The Importance of Being Floppy
By John Yip Hon Kay

A friend of mine once told me that organic chemists are people who try to reproduce what God has already made, while inorganic chemists make molecules that the Providence did not bother to create. Like many other general statements, it is an exaggeration. In fact chemists have been looking for similarity between organic and inorganic compounds. For example, there is a continuous search for organic compounds that exhibit superconductivity as some copper oxides. And it is a triumph for inorganic chemistry to reproduce what God has already made, as some copper oxides. And it is a triumph for inorganic chemistry to prove my hypothesis, we had done a lot of variable temperature and 2-D NMR studies. I would not bore you with all the details; suffice to say our low temperature EXSY (exchange spectroscopy) study clearly shows that there is an exchange between Phax and Pheq rings, a telling sign for cyclohexane-like ring inversion. Based on these results we arrived at the conclusion that the gold ring flips like cyclohexane in solution. Unlike the organic molecule, the gold ring is floppy and the inversion, explaining why there is only one sharp 31P signal. To prove my hypothesis, we had done a lot of variable temperature and 2-D NMR studies. I would not bore you with all the details; suffice to say our low temperature EXSY (exchange spectroscopy) study clearly shows that there is an exchange between Phax and Pheq rings, a telling sign for cyclohexane-like ring inversion. Based on these results we arrived at the conclusion that the gold ring flips like cyclohexane in solution. Unlike the organic molecule, there is only one explanation for these contradictory 1H and 31P NMR results: the gold ring is floppy and the fluxional process is the same as the ring inversion of cyclohexane. In the ring inversion, the diastereotropic Ph rings switch their positions and this would explain why the 1H NMR signals are very broad. On the other hand, the P atoms in the corners remain unchanged throughout the inversion, explaining why there is only one sharp 31P signal.

Recently my graduate student Prabha studied the reaction between Me3AuCl (a common starting material for gold(I) complexes) and a bidentate phosphine 9,10-bis(diphenylphosphino)anthracene (PAuP). A bright yellow solid was isolated from the reaction and the X-ray crystal structure of the compound (solved by Prof. J.J. Vittal) shows a gold ring composed of three Au(I) atoms and three PAuP. The ring is puckered, showing a chair conformation very similar to cyclohexane. A perchlorate ion is trapped in the ring. There are two sets of phenyl groups in the gold ring: the ones sticking inwardly (Phin) and the ones pointing outwardly (Phout). Like the protons in cyclohexane, the Pheq and Phax are diastereotopic.

We were overjoyed when we saw the crystal structure as puckered metalacycles are rare. However, we did not start to write a paper on it because we had problems interpreting the NMR spectra of the complex. We found that the 31P NMR spectrum showed only one sharp signal but the 1H NMR signals were broad and unresolved. I had Prabha repeat the 1H NMR three times and was convinced that the broad 1H NMR signals were real. Then it occurred to me that there is only one explanation for these contradictory 1H and 31P NMR results: the gold ring is floppy and the fluxional process is the same as the ring inversion of cyclohexane. In the ring inversion, the diastereotropic Ph rings switch their positions and this would explain why the 1H NMR signals are very broad. On the other hand, the P atoms in the corners remain unchanged throughout the inversion, explaining why there is only one sharp 31P signal.
Carbon is one of the building blocks of life and for those who study carbon in its many incarnations, it is indeed fortunate that it has isotopes. The major stable-isotope is carbon-12, the minor isotope (~0.1%) is carbon-13 and the ratio of these isotopes in any compound is a fundamental tracer of the processes involved in the compound’s formation. The third isotope is carbon-14, radiocarbon, which has the additional advantage of undergoing radioactive decay.

The isotopic fingerprints imparted by compounds by the chemical processes that led to their formation have provided a wealth of information in a multitude of disciplines. The stable-isotope composition of carbon dioxide and methane in the atmosphere traces the sources and fates of ‘greenhouse gases’ and compound-specific isotope analyses trace the origin of petroleum. In other fields, the isotopic composition of Egyptian mummies has provided information on their diet and the isotopic composition of carbonates in Martian meteorites has added fuel to debates on the possibility of life on other planets. Radiocarbon dating has provided ages on everything from the earliest humans to the Shroud of Turin.

Since arriving at the Chemistry Department, Dr. Bird has found another place to use biogeochemical techniques, including carbon isotope analyses – a 22 metre-thick pile of bird and bat excrement (guano) in a cave in Borneo. This may not sound like an attractive target for research but the guano in Niah Cave (northern Sarawak) may archive a goldmine of environmental information. Dr. Bird visited the cave in April, as part of an archaeological expedition. The human skull was found in the deposits in the cave in 1955 but the age of the ‘Niah Skull’. Dr. Bird took samples from the pile of guano deep in the cave for radiocarbon dating, and the dates suggest that the guano is 30,000 years old 4 metres down into the deposit. Therefore the whole pile of guano might represent over 100,000 years of accumulation.

Guano is ultimately derived from vegetation. The vegetation was eaten by insects, the birds and bats ate the insects, and deposited the residue of their meal in the cave. Different types of vegetation have distinctive carbon-isotope compositions and so the pile of guano represents a long record of vegetation and climate change in the region, as well as a bad smell. In addition, the layers of guano would have trapped material blown into the cave as they accumulated slowly. This material would include dust blown from the Himalayas during dry climatic periods and fine soot from biomass burning. Thus the guano also should contain a long record of biomass burning and changes in global aridity.

The pile of guano has the potential to be one of the few long records of environmental change in the Indonesian archipelago – a region of vital importance to global climate. The results will also assist in understanding the genesis of the smoke haze that periodically obscures Singapore. Extracting the environmental records hidden in the guano is the task ahead, but in common with much modern environmental research, this task comes down to the application of knowledge derived from basic research in Chemistry.
Dr Sim Wee Sun awarded the DuPont Asian and European Young Professor Award

Congratulations to Dr Sim Wee Sun who has recently been awarded the DuPont Young Professor Award!

This prestigious Award, sponsored by the DuPont Fellows Forum and the DuPont Corporate Centre for Collaborative Research and Education, is designed to provide startup grants to help outstanding young university faculty members launch their research careers. In recent years, between ten to fourteen Young Professor grants have been awarded annually in the United States on a competitive basis. The success of this programme has prompted DuPont to extend the award to include nominations from Asia and Europe in 2001. This year, the Selection Committee has received 36 nominations for the Asian and European Young Professor grants, and 4 awards have been made. The grant will provide funding of US$25,000 per year for up to three years to support highly original research programmes of value to DuPont.

Wee Sun graduated with a B.Sc. (First Class Honours) degree in Chemistry under the Direct Honours programme from NUS in 1992. He received funding from the Cambridge Commonwealth Trust and a Benefactor’s Scholarship from St John’s College at Cambridge to pursue PhD at the University of Cambridge under the supervision of Professor David A. King, FRS. He was subsequently awarded an Oppenheimer Research Fellowship to conduct postdoctoral work at Cambridge before joining NUS as a Faculty member in 1997.

Wee Sun’s research focuses on the application of modern surface analytical techniques to study the interaction of solid surfaces with adsorbed molecules. He aims to gain molecular-level understanding and control of technologically relevant surface processes that are of crucial importance in the fields of heterogeneous catalysis, microelectronics and thin film technology. The DuPont Young Professor grant will be used to support his research programme in which the surface chemistry of self-assembled thin organic films will be studied in detail in an effort to understand and develop their role in advanced semiconducting and light emitting devices.

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Chemistry Graduate Students Form Club! http://www.chemistry.nus.edu.sg/cgc/cgsc.htm

The wisdom inherited from our ancestors has always been deeply embedded in us – Man cannot live and work alone. We all depend on one another. In today’s world, in which the pace towards globalization keeps increasing with time, networking is becoming even more important. Now, it is no longer sufficient to network within a small local community. We need to form multinational, trans-national networks to keep up with the pace of globalization. Based on this ambition and far-sightedness, the Chemistry Graduate Club (CGC) has been formed by the Department of Chemistry’s large cohort of academic and social lives on campus through creative and full utilization of existing resources, and exposure to the chemical industries. With this mission in mind and a shared vision to develop the club into a constantly forward-looking club that brings together its graduates, the Department and chemical industries in Singapore, the team has already started to organize activities, with the first being a friendly soccer game between graduates and staff and a logo competition. Expect more activities in the months to come......

By Goh Ho Wee
Chair of CGC
Appreciation Dinner

In conjunction with the NUS Quality Service Day on the 8th of November, the Department organized an Appreciation Dinner at Raffles Town Club.

The Department is rapidly moving into a new phase of development and is now placing a lot of emphasis on the development of her people, the international impact of work, and the educational support in this knowledge-based economy. Our present success owes a great deal to our pioneers who have contributed to the Department’s development in a very difficult period of its history when we strove to gain international treatment to determination of protein structures.

Seven Japanese scientists have been invited to participate in the Symposium. Local invited speakers include those from the Department of Chemistry, Department of Biological Sciences, Department of Chemical and Environmental Engineering, Department of Civil Engineering, the Environmental Technology Institute, etc.

Chemistry alumni, especially those in industry, are especially welcome to participate. There is no registration fee. Please view the website http://www.chemistry.nus.edu.sg/chmjsps.htm for updated information, including registration details.
The vision of the Department’s outreach programme has slowly been defined to meet the challenges of the 21st Century for NUS and Singapore. Our theme is establishing and maintaining “A premier outreach programme that is continually relevant to the Department’s teaching and research, locally and globally”. In pursuit of this vision, the members of the Department’s outreach committee has set up the requirements for establishing a credible outreach programme into three broad areas that are **recruitment**, **nurturing** and **aftercare**.

### Recruitment

The agenda in **recruitment** is to excite those choosing to study at NUS to consider the wonderful world of Chemistry. We have divided schools, junior colleges (JCs) and polytechnics into geographical groupings and created teams into GSNs (Geo-Specific Networks) to continually reach out to schools in Singapore. It has been fortuitous that NSTB and MOE have also thought along these lines. Therefore when the call came for participation in a pilot project called the “Teacher’s-Aides” programme to the northern school cluster to support teachers with our research expertise in 2002, the Department was well positioned to not only meet the expectations for the pilot project but had in place the organizational structure to implement the full programme in 2003. Also, with a revised script in hand, we will continue to visit schools and JCs to impart to them the necessity of a good foundation in Chemistry as a good career choice as well as a springboard to excelling in the life sciences so important to Singapore today.

### Nurture

In **nurture**, the committee endeavors to grow the interest of students in Chemistry during the time they are with NUS-Chemistry. Our most immediate task is to implement a bonding programme with our students from level 1, intensifying through levels 2, 3 and 4 by all staff of the Department. We are also asking our adjunct staff to participate more fully in imparting their work experience in the industry to our students and increase student placements to build industrial relationships. Finally we are creating a consultancy format in collaboration with the university’s Industry and Technology Relations Office (INTRO) to make it easier for staff to interact with industry, taking into account legal and IP (intellectual property) ownership issues.

### Aftercare

The **aftercare** programme seeks to build a lifelong relationship with the Department’s alumni. We know and are pleased that many of you identify very much with your alma mater department. We would like that identification to continue and in fact increase, and we solicit you to participate actively. Only through you can the Department increase its profile and prestige of Chemistry among our graduates and the public. We urge you to consider joining our alumni activities and if willing, sit on a Departmental advisory committee on alumni affairs. We are also looking into alumni being involved in scholarship and curriculum review committees and advise on the evaluation of teaching in the Department.

These are indeed exciting times for the Department and we are certain, as our former students, you would like to see these programmes succeed. Please feel free to contact us to give your feedback and input, and most of all, join us in bringing this programme forward.

### To alumni and friends of the Department of Chemistry,

The vision of the Department’s outreach programme has slowly been defined to meet the challenges of the 21st Century for NUS and Singapore. Our theme is establishing and maintaining “A premier outreach programme that is continually relevant to the Department’s teaching and research, locally and globally”. In pursuit of this vision, the members of the Department’s outreach committee has set up the requirements for establishing a credible outreach programme into three broad areas that are **recruitment**, **nurture** and **aftercare**.

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These are indeed exciting times for the Department and we are certain, as our former students, you would like to see these programmes succeed. Please feel free to contact us to give your feedback and input, and most of all, join us in bringing this programme forward.

Our best wishes for the holiday season and 2002.

From: Eugene Khor (Chairman) and the Outreach Committee

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**Members in the Outreach Committee:**

Chair: A/P Eugene Khor (chmkhore@nus.edu.sg)

Recruitment:  
A/P Loh Teck Peng (chmlohtp@nus.edu.sg)
Dr Fan Wai Yap (chmfanwy@nus.edu.sg)
Dr Ryan Bettens (chmbetts@nus.edu.sg)
Dr Leong Lai Peng (chmllp@nus.edu.sg)

Student Counsellor: Dr Sim Wee Sun (chmsimws@nus.edu.sg)

UROPS: Dr Loh Kian Ping (chmlohkp@nus.edu.sg)

Industrial Relations: A/P S. Jaenicke (chmsjs@nus.edu.sg)

Graduate Programme: A/P Xu Guoqin (chmxgq@nus.edu.sg)

Graduate Club: A/P Chuah Gaik Khuan (chmckg@nus.edu.sg)

Alumni Network: Dr Chin Wee Shong (chmcws@nus.edu.sg)
Coming to the National University of Singapore must have been the best decision that I have made. Why? As it opens up opportunities for instance studying yet in another institute for one semester under the Student Exchange Program (SEP). So what I did was to receive all with open arms when I arrived at the University of Hong Kong (UHK) in the autumn of 2000.

To me, Hong Kong is definitely not just another city like Singapore, as many have told me before. It has the skyline of not just the concrete skyscrapers but also the natural landscape of the mountainous hills and of the coastline. You just have to explore! For example, how often do you hear of people canoeing by the Sandy Bay to the Aberdeen? Well, my friends and I did just that under the guidance of our canoeing instructor. It was a time when we saw much beautiful coastlines and a waterfall which was how Hong Kong, the fragrant harbor got its name from.

I was thankful that I got to stay in the St. John’s College in UHK for a rental of $500 a month. Well, my friends and I did just that under the guidance of our canoeing instructor. It was a time when we saw much beautiful coastlines and a waterfall which was how Hong Kong, the fragrant harbor got its name from.

In the Earth Sciences elective, I was able to marvel the mother nature of Hong Kong and to learn about the formation of the rocks at the same time. We went to the Ninepin Group Islands where we saw the magnificent columnar joints and sea arch. We went to the Lamma Islands to study the sea cliffs and there was the Lai Chi Chong field trip week where we scaled the highest peak of Sai Kung, the Shek Uk Shan. The knowledge I got from this course was about navigation in the day, the study of geological and topographic maps and finally the habit of keeping a field book!

As for the architecture module, it allowed me to take advantage of the All Arts Scheme of UHK where every student is given HKD2000 to watch cultural events upon submission of the reviews of the event you went. I find this a very meaningful initiative and must be complimented. In my course with architecture, I had learnt the outlook of an architect and what architecture discipline is all about. For instance the use of a sketchbook was very interesting as I got to sketch down the kinds of landscapes, which fascinated me. Hence, it was different from just taking photographs. It was equally inspiring to watch performances such as the Opera Tosca, the American Ballet Theatre and the Vagina Monologues and the many exhibitions at the Hong Kong Cultural Center in Kowloon.

What must be mentioned were the advanced experimental techniques and instruments that I learnt in the “Organometallics” and “The Modern Chemical Instrumentation and Applications” chemistry modules. In the former, there was a mini project which we were paired up to synthesize a compound from scratch. The title of my project was “The Preparation of Analysis of W(dppe)(CO)4” It was a project that encompassed doing literature research to find different methods of synthesis, over at the ninepin group islands field trip. We were introduced to the natural formation of the columnar joints seen in the background. This was one of the few places in the world where one can find such columnar joints.

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During my undergraduate days, I had always wondered what career prospects lay ahead for me. I had imagined myself to be a typical chemist – mixing concoctions in the lab and “poof!” all my hair will stand on end. I had also fancied teaching or even continuing my studies, after all, my supervisor had offered to take me in. Anyway, none of these happened.

Instead, I became an applications chemist for a scientific instrument company. As with all foreign students who had graduated from the National University of Singapore, I was obliged to serve a 3-year bond working in Singapore. Upon completion of my bond, I was faced with a difficult decision – to stay in Singapore or return home to Malaysia. It was difficult because I had a good job and many friends in Singapore. Eventually, after weighing the pros and cons, I decided to go home. Many people asked why. I had wanted to be closer to my family and to enjoy a slower pace in life. Now it has been 4 years since I came home and people ask me if I regret my decision. Well, no. I may have earned less financially and started from scratch but the quality of life has improved tremendously and I definitely feel less pressure here.

There are plenty of job opportunities available for chemistry graduates in Malaysia. Being an agricultural country, Malaysia has many food, oil palm, wood and rubber factories which need experienced chemists not just for quality control but also R&D laboratories. A chemist’s responsibilities include daily routine analysis, implementation of GLP, GMP, ISO policies, audits, calibration and maintenance of laboratory equipment and troubleshooting when flaws appear in the products. It is indeed a heavy workload and frequently requires 10-hour workdays on the average. There are also industries which depend on agricultural products as raw material. Such industries include margarine and soap factories, paper and plastic products and glove and medical manufacturers. These industries require chemists and those producing food, pharmaceutical and herbal products also require graduates from medical and biological sciences especially pharmacists and microbiologists.

For those who do not fancy a laboratory-based career, they may also work with companies that supply scientific equipment or biological reagents. These companies may be a branch of the parent companies or local distributors and supply equipment such as chromatography systems, spectrometers, measuring equipment and ultrapure water systems. These jobs are not laboratory-based. They require the person to go and meet customers whether for sales, problem-solving, training or service. Here, customer service is very important and can only be learnt on the job. It requires much patience and diplomacy especially when faced with angry, fussy and rude managers and equipment that just does not respond to your tender-loving touch. This brighter side of this job line is that it enables the person to travel widely and visit interesting places. Do take note that interesting places do not always mean tourist attractions. It may be an oil palm estate in Hutan Melintang (Do you know where that is?) where you have to spend a night, a commercial laboratory analyzing bunker fuel in Port Klang (which means your Proton car is the only car among the tankers and cabins), a MINDEF ammunitions depot in the middle of the jungle of Selangor or a petroleum processing depot where you have to cycle to the laboratory, wearing safety boots and hard hat, cars are not allowed.

Graduates who prefer to further their studies would find the local universities an ideal choice. Currently there are plans to build universities, whether public or private, in every state in Malaysia. Hence, there are opportunities for post-graduate work or even research assistants. The local universities also have various collaborative partnerships with private companies to carry out research projects. Foreign universities are also mushrooming in the Klang Valley, Penang and East Malaysia. These universities require lecturers and tutors whether on a full-time or part-time basis and provide opportunities for those with job experience and post-graduate qualifications.

One cannot really complain that there is a lack of career prospects in Malaysia. The opportunities are there but for a returning Malaysian, as in my case, financial consideration is, of course, a major one. Some may also have to consider uprooting their families. Once these hurdles are overcome, it is truly a joy to settle down in Malaysia and make new friends again.
Season’s Greetings from Alumni

To:  Ms Chan Yin Lai, Ms Tan Soh Cheng, Ms Serene Lam, Ms Siew Hui (BSc. Sheares Hall ’89 - ’92):
“Hey gals! Miss you much. May you have a wonderful X’mas and a bright 2002 ahead!!”
Best Wishes from Gwendolyn Neoh, 1992

To: B Sc Chem B Class of 94’
“Hi friends, hope you are not too badly affected by today’s economic climate. Anyway, life must go on.....I hereby wishing all of you a Merry Christmas and A Happy 2002 ....... Btw, I’m leaving with my husband and children for Arizona, USA in mid 2002 for 2 years. Hope to catch up with you before I leave.....Take care.”
From: Sally Oh (salad711@yahoo.com)

To: the BSc Class of ’95 and the BSc(Hons) Class of ’96
“Wishing one and all every success and happiness in the New Year ahead; may our zest for life and all its wonders grow with each passing year.”
Audi Fong (audifong@yahoo.com), BSc 1995, BSc (Hons) 1996, PhD 2001

To: B. Sc (Chemistry) ’87
“Time has flied and is still flying
How many years have we not looked back
If time permits us to keep flying
Please drop me a mail”
From: Alice Chen (alice@italsing.com.sg)

To: B.Sc Hons Class of ’89
Merry Christmas and Let’s get Together. We are now working in the same company : SSMC Pte Ltd and would like to renew contact with all our classmates.
From: Yeo Sock Khim (sock.khim.yeo@philips.com) and Paul Tan (paul.tan_2@philips.com)

To: Chem B Class ’91, graduated in 1991
Have a merry Christmas. It’s been 10 years since we graduated together. Do press on during this challenging period and learn as much experience as we need to. Be prepared to reap better harvest when the ‘storm’ is over. We can make it.
From: Samuel (samlsp@singnet.com.sg)

To: B Sc Class of ’89, Shearites and Eusopheans
“Long time hasn’t heard from anyone ! Doing well, Healthy and Happy, I hope. Best Wishes Always...”
From: Chang Geok Lan (geoklan@gift-at-net.com)

To: B.Sc Honours Class of 1970
“Christmas Greetings to all my classmates wherever you may be!”
From: Lean Lam Keat ( Paul ) (lean_paul @ hotmail.com)

To: ChemConnections
Dear fellow friends of B.Sc ‘86,
“It has been 15 long years since we graduated in 1986. My Christmas wish is : May the Peace and Joy of Christmas prevail in your home. Do write to me at xtina@pacific.net.sg.”
From: Christina Lim

Specially to All BSc class of 2000:
“Dear friends, it has been more than a year since we have last parted. How have all of you been doing? Anyway, in this festive season, I would like to send my warmest greetings to each and everyone of you... May you continue to strive hard for knowledge for a bigger world out there and may you continue to live life to the fullest and happiest each day! Merry Christmas! :) “
With regards from: Eileen Chia (2000 gradund)