted wisdom in the chemical education community. Many first-year university textbooks try to take these ideas into account in their design.

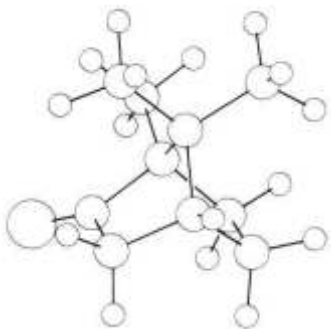
The focus of this paper is the sub-microscopic level, but before we move on, we might reflect upon potential interaction between this level and the symbolic level.

The artist Magritte drew attention to this issue

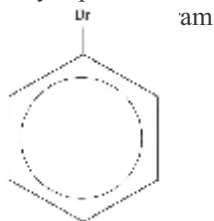


“Ceci n'est pas une pipe” means “This is not a pipe. Rather, it (the painting) is a representation of a pipe.

In our context, the following is not a drawing of camphor. Nor is it a molecule of camphor. Rather, it is a representation, with contained information, of a camphor



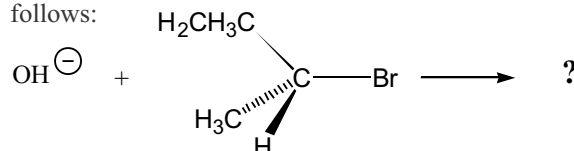
I hope to convince you that this issue is important, and that teachers need to maintain a high level of consciousness about the distinction between a reality and its representations. There is evidence that students engage in chemical deduction by operating on symbolic representations, rather than on visualisations of the reality that they represent. For example, when confronted with



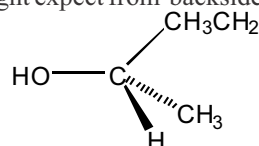
a student described by Kleinman et. al. (1987)

declared that bromobenzene does not have a plane of symmetry because 'B' and 'r' are different. Just as the words *mother*, *car*, *football* and *traffic light* should evoke images of a reality rather than of the words themselves, so students need to be able to see beyond drawings of structures of molecules to the 'reality' that they represent.

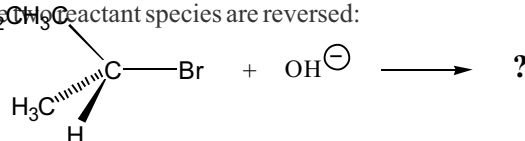
In somewhat similar vein, Ladhams Zieba (2004) asked 18 second-year university students to draw the product species most likely to be produced from the substitution reaction of 2 bromobutane represented as follows:



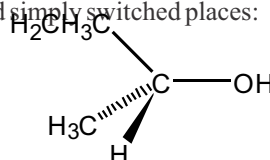
Ten of them drew the inverted substitution product that you might expect from 'backside attack' in an S_N2 reaction:



The other eight students drew a variety of responses. Seventeen other students were asked the same question, about the same reaction, now represented by an equation in which the positions of the formulas of the reactant species are reversed:



Eight of the students drew a substitution product without inversion, as though the hydroxide and bromide had simply switched places:

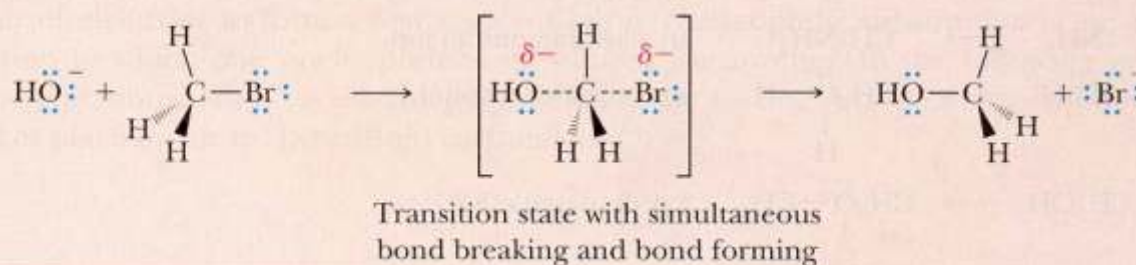


Only one of the others suggested inversion of the substituted butane. Obviously, these students are operating on the written representations, rather than on a visualised reaction mixture at the molecular level, with its multitude of possible collisional orientations. The consequence was that the predicted product of a reaction generally depended on how the representations of the reactive species were arranged on paper in a chemical equation!

Further research evidence obtained by Ladhams-Zieba demonstrated that we can provide confusing cues to our students if we do not clarify the distinction between a substance and its molecules. In our discussions about nucleophilic substitution reactions, we usually (and for good reason) portray a tetrahedral distribution of bonds around the carbon atom at which substitution takes place – as in the following extract from a textbook:

MECHANISM An S_N2 Reaction

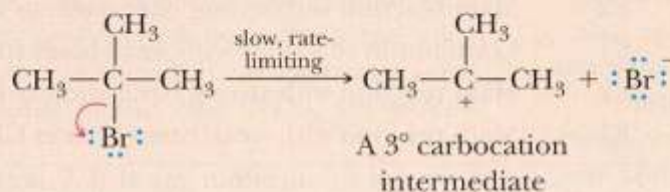
The nucleophile attacks the reactive center from the side opposite the leaving group, which results in inversion of configuration.



And in discussion of elimination reactions, we usually portray a planar arrangement of bonds in the substrate molecule:

MECHANISM E1 Reaction of 2-Bromo-2-methylpropane

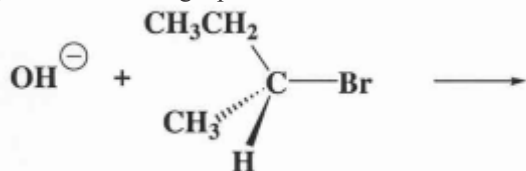
Step 1: Rate-limiting ionization of the C—Br bond forms a carbocation intermediate.



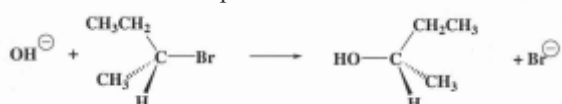
Step 2: Proton transfer from the carbocation intermediate to a molecule of solvent (in this case, methanol) gives the alkene.



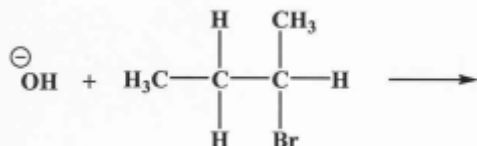
The researcher asked third-year students in a highly reputable university to predict the products of a reaction represented in a partial equation by un-named structural representations. The reactants were 2-bromobutane and hydroxide ions. Of those who were given the following representation



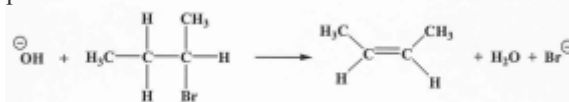
the most common response was a substitution reaction:



Most of those presented with a partial equation showing the substrate with a square planar appearance



predicted a substitution reaction:



Of course, the product of reaction between two substances does not depend on how one of them is drawn! We see once again evidence that the students are operating on the representations on the page, rather than on a visualised reality that the drawings represent.

Furthermore, some of the language that chemists (and chemistry teachers) commonly use has the potential to confuse students by not clearly distinguishing between whether we are talking about the macroscopic level or the sub-microscopic level of atoms and molecules. There is plenty of research evidence that some students attribute to atoms and molecules the properties (such as colour, malleability, density, expansion on heating) of the substances. Is this confusion at least partly due to lack of differentiation in the language that we use:

- When we refer to 'the structure of water', do we clarify whether we are referring to the arrangement of molecules within the substance water, or to the

arrangement of atoms within each of its molecules?

- Do we sometimes say that methane has tetrahedral shape, when we mean that methane molecules have tetrahedral shape (while methane has the shape of its container)?
- Do we ever draw the structure of a water molecule and say “This is water”? No water is a colourless liquid that dissolves sugar.
- If we say that oxygen expands when heated, do we make sure that our students are visualising the substance oxygen, and not a molecule of oxygen?
- When we say that copper is malleable, do we clarify that we are talking about the substance copper, and not a copper atom?
- Since the statement “Water consists of hydrogen and oxygen” is seen so commonly, is it surprising that many students believe that the bubbles seen in boiling water are the substances hydrogen, $H_2(g)$ and oxygen, $O_2(g)$? It takes little extra trouble to be precise in our language and encourage useful visualisation by saying “Each water molecule (of the trillions darting around in a glass of water) has two hydrogen atoms and one oxygen atom bound together”?

Of course, in each of the cases above, we know what we mean. the issue is whether the novice chemist (the student) understands our language unambiguously.

Two levels of the sub-microscopic world - Jensen

Jensen (1988a, b) has taken Johnstone's model further. While recognising both the macroscopic level (which he labels *molar*) and the sub-microscopic level, Jensen points to a significant distinction between two layers of the sub-microscopic world; we use one (which he calls *molecular*) when we consider the properties and structure of molecules, and another (*electrical*) when we model electron disposition within a molecule. Properties of dioxygen appropriate to each of these three levels are identified, for illustrative purposes, in the following table.

| | |
|-------------------|---|
| molar | Colourless, odourless, paramagnetic, highly reactive gas, essential for most life, composing 21% of atmosphere by volume, mp = 54.8 K, bp = 90.2 K |
| molecular | Diatomic O_2 molecule, non-polar, O-O bond length = 121 pm |
| electrical | 
or
$(s_{2s})^2(s_{2s}^*)^2(p_{2px})^2(p_{2py})^2(s_{2p})^2(p_{2px}^*)(p_{2py}^*)$ |

Examples of each of Jensen's three levels of chemical operation, as applied to dioxygen.

You may have recognised that we have already encountered these three levels of chemistry operation in the context of understandings about benzene, on page 2.

Perhaps the simplest way to think about Jensen's two levels of the sub-microscopic world is that the *molecular* level refers to what we might see when observing a molecule as though from a neighbouring molecule, while the electrical level is concerned with 'observations' of electron distribution from within the molecule – and which I therefore prefer to refer to as the *intramolecular* level. The correspondence between the propositions of Johnstone and Jensen, as well as the labels adopted for this paper, are displayed in the following table.

| Johnstone | Jensen | Preferred labels |
|-----------------|------------|------------------|
| Macroscopic | Molar | Macroscopic |
| Sub-microscopic | Molecular | Molecular |
| | Electrical | Intramolecular |

Correspondence between the levels proposed by Johnstone and those proposed by Jensen, along with the labels used in the remainder of this paper.

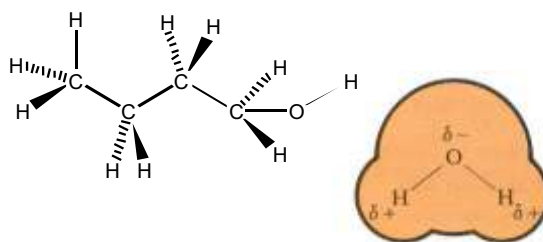
Of course there are interdependencies amongst chemists' operations at these three levels. For example, the macroscopic observation that ammonia is very soluble in water may be rationalised at the molecular level on the grounds that the ammonia molecule has a permanent charge separation (ie, is a dipole), and this in turn can be modelled at the intramolecular level by consideration of unequal electron distribution between nitrogen and hydrogen atoms.

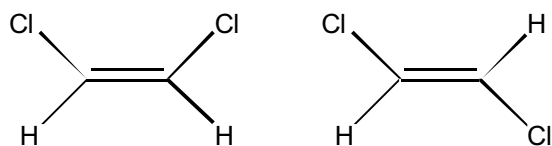
It seems obvious that students would be assisted if teachers and textbooks were explicit in announcing when they are modelling at the molecular level and when they in intramolecular mode, so that students would develop these ways of thinking more consciously.

The molecular level – a further refinement

There is a further distinction between layers of operation at the molecular level that should be explicitly recognised. This concerns whether our visualisation engages images of single molecules, or images of many particles. There is both research and experiential evidence to support the view that students would benefit from a consciousness about which of these distinct types of image are used for particular purposes.

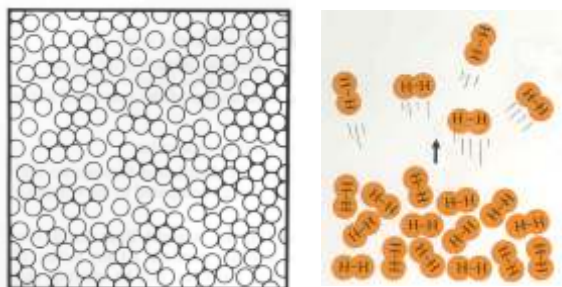
Sometimes at the molecular level we find it useful to visualise an image of one particle for a particular purpose. We do this when we want to indicate, for example, connectivity, bond angles, cis-trans isomerism, stereochemistry, or molecular polarity.



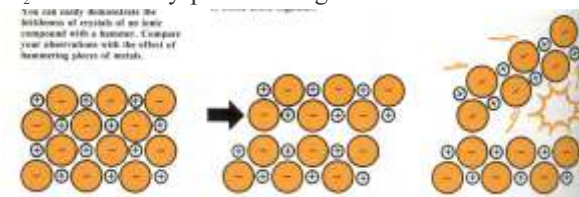


Single-particle representations that are commonly used to portray connectivity and bond angles, molecular polarity, and cis-trans isomerism, respectively.

On the other hand, for some purposes we need to use pictures with many atoms, ions or molecules to develop sensible understanding of phenomena. For example, it is impossible to represent changes of state, diffusion of gases, solubility of a solid in a liquid, optical activity, or many other phenomena by other than many-particle pictures.



Portrayal of the liquid state and of vaporisation of liquid H_2 demand many-particle images.

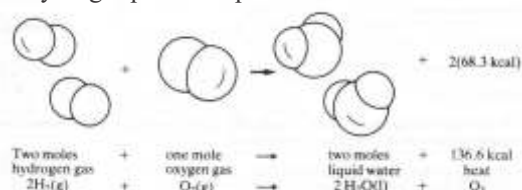


A many-particle representation that rationalises the brittleness of an ionic crystal.

Does it matter?

There is convincing research evidence that the conscious distinction between single-particle images and many-particle images at the molecular level is significant, and that use of the inappropriate mode can inhibit understanding. For example, Ben-Zvi *et al.* (1987) have shown that some school students in Israel have responded to a question asking whether N_2O_5 is a possible product of a chemical reaction between the elements N_2 and O_2 by saying "No. Where from did we get three additional oxygen atoms?" Obviously these students did not engage a many-particle picture of a reaction mixture containing nitrogen and oxygen.

Ben-Zvi attributes blame to common textbook diagrams, such as the one reproduced below, which portray single-particle representations of a reaction.

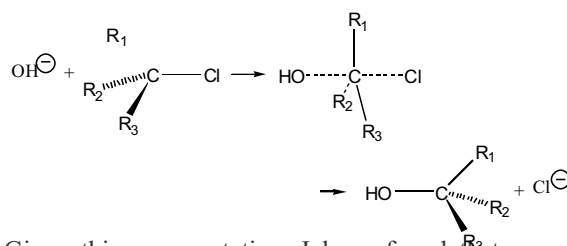


Copy of diagram showing conflict between the symbolism $O_2(g)$ and representation of one molecule - from Ben-Zvi *et al.* (1987)

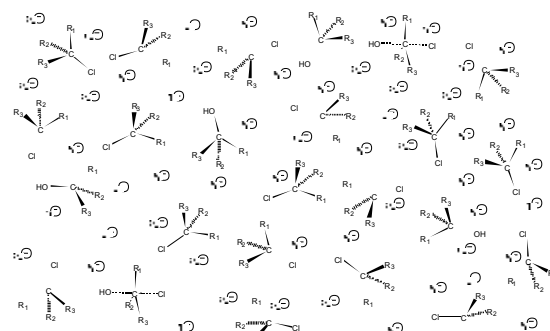
Perhaps we instructors and textbook writers should

more commonly use many-particle pictures to portray reaction mixtures at the molecular level. Such diagrams are not common in textbooks, but they certainly are becoming more popular in computer representations. Even so, we should not presume that our students will automatically recognise the significance of using many-particle images for specific purposes.

Sometimes it is hazardous (cognitively speaking) to use single-particle pictures for instructional purposes. For example, textbooks commonly say that the rate of an S_N2 substitution reaction depends on the concentration of both the substrate and the nucleophile, and then use a single-particle representation of the reaction mechanism:



Given this representation, I have found that many students, even at the university level, say that what is meant by 'the rate of the substitution reaction' is how fast the portrayed event proceeds. But how fast this single event proceeds is not what is meant, and indeed there is no sense to be made from a statement that the rate of this event is dependent on the concentrations of both reactants. Of course, the 'rate of reaction' refers to how many such reaction events occur per second. The teacher whose PCK recognises this will use diagrams (or dynamic computer graphics) indicating many such events occurring in a reaction mixture – not simultaneously.

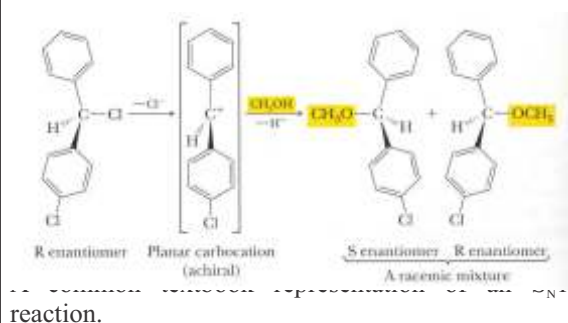


A multi-particle representation of an S_N2 substitution reaction mixture, that attempts to capture an instant in time. Some reactant species are present, as are some product species and a few intermediate species. A better representation, achievable now with computer graphics, can show the changing relative amounts of reactant species and product species, and a relatively constant 'concentration' of intermediate species.

Perhaps too, we should refrain from using commonly used language that implies a single-particle event - such as "The nucleophile OH^- uses its lone pair electrons to attack the alkyl halide carbon 180 away from the departing halogen. This leads to a transition state". This suggestion of single-particle images is probably enhanced by computer representations

which portray one nucleophile molecule arriving on screen and, with apparent pre-ordained objective, attacking the only substrate molecule shown from the appropriate orientation.

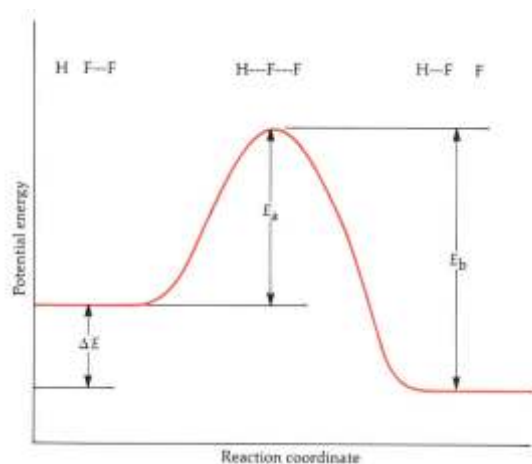
Ladhams Zieba (2004) has found that university students can be confused when a single-particle representation of an S_N1 substitution reaction leads to a racemic mixture of products.



How can we get two molecules of product from only one molecule of substrate compound? The teacher with PCK in this area, will realise the benefit of representing this situation with a drawing or simulation containing many particles undergoing substitution, half of which give rise to one enantiomer, and half to the other.

To yet another example. Of the two diagrams usually used in conjunction to account for the temperature dependence of reaction rates, one refers to single-particle events, and the other refers to many-particle situations.

The activation energy profile diagram is a story about a single reaction event.



particles involved in an event initiated by collision between one H atom and one F_2 molecule.

However, the Boltzmann distribution diagram refers to the average energies of many particles.

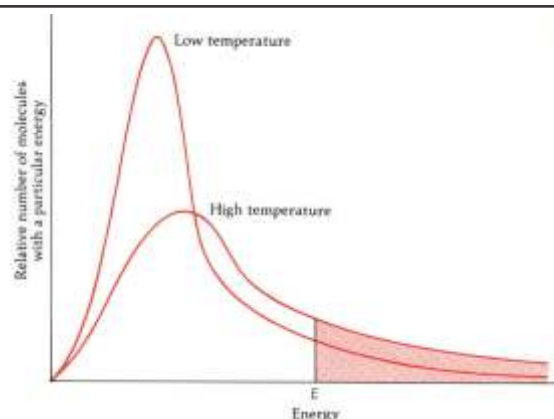


Diagram portraying the distribution of energies of molecules in a system at two temperatures.

Reconciliation between these two diagrams is not simple.

An expanded framework

It may be useful for students to be aware of the several layers of observation and imagination in which chemists engage. The following table shows the layers in this framework.

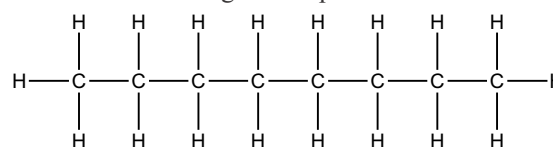
| Johnstone | Jensen | Current framework |
|-----------------|------------|----------------------------------|
| Macroscopic | Molar | Macroscopic |
| Sub-microscopic | Molecular | Molecular, single-particle image |
| | | Molecular, many-particle image |
| | Electronic | Intramolecular |

A portrayal of correspondence between levels of operation in chemical thinking from Johnstone and Jensen with the current work.

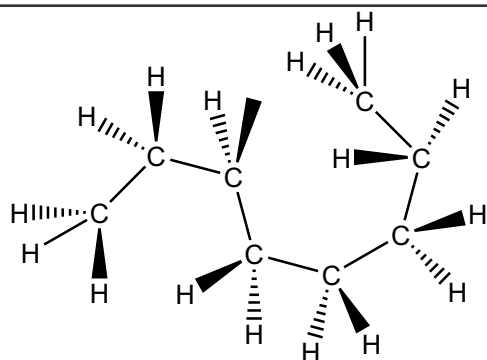
Diagrams (as well as animations and simulations) and language

I have tried to make a convincing argument that visualisation of a 'reality' is important for quality understanding of chemistry. And I have further suggested that to achieve this, we need to be careful not only in our selection of representations in the classroom, but also in the selection of the language that we use.

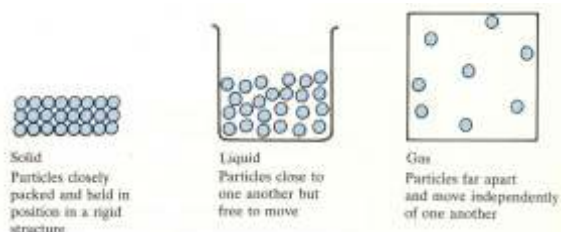
Over and above what has been said, it is also important to consider the quality (as well as the type) of the representations that we use. For example, to encourage a quality image of an octane molecule, which of the following is more powerful?



or a fluctuating (twisting and folding) version of



A set of diagrams commonly used to compare the solid, liquid and vapour states of substances is the following:



How well do these diagrams represent our shared beliefs about the relative volumes of liquid and solid states (at least, of water), of the rapid movement of particles, and of the number of particles per apparent volume of the vessels?

And in common representations, like the one below, of S_N2 substitution reactions, is there not a suggestion of pre-ordained attack by the OH^- ion at the correct orientation relative to the alkyl chloride – rather than just one of the billions of collisions happening with statistical variation of energies and orientations?

We also need to be careful in our use of language. In chemistry we have invented many words that are particular to our discipline and are not used elsewhere – such as electronegativity, standard reduction potential, enthalpy, cation, molecular orbital, and carboxylic acid. We may use these words in the classroom, but do our students understand what we mean by them. Conversely, the students may use them, but do they know their meaning, or are they used in the way that a parrot can remember and say them? It is important to have some sense of which is the case. There is a distinction between the scientifically correct definition of any of these terms and an explanation that is useful to our students. For example, the IUPAC definition of *polarity* is:

“When applied to solvents, this rather ill-defined term covers their overall solvation capability (solvation power) for solutes (i.e. in chemical equilibria: reactants and products; in reaction rates: reactants and activated complex; in light absorptions: ions or molecules in the ground and excited state), which in turn depends on the action of all possible, nonspecific and specific, intermolecular interactions between solute ions or molecules and solvent molecules, excluding such interactions leading to definite chemical alterations of the ions or molecules of the solute. Occasionally, the

term solvent polarity is restricted to nonspecific solute/solvent interactions only (i.e. to van der Waals forces).”

This is hardly useful to our students. Repackaging this definition in a way that has meaning to students, as well as being free of significant errors of commission or omission is a challenge (and is an example of PCK).

We also use in Chemistry words that have different meaning in contexts outside of chemistry. Some such words in the English language (there may be a different set in the Croatian language) include: preparation; concentration; hard; volatile; attractive (forces); migration; fusion; reduction; strong; weak; saturated; dispersion; complex; basic; spontaneous. When we use these words, are we sure that our students are not using the other meanings, or at least are somewhat confused? There is a mass of research evidence that suggests that we cannot presume that.

Conclusion

The intent of this paper is to encourage us all to think carefully about the messages that we transmit in our classrooms. The challenge is perhaps bigger than we might think. We need to work hard to avoid the mis-match between teacher intent and student understandings portrayed in a cartoon presented by Kleinman et al (1987) and re-presented here:



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Kandiah Award for Basic Chemistry - 2012

Ms. Pathira Kankanamge Vinitha Ranji from the Open University of Sri Lanka has been awarded the Kandiah Award for Basic Chemistry in recognition of her research on “*Bioactivity Directed Chemical Investigation of Fungal Extracts : Citriquinones A & B from *Penicillium citrinum* and Butyrolactone I & (+)- Geodin from *Aspergillus terreus**”. The research was carried out under the supervision of Prof. G.M.K.B. Gunaherath, Dept of Chemistry, The Open University of Sri Lanka, Prof. S.C. Wijeyaratne, Dept. of Botany, University of Sri Jayawardenapura and Dr K.H. Jayawardena, Dept of Zoology, The Open University of Sri Lanka.

Miss P.K.V. Ranji is an old girl of Sanghamitta Girls College, Galle and is currently reading for her MPhil degree in Natural Products Chemistry at the Open University of Sri Lanka. She is also a member of the Sri Lanka Association for the Advancement of Science.

Kandiah Award for Basic Chemistry - 2012

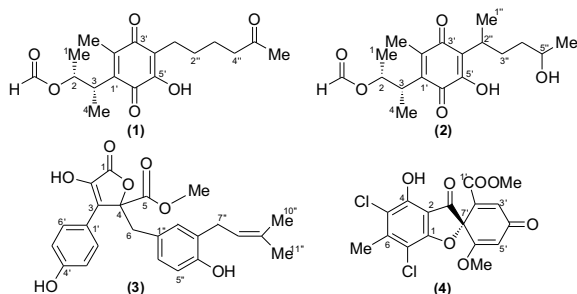
Bioactivity Directed Chemical Investigation of Fungal Extracts: Citriquinones A and B from *Penicillium citrinum* and Butyrolactone I and (+)-Geodin from *Aspergillus terreus*

Pathira Kankanamge Vinitha Ranji

Department of Chemistry, The Open University of Sri Lanka, Nawala, Nugegoda.

Abstract

As part of an ongoing search for new bioactive natural products from fungal species inhabiting diverse environments, bioactivity guided fractionation of the extracts of two terrestrial fungal species *Penicillium citrinum* and *Aspergillus terreus* was carried out. Two new benzoquinones; citriquinone A (1) and citriquinone B (2) were isolated from *P. citrinum* while, two known metabolites butyrolactone I (3) and (+)-geodin (4) were isolated from *A. terreus*. The chemical structures of these were elucidated by extensive usage of spectroscopic data. Citriquinone A (1), butyrolactone I (3) and (+)-geodin (4) exhibited significant antibacterial activity against *Bacillus* sp. while Citriquinone A (1) exhibited cell migration inhibitory activity (CMIA) against human cancer cell line, HEP 2.



Keywords: *Aspergillus terreus*; *Penicillium citrinum*; Citriquinone A and B

Introduction

Fungi play an important role in the environment and have the ability to exploit almost all niches, both natural and man-made. They have been found to

produce unique complex molecules as secondary metabolites¹. Since most of these natural products have evolved because of microbial “stress tolerance”^{2,3} microbes are the most fitting and promising source for novel antibiotic, antifungal and anticancer drugs. Thus the importance of research aimed at drug discovery from fungal sources inhabiting diverse environments, is undeniable.

Methodology

The present study is on bioactivity directed fractionation of the metabolites of two terrestrial fungal species, which showed significant antibacterial activity against gram positive bacteria. One fungal culture was originated from a soil sample collected from the garden of the Botany Department of University of Sri Jayewardenepura while the other was from a soil sample associated with roots of *Suveda maritima* plant collected from Puttalam District. These cultures were identified as *Penicillium citrinum* and *Aspergillus terreus* respectively by studying their molecular characteristics⁴.

Investigation of *P. citrinum*

Extraction and Bioactivity Directed fractionation

A homogeneous spore suspension of the fungal culture, *P. citrinum* was made in sterile distilled water and 1 mL aliquots were inoculated into 80 glass bottles (350mL) containing 40 mL of PDA. Then the bottles were incubated for 21 days at 30 C. At the end of 21 days, secondary metabolites of these cultures were extracted into MeOH and the extract was concentrated to ~1/5 of its volume to remove MeOH and partitioned with EtOAc. The EtOAc extract (1.27 g) was dissolved in 80% aqueous-methanol and partitioned between

hexane. The 80% aqueous-methanol fraction was diluted to a 50% aqueous-methanol solution, by adding water and then partitioned with CH_2Cl_2 . The hexane and CH_2Cl_2 layers were evaporated to dryness under vacuum at 40 °C to yield the hexane fraction (0.22 g) and CH_2Cl_2 fraction (0.99 g). The CH_2Cl_2 fraction, which showed antibacterial activity, was further fractionated by silica gel column chromatography followed by preparative TLC to yield two new natural compounds, citriquinone A (**1**) and citriquinone B (**2**).

Antibacterial Assay

In order to direct the fractionation each and every extract/ fraction and isolated compounds (dissolved in MeOH) were subjected to bioassay and antibiotic activity against *Bacillus* sp., was determined using Kirby-Bauer Disc Diffusion method⁵.

Cell Migration Inhibition Assay on Cancer Cells

Human cancer cell line, HEp 2 (Epidermoid carcinoma, larynx, adherent, monolayer) was established *in-vitro* in complete growth medium (Dulbecco's modified Eagle's medium, 10% fetal bovine serum), supplemented with antibiotics in plastic tissue culture flasks using standard methods. Cells were transferred into 96 well plates with clear bottoms, incubated overnight at 37 °C with 5% CO_2 in a humidified incubator. After 12 hours (at confluence stage) a scratch was performed along the vertical axis of each well by inserting and pulling a sterile micropipette tip (2 – 20 μL) towards the user and scratch was washed with fresh medium⁶. From an initial investigation it was found that the appropriate concentration of DMSO to be used as the carrier of extracts, fractions and compounds without affecting the cell growth is 1% DMSO in growth medium. Samples were prepared by dissolving them in appropriate volumes of DMSO and mixing with the growth medium (total volume 200 μL). Subsequently, these were introduced into each well. 1% DMSO in growth medium was used as the control. An inverted fluorescence microscope was used to visualize cells and the healing/inhibition of the scratch. Images were

captured on a digital camera using a 10 × objective. Plates were incubated for 24 hours and images were recaptured in the same way.

Investigation of *A. terreus*

Extraction, Bioactivity Directed fractionation and structure elucidation

A homogeneous spore suspension of the fungal culture *A. terreus* was made in sterile distilled water and 1 mL aliquots were inoculated into 85 glass bottles (350 mL) containing 40 mL of PDA. Then bottles were incubated for 21 days at 30 °C. Secondary metabolites were extracted into MeOH and the extract was concentrated to ~1/5 of its volume to remove MeOH and partitioned with EtOAc. The EtOAc extract (2.07 g) was dissolved in 80% aqueous-methanol and partitioned with hexane. The 80% aqueous-methanol fraction was diluted to a 50% aqueous-methanol solution, and then partitioned with CH_2Cl_2 . Each organic layer was evaporated to dryness under vacuum at 40 °C to yield the hexane fraction (0.38 g) and CH_2Cl_2 fraction (1.33 g). Antibacterial CH_2Cl_2 fraction was further fractionated by repeated column chromatography over Sephadex-LH20 and SiO_2 followed by preparative TLC to yield two compounds, (**3**) and (**4**).

Results and Discussion

Investigation of *P. citrinum*

Citriquinone A (1**):** Afforded as a yellow solid, $[\alpha]_D = -6.35$ (c 0.524, CHCl_3). High resolution ESI(±)MS analysis gave pseudomolecular ion at m/z 337.1646 $[\text{M}+\text{H}]^+$ (calculated for $\text{C}_{18}\text{H}_{25}\text{O}_6$, 337.1644) revealing the molecular formula to be $\text{C}_{18}\text{H}_{24}\text{O}_6$. The IR spectrum showed absorptions at ν_{max} 3430(br), 2862(sh) and 1717 cm^{-1} suggesting the presence of a hydroxyl group, hydrogen atom bonded to a carbonyl carbon and a ketone carbonyl respectively while the peak at ν_{max} 1637 cm^{-1} together with the ^{13}C NMR signals at δ 187.02 and 182.94 suggested the presence of a 1,4-benzoquinone system.

Table 1: NMR data of **1** (600MHz, CDCl_3) and **2** (400MHz, CDCl_3)

| Position | 1 | | | 2 | | |
|----------|-----------------------------------|---------------------|-------------------------|-----------------------------------|---------------------|-----------------|
| | δ_{H} (m, J (Hz)) | δ_{C} | gHMBC | δ_{H} (m, J (Hz)) | δ_{C} | gHMBC |
| 1 | 1.34 (3H, d, 6.0) | 19.02 | 4, 3, 2 | 1.35 (3H, d, 4.0) | 19.24 | 2,3 |
| 2 | 5.46 (1H, m) | 72.83 | 4, 3, 1', 2-OCHO | 5.46 (1H, m) | 73.10 | 2-OCHO |
| 3 | 3.04 (1H, m) | 40.04 | 2', 6' | 3.05 (1H, m) | 40.30 | 1, 2', 6' |
| 4 | 1.23 (3H, d, 7.2) | 15.42 | 1, 3, 2, 1' | 1.25 (3H, d, 8.0) | 15.63 | 2, 3, 1' |
| 2-OCHO | 7.84 (1H, s) | 160.19 | 2 | 7.86 (1H, s) | 160.47 | 2 |
| 1' | | 140.23 | | | 140.18 | |
| 2' | | 144.84 | | | 145.50 | |
| 3' | | 187.02 | | | 187.17 | |
| 4' | | 150.75 | | | 123.70 | |
| 5' | | 119.89 | | | 150.70 | |
| 6' | | 182.94 | | | 183.36 | |
| 2'-Me | 2.07 (3H, s) | 12.53 | 2, 3, 4, 1', 2', 3', 6' | 2.07 (3H, s) | 12.91 | 1', 2', 3' |
| 5'-OH | 7.05 (1H, s) | | | 7.13 (1H, s) | | 4', 5' |
| 1'' | 2.39 (2H, t, 7.8) | 22.60 | 3'' 2'', 5', 4', 3' | 1.19 (3H, d, 8.0) | 18.47 | 4', 3'' |
| 2'' | 1.43 (2H, m) | 27.51 | 1'', 4'', 5' | 3.01 (1H, m) | 29.97 | 1'', 3', 4', 5' |
| 3'' | 1.57 (2H, m) | 23.58 | 1'' 2'', 4'', 5'' | 1.63 (2H, m) | 30.50 | 2'' |
| 4'' | 2.43 (2H, t, 7.8) | 43.36 | 1'', 2'', 5'' | 1.23 (2H, m) | 37.90 | 2'' |
| 5'' | | 209.16 | | 3.74 (1H, m) | 68.39 | 3'' |
| 6'' | 2.11 (3H, s) | 29.91 | 3'', 4'', 5'' | 1.14 (3H, d, 4.0) | 23.63 | 4'', 5'' |

¹³C assignments were made with the help of both gHSQC and gHMBC experiments

The ^1H and ^{13}C NMR together with HSQC data (Table 1) showed the presence of four methyls, of which two are secondary [δ_{H} 1.34 d, ($J = 6.0$ Hz) and 1.23 d, ($J = 7.2$ Hz); δ_{C} 19.02 and 15.42] and two are tertiary (δ_{H} 2.07 and 2.11 s; δ_{C} 12.53 and 29.91), four methylenes, three methines, of which one is a formyl group (δ_{H} 7.84 s; δ_{C} 160.19) and seven quaternary carbons of which three are carbonyls (δ_{C} 182.94, 187.02 and 209.16). The ^1H - ^1H COSY spectrum of **1** showed, that the multiplet at δ 3.04 correlates with the methyl protons at δ 1.23(d) and with the multiplet at δ 5.46, which correlates with the methyl group at δ 1.34, revealing the spin system $\text{CH}_3\text{-CH-CH-CH}_3$ (Figure 1). The singlet appearing at δ 7.84 in the ^1H NMR spectrum showed HMBC correlation to the oxygenated methine carbon at δ 72.83 and the proton attached to that oxygenated methine carbon (δ_{H} 5.46) showed HMBC correlation to the carbonyl carbon at δ 160.19 indicating the presence of a HCO_2 group (Figure 1). The ^1H - ^1H COSY spectrum further showed that the multiplet at δ 1.43 ($\text{CH}_2\text{-2''}$) correlates with the triplet at δ_{H} 2.39 ($\text{CH}_2\text{-1''}$) and with the multiplet at δ_{H} 1.57 ($\text{CH}_2\text{-3''}$), which correlates to the triplet at δ_{H} 2.43 ($\text{CH}_2\text{-4''}$), revealing the spin system $\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2$ (Figure 1). The singlet appearing at δ 2.11 in the ^1H NMR spectrum depicted a methyl group adjacent to a carbonyl carbon, which showed HMBC correlations to the carbonyl carbon at δ 209.16 and to the methylene carbon at δ 43.36 (C-4'') suggested the presence of a CH_3CO group attached to the $-\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2-$ spin system (Figure 1). Methyl protons at δ 2.07 showed HMBC correlations to the carbonyl carbon at δ 187.02 (C-3'), 144.84 (C-2') and 140.23 (C-1') placing it at C-2', while the methyl protons at δ 1.23 showed HMBC correlations to carbon at δ 140.23 indicating the connectivity between C-3 and C-1'. Protons appearing at δ_{H} 3.04 showed HMBC correlations to carbonyl carbon at δ 182.94 (C-6') and 144.84 (C-2') while protons at δ_{H} 2.39 showed HMBC correlations to carbons at δ 187.02 (C-3'), 150.78 (C-4') and 119.89(C-5'). These evidence collectively suggested the connectivity of the molecular fragments to the 1,4-benzoquinone ring system as shown in Figure 1.

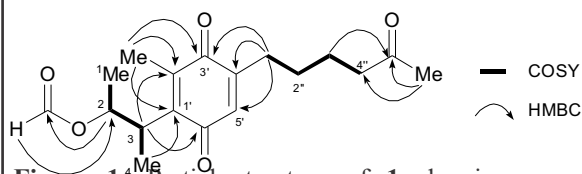


Figure 1: Partial structure of **1** showing some important COSY and gHMBC correlations

As there is no evidence for vinylic H atoms, it is suggested that the hydroxyl group is located at the 5' position of the quinone ring system. Thus, the structure of **1** was elucidated as 3-(5-hydroxy-2-methyl-3,6-dioxo-4-(5-oxohexyl)cyclohexa-1,4-dienyl)butan-2-yl formate (**1**) and stereochemistry of C-2 and C-3 positions were assigned as *R* and *S* respectively comparing the coupling constants of reported citrinin

derivatives having similar chiral centers^{7,8}.

Citriquinone B (2): Afforded as a yellow solid, m/z 337 $[\text{M-H}]^-$, $[\alpha]_{\text{D}} = -15.57$ (c 0.136, CHCl_3). The molecular formula of **2** was established as $\text{C}_{18}\text{H}_{26}\text{O}_6$ by a combination of low resolution ESI ($\pm$) MS and NMR data. The ^1H NMR and ^{13}C NMR spectra of **2** revealed a close relationship to **1** except for the absence of a ketone carbonyl (δ_{C} 209.16) and presence of an additional methyl group (δ_{H} 1.19; δ_{C} 18.47) (Table 1). Comparison of molecular formula and ^1H - and ^{13}C -NMR spectra of **2** with those of **1** revealed that **2** differed from **1** only in the side chain attached to the C-4' position of the benzoquinone moiety. The ^1H - ^1H COSY spectrum showed that the methyl doublet at δ 1.19 correlates with the methine protons at δ 3.01(m) while the methyl group at δ 1.14(d) correlates to the methine protons at δ 3.74(m), revealing the presence of two CH_3CH spin systems (Figure 2). The presence of $\text{CH}_2\text{CHCH}_2\text{CH}_2\text{CHCH}_3$ system was evident by HMBC correlations (Figure 2). The secondary methyl group at δ_{H} 1.14 ($\text{CH}_3\text{-6''}$) showed HMBC correlation with the oxygenated carbon at δ 68.39 (C-5'') and the methylene carbon at δ 37.90 (C-4'') while the methylene protons at δ 1.23 ($\text{CH}_2\text{-4''}$) showed HMBC correlations with the methine carbon at 29.97 (C-2''). The secondary methyl group at δ_{H} 1.19 ($\text{CH}_3\text{-1''}$) showed HMBC correlation with the methylene carbon at δ 30.50 (C-3'') while the methine protons at δ 3.01 showed HMBC correlations with the methylene carbon at δ 37.90 (C-4''). HMBC correlation between δ_{H} 1.19 ($\text{CH}_3\text{-1''}$) and δ_{C} 123.70 (C-4') established the connectivity of $\text{CH}_2\text{CHCH}_2\text{CH}_2\text{CHCH}_3$ spin system to the benzoquinone ring (Figure 2). Thus the structure of **2** was established as 3-(5-hydroxy-4-(5-hydroxyhexan-2-yl)-2-methyl-3,6-dioxocyclohexa-1,4-dien-1-yl)butan-2-yl formate.

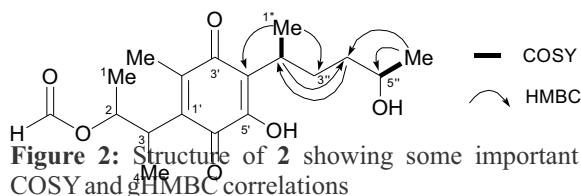


Figure 2: Structure of **2** showing some important COSY and gHMBC correlations

Presence of stereoisomers as a mixture was evident by the fine splitting of the methyl signals at δ 1.19 and 1.25 and fine doubling of some of the ^{13}C NMR signals. Further attempts are being made to separate the stereoisomers of citriquinone B.

Bioactivity Studies

Antibacterial Assay

CH_2Cl_2 extract and citriquinone A (dissolved in MeOH) found to be showing antibacterial activity against *Bacillus* sp., when subjected to antibacterial assay (Table 2).

Table 2: Fractions obtained from solvent partitioning and their activity against *Bacillus* sp.

| Fraction | Dose ($\mu\text{g}/\text{disc}$) | Diameter of Clear Zone (mm) |
|-------------------------------|------------------------------------|-----------------------------|
| Hexane | 500 | - |
| CH_2Cl_2 | 500 | 9.5 |
| 50% aqueous MeOH | 500 | - |
| Citriquinone A | 250 | 16 |
| Positive control: Amoxicillin | 25 | 12 |

Cell Migration Inhibition Assay on Cancer Cells

The EtOAc extract, Hexane fraction, CH_2Cl_2 fraction and **1** were subjected to cell migration inhibition assay on cancer cell line HEP 2.

Table 3: Results of Cell Migration Inhibition Assay

| Fraction | Dose (mg / mL) | Growth effect |
|-----------------------------|----------------|---------------|
| Hexane | 0.5 | Toxic |
| CH_2Cl_2 | 0.5 | Inhibition |
| Citriquinone A (1) | 0.5 | Inhibition |

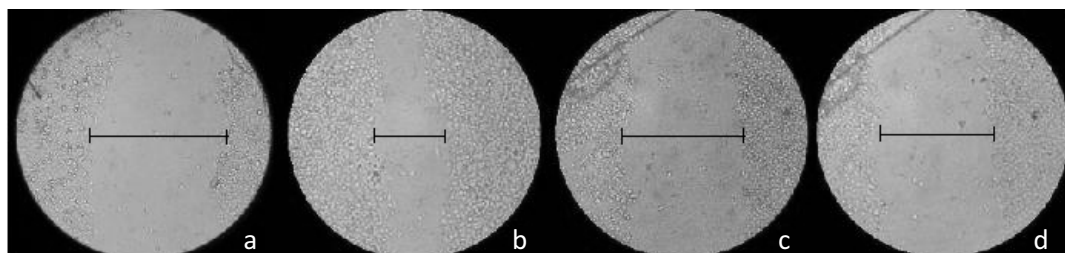


Figure 3: Cell migration inhibition assay data of **1**: Image of the scratch; (a) with control, before incubation (b) with control, after incubation (c) with citriquinone A, before incubation (d) with citriquinone A, after incubation

EtOAc extract at higher concentrations (≥ 1.5 mg/mL) and hexane fraction were found to be toxic to the cells thus detaching the cells from the surface. By comparing the width of the scratch, before and after incubation, it was revealed that CH_2Cl_2 fraction and **1** had inhibited growth/ cell migration of the cells when compared to the control (See Figure 3). Thus the results revealed that **1** is having potential anticancer activity, and further studies relating to the evaluation of the anticancer properties of citriquinones would be much beneficial for the mankind.

Investigation of *A. terreus*

The structures of (**3**) and (**4**) were established as butyrolactone I and (+)-geodin respectively by extensive usage of spectroscopic data (Table 4) and confirmed by comparison with reported values⁹⁻¹¹.

Table 4: NMR data of **3** and **4** (400MHz, CDCl_3)

| 3 | | | | 4 | | | |
|----------|------------|------------------------|--------------------|----------|------------|------------------------|----------------|
| Position | δ_c | δ_H (m, J (Hz)) | gHMBC | Position | δ_c | δ_H (m, J (Hz)) | gHMBC |
| 1 | 169.44 | - | - | 1 | 165.44 | - | - |
| 2 | 137.44 | - | - | 2 | 109.47 | - | - |
| 3 | 128.26 | - | - | 3 | 193.37 | - | - |
| 4 | 85.77 | - | - | 4 | 149.35 | - | - |
| 5 | 170.21 | - | - | 5 | 114.74 | - | - |
| 6 | 38.58 | 3.39(2H, m) | 4, 1'', 3, 2'', 5 | 6 | 146.59 | - | - |
| 1' | 121.90 | - | - | 7 | 108.86 | - | - |
| 2', 6' | 129.33 | 7.54(2H, d, 8.8) | 3, 4' | 6-Me | 18.76 | 2.56(3H, s) | 5, 6, 7 |
| 3', 5' | 115.78 | 6.84(2H, d, 8.8) | 1', 4' | 1' | 165.39 | - | - |
| 4' | 157.46 | - | - | 2' | 137.03 | - | - |
| 1'' | 124.20 | - | - | 3' | 137.56 | 7.12(1H, s) | 1', 2', 5' |
| 2'' | 131.66 | 6.45(1H, d, 2.0) | 7'', 6, 6'', 4'' | 4' | 184.98 | - | - |
| 3'' | 126.91 | - | - | 5' | 104.45 | 5.80(1H, s) | 3', 4', 6', 7' |
| 4'' | 153.39 | - | - | 6' | 167.88 | - | - |
| 5'' | 114.52 | 6.47(1H, d, 8.0) | 1'', 3'', 4'' | 7' | 84.50 | - | - |
| 6'' | 128.95 | 6.54(1H, dd, 2.0, 8.0) | 6, 2'', 4'' | 1'-OMe | 57.03 | 3.68(3H, s) | 1', 2' |
| 7'' | 28.43 | 3.08(2H, d, 7.2) | 8'', 3'', 9'', 4'' | 6'-OMe | 53.15 | 3.73(3H, s) | 5', 6' |
| 8'' | 121.82 | 5.05(1H, t, 6.0) | 10'', 11'' | | | | |
| 9'' | 133.30 | - | - | | | | |
| 10'' | 17.61 | 1.57(3H, s) | 11'', 8'', 9'' | | | | |
| 11'' | 25.63 | 1.63(3H, s) | 10'', 8'', 9'' | | | | |
| 5-OMe | 53.40 | 3.72(3H, s) | 5 | | | | |

Bioactivity Studies

Antibacterial assays carried out in different concentrations, revealed that both compounds are active against *Bacillus* sp. while **4** found to be more active than an equivalent dose of Amoxicillin (Table 5).

Table 5: Activity of **3** and **4** against *Bacillus* sp.

| Test Sample | Dose ($\mu\text{g}/\text{disc}$) | Diameter of Clear Zone (mm) |
|-------------------------------|------------------------------------|-----------------------------|
| 3 | 150 | 12.5 |
| 4 | 25 | 18.0 |
| Positive control: Amoxicillin | 25 | 12.5 |

Acknowledgement

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POST GRADUATE RESEARCH IN SRI LANKA (a student perspective)

Dr. A A P Keerthi

*Faculty of Medicine / South Asian Institute of Technology and Medicine, Malabe***Preamble**

To date the Institute of Chemistry Ceylon has been playing a leading role in the tertiary education system in Sri Lanka producing chemistry special graduates more than the national universities. Majority of these graduates may join the private or government sector, self-employment (i.e. tuition and own business) or seek opportunities to read for higher degrees in the field of chemistry or any other subject areas. The latter may select the M.Sc.s, MBAs etc., or search for more exciting experience involving novel hypothesis and findings via registering for the research based higher degrees such as M. Phils and PhDs. These types of research programmes are directed to highly specified subject areas and need to have a good financial support. The only available options for a financial support are either a scholarship from a foreign or local university/research institute. Realistically, other than academic achievements and satisfaction gained by a student both these options is not financially fruitful. In spite of the challenges faced by these young graduates, they sacrifice the most valuable and critical era of their lives and not being given sufficient recognition.

What are the challenges faced by a young graduate who embarks on a research programme? How does one become a successful researcher? How does one find a supervisor or identify your project? What should one expect from your supervisor? How to handle difficult situations? These are some of the thoughts related to a research project that I wish to highlight in this report.

Choice of research field/topic, Do you really need it?

A student who wishes to engage on a postgraduate degree or research programme needs to be careful on selecting his/her research field. It is better if the research is your own field of interest, an area which is more familiar and in which it is more suitable to your expertise. Senior teacher's advice may help on your decision making but no extrinsic factors should come into play. A total commitment on your research work is essential.

How do you find a supervisor?

A success of a research programme/project depends on your supervisor to a greater extent. What are the points you need to consider in this regard?

The supervisors' field of expertise and interest should be in line with your research interest. His/her previous project records, successful projects, number of successful post graduate degree students, number of publications of his/her students' credit from each project/degree and the number of unsuccessful project/degrees, will reflect the actual capabilities of a supervisor.

Expert collaborators are needed to support the research project and the students when necessary. Professional supervisors always openly express their role and that of his/her collaborators. Collaborators contribution to the project is very significant, such as scheduled plans for the future, what is expected from a research student and any specific training or skills that the student should master before commencing the research. Confidence of a supervisor will help to counter numerous scientific challenges that await you.

Start and the progress of a research

It is necessary to collect and study the relevant literature prior to commencing the research and before submitting the research proposal. This will help you to understand the depth of your research study. Gathering literature is a never ending exercise that continues throughout the research work and it is more beneficial towards the end. The detailing of the research proposal can be worked out based on the literature and a series of discussions with your supervisor/s. A well prepared research student could gain the supervisors confidence by actively participating (i.e. well prepared ahead, questioning and answering, progress of the literature reading and the research and etc.) in these discussions/meetings.

Before starting a research there are list of things that a student and the supervisor should discuss together, such as availability of procedures (i.e. synthetic and analysis) equipment and chemicals in Sri Lanka. These requirements should be sent to the relevant officials for further actions. Maintenance of stocks of adequate chemicals and relevant equipment will ensure a smooth flow of laboratory work. Availability of more than one source of funds to support the research would be an added advantage, especially in our country where finances for research grants are sometimes insufficient.

It may be necessary to optimize the proposed experimental protocols by doing several trials subsequent to the experimental protocol which can be amended after discussing with supervisor/s. At every level it is necessary to accept both positive and negative results evenly. It is not important to have concrete predictions on results other than the hypothesis such as predictions otherwise it can hinder wide open discussions based on results. It is a misconception that all negative results are useless. Failures are the pillars of success. There are some instances where researchers have achieved heights on so called negative results. Visionary supervisors always encourage their students to make use of the negative results.

Regular lab/field visits of a supervisor will helpful to a student to improve his/her lab/field skills, motivation, productivity, credibility and confidence about the work. Working in a research group with

other researchers (i.e. multidisciplinary research group) at different levels and the exposure of a research background would have a great impact on a new research student.

Lab record book

Keeping records and maintaining a lab record book are extremely important in the case of laboratory/field work and experiments.

Maintaining a lab book with page numbers, experiments or field work numbering, date, sample labelling according to the experiment/field number and same as for the results are good practices of an excellent student and a researcher. This is very useful in future for the relevant student, new students who want to continue the research work and the supervisor. For an example his/her future use (i.e. dissertation/thesis/report writing) and supervisor to find out the drawbacks, to upgrade, to venture new avenues out of the research projects, publications etc. Some may prefer to maintain record books only for the results. However, incorporating all the rough work on the record book may help the student to trace some genuine mistakes. Alternatively a separate record book can be maintained for this purpose.

First-class supervisors always do unexpected visits to the lab bench or experimental field and do on the spot check of the progress, record books or field notes, results, statistics and etc. There supervisor's guidance, instructions and questions are very helpful to sharpen the student's research skills, communication and teaching abilities as well as the personality.

These occasions could be very productive discussion platforms for the student and the research team. It is good for the students to expect regular supervision sessions so that they are motivated and prepared at anytime. From the students' point of view keeping records on this type of scientific discussions would be an added advantage. Sometimes students may be reluctant to have unexpected lab visits at the postgraduate level, but to work with such supervisor is an asset.

Progress report

Once the research programme has started the student is bound to work within the specific deadlines. This will help the student to plan the programme or the work load ahead and also for funding agencies, supervisors and the institute/university to monitor your progress. It is the student's duty to submit progress reports periodically to all interested parties.

Progress reports should monitor without exposing much raw data to the public. Students are always given feedback on his/her progress after reviewing their reports.

It is important to address issues, mistakes and further work that a student could do to improve the quality of the research. These can be taken as constructive criticisms. Apart from funding agencies, other stakeholders are also seeking progress reports. Uninterrupted research reports could ensure continuation of the funding in case of leading to a higher degree (i.e. M.Phil. to Ph.D.).

Publications

Publications are one of the major outcomes of a research which is an asset for student, supervisor and science community. Once a student have reasonable results supervisor always encourage writing a paper. Laying foundation for a paper will show the needing results, missing or mislaid parts and things that needs to be done further to have a complete set of results to write a good discussion on the research. In case of journal article it is very important to build up arguments and forward discussion leading to conclusions.

Writing abstract needs more proficiency as it has to be summarized to a few paragraphs (i.e. maximum 1 A4 page). Oral presentations are very important part of a research project. As with most personal **skills oral communication cannot be taught**. Supervisor/instructors can only point the way. So as always, practice is essential, both to improve your skills generally and also to make the best of each individual presentation you make. During the research programme a student get several chances to present their results such as group, departmental, progress review, symposiums, seminars and conferences. Those are valuable chances for a student to build up their communication skills, confidence, quick thinking ability and mostly to defence their final thesis.

The material of your presentation should be concise, to the point and tell an interesting story (i.e. story is consistent and flows smoothly). In addition to the obvious things like content and visual aids, the following are just as important as the audience will be subconsciously taking them in:

- **Your voice** - *how* you say it is as important as *what* you say
- **Body language** - a subject in its own right and something about which much has been written and said. In essence, your body movements express what your attitudes and thoughts *really* are.
- **Appearance** - first impressions influence the audience's attitudes to you. Dress appropriately for the occasion.

Prepare the structure of the talk carefully and logically, just as you would do for a written report. What are:

- the objectives of the talk?
- the main points you want to make?
- Presentations should highlight results/outcomes of the research.

The supervisors' role is to guide you in the preparation of the manuscript and it should also focus on improving your scientific language and expression while retaining your individuality. Contributions of collaborators and supporting staff should always be duly acknowledged.

Student teacher relationship

It is always necessary to have a good mutual relationship between the teacher and the student. It is important the student to consider his/her supervisor as a senior respected academic and a mentor. Student should never underestimate or compare his/her supervisors' with other supervisors. Students should win the confidence of the supervisor throughout his/her research work and not by other means. It is not

necessary to be a favourite or a close friend of your supervisor. Good supervisors always keep their distance from the student and never assign tasks other than those related to the research work. The supervisor should be a role model encouraging the students to develop good academic practices such as punctuality, professionalism etc.

Generally, at the initial stage of the research students depends more on supervisor(s) and with time, after successful training he/she begins to exhibit his/her individuality and scientific maturity.

How to handle problems

Unavoidable arguments, problems or situations can arise between supervisors and student. Some of these may be beyond students' control. It is always advisable to consult a respected senior member of the staff or higher officials such as Dean of the postgraduate institute/faculty etc. It is a duty of all the parties to resolve such situation with minimal damage to the research; student and supervisor(s). Supervisor should always play a mature role in such situations.

Scientific arguments between supervisors, students and research group are essential for progress. These types of arguments should be presented along with supporting scientific evidence such as literature, calculations or results. Counter arguments should be critically evaluated before reaching conclusions. It may be useful to remember that the student may not be correct and it is the supervisors' role to indicate the student where he/she has gone wrong. This will certainly contribute to the success of the research project.

Thesis

Before start writing the thesis it is necessary to identify guidelines of the relevant postgraduate faculty or university regarding the procedures to be followed.

It is wise to start with literature review. It is advisable to discuss the flow of the thesis at frequent intervals by giving drafts of sections/chapters for correction and receiving feedback of the supervisor. This practice is very good till the end of the

thesis/dissertation completion and also for the supervisor. Then the supervisor has a good idea about the content and the flow of the story. This avoids the repetitions and mistakes done in conclusions/summary/linked chapters etc.

Once the thesis was prepared it is a common practice to request soft copies of the thesis or document for perusal. This may be subjected to screening by search engines which would point where any incorrect procedures such as plagiarism could be detected. Plagiarism should never be resorted to in the preparation of a thesis or a publication. Already published material can be incorporated to your thesis giving relevant credits to authors.

Unexpected genuine mistakes can be observed when writing your thesis and the necessary alterations can be done by further lab work and analysis. The lab record book, results, statistics and records of discussion with supervisor(s) are very important for the thesis writing. Amendments and corrections of the thesis should be done according to the supervisors' comments. Rehearsals for the final thesis defense are often arranged by the supervisor. At this point the student should have the self confidence to realize that he/she is the most knowledgeable and an expert on his/her research project. High-quality supervisors always lead the research students to this point of excellence.

The postgraduate research or degree cannot just simplify to a qualification. It is important to mold professional qualities together with career development. After successful completion of your research the supervisor-student relationship takes on to a new dimension. It becomes a lifelong relationship with more professional respect for one another. However, you should remember that although now you are an individual in your own right, your supervisor will always stand out as a teacher and will be there for you.

(Special thanks: Prof. E R Jansz, Prof. S Goonewardene, Wageesha, Thushari)

Students' Talent Show - AURA IV



Aura IV held on 20th July at Janakala Kendraya, Battaramulla, turned out to be a fascinating, entertaining, well organized and splendid performance by our students at all Levels in the form of Dance, Song, Drama and Orchestra etc. Our congratulations to them!



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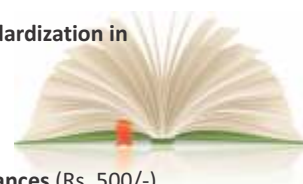
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RSC NEWS

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 | Number |
|---|------------------|
| CChem, FRSC | 11 |
| FRSC | 05 |
| CChem, MRSC | 10 |
| MRSC | 20 |
| AMRSC | 08 |
| Affiliate /Under Graduate. | <u>06</u> |
| Total Membership as at July 2012 | <u>60</u> |

2. Committee of Management

The following were elected to the Committee at the 51st Annual General Meeting held on 27th July 2012.

| | |
|-----------------|--------------------------|
| Chairman | - Dr. M P Deeyamulla |
| Vice Chairman | - Mr. W J P D Jayalath |
| Chairman Elect | - Mr. I M S Herath |
| Hony. Secretary | - Dr. Positha Premaratne |
| Hony. Treasurer | - Prof. W S Fernando |

Committee Members - Prof. Sudantha Liyanage
Mr. W A P Silva
Mr. S Perasiriyan
Mr. R M G B Rajanayake
Mr. Sulith Liyanage

3. Committee Meetings

There were 12 Committee Meetings held during the period, July 2011 to July 2012. 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 2011/2012 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) Contribution for the Interschool Chemistry Quiz

(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 IYC Challenge project at Eastern Province.

4.4 Inter - University Chemistry Competition.

4.5 Teacher training program.

4.6 Advanced Level chemistry seminar.

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

4.8 Book donation program.

4.9 Popular Lectures.

4.10 Industrial Visit.

4.11 Writing Monographs by few committee members.

4.12 Newton A. Dias Weerasinha Memorial Scholarship 2011/2012

4.13 Popularisation of Chemical Science and Teacher training programme and book donation programme at Trincomalee.

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/SriLanka/index.asp.

Dr. Positha Premaratne
Hony Secretary

Chemical Education Workshop



Annual Dinner & Induction of the New President: Dr. S Mohanadas





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