Guide for contributors to the Australian Journal of Education in Chemistry

Introduction

The Australian Journal of Education in Chemistry publishes refereed articles contributing to education in Chemistry. Suitable topics for publication in the Journal will include aspects of chemistry content, technology in teaching chemistry, innovations in teaching and learning chemistry, research in chemistry education, laboratory experiments, chemistry in everyday life, news and other relevant submissions.

Manuscripts are peer reviewed anonymously by at least two reviewers in addition to the Editors. These notes are a brief guide to contributors. Contributors should also refer to recent issues of the Journal and follow the presentation therein.

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2. On another separate page provide an abstract of 50 to 100 words;

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In this issue ..........

John Webb describes the ‘progress’ of chemical weapons since World War I, and international efforts to prevent their use, especially in the context of a world facing increased incidence of terrorist attacks. In discussing challenges to the 1997 Chemical Weapons Convention, he urges the adoption of codes of conduct and professional training for chemists and their biological and biotechnology counterparts.

The 2003 Nobel Prize in Chemistry was awarded for research into how water and ions move through cell membranes. In a paper that may be of wide-reaching significance for teachers, Lim and Lee discuss the chemistry behind this work in relation to the high school chemistry curriculum. In considerable detail, they demonstrate how this chemistry can be used to show that chemistry is relevant to the wider world, that simple fundamental concepts are essential to cutting-edge research, and that chemical knowledge is dynamic and evolving.

Desktop computers have been used by students in a computational and theoretical chemistry module introduced into the University of Mauritius curriculum. Ramasami describes the basis of the course, and presents some calculation outcomes for the gauche- and trans-conformers of ethane and 1,2-disubstituted ethane compounds using molecular mechanics on the desktop computer.

The ACELL laboratory experiment in this issue was developed by Wajrak and Boyce. Rather than simply provide a recipe for RP-HPLC separation of a mixture of preservatives, students are required to determine experimentally the optimum conditions for separation. In this way, they claim, students will not only develop deep understanding of the technique, but they will gain experience in method development as well.

As in studies in other topics, Ceyhun and Karagolge found that even though some Turkish higher education students can successfully do calculations of electrochemical cell potentials, they have misconceptions about the processes occurring in cells. In particular, the mode of charge transfer through aqueous solutions was poorly understood. They point the finger at imprecise textbook and instructor language which is open to misinterpretation by students. Misconceptions were reduced by use of computer animations of the cell processes.

While classroom demonstrations of chemiluminescence have become popular in recent years, one long-known reaction that uses cheap and easily available reagents seems to have escaped attention. Barnett and others describe the reduction of high oxidation state manganese species with emission of red-orange light. Whether from Mn(III), Mn(IV) or Mn(VII) species, the same wavelength of light is emitted by an excited Mn(II) species as it phosphoresces. Significant student exploration of the conditions is possible.

Sarma draws attention to the difficulty of coping with a vast array of technical terms in chemistry. To help understand these terms better, he presents a taxonomy of terms that apply to chemistry at the macro level, with discussion of how their meaning relates to the origin of their roots – mainly from the Greek or Latin.

Molecules of polycyclic compounds have two or more rings that share carbon atoms. Taherpour perceives a problem for chemistry students in determining the number of rings in molecules of these compounds using rules that hypothetically break some of the bonds to form open-chain compounds. A new method is proposed, based on determination of the ‘degrees of unsaturation’.

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Editorial
The importance of demonstrations in chemistry

David Treagust and A. Chandrasegaran

For over a century, laboratory work has been used in teaching and learning of school science. With the popularity of the constructivist-informed teaching approaches since the 1980s, teachers often emphasised the role of hands-on experiences in learning science, including chemistry. There are occasions when demonstrations are preferred to laboratory work in teaching science, because they are a less expensive or a safer way of providing students with experiences of laboratory experiments. Further, lecture-demonstrations can be fun, students like them because they are attention getting, they provide breaks from lectures and provide concrete examples in chemistry (Bodner, 2001). Students do report that demonstrations helped them understand the theories behind the chemistry (Walton, 2002). At the secondary school level especially, laboratory demonstrations in the teaching of chemistry can provide colourful, surprising or dramatic effects—such as burning a piece of magnesium ribbon before a junior class of science—that can motivate students.

Unfortunately, lecture-demonstrations do not always help students develop an understanding of the concepts being demonstrated (Bodner, 2001). Reasons are that students come to the practical classes with their own ideas and do not observe the phenomena as expected by their teacher. Similarly, the teacher/instructor expects the demonstration to be self-evident and does not realise that the students do not share this theoretical perspective. For demonstrations to be effective, research has shown that the central importance of the instructor is as a mediator of student learning and an interpreter of the content of science because all that is being demonstrated is not obvious.

To make demonstrations more student-centred, teachers/instructors may consider using Predict-Observe-Explain (POE) activities. POE activities can be a very useful way to juxtapose demonstrations with explanations. In a POE activity, students are first asked to predict what would happen next in a demonstration. Subsequently, they have to observe the demonstrations carefully and finally to explain what they have observed. The teacher/instructor can have a follow-up group or whole-class discussion with the students to discuss their observations and explanations. Discrepant events play a key role in the POE model, but it is intended inconsistency of the model rather than unrecognised inconsistency (Fensham & Kass, 1988).

In an action research study with first year university chemistry students at the Udonthani Rajabhat University, Thailand, Chaimaneewong (2005) designed, developed and trialed three POEs to teach key concepts for the rate of reaction based on inconsistent or discrepant events in chemistry. The Rajabhat University’s chemistry curriculum has been developed from English language textbooks for more than 30 years. What is stated in the books will be translated, rearranged and used by instructors to explain concepts to Thai students in the classroom. The foreign textbooks contain a tremendous amount of facts, principles, rules, laws, theories and exercises in almost the same fashion, such that only the most intelligent readers can grasp the concept. Thai teachers inevitably use the same sequence of course structure for describing the content to students, while students passively listen and take notes.

Three main tasks were conducted in Chaimaneewong’s study. The first task involved the optimization on the three POE models for three types of chemical reactions—acid-base neutralization, an iodine clock reaction and a decomposition reaction—to meet the POE model’s criteria. Students’ preinstructional conceptions were the most important clues used to guide this development. The cycle of plan, act, observe and reflection in action research was continuously employed until the students had developed a scientific understanding of the notion of a chemical reaction. The second task was the implementation of the optimized POE models with two classes of about 33 students. The last task was the assessment of the three POE models. The students’ responses were collected and presented by means of exploratory data analysis. The results showed that the students who encountered anomalous data were able to construct their own knowledge after responding to the POE models. The students were also asked to respond to an attitude test which produced a mean average of 4.17 (out of 5) indicating students had a high positive attitude towards the POE model.

References


Professional Ethics in Support of Chemical Disarmament:
A Challenge for Chemical Education

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Dedication
This paper is dedicated to a distinguished Tasmanian chemist, Dr. Peter Dunn whose contributions to chemical defense and international peace were recognized during his lifetime by the awards of the Order of Australia in 1992 for service to international relations, the Anzac Peace Prize of 1989, an honorary Doctor of Laws from the University of Tasmania in 1997 and an honorary Fellowship of the RACI. His professional life was based at the Defence Science and Technology Organization’s facility at Maribyrnong, Melbourne (1951-1993). The obituary published by the RACI in September 2000[1] reports also on his work with the United Nations, extending from 1984 when he was the chemist appointed to the UN team sent to Iran to investigate the alleged use of chemical weapons (CW) in the Iran-Iraq war. Subsequent missions to Iran, Iraq and Kurdistan over the next few years provided evidence of the additional use of chemical warfare agents.

After the first Gulf War, he was appointed as a Commissioner of the United Nations Special Commission on Iraq (UNSCOM) and played a major role in overseeing the destruction of the chemical weapons stockpiles discovered in Iraq including as team leader of the first UNSCOM CW inspection. He continued as the Coordinator of the Chemical and Biological Weapons Working Group of UNSCOM from 1993 until 1997.

Peter Dunn summarized his career as ‘protection of personnel and equipment and the promotion of peace and safety through global chemical weapons disarmament’. In a series of talks and articles in the RACI’s journal, Chemistry in Australia, he raised the awareness of the Australian chemical professional community to the realities of chemical warfare and the pressing need to support national and international measures to prevent it. His presentation at the 6th annual Professors and Heads of Departments of Chemistry Conference, Canberra in 1996 was the inspiration for the project reported in this paper.

Introduction and Historical Perspective
The first World War, 1914-1918 is often referred to as the ‘chemical war’ since it was the first occasion for the systematic and extensive use of toxic chemical substances as agents of warfare, beginning in 1915 with the use of chlorine.

‘The 22nd of April 1915 had been a warm and sunny day, but towards the end of the afternoon a breeze sprang up. It came from the north, from behind the German lines, blew across No Man’s Land, and gently fanned the faces of the Allied soldiers in position around the village of Langemarck, near Ypres. At five o’clock, three red rockets streaked into the sky, signaling the start of a deafening artillery barrage. High explosive shells pounded into the deserted town of Ypres and the villages around it. At the same time the troops sheltering near Langemarck saw two greenish-yellow clouds rise from the enemy’s lines, catch the wind, and billow forwards, gradually merging to form a single bank of blue white mist. German pioneers were opening the valves of 6,000 cylinders (of liquid chlorine) spread out along a four mile front the breeze stirred again, and one hundred and sixty tons of it, five feet high and hugging the ground, began to roll towards the Allied trenches. Chemical warfare had begun [2].

This first use of chlorine as a chemical warfare agent caused an estimated 5,000 deaths, an additional 10,000 causalities and widespread demoralization of the troops. This first use of a chemical weapon in World War I, was the beginning of the transformation of the battlefield into a contest of increasing levels and diversity of chemical armaments, delivery systems, protective clothing and equipment that extended to the end of the conflict. The chemical industries and professions on both sides of the conflict were immediately and extensively engaged in technical aspects of production, protection against, and detoxification of chemical warfare agents.

‘A chemical arms race developed, in the rush of which there was no time to worry about ethics. Soon, virtually every leading chemist in Britain was at work on some aspect of gas warfare. Thirty three different British laboratories tested 150,000 known organic and inorganic compounds in an attempt to develop the most poisonous war gas possible...In a short time, chemical weapons moved from the fringes of war to its very heart’ [3].

The agents used during WW1 included phosgene, mustard gas, cyanide and lewisite but not the nerve agents (tabun, soman sarin) that were developed in German laboratories just prior to and during the second World War [2,3]. All of these substances fit the definition of chemical warfare agents as being those chemical substances which are intended for use in military operations to kill, seriously injure or incapacitate humans because of their physiological effects. This definition excludes herbicides, smoke and flame agents.

The use of poison gas in warfare during 1915-1918 was widely seen as repugnant, a mood captured in the famous poem by Wilfred Owen:

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The use of chemical warfare agents continued to increase through the war, with sulphur mustard, 2,2'-di(chloroethy1)disulphide (which was, and sometimes still is, referred to as ‘mustard gas’) becoming the most widely used, indeed on a massive scale. It has been estimated that 1/6 of all British casualties in the last 18 months of the war were the result of chemical warfare. Overall, it is estimated that some 124,200 tonnes of phosgene (carbonyl chloride, Cl₂CO, quickly replacing chlorine as the volatile CW agent used), mustard and other chemical agents had been released and more than 90,000 had suffered painful deaths due to exposure to them. Those injured by CW numbered 1.3 million [5]. One particular incident is worth noting:

On 14 October (1918), during the final Allied offensive, British mustard shells rained down into a shattered Belgian village called Werwick, causing heavy casualties among the exhausted 16th Bavarian Reserve Infantry. A few days before the Armistice, a trainload of the men wounded in the Werwick attack were shipped back to Germany. Among them, blinded and humiliated, was a twenty-nine year old corporal, whose injuries helped determine him to avenge the German defeat: Adolph Hitler [6]  

The development of chlorine as a chemical weapon, and the subsequent management of the German chemical warfare programme, is generally attributed to one of the giants in the development of modern chemistry, Fritz Haber who was, in 1914, the Director of the Kaiser Wilhelm Institute in Berlin and acknowledged as Germany’s leading industrial chemist. However, by 1918, ‘fearing that he would be tried as a war criminal, Fritz Haber donned a false beard and as the war ended he took off for Switzerland: so too did Carl Duisberg, head of the German chemical industry. Neither in the end was tried (for war crimes). Indeed, in 1919 Haber was honored with the Nobel prize for his work on the synthesis of ammonia, a decision which outraged the scientific world.’ [6]

The chemical arms race continued in the intervening years leading up to the second World War. The nerve gas agents appeared. Tabun (O-ethyl N,N-dimethyl phosphoramidocyanidate known as GA) was developed in 1936 and, later, sarin (GB) which was also an organophosphorus compound (isopropyl methyl-phosphonofluoridate) but had ten times the toxicity of tabun. Although stocks of these agents were discovered in Germany at the end of the war, these chemical warfare agents were not used during the conflict. Some analysts refer to Hitler’s exposure to chemical warfare in WW1 as a critical factor in their being held back from first use. It was estimated that German production capacity of tabun reached several tonnes per month and that, at war’s end, a facility for the production of 500 tonnes per month of sarin was nearing completion. It is striking that the Allies were somewhat unaware of this German development in the production and weaponisation of such highly toxic nerve agents.

Sarin became widely known in recent times through its use in 1995 by the Aum Shinrikyo sect in the Tokyo subway terrorist attack [7]. Its name is reported [2] to derive from the names of the scientists who discovered it in 1938: Schrader, Ambros, Rudinger and van der Linde. Other nerve gases include soman (GD), and VX whose discovery in military establishments in the mid-1950s was a result of the pesticide research by ICI (UK). Ricin, a toxin extracted from the seeds of the castor oil plant, is also known from its modern usage to assassinate a Bulgarian write-in-exile, in London in 1978. The molecular structure of the ricin protein is known to at least 2.5 A [8].

Instances of the use of chemical warfare agents continued to accumulate e.g. Japan’s use from 1937 of ‘mustard gas’ in the war with China, Italy’s use of mustard gas in 1935-36 during its invasion of Abyssinia (Ethiopia), French and Spanish use of poison gas in 1925 in Morocco to subdue rebellions, among others. However, by far the most startling use was Iraq’s deployment of nerve gas agents in addition to sulphur mustard, in the war against Iran and in internal conflicts in the Kurdistan region.

‘In the spring of 1984, a familiar and terrible type of fatality began to reappear in the casualty lists of the latest Middle East war. A United Nations report described one typical victim, an Iranian soldier: ‘Sourab Norooz, age 24, exposed [in March 1984] at Majnoon...crepitation [a grating, crackling sound] due to gas in the chest wall, probably resulting from gas gangrene...the patient died that night’….one of the first pieces of evidence from the Iran-Iraq war was proving that Saddam Hussein was using mustard gas’[9]

Nerve agents were also employed in this conflict: In 1984, tabun, known for over 40 years was used for the first time in a battlefield, near Basra in the south of Iraq. Subsequently Iraq became interested in the production of both sarin (GB) and VX. Later, in 1988, a cocktail of chemical warfare agents was used at Halabja against a Kurdish community. Sarin caused approximately 5000 deaths in 5 minutes in the attack at Halabja. The US State Department estimated that 20,000 Iranian soldiers died from chemical weapons during this 1983-1988 war. Dr. Peter Dunn’s key role in the confirmation of the use of chemical weapons in this war has already been referred to above [1,10]. Some striking details of this event have been reported by Richard Butler, Executive Chairman of UNSCOM from 1997-1999 and Australia’s Ambassador for Disarmament in Geneva from 1984-1988 at the time of the investigation of the use of chemical weapons by Iraq in the war with Iran [11].

Disarmament initiatives
This brief history of the development and use of chemical weapons makes for sobering reading, especially for a
professional chemist. Following the First World War, and the widespread revulsion against these weapons (rather tragically described by Fritz Haber as “A higher form of killing”), various disarmament initiatives emerged. In May 1925, under the auspices of the League of Nations, the Geneva Protocol was agreed to, and thirty-eight powers signed, including the United States, France, Germany, Italy, the British Empire, Japan and Canada. The USSR, barely established at that time, did not attend the Geneva conference. This Protocol, a formal document signed in name of governments, reads in part as follows:

*Whereas the use in war of asphyxiating, poisonous or other gases, and of all analogous liquids, materials or devices, has been justly condemned by the general opinion of the civilized world; and*

*Whereas the prohibition of such use has been declared in treaties to which the majority of Powers of the world are Parties; and*

*To the end that this prohibition shall be universally accepted as a part of International Law, binding alike the conscience and practice of nations;*

*Declare: That the High Contracting Parties, so far as they are not already Parties to Treaties, prohibiting such use, accept this prohibition, agree to extend this prohibition to the use of bacteriological methods of warfare and agree to be bound as between themselves according to the terms of this declaration…*[12]*

Such treaties require ratification by the governments who sign before they enter into force. The Protocol was signed promptly by France (1926) and the UK (1930) but Japan ratified it only in 1970 and the USA in 1975. In 1956, the British renounced the use of chemical weapons and proceeded to dump their stocks at sea, in deep waters off the Inner Hebrides. Disarmament debate was dominated in the years post-World War II by the issues of nuclear weapons development, testing and potential use. In 1968, discussions began at the Disarmament Conference in Geneva concerning chemical and biological weapons. The Biological Weapons Convention (BWC) was concluded relatively quickly, opening for signature in 1972, but was seriously flawed, since it did not include effective compliance, monitoring or verification procedures (including the crucial component of ‘unannounced inspections’). Debate, discussions and dissent continue to the present time to develop it into a more effective disarmament instrument.

**Chemical Weapons Convention (CWC)**

However, in contrast, the Chemical Weapons Convention does include what are generally regarded as effective verification provisions, including challenge inspections. It entered into force in 1997 after long, protracted and at times interrupted discussions [5]. In September 1992, a text was agreed to by the Conference on Disarmament, and, when it was opened for signature in January 1993, 130 countries signed in the first three days. The Chemical Weapons Convention’s full title is the Convention on the Prohibition of the Development, Production, Stockpiling and Use of Chemical Weapons and on their Destruction.

It consists of 24 Articles, extending to 46 pages of text followed by three times that length of several Annexes concerning the schedules of chemical substances, verification and inspections regime and the protection of confidential information. In support of the Convention, the Organisation for the Prohibition of Chemical Weapons was established in The Hague, the Netherlands. Its staff includes 200 inspectors involved in inspections of civilian and military chemical plants around the world [13].

The CWC is recognized as one of the 25 ‘core treaties’ essential for security for all. In June 2003, Timor Leste became the 152nd State Party to sign and ratify the Convention.

The Convention aims to ensure the:

- destruction of stockpiles of chemical weapons
- destruction of former CW production facilities (or their conversion to peaceful uses)
- routine inspections of chemical weapons production facilities
- training of national staff
- establishment of controls on exports, managed by the national Authority
- promotion of international cooperation in the peaceful uses of chemistry
- cooperation with professional chemical groups such as the international Union for Pure and Applied Chemistry (IUPAC).

**Challenges to the effectiveness of the CWC**

In April 2003, the first Review Conference of the CWC was held at the OPCW. In preparation for this, IUPAC hosted a Workshop in Bergen, Norway: Impact of Scientific Development on the Chemical Weapons Convention, the Proceedings of which were published by IUPAC [15]. Challenges to the effective implementation of the CWC come from several directions from advances in science and technology [16]:

- Changes in the chemical industry with the emergence of smaller, more flexible reactors, including the use of microreactors.
- Scientific advances in genomics (the completion of the human genome project) and proteomics allowing the targeted design of new drugs but, at the same time, the possible discovery of completely new toxins not specifically identified in the Convention. Progress in bioprospecting, where bioactivities are assayed could also reveal new agents of chemical warfare potential.
- Further, the blurring of the distinction between biological and chemical weapons is increasing, while the international treaty status of the two classes of weapons differs significantly, e.g. regarding inspections [13,14].
- Additionally, some of these developments raise the possibility of chemical weapons capability being employed by terrorist groups not just by so-called ‘rogue’ States.

Furthermore, the preparedness of civil society to respond
to a terrorist use of chemical or biological weapons is a matter of concern, as noted in the consideration of such a scenario [17]. Finally, the Convention is faced with the ambiguity of the provisions relating to the prohibition of use of incapacitating chemical substances, as exemplified by the recent use of a fantany derivative in the Moscow hostage siege which raises the question of the permitted use of such toxic chemicals.

With the series of recent terrorist attacks in many countries, concern has increased regarding how to strengthen the Conventions and so limit the likelihood of terrorist use of chemical and biological weapons. The anthrax incidents of 2001-2002 in North America heightened these concerns. It is worth noting that, during the Chemical Education Conference in Tasmania, reports appeared of the interception of a letter addressed to the White House, USA containing a vial of ricin, the second such vial identified moving through the US Post Service (the first being in October 2003) [18].

Response of chemical profession: Codes of Conduct
The Royal Australian Chemical Institute has engaged with these issues through the hosting, in Melbourne in May 2001, a regional workshop and symposium to increase professional awareness of the CWC in Australia and in the region. The program included a demonstration inspection of a Discrete Organic Chemical (DOC) facility at an industrial site. To deliver this program, the RACI joined with the OPCW, the Department of Foreign Affairs and Trade (DFAT), Australian Safeguards and non-Proliferation Office (ASNO), Defence Science and Technology Organisation (DSTO), the Australian Agency of International Development (AusAID) and the Plastics and Chemicals Industries Association (PACIA).

The United Nations has also entered the debate. Within the UN system, responsibility for the debate concerning codes of practice has been assigned to the United Nations Educational, Scientific and Cultural Organisation (UNESCO). The response and initiatives of the UN were considered at a meeting in early 2003 in Paris at UNESCO headquarters [19]. In addition to other aspects, the UN encouraged ‘proposals to reinforce ethical norms, and the creation of codes of conduct for scientists, through international and national scientific societies, and institutions involved in teaching of science and engineering skills related to weapon technologies.’ Disciplines of immediate concern include chemistry, biochemistry, molecular biology and biotechnology as well as physics and engineering related to nuclear devices.

Professional chemists have some degree of awareness of codes of conduct, also called codes of practice, particularly related to safety in the chemical workplace, be it educational, industrial or commercial. The safety aspects of all usage of chemicals at work within Australia come under the purview of the National Occupational Health and Safety Commission (NOHSC). The national Hazardous Substances Regulatory Package includes a National Code of Practice for the control of workplace hazardous substances [20]. The Code takes the form of a detailed set of guidelines for particular chemical substances. These include handling and labeling of hazardous substances, the control of scheduled carcinogenic substances, preparation of material safety data sheets, safe use of synthetic mineral fibers, inorganic lead, vinyl chloride, ethylene oxides or timber preservatives as well as the safe removal of asbestos. As noted elsewhere [21],

‘From a profession viewpoint, chemists need to be familiar with their legal obligations with regards to hazardous substances and dangerous goods, be proactive in ensuring worker safety and always ensure that hazard identification, risk assessment and risk-management procedures are undertaken in a constructive, proactive manner to maintain both process efficiency and worker safety.’

Considered in a broader context, chemistry, like many professions, presumes that a chemist’s professional identity includes training and education in professional knowledge and practice as well as practicing within the code of the profession. Such codes vary across professional groups, ranging from a statement of ideals to a statement of minimum standards. A recently published analysis of various codes for social workers, counselors, nurses, psychologists, accountants, teachers as well as the chemists (through the RACI) identified three general sets of values embedded in professional codes [22]. The first is ethical behaviour (honesty, confidentiality, compliance with standards etc). The second, professionalism, covers a wide range of behaviors (competence, dedication, quality practice, respect, due care etc.). The third general class of values related to the advancement of the profession through ongoing professional development and commitment to improving practice, mentoring beginning practitioners, raising the standards of the profession etc.

For professional chemists, the RACI provides a Code of Ethics in its By-law 22 which has been summarized as follows [22]:

‘...the RACI’s Code of Ethics (By-law 22) is less detailed than many others but is consistent with their values (see above). For example, members of the Institute are bound to advance the honour, integrity and dignity of the profession of chemistry’. Competence, honesty, integrity, objectivity, independence and tolerance will be measures of their professionalism. They are exhort to respect their clients, colleagues, employers and employees, and to advance their subordinates. Responsibility for the welfare, health and safety of the community is an overarching principle’

Initially, entry to a profession was by the taking of an oath. Perhaps the most widely recognized such oath is that of the medical profession, the Hippocratic Oath. As an ancient oath of uncertain origins, it reads somewhat archaic in style though many of the commitments taken under it resonate with more modern expressions of such professional oaths. Thus [23],

I swear by Apollo the healer...I will use my power to help the sick to the best of my ability and judgement; I will abstain from harming or wronging any man by it....I will be chaste and religious in my life and in my practice...I
will not cut, even for the stone, but I will leave such procedures to the practitioners of that craft...whatever I see or hear, professionally or privately, which ought not to be divulged, I will keep secret and tell no one...

Its persistence through subsequent history has given it a central status in discussions of codes of conduct and professional behaviour [23,24]. Thus, the oath ‘foreshadows...the paradigm of a profession (one professing an oath) as an ethically self-regulating discipline among those sharing specialized knowledge and committed to a service ideal’[23], an inspiration that has been taken up increasingly by professions over the past two decades [24].

The issue of professional ethical standards has emerged also in the discussions within Australia concerning the desirability of generic graduate attributes in graduates from Australian universities. The graduate attributes encompass intellectual and professional attributes as well as values, expressed generically as ‘understanding of and commitment to professional ethical standards’[22].

Given these desirable attributes for graduates, including those in chemistry, how can they be encouraged and developed? A variety of pedagogical approaches and strategies can be considered, recognizing that the goal is different from that of acquiring technical knowledge and skills. One issue for debate is whether to include such material in a special teaching unit or whether they should be incorporated into academic and professional units. Specific approaches could include the use of case studies, development of project and problem-based learning, mentoring by staff or, preferably, a combination of several of these teaching strategies [22,26,27].

Projects concerning Codes of Conduct

In the specific context of supporting chemical disarmament, the Federation of Asian Chemical Societies (FACS) has recently adopted a regional project with a focus in professional ethics in support of chemical disarmament. The member societies are being invited to participate, through a nominated representative, in the collection and comparison of codes of conduct and the identification of relevant courses and training materials. The goal of the project is to eventually have available appropriate training materials for use in professional development workshops for chemists throughout the region.

The impact of any such codes of conduct will be greatly strengthened by a research-based understanding of the knowledge and attitudes of professional scientists towards chemical and biological weapons issues. Approaches have been validated for such studies in the case of public attitudes in Australia towards biotechnology [28-30].

This FACS project links in with the parallel Ethics Project of the Organization for the Prohibition of Chemical Weapons, initiated in 2002 [5]. The author is the Australian representative to this Project, which has taken some time to get underway. Strong expressions of support have come from Presidents of IUPAC for these projects.

Other related projects include that of the Pugwash Conferences on Science and World Affairs [31], well-known for its being awarded the Nobel Peace Prize in 1995. Pugwash has initiated a series of meetings to develop the support and appropriate approaches for such codes. In parallel, the International Committee of the Red Cross (ICRC) has such codes of ethics included in the scope of its project entitled Biotechnology, Weapons and Humanity [32]. A particular focus of this is the development of codes of conduct for biological scientists, a key topic to be discussed at the Annual Meeting of States Parties of the BWC in 2005.

It is important to note that the discussions regarding ethics in support of chemical disarmament can also be applied, and perhaps with even greater urgency, to ethical education in support of the Biological Weapons Convention. As noted earlier, the boundary between ‘chemical weapons’ and ‘biological weapons’ is becoming less distinct. A concerted approach, including chemists and their biological and biotechnology counterparts, offers the greatest benefit in supporting disarmament.

While codes of conduct are no guarantee that no scientists will work on chemical or biological weapons, they do offer crucial support to disarmament and the fight against CB terrorism. The codes, highly visible and supported strongly at every level, will make it less likely that scientists will inadvertently contribute to such activity. They will increase the awareness of scientists of the types of chemicals used as CW precursors and help them notice any suspicious activity that should be referred to the relevant authorities. It is an “educational imperative”[27] for the community of chemical and biological scientists and technologists.

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12. Reference 2, p. 45.

Using the 2003 Nobel Prize for Chemistry to illustrate fundamental concepts in the secondary school curriculum

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Abstract

The Nobel Prize in Chemistry for 2003 was awarded jointly to Peter Agre and Roderick MacKinnon for their discoveries of how water and ions move through cell membranes. The water and ion channels through the lipid bilayer membranes allow cells to regulate their volume and internal osmotic pressure. In addition, the ion channels allow cells to generate and transmit electrical signals, which is required for the operation of the nervous system. This paper discusses the work, which led to this Nobel Prize, its significance to society, and the connections to concepts in the secondary school curriculum. Specific topics covered in representative secondary school syllabi are given in the appendices.

Introduction

Learning is enhanced if the student is able make a connection to the subject matter (p. 7 of Ref 1). This paper uses the 2003 Nobel Prize to illustrate some aspects of the high school chemistry curriculum in order to show that chemistry is relevant to the wider world, that simple fundamental concepts are essential to cutting-edge research, and that chemical knowledge is not static, but evolving and improving. Note that the work celebrated by this Nobel Prize has been in progress since 1988, which is during the lifetime of the senior high school student.

The 2003 Nobel Prizes

The 2003 Nobel Prize in Chemistry was shared between Peter Agre and Roderick MacKinnon for their work on how water and ions move through cell membranes. It is worth noting that this Chemistry Nobel Prize was awarded to two medically-trained scientists, while the Nobel Prize in Physiology or Medicine was awarded to Paul C. Lauterbur and Sir Peter Mansfield, who have backgrounds in chemistry and physics, “for their discoveries concerning magnetic resonance imaging” (2, 3), confirming that chemistry is indeed the “central science”. This paper discusses the Nobel Prize in Chemistry.

What Are Membrane Channels? (2-4)

A cell can be imagined as a porous “sack”. How do water molecules and aqueous ions pass through the hydrophobic interior of the cell wall or membrane, which is a lipid bilayer (Fig. 1)?

The existence of special “water channels” has been postulated since the 1840s by Brücke (5), Pfeffer (6), Ostwald (7) and others. In the 1950s, Sidel and Solomon demonstrated the existence of channels that are able to selectively and rapidly transport water through the membrane of red-blood cells, and that ions and other solutes are excluded from the channel (8). However, the protein(s) responsible was not identified. Further, it was unclear if these channels passed water to the exclusion of all other species, or if they could switch between water transport and other transport modes. As late as 1987, the mechanism of their operation was still unclear (4).

Figure 1. Schematic diagram of lipid bilayer cell membrane. A membrane channel allows water (darker circles) and aqueous ions (lighter circles) to pass through the hydrophobic bilayer.

In 1890, Ostwald had also postulated that biological electrical signals were due to ion transport in and out of cells (7). Hodgkin and Huxley showed that electrical signals along nerves were due to the transport of mainly sodium (Na+) and potassium (K+) ions through nerve cell membranes (9). Skou showed in 1957 that ions could be pumped across a membrane against a concentration gradient (10). In 1977, Ross et al. identified a protein, which acts as the ion channel. It was shown that some channels could pass the larger potassium ions while blocking the smaller sodium ions (11). However, the mechanism of ion transport through the protein channel was unknown.
Water Channels (2, 3, 12-14)

Like Sidel and Solomon, Agre and coworkers studied the transport of water through the membrane of red-blood cells. The CHIP28 protein from the membrane of blood cells and renal tubules was isolated in 1988. In 1991, the peptide sequence of CHIP28 was determined, and CHIP28 was postulated to be the water channel. The following year, control experiments proved that CHIP28 was, indeed, the water channel. CHIP28 was renamed Aquaporin 1 (AQP1) meaning “water pore”. Between 2000 and 2001, high-resolution 3D structures of AQP1 were obtained using X-ray crystallography, which in turn, enabled detailed atomistic computer simulations (14-16) of how AQP1 functions.

Ion Channels (2,3,17-21)

While much was known about the existence of ion channels, again the breakthrough came in the form of high-resolution 3D structures of a K+ channel protein, KcsA in 1998 (22). Subsequent studies on KcsA and other ion proteins showed that two of the α-helices that form part of the protein are a “gate” that can change position by about 30°, moving 20 angstroms (2 nm) to “open” and “close” the ion channel.

Why A Nobel Prize In Chemistry?

Knowledge about the structure and function of membrane channels is of importance and significance in biology and medicine. For example, failure of channel function can lead to renal failure, inability to maintain body fluid balance and diseases of the nervous system. Information about the membrane channels will enable design of drugs that can better target these channels.

Why, then, should this be a Nobel Prize in Chemistry? The answer is that although the discoveries about membrane channels are important to biology and medicine, the work itself is grounded in chemistry. The isolation and purification of proteins (polymers composed of amino acids) are chemical methods, as is crystallisation and the determination of molecular structure using X-ray diffraction, electron diffraction, and NMR. The remainder of this paper discusses how the Nobel-Prize-winning work can be used to illustrate fundamental chemical concepts in the Australian secondary-school chemical curriculum. Specific topics covered in representative secondary school syllabi are given in the appendices.

Links to Scientific Literacy and the History and Philosophy of Science

There has been recent discussion on the nature of scientific literacy (23-25). The Analytical Chemistry section of the VCE Study Design (Unit 3) makes the distinction between knowledge, theory and evidence (26), as does the HSC Chemistry syllabus (27), and others. The work of Sidel and Solomon, amongst others, and even the early (pre-1992) work of Agre had postulated the existence of water channels. The crucial experiments, which provided evidence for water channels, were published by Agre in 1992 (2, 3, 12); both natural and artificial cells without the CHIP28 protein were unable to absorb water; those with CHIP28 absorbed water rapidly. In addition, water absorption was blocked by the presence of mercury (2, 3). This can be used to illustrate the difference between Aristotelian science and the modern practice of science. Aristotle (c 384-322 BC) had taught that science was based on induction and belief (28, 29), without need for experimental verification, probably because that was beyond the abilities of the ancients. In contrast, the experiment-based philosophy can be traced back to (28, 29):

- Novum organum by Francis Bacon (1561-1626), which recommends that science be based on induction and experimentation (28, 29);
- Philosophiae naturalis principia mathematica (the mathematical principles of natural philosophy, 1687) by Isaac Newton (1642-1727), where theories are based on observation and used to make predictions (29).

The key concept here is that of appropriate experimental design, incorporating control experiments. Note that more recently, Karl Popper (1902-1995) expounded that experiments can only disprove scientific theories (28).

A second link of the 2003 Nobel Prize to Scientific Literacy and the History and Philosophy of Science is in the use of representations such as the Figures in this paper to model reality. A particular feature of chemistry and the other molecular sciences is a three-fold description (representation) of matter (30, 31):

- The macroscopic or observation-based description;
- A pictorial description whereby chemical substances are depicted as molecules consisting of atoms (shown as balls) connected by bonds (shown as lines);
- An abstract “code”-based (chemical formulae) description, as shown in Fig. 5. Often this is used within the context of a chemical equation.

No one has directly observed atoms, in the way that biologists have observed living organisms. Nevertheless, these representations (models) are so useful and powerful in chemistry that most chemists discuss or think of these models as if they are reality (as opposed to being a description of reality) (31). Computer modeling (15, 16) based on the work of Agre has enabled scientists to visualise how the water channel functions.

Links to the Atomic Theory

Previous Nobel-Prize-winning work on membrane channels (9, 10) had been based on macroscopic observations: whether a phenomenon could be observed in the laboratory, without knowledge at the microscopic level. The work of Agre and MacKinnon determined the spatial arrangement of atoms within the protein molecules that formed the membrane channels. Macroscopic isolation of the membrane proteins was insufficient: knowledge of individual atoms and groups of atoms was needed to investigate how the proteins function. Hence this work relies on the Atomic Theory of matter.
Furthermore, individual atoms consist of electrons around a central nucleus. Gain or loss of electrons results in the formation of charged species (ions). Unequal “sharing” of electrons between atoms gives rise to species (polar groups and molecules) with partial charges. The non-polar tails of the lipids form a hydrophobic interior of the bilayer cell wall that is a barrier to the passage of polar (e.g., water) and ionic species. The membrane channel proteins form a “tube” with a hydrophilic interior to allow passage of water or ions (Figs 1 and 2).

Atoms, ions and molecules have size. In AQP1, KcsA and other membrane channels, there is a “filter” region formed by the constriction of the hydrophilic passage through which water or ions pass (Fig. 2). This filter acts to exclude larger neutral molecules or ions from passing (15, 16, 22).

Figure 2. Schematic diagram of AQP1, showing the positive residues (represented by the oval) in the narrow “filter” region of the channel.

In AQP1, the “filter” region also has positively-charge residues (groups attached to the protein backbone). The interatomic forces between the positive residues and species in the channel (a) repel cations, especially hydrated H⁺ or H₂O⁺, which are the same size as or smaller than neutral water, and (b) cause the water molecules to be orientated differently in the top and bottom of the channel (Fig. 2) (15, 16).

Links to the Theory of Acids and Bases
A Bronsted-Lowry acid is a proton donor; a Bronsted-Lowry base is a proton acceptor. The Grotthaus mechanism of “proton hopping” (Fig. 3) is an example of a concerted acid-base reaction in which all the orientated water molecules are amphoteric (act as both acids and bases). The water molecules simultaneously gain and lose one proton, so that they remain neutral H₂O. The presence of a charged region in the AQP1 channel causes the water molecules to be orientated differently in the top and bottom of the channel (Fig. 2), thus preventing the Grotthaus mechanism (15, 16).

Figure 3. The Grotthaus mechanism for “proton hopping”, whereby orientated water molecules accept a proton in one region (top) while releasing a proton elsewhere (bottom). The water molecules remain neutral.

Links to Water as a Solvent
Water is a polar molecule, which can solvate (dissolve) ions by favourable intermolecular interactions. The slightly positive hydrogen atoms in water can be orientated towards anions while the slightly negative oxygen atoms can be orientated towards cations (see Fig. 4). The formation of a solvent shell around a solvated ion overcomes the cation-anion attractive forces which would otherwise result in the (re)formation of the salt.

Figure 4. Schematic representation of solvation of ions. (a) Solvation of a cation. (b) Solvation of an anion.

The K⁺ channel protein, KcsA, has oxygen atoms on the sides of the “filter” region which are spaced so that they are at the same distances as the oxygen atoms in the water solvation shell surrounding aqueous K⁺. The similarity of environment allows K⁺ to move easily from water into the membrane channel. Although Na⁺ has similar properties to K⁺, it has smaller size, so that the oxygen atoms in the “filter” region are at distances too large to form favourable interactions with Na⁺.

Links to Surfactants (Lipids)
A surfactant is a molecule with a polar (often ionic) “head” and one or more non-polar hydrocarbon “tails”. Surfactants are the active ingredient in soaps and detergents (see Fig. 5).
Figure 5. Examples of surfactants. In each case, the non-polar tails have been indicated by boxes. (Top) Sodium palmitate, a soap. (Centre) Sodium lauryl sulfate, an ionic surfactant in toothpaste. (Bottom) Phosphatidylcholine, a common lipid found in cell membranes.

At sufficient concentrations, surfactants form macromolecular structures where the non-polar, tails associate with each other through van der Waals forces to form hydrophilic regions, with the polar heads being solvated in water. These structures are called micelles and bilayers (Fig. 6). These structures are dictated by the various intermolecular ionic, polar and non-polar interactions between the surfactants and the solvent, as well as the shapes of the surfactants. The lipids in the cell walls are usually biological surfactants with two hydrophobic tails. The bulky lipid tails (Fig. 5) favour the formation of bilayers, which has smaller curvature than micelles (Fig. 6).

Figure 6. At sufficient concentrations, surfactants in water solution will form micelles (top) and bilayers (bottom).

Links to Molecular Shape

Proteins are composed of amino acids joined together in a backbone of carbon and nitrogen atoms, with side chains called residues. The bonds around each of these atoms are arranged in 3-dimensional space, giving rise to characteristic molecular geometries or structures.

Figure 7 shows a small part of the K⁺ channel protein, KcsA (22). For clarity, most of the hydrogen atoms are not shown, but Fig. 7 clearly shows that bonds are arranged in very specific directions relative to each other. Some of the carbonyl oxygen atoms and the amine (nitrogen) atoms in the amino acids along the protein backbone are indicated by solid and hollow arrows respectively. The dashed lines are hydrogen bonds (intermolecular forces) which hold this part of the protein in an α-helix (see Fig. 8). The α-helical structures form rigid frameworks for the protein.

Figure 7. A small part of the of K⁺ channel protein, KcsA (22). The dashed lines are hydrogen bonds, which hold this part of the protein in an α-helix (see Figure 8). The solid arrows indicate the carbonyl oxygens and the hollow arrows indicate the amine (nitrogen) atoms in the amino acids along the protein backbone.

Figure 8. Part of the of K⁺ channel protein, KcsA (22), surrounding the portion shown in Figure 7. The left-hand structure shows the amino acid backbone. The right-hand diagram is a space-filling model, showing structure of the α-helix.

Links to High-School Biology

Cells are fundamental “building blocks” for all living organisms larger than viruses. The cell is a porous “sack” consisting of a lipid bilayer cell membrane, incorporating various proteins, some of which are the media for transport of water, ions and nutrients through the cell wall.

Amongst other concepts, which can be illustrated, the “pumping” of water through cell walls and along capillaries is the source of the osmotic pressure that can push water from ground level to branches and leaves high in the tree canopy.
Links to High-School Physics

Diffraction is a characteristic wave behaviour. Waves entering a regular array are diffracted to emerge from the lattice in special directions, which depend on the wavelength and the lattice spacing, as predicted by Bragg’s Law. This can be seen by, for example, the diffraction of water waves by the regularly-spaced piers or pylons under a wharf.

X-rays, high-energy electrons and high-energy neutrons exhibit diffraction when passing through a crystal. Analysis of the diffraction pattern yields the spatial arrangement of atoms in the crystal, which was the method used to determine the molecular structure of the water- and ion-channel proteins.

Use of monochromatic radiation (light of only one wavelength) increases the resolution of the diffraction pattern and hence the accuracy and precision of the resultant molecular geometry determination. Synchrotron x-ray radiation was used, especially for determination of the ion channel structure, because it is a very intense source with an extremely narrow range of wavelengths.

Nobel Laureates as Role Models

Although government policy envisages a technologically-based Australia, the media does not present many scientists as role models. Discussion of Nobel Laureates in the classroom partially remedies this lack. Other scientist role models include inventors, and CSIRO and university scientists. The Journal of Chemical Education’s website has a list of (mainly American) female and “minority” role models. http://jchemed.chem.wisc.edu/JCEWWW/Features/eChemists/index.html.3

Summary

Discussion of the work of Peter Agre and Roderick MacKinnon, which led to their 2003 Nobel Prize in Chemistry can be used to illustrate several fundamental concepts in chemistry. These include discussions of the philosophy of the scientific method, the atomic theory, periodic properties, the Bronsted-Lowry theory of acids and bases, intermolecular forces, the solvation of ions by water, the nature of surfactants, and molecular shape. Topics in the biology and physics syllabi can also be covered. Specific topics covered in representative secondary school syllabi are given in the appendices. Finally, discussion of the Nobel Prize can demonstrate that chemistry is an evolving discipline with new knowledge being constantly discovered at the frontiers of science.

Further reading

Readers may find the review articles of References (2, 3, 21) and their lists of references particularly useful. References (2, 3) can be downloaded from the Nobel Foundation’s website: http://www.nobel.se/.3

Dr Schulten, Dr Tajkhorshid, Dr Stroud, Dr de Groot and Dr Grubmüller have produced very good animations (15, 16) of the structure and function of the water channel, which can be found at http://www.mpibpc.gwdg.de/abteilungen/073 and http://www.ks.uiuc.edu/~emad.3

References (13, 14, 17-20) are some of the primary and review literature describing the work of Agre and MacKinnon.

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NOTES

1 Note that Hodgkin and Huxley shared the 1963 Nobel Prize in Physiology or Medicine with Australian, Sir John Carew Eccles, for their discoveries concerning the ionic mechanisms involved in excitation and inhibition in the peripheral and central portions of the nerve cell membrane (9).

2 Francis Bacon’s 1620 Novum organum refers to a new organon (28, 29), to distinguish it from Aristotle’s organon.

3 Unless otherwise noted, web links were checked on 1 December 2004.

4 A new VCE Chemistry Study Design is due to be released in 2005. It is expected that topics like atomic theory, acid-base theory, chemistry of water and the concept of molecular shape will all be part of the new Study Design.

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Appendix I. The 2003 Nobel Prize for Chemistry is relevant to the following topics in the Victorian VCE syllabus.
This Appendix is a non-exhaustive list of topics in various state syllabi in which the 2003 Nobel Prize for Chemistry can be discussed. This paper and this Appendix is intended to provoke ideas of how readers might discuss the 2003 Nobel Prize for Chemistry can be discussed in their own syllabus.4

VCE Chemistry (26) Unit 1
Introduction to materials

• formation of ions
• interatomic and intermolecular forces

Water
• the importance of water as a solvent and the importance of its solvent properties in living systems

Chemistry of surfaces
• the action, at a molecular level, of surfactants

VCE Chemistry (26) Unit 4
Food chemistry
• importance of molecular shape (as determined by primary, secondary and tertiary structures) in determining the function of proteins

The periodic table
• atomic and ionic radius

VCE Biology (32)
Unit 1, Outcome 3
• formulation of hypotheses based on observations
• use and need for controls in the design of experimental investigations

Cells in their environment
• cell structure
• structure, function and properties of cell membranes

VCE Physics (33)
Wave-like properties of light
• diffraction

Interactions of light and matter
• diffraction

Synchrotron and applications
• Synchrotron radiation
diffraction from crystals and Bragg’s law structure of materials

Appendix II. The 2003 Nobel Prize for Chemistry is relevant to the following objectives and outcomes in the NSW HSC syllabus. (27)
Prescribed Focus Area 1. History of chemistry
• H1. evaluates how major advances … have changed the direction or nature of scientific thinking

Prescribed Focus Area 5. Current issues, research and developments
• P5. describes the scientific principles employed in particular areas of research in chemistry

Domain: Knowledge 6. Atomic structure and periodic table
• P6 explains trends and relationships between elements in terms of atomic structure and bonding

Domain: Knowledge 9. Carbon chemistry
• P9. relates … the unique nature of carbon chemistry

Appendix III. The 2003 Nobel Prize for Chemistry is relevant to the following topics in the International Baccalaureate (IB) syllabus.

Human Biochemistry option
Both the Chemistry and Biology curricula in the International Baccalaureate (IB) have (Human) Biochemistry options. Discussion of the 2003 Nobel Prize for Chemistry would be relevant to fundamental chemical concepts and also to the (Human) Biochemistry optional study.
A Learning Experience: Conformational Studies of Ethane and 1,2-Disubstituted ethanes using Molecular Mechanics

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Abstract
Computational chemistry involves the use of computers for investigating chemical systems. It is becoming increasingly important for research and is being integrated in the chemistry curriculum. More interestingly computational chemistry can now be explored using desktop computers. A computational and theoretical chemistry module was introduced at the University of Mauritius. Among the computational laboratory assignments, students obtained the gauche-trans energy difference of ethane, 1,2-disubstituted ethanes and their energy profiles in the gas phase using molecular mechanics method. The feedback from the students was promising for the development of computational chemistry at both research and teaching levels. The module is now running successfully for four years already.

Introduction
Computational chemistry is a mathematical tool to investigate chemical systems in terms of molecular structure, properties, reactivity and kinetics (1). Computational chemistry is particularly useful in investigating problems, which are either difficult or sometimes inaccessible at experimental levels. The basis of computational chemistry is to set up the Schrödinger equation for the system under investigation and then solving the equation. The equation set up is generally solved using mathematical algorithms and these algorithms are now commonly available in commercial software. Sometimes these algorithms require very large number of calculations to be computed. Thus with explosive growth of computer power, computational chemistry is benefiting to full advantage and accurate computational calculations can be done on desktop computers. Molecular mechanics (MM) and electronic structure methods are two areas in computational chemistry for investigating the structure of molecules and their reactivity. Computational chemistry is a widely used research tool and it is also finding its way in the mainstream chemistry curriculum (2-6).

Conformational analysis is the study of the rotamers resulting from the free rotation about a single bond of a group of atoms in a molecule. Rotamers of a given molecule can have different physical and geometric properties. The 1,2-disubstituted ethanes, XCH₂CH₂X, are among the simplest molecules exhibiting internal rotation and the torsion potential plays an important role in conformational analysis (7-12). The most interesting feature of these species is that they have two stable conformers termed as the gauche and trans forms. There have been various attempts to calculate the gauche-trans difference using experimental (7-10,12) and computational methods (8,9,11,13-15).

Computational chemistry was unknown at the University of Mauritius (16) having a Department of chemistry running undergraduate and postgraduate degrees. To meet international standard, computational and theoretical chemistry were offered as an elective module for the first time in the year 2001. The response for this module was quite interesting as could be interpreted from the students survey questionnaire. A computational laboratory was set up using sufficiently powerful desktop computers running Windows 98 operating system and commercial software such as Chem Office (17) and Gaussian 03W (18). The elective module was for 45 h running over one semester of 15 weeks. Out of the 45 h, 30 h was used for lectures and 15 h for computational laboratory experiments. The module was assessed by 1 h class test (10%), three computational assignments (15%) and 2 h written examinations (75%). This paper reports a learning experience from 22 second year students of BSc (Hons) Chemistry of the year 2002 from the University of Mauritius. They obtain the gauche-trans energy difference of ethane, 1,2-disubstituted ethanes and their energy profiles. The 1,2-disubstituted ethanes considered for this study were butane, 1,2-difluoro ethane, 1,2-dichloro ethane, 1,2-dibromo ethane, 1,2-diodo ethane, 1,2-dicyano ethane, 1,2-ethane diol, 1,2-dimethoxy ethane, 1-bromo-2-chloroethane and 1-bromo-2-chloropropane. The results obtained compare satisfactorily with findings in the literature. A questionnaire, apart from oral questions, was used to investigate the student’s understanding and reactions to this study and an analysis of the completed forms indicates that we had a promising start. The oral questions and the questionnaire used are given in the Appendix (available from the author).

Methods
Molecular mechanics is the computational method, which is available in Chem Office and is used in this work to obtain the energy of the rotamers of ethane and 1,2-disubstituted ethanes. Molecular mechanics is a method that has been applied to many classes of compounds and unlike quantum mechanical methods, electrons are not included in calculations. The latter is justified using Born-Oppenheimer approximation (1). Molecular mechanics assumes that the electrons in a system find their optimum distribution and thus a molecule is considered to be a collection of masses that are interacting with each other via harmonic forces. Mathematical potential energy functions having constants to be determined using experimental data are used to describe these interactions and a force field describing the total energy is set up using these functions. The total energy (equation (1)), \( E_{\text{T}} \), is made
of several terms, one of which is attributed to stretching \((E_s)\), one to angle bending \((E_b)\), one to van der Waals interactions, \((E_{vdW})\), one to torsional interactions \((E_t)\) and one to electrostatic interactions \((E_e)\) \(\text{(1)}\).

\[
E_T = E_s + E_d + E_t + E_{vdW} + E_e
\]

---

**Stretching energy**

This term arises due to bond stretching or compression and is assumed to be harmonic in behaviour. The general form of this term is as given by equation \(\text{(2)}\).

\[
E_s = \frac{1}{2} k_s (x - x_o)^2
\]

\(k_s\) is force constant, \(x_o\) is the natural bond length, and \(x\) is the actual bond length.

---

**Angle bending energy**

This term arises due to changes in bond angle and is again assumed to be harmonic in behaviour. The general form of this term is as given by equation \(\text{(3)}\).

\[
E_b = \frac{1}{2} k_\theta (\theta - \theta_o)^2
\]

\(k_\theta\) is a constant, \(\theta_o\) is the natural bond angle, and \(\theta\) is the actual bond angle.

---

**Torsional energy**

This is a very important term for the molecules under study and it arises due to internal free rotation about a bond. The general form of this term is as given by equation \(\text{(4)}\).

\[
E_t = \sum_{n=0}^{\infty} \frac{V_n}{2} \left[ 1 + \cos(n\omega - \gamma) \right]
\]

\(\omega\) is torsional angle, \(V_n\) is a constant related to barrier height, \(n\) is the multiplicity that is the number of minimum points in a 360° rotation and \(\gamma\) is the phase factor which determines where the torsion angle pass the minimum.

---

**van der Waals energy**

The term arises due to electrostatic repulsion between pairs of electrons and it is a short-range repulsion. A modified form of the Lennard-Jones 6-12 potential as given by equation \(\text{(5)}\) is generally employed.

\[
E_{vdW} = \varepsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \right]
\]

\(\varepsilon\) is well depth, \(\sigma\) is the collision diameter, and \(r\) is the distance between the pairs of electrons.

---

**Electrostatic energy**

The term arises due to electrostatic interactions between charges on non-bonded atoms. The general form of this term is as given by equation \(\text{(6)}\).

\[
E_e = \sum_i \sum_j \frac{q_i q_j}{D r_{ij}}
\]

\(q_i\) and \(q_j\) are the charges involved, \(r_{ij}\) is the distance between the charges and \(D\) is the dielectric constant.

---

However apart from these terms, depending on the complexity of the molecule there can be other terms referred as cross terms and one such term is the bending-stretching energy. It is found that if the bond angle is decreased, the neighbouring atoms are stretched to reduce interactions between the 1,3 atoms. The general form of this term is as given by equation \(\text{(7)}\).

\[
E_{bs} = \frac{1}{2} k_{bs} \left[ 1 - l^2 \right] \left[ 1 - l^2 \right] \left[ \theta - \theta_o \right]
\]

Once the force field has been formulated, the constants have to be determined using available experimental data, a process known as parameterisation then can be used. Chem3D uses a modified version of Allinger’s MM2 force field. For this work, 22 students were grouped in pair to work on ethane and a given 1,2-disubstituted ethane. Each group had to vary the dihedral angle, \(\theta\) (see Figure 1), in steps of 5° from 0° to 180° and for each conformation, minimisation is carried out to obtain the different energy terms and the total energy. The results from the different groups were compiled in one computational laboratory session and these results were analysed. In the same session oral questions were asked to each student and then finally students were required to fill the student evaluation form.

---

**Results and discussion**

The different energy terms for varying dihedral angle obtained for 1,2 dibromoethane are given in Table 1. The energy profile obtained is illustrated in Figure 2.

---

The gauche–trans energy differences for ethane and the 1,2-disubstituted ethanes studied are given in Table 2. It is to be noted that minimum energy for the gauche conformation does not occur at 60° in all profiles and this may be explained on the basis the calculations are done for discrete conformers in the gas phase and hence do not take into account intermolecular interactions. As a rule of thumb, gauche–trans energy difference decreases as the size of the substituent increases except for more polar molecules where there is a preference for the gauche form. The abnormal gauche–trans energy of fluorine has been noted by previous workers even experimentally \(\text{(7)}\). Thus it can be found that the results obtained agree satisfactorily with the literature.
Table 1: Energy terms for 1,2-dibromoethane

<table>
<thead>
<tr>
<th>Dihedral angle °</th>
<th>E₁</th>
<th>E₂</th>
<th>E₃</th>
<th>E₄</th>
<th>E₅</th>
<th>E₆</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>kJ/mol</td>
<td>kJ/mol</td>
<td>kJ/mol</td>
<td>kJ/mol</td>
<td>kJ/mol</td>
<td>kJ/mol</td>
</tr>
<tr>
<td>0.0</td>
<td>0.80</td>
<td>13.40</td>
<td>0.87</td>
<td>10.40</td>
<td>11.90</td>
<td>10.64</td>
</tr>
<tr>
<td>5.0</td>
<td>0.78</td>
<td>13.52</td>
<td>0.85</td>
<td>10.02</td>
<td>11.75</td>
<td>10.63</td>
</tr>
<tr>
<td>10.0</td>
<td>0.75</td>
<td>13.57</td>
<td>0.82</td>
<td>9.05</td>
<td>11.40</td>
<td>10.61</td>
</tr>
<tr>
<td>15.0</td>
<td>0.74</td>
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<td>7.80</td>
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<td>0.74</td>
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<td>10.54</td>
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<tr>
<td>25.0</td>
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<td>12.15</td>
<td>0.70</td>
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<td>0.16</td>
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<tr>
<td>180.0</td>
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<td>1.84</td>
<td>0.26</td>
<td>0.03</td>
<td>3.89</td>
<td>6.94</td>
</tr>
</tbody>
</table>

Where:

- E₁ is stretching energy
- E₂ is bending energy
- E₃ is stretching-bending energy
- E₄ is torsional energy
- E₅ is 1,4 Van der Waal’s interactions energy
- E₆ is dipole-dipole interactions energy

Table 2: Energy of gauche and trans conformers of ethane, 1,2-disubstituted ethanes and the energy difference

<table>
<thead>
<tr>
<th>Substance</th>
<th>Energy of gauche conformer</th>
<th>Energy of trans conformer</th>
<th>Energy difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethane</td>
<td>3.42</td>
<td>3.42</td>
<td>0.00</td>
</tr>
<tr>
<td>Butane</td>
<td>12.70</td>
<td>9.10</td>
<td>-3.60</td>
</tr>
<tr>
<td>1,2-difluoroethane</td>
<td>13.70</td>
<td>16.25</td>
<td>-2.55</td>
</tr>
<tr>
<td>1,2-dichloroethane</td>
<td>21.08</td>
<td>14.16</td>
<td>-6.92</td>
</tr>
<tr>
<td>1,2-dibromoethane</td>
<td>19.13</td>
<td>13.27</td>
<td>-5.86 (5.89)</td>
</tr>
<tr>
<td>1,2-diiodoethane</td>
<td>8.00</td>
<td>5.19</td>
<td>-2.81</td>
</tr>
<tr>
<td>1,2-ethanediol</td>
<td>11.88</td>
<td>8.57</td>
<td>-3.31</td>
</tr>
<tr>
<td>1,2-dicyanoethane</td>
<td>26.80</td>
<td>18.84</td>
<td>-7.96</td>
</tr>
<tr>
<td>1,2-dimethoxy-ethane</td>
<td>41.79</td>
<td>40.34</td>
<td>-1.45</td>
</tr>
<tr>
<td>1-bromo-2-chloroethane</td>
<td>19.19</td>
<td>13.69</td>
<td>-5.50</td>
</tr>
<tr>
<td>1-bromo-2-chloropropane</td>
<td>23.58</td>
<td>19.95</td>
<td>-3.63</td>
</tr>
</tbody>
</table>

Conclusions

This work is one of the assignments of the computational and theoretical chemistry module at the University of Mauritius. Students obtained the gauche–trans energy difference of ethane and 1,2-disubstituted ethane using molecular mechanics method. The results obtained compare satisfactorily with literature findings and further the feedback for the students was interesting. We guessed...
that it was a promising start and in fact this is the fourth year that computational and theoretical chemistry module is running as an elective for BSc (Hons) Chemistry students. Another assignment, as suggested by the students, is in progress to obtain the gauche-trans energy difference for the compounds studied in different solvents. These studies would definitely be in line with an extract with Sir John Pople’s Nobel prize speech (19): “…the fact that mathematics has invaded chemistry, that by means of theoretical calculations we can predict a large variety of chemical phenomena”.

Acknowledgements
The author is grateful to The University of Mauritius Research Fund for supporting this work and second year students of BSc (Hons) Chemistry of the year 2002 for the participation. The author is also grateful to anonymous reviewer and colleagues whose constructive criticisms have improved the manuscript.

References

Continuation from page 9:

Professional Ethics in Support of Chemical Disarmament:
A Challenge for Chemical Education

31. Pugwash web site: http://www.pugwash.org/
The determination of the best separation conditions for a mixture of preservatives of varying polarity using HPLC: An ACELL experiment.1

Magdalena Wajrak and Mary Boyce

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Introduction

Chromatography is a fundamental component of most analytical chemistry units in undergraduate science programs. Many gas chromatography (GC) and high performance liquid chromatography (HPLC) experiments tend to focus on the quantitative aspect of the technique (determination of benzoic acid in coca cola or ethanol in wine) [1-3]. However, these experiments do not actively develop students understanding of the separation processes involved and method development (ie development of best separation conditions) is limited due to time constraints. To address these issues we have been active in developing experiments that promote understanding of the separation mechanisms involved [4,5].

This aims of the experiment described here are to (i) extend and develop students understanding of the mechanisms of separation in reversed phase (RP) chromatography (ii) provide students with some experience in method development and (iii) expose students to appropriate tools that can facilitate method development.

Students are required to determine the best separation conditions (ie mobile phase conditions) to separate a complex mixture including the non-polar paraben based preservatives and the polar preservatives, sorbic acid (2,4-dihexenoic acid) and benzoic acid using RP–HPLC system. The introduction of an ion-pairing reagent is necessary to resolve the mixture. A modelling package, DryLab®, is used to simulate the separation and determine the best conditions (ie the amount of pairing reagent required to resolve the mixture).

Preservatives were chosen as it has immediate relevance and also because the commonly used preservatives fall into two categories, the non-polar and closely related parabens and the polar organic acids. The parabens are easily resolved by reversed phase HPLC but the acids and the parabens are difficult to resolved simultaneously by RP-HPLC, hence the need for an ion-pairing reagent.

Acknowledgements

The original idea for this experiment came from a paper by Boyce and Spickett entitled ‘Separation and Quantification of Preservatives Using Ion Pair HPLC and CZE: An Extended Investigation of Separation Mechanisms’ [5]. The experiment has been adapted to include a modelling component and the capillary zone electrophoresis (CZE) component has been removed. The authors wish to thank: Mr Mark Bannister, laboratory technician from Edith Cowan University, for his help in setting up this experiment. In addition, thanks must also go to the members of the ACELL team for useful feedback and suggestions.

Educational Template

Section 1 - Summary of the Experiment

1.1 Experiment Title

The determination of best separation conditions for a mixture of preservatives of varying polarity using HPLC.

1.2 Description of the Experiment

In this experiment students are required to determine the best separation conditions (ie mobile phase conditions) to separate a complex mixture including the non-polar paraben based preservatives and the polar preservatives, sorbic acid (2,4-dihexenoic acid) and benzoic acid using RP–HPLC system. The main aims of the experiment are to (i) promote student understanding of the mechanisms of separation in chromatography, in this case RP and ion pair (IP)-RP separations and (ii) to expose students to modern tools, in this case a modelling package, used to facilitate the process.

1.3 Course Context and Students’ Required Knowledge and Skills

At ECU our students complete a Bachelor of Technology (Applied & Analytical Chemistry) Degree. This degree has a significant TAFE component in first and second year and as a result our chemistry majors have good hands on instrumentation skills. In third year, our students complete several analytical chemistry units at ECU, one of which is Analytical Chemistry I* where the main emphasis is on chromatographic techniques including HPLC, gas chromatography and capillary electrophoresis. The theory of chromatography is covered in some detail and includes a discussion on RP and IP separations. In the laboratory, students complete introductory HPLC based experiments that focus on proper use and maintenance of HPLC instrumentation, quantitative measurements and the recording and generating of data such as retention times, peak widths, etc.

1 The complete documentation for this experiment is freely available on the ACELL web site [www.apcell.org]. It includes the educational template, a set of student notes, demonstrator notes and technical notes to allow ready implementation into a new laboratory.
The experiment described here is one of a few extended activities that students complete in the final weeks of semester. Therefore, it is assumed that students will have the skills (with some help if required from the demonstrator) to operate the pump system, UV-VIS detector and the HPLC software. In other words students are not generally preoccupied with how to inject the sample or get the computer to take in the data.

*Some students will be taking chemistry as a supporting major and will not have done the TAFE component and therefore introductory HPLC experiments are vital for these students.

1.4 Time Required to Complete
Prior to Lab 30min for reading
In Laboratory 3 hours for laboratory work

After Laboratory 2 hours for analysis of results, report writing and answering questions.

 Providence
The original source of this experiment is a paper by Boyce and Spickett entitled ‘Separation and Quantification of Preservatives Using Ion Pair HPLC and CZE: An Extended Investigation of Separation Mechanisms’ [5]. Two main modifications have been made from the original paper; inclusion of modelling component using DryLab® software and the removal of capillary zone electrophoresis component.

 Other Comments
Although butyl paraben (butyl 4-hydroxy-benzoate) is also a common non-polar preservative, we have not used it in this experiment due to time constraints. Butyl paraben is the heaviest of the parabens and would have taken over 10min to come off the column.

<table>
<thead>
<tr>
<th>Learning Outcomes</th>
<th>Process</th>
<th>Assessment</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>What will students learn?</strong></td>
<td><strong>How will students learn it?</strong></td>
<td><strong>How will staff know students have learnt it?</strong></td>
</tr>
<tr>
<td><strong>How will students know they have learnt it?</strong></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Theoretical and Conceptual Knowledge

<table>
<thead>
<tr>
<th>Statements</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>Students will gain a deeper understanding of the separation mechanism in RP chromatography.</td>
<td>Students will run a mixture containing polar and non-polar preservatives on a C18 column using a polar mobile phase and identify the peaks on the resulting chromatogram. The separation and elution order of the non-polar preservatives provide a classic example of how such solutes are resolved by RP chromatography. The inability to resolve the polar solutes under the same conditions also highlights the limitations of the RP conditions.</td>
</tr>
<tr>
<td>Students are required to label the peaks in the chromatograms recorded and hence explain the elution order observed. The students will discuss and explain their results with the demonstrator. The demonstrator can then probe students understanding and clarify any misconceptions the students may have.</td>
<td></td>
</tr>
<tr>
<td>Students will learn how separation mechanisms can be cleverly manipulated to provide better resolution – in this case the addition of a pairing reagent to the mobile phase to separate the polar preservatives.</td>
<td>Students will add pairing reagent (at different concentrations) to the mobile phase in an attempt to resolve the coeluting polar solutes. They will determine the identity of the peaks recorded for each chromatogram recorded by running individual standards of the solutes.</td>
</tr>
<tr>
<td>Each student group will determine the elution order and identify the components separated under the various conditions. The students will discuss and explain the elution order observed with the demonstrator. The demonstrator will also probe students understanding. In addition students are required to complete post lab questions which are assessed and returned to students for feedback.</td>
<td></td>
</tr>
<tr>
<td>Students get an opportunity to apply and consolidate theory learnt in lectures in the laboratory environment.</td>
<td>Students completing the experiment must use separation and chromatography theory to explain their results.</td>
</tr>
<tr>
<td>The feedback received from the laboratory write-up and the final examination mark.</td>
<td></td>
</tr>
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### Scientific and Practical Skills

<table>
<thead>
<tr>
<th>Provide students with more experience in the use of HPLC instrumentation</th>
<th>Students are required to vary the mobile phase, condition the column between changes in mobile phase and carry out a number of separations in completing this experiment</th>
<th>Students will build on instrumentation skills already developed. Students will concentrate on explaining their results rather than how to use the injection loop or the HPLC software.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Expose students to the use of a chromatographic modelling package.</td>
<td>Students will use the modelling package to determine best separation conditions for the mixture under investigation. Students will take their experimental data, insert it into the modelling package, model the separation and hence predict best separation conditions. They will then test the predicted conditions experimentally.</td>
<td>Students will complete a simulation and obtain best separation conditions for their data.</td>
</tr>
<tr>
<td>Recording, extracting and calculating relevant scientific data including retention times and peak widths.</td>
<td>Students will use appropriate formulas to work.</td>
<td>Students will obtain ‘reasonable’ data typical for HPLC.</td>
</tr>
<tr>
<td>Students will better appreciate how the quality of resolution will be compromised by budget (eg. time and chemical costs).</td>
<td>The modelling package will allow students to view the resolution and retention times of the analytes under different conditions. While best resolution might be achieved at longer run times, students will also be able to determine conditions that support short run times but with poorer resolution.</td>
<td>What “best separation conditions” means will be discussed by the students and demonstrator – are all analytes of interest quantitatively, will a short run time resolve the key analyte of interest – what is the cost of the separation.</td>
</tr>
</tbody>
</table>

### Generic Skills

<table>
<thead>
<tr>
<th>Students will further develop their report writing skills.</th>
<th>Students will be asked to prepare a clear, well-structured, formal report.</th>
<th>The report will be marked according to the criteria given in experimental notes and written feedback will be provided with respect to those criteria.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Students will get the opportunity to participate in group discussions and work as a team.</td>
<td>Students will be encouraged to discuss questions ‘in the lab’ and their results within the group prior to writing up the final report.</td>
<td>The demonstrator will actively participate in students’ discussions. As part of the scientific report students will be required to give a written account (as part of the formal laboratory report, which is assessed) of the questions discussed during the laboratory session.</td>
</tr>
<tr>
<td>Students will develop new and industry relevant computer skills.</td>
<td>Students will use, DryLab®, a computer package to determine best separation conditions.</td>
<td>Be familiar with a HPLC modelling package.</td>
</tr>
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</table>
Explanatory notes to Student Learning Experience

This experiment was presented at the APCELL workshop in 2002. The exercise and associated documentation was revised, incorporating suggestions from workshop participants. The version presented here includes further changes in response to the 2002 student feedback, and to comments from the APCELL referees.

3.1 Did this experiment help you to understand the theory and concepts of the topic? If so, how, or if not, why not?
S1: I didn’t feel it increased/improved my prior understandings.
S2: Yes, helped clarify my understanding of mobile/stationary interaction.
S3: Yes.
S4: Yes - experiment was based on theory rather than learning analytical/instrumental techniques.
S5: Most definitely. The demonstrator was terrific at asking leading questions.
S6: Yes

3.2 How is this experiment relevant to you in terms of your interests and goals?
S1: Not particularly relevant – Not my area of expertise/interest. However, found it interesting to do something different.
S2: Not relevant, but it was fun to think.
S3: It broadened my outlook. Not directly relevant to me.
S4: Interested in food and instrumentation so very relevant experiment.
S5: I want to incorporate HPLC experiments in Second Year analysis of biological molecules.
S6: Very – formulation analysis.

3.3 Did you find this experiment interesting? If so, what aspects of this experiment did you find interesting? If not, why not?
S1: Yes. Conceptually interesting. Good to have discussion.
S2: Interesting because students should be able to see industrial/employment relevance.
S3: I am surprised it’s aimed at second half of 3rd year. I’d see it as a good early HPLC experiment followed by a more demanding one.
S4: Yes – learning a different way of separating compounds.
S5: I am an organic chemist, so it was very interesting (structure-polarity relationships, etc).
S6: How the instrument works. What is good separation. Software is cute. Bit expensive.

3.4 Can the experiment be completed comfortably in the allocated time? Is there time to reflect on the tasks while performing them?
S1: Ran a bit short of time in making sol’s, conditioning.
S2: I think it’s suitable for a 3 hour lab but 90 minutes was really rushed.
S3: I think so.
S4: We were pushed for time in out 90 minutes. Yes – because it takes time for each run so you have time to reflect and discuss.
S5: Hard to tell without doing the experiment in full.
S6: Yes.

3.5 Does this experiment require teamwork and if so, in what way? Was this aspect of the experiment beneficial?
S1: Not necessarily. Discussion in the group was helpful.
S2: Teamwork helps to get ideas out.
S3: Not really!
S4: Not required at all but we discussed results amongst the group.
S5: The discussions were extremely beneficial. I would have been less confident doing it on my own.
S6: Discussing separation theory.

3.6 Did you have the opportunity to take responsibility for your own learning, and to be active as learners?
S1: Yes.
S2: It was a bit easy to “cruise” and let more vocal members of the group to continue talking.
S3: A bit – demonstrator took control.
S4: Yes.
S5: Yes, needed to take risk to make suggestions.
S6:

3.7 Does this experiment provide for the possibility of a range of student abilities and interests? If so, how?
S1: Don’t really know. Haven’t thought about it.
S2: I think not-too-enthusiastic students can hide in the group and vocal students can dominate.
S3: I feel not very demanding for very bright students. It’s really routine analytically.
S4: Yes – actual experiment wasn’t difficult – more the interpretation but this (I assume) could be taken away from the lab and worked through.
S5: Yes.
S6: Not really.

3.8 Did the laboratory notes, demonstrators’ guidance and any other resources help you in learning from this experiment? If so, how?
S1: Didn’t get much opportunity to read them. Can’t really comment.
S2: Didn’t really get to see.
S3: The demonstrator was very pleasant and enthusiastic which was more than half the enjoyment. I might find it harder with a frumpy demonstrator or no demonstrator.
S4: Yes – demonstrator guided us along.
S5: N/A.
S6: Yes example chromatograms.

*to continue on page 31*
Chemistry Students’ Misconceptions in Electrochemistry

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Abstract
In this study, by taking into account Garnett and Treagust’s study of students’ misconceptions in electrochemistry, a variety of tests were applied to students to determine what kinds of misconceptions in electrochemistry were found in Turkish higher education. These questions were administered to 40 Chemistry Education students after their electrochemistry instruction. This confirmed most of the misconceptions reported and identified of several new ones, including the notions that electrons can flow through aqueous solutions without assistance from the ions and that only anions constitute a flow of current in electrolyte solutions. Chemistry education students suggested two mechanisms for electron flow in electrolyte solutions and the salt bridge: electrons can either attach themselves to ions in solutions or they can flow by themselves without assistance from the ions. Analysis of the text books used by chemical education students suggests a source of these misconceptions were mistakes or misleading statements in the texts, which can be misinterpreted or over generalized to inappropriate situations. Most students demonstrating misconceptions were still able to calculate cell potentials correctly, which is consistent with research suggesting that students capable of solving quantitative examination problems often lack of understanding of the underlying concepts. Animations are a part of computer-assisted learning that improve students’ motivation and encourage students to adjust the rate of their learning according to their capacity and reduce misconceptions.

Introduction
Electrochemistry is the study of the relationships that exist between chemical reactions and the flow of electricity. Included here are electrolysis reactions, in which nonspontaneous changes are forced to occur by the passage of electricity through chemical systems. Also included are spontaneous oxidation-reduction reactions (redox reactions) that are able to supply electricity. Chemical reactions are also accompanied by absorption or evolution of heat (the heat effect of the reaction) and don’t involve electrical energy. Electrochemistry deals with reactions proceeding at the expense of external electrical energy or serving as a source of this energy. Such reactions are known as electrochemical reactions (1). Several researchers have documented students’ misconceptions in electrochemistry. One reason for the interest in studying educational aspects of electrochemistry is that surveys of students and teachers suggest that students find this topic difficult (2), and research confirms that students’ beliefs about problem complexity affect their performance and learning. Several articles have promoted pedagogical suggestions or opinions about more effective methods of teaching electrochemistry (3, 4); but few, if any, of these have actually been tested.

Allsop and George (5) reported that students had difficulty using standard reduction potentials to predict the direction of chemical reactions and were unable to produce an acceptable diagram of an electrochemical cell; 12% of these students stated that a salt bridge provides a pathway for the flow of electrons. Ogude (6) noted that although many students can solve the quantitative electrochemical problems that appear on chemistry exams, few were able to answer qualitative questions requiring a deeper conceptual knowledge of electrochemistry. Also in this Ogude’s study, 32% of undergraduate students consistently replied that electrons can not flow in the electrolyte and 29% consistently replied that electrons can flow in the electrolyte; 43% were inconsistent in their responses. Similar results were found (7) where 30% of students suggested that ions flow to complete the circuit in the electrolyte solution while 62% suggested that electrons flow in the electrolyte.

There are two major reasons that students experience problems with these concepts: the topics are very abstract, and the language of chemistry is new. Teachers use words from everyday language that have different meanings in the scientific context called “portmanteau words” (8). Garnett and Treagust (9) probed student misconceptions about oxidation-reduction reactions and electrochemical and electrolytic cells through interviews with high-school students in Australia. They reported several common misconceptions about oxidation-reduction reactions, electrochemical cells, and electrolytic cells. Misconceptions about the flow of current in electrolyte solutions and the salt bridge include the notions that,
- electrons move through the electrolytes and the salt bridge, carried or transferred by cations and anions;
- protons move through the electrolytes and the salt bridge, even in neutral or basic solutions; and
- ion movements in solution do not constitute an electrical current.

Recent research has focused on students’ conceptual difficulties with electrochemistry (5, 6, 10, 11).

The first part of this article focuses on students’ misconceptions and proposed mechanisms related to current flow in electrolyte solutions and the salt bridge (summarized in Table 1), and on likely sources for these misconceptions. The second part reports the results of a study to determine whether teaching to actively confront the misconception that electrons flow in solution using computer animations will decrease the number of students consistently harboring this misconception.
**Investigation and Evaluation**

**Current flow through Electrolyte Solutions:**

Students recognize that current cannot flow without a closed circuit, and many believe that only electron flow can complete this circuit. Consequently, many students cling to the notion that electrons flow from the anode to the cathode along the wire and are then released into the electrolyte at the cathode, traveling through the electrolyte solutions and the salt bridge to reach the anode. This is represented as misconception 2a (Table 1), which was held in one form or another by eight of the 15 students.

Of those who believed that electrons flow through the salt bridge, two stated that anions in the electrolyte solutions and the salt bridge help transfer the electrons (misconception 2b), three stated that cations transfer the electrons through the salt bridge (misconception 2c) and three stated that the electrons flow through solution without any assistance from anions or cations (misconception 2d).

Three students who correctly stated that ions flow through solutions and the salt bridge to complete the circuit suggested that it is the flow of anions in solutions that completes the circuit, and cation flow does not constitute a current (misconception 2e).

In their responses to questions about electrochemical and electrolytic cells, seven of the 15 students responded with comments suggesting that the electrodes have net positive and negative charges. Some believed that the anode is positively charged (misconception 3b); they interpreted anion flow toward the anode as suggesting that the anode is positively charged and cation flow toward the cathode as suggesting that the cathode is negatively charged.

**Mechanisms for Electron transfer through Electrolyte Solutions:**

Seven of the eight students who stated that electrons flow in electrolyte solutions and the salt bridge suggested possible mechanisms for the flow of electrons. Five stated that electrons are transferred from the cathode to the anode by the ions in solution (misconception 1b). Four of these students stated that cations (Ag⁺ and NH₄⁺ in the galvanic cell and Al³⁺ in the electrolytic cell) assisted in the transfer of electrons from the cathode to the anode (misconception 2c) while one student stated that anions help in the transfer of electrons from cathode to anode. None of the students in this study demonstrated misconception 1a; this misconception was originally reported by Garnett and Treagust (10). A student suggested that electrons are transferred back and forth from anion to cation as they travel in solution from the cathode to the anode. Three students who stated that electrons flow in electrolyte solutions and the salt bridge suggested that the electrons receive no assistance from ions and travel as free electrons from the cathode to the anode (misconception 2e).

In contract to Garnett and Treagust’s students, none of our students suggested that electrons travel in solution as free electrons from the cathode to the anode (misconception 2e).

Table 1: Common misconceptions found in students investigated

<table>
<thead>
<tr>
<th>Common misconception</th>
<th>Student responses</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Statement of Misconception</strong></td>
<td></td>
</tr>
<tr>
<td>Current flow through Electrolyte Solutions:</td>
<td></td>
</tr>
<tr>
<td>2a: Electrons enter the solution from the cathode, travel through the solutions and salt bridge, and emerge at the anode to complete the circuit.</td>
<td>24</td>
</tr>
<tr>
<td>2b: Anions in the salt bridge and the electrolyte transfer electrons from the cathode to the anode.</td>
<td>6</td>
</tr>
<tr>
<td>2c: Cations in the salt bridge and the electrolyte accept electrons and transfer them from the cathode to the anode.</td>
<td>9</td>
</tr>
<tr>
<td>2d: Electrons can flow through aqueous solutions without assistance from the ions.</td>
<td>9</td>
</tr>
<tr>
<td>2e: Only negatively charged ions constitute a flow of current in the electrolyte and the salt bridge.</td>
<td>24</td>
</tr>
<tr>
<td>3b: The anode is positively charged because it has lost electrons; the cathode is negatively charged because it has gained electrons.</td>
<td>none</td>
</tr>
<tr>
<td><strong>Mechanisms for Electron transfer through Electrolyte Solutions:</strong></td>
<td></td>
</tr>
<tr>
<td>1a: Electrons move through solution being attracted from one ion to the other</td>
<td>none</td>
</tr>
<tr>
<td>1b: Electrons move through solution by attaching themselves to ions at the cathode and are carried by that ion to the anode.</td>
<td>15</td>
</tr>
<tr>
<td>2c: Cations in the salt bridge and the electrolyte accept electrons and transfer them from the cathode to the anode.</td>
<td>12</td>
</tr>
<tr>
<td>2e: Only negatively charged ions constitute a flow of current in the electrolyte and the salt bridge.</td>
<td>9</td>
</tr>
</tbody>
</table>

**Probable sources of misconceptions for students:**

Garnett and Treagust (10) proposed two origins of student misconceptions concerning the flow of current in electrolyte solutions and the salt bridge:

- Students’ interpretation of the language of science – students interpret the terminology used in the textbook or by the instructor in a manner consistent with everyday usage, but inconsistent with scientific usage and
- Students applying information too generally, over-generalizing a scientific statement to situations where it is inappropriate. From these proposed origins, Garnett et al. (9) drafted suggestions for improving the chemistry curriculum that included the following ideas:

- Teachers and curriculum developers need to select explanatory language with care, and be particularly cautious in selecting language having everyday
meanings that differ from meanings in a scientific context and
- Teachers and curriculum developers need to be cautious in making unqualified, generalized statements about concepts because students tend to interpret the statements literally, and apply them more extensively than is intended.

Ogude and Bradley (6) attributed student misconceptions concerning current flow in electrolyte solutions and the salt bridge to two factors:

1. Reference by textbooks or the instructor to continuity of current and established belief in the electronic nature of current electricity and
2. Careless discussion of electrode processes (textbooks with obvious mistakes or misleading statements result in student misconceptions).

Ogude and Bradley suggested that a major source of misconceptions comes from imprecise or inappropriate language used by textbooks and instructors in explaining electrochemical concepts and this study is no exception. More than half of the students in this interview study suggested that electrons flow in electrolyte solutions and the salt bridge to complete the circuit. Analysis of the two textbooks used by these students (12, 13) revealed that all have comments that, while not technically incorrect, may be misinterpreted to suggest that electrons do flow through electrolyte solutions and the salt bridge.

For example,

1. “In a solution of an electrolyte, or in molten salt such as sodium chloride, however, electrical charge is carried through the liquid by the movement of ions. The transport of electrical charge by ions is called electrolytic conduction, and it is able to occur only when chemical reactions take place at the electrodes” (12).

Rendition: If students interpret “electrical charge” as “electrons” instead of as “the inherent charge of the ions”, the first sentence could lead to misconceptions 2b and 2c and the second sentence could foster misconception 1b about the transfer of electrons through electrolyte solutions and the salt bridge.

2. This task is accomplished through a galvanic (or voltaic) cell, which is merely a device in which electron transfer is forced to take place through an external pathway rather than directly between reactants (13).

Rendition: Electrons are being transferred from the reductant to the oxidant, but “electron transfer through an external pathway” can be misinterpreted as suggesting that electrons flow throughout the entire circuit including the electrolyte solutions and the salt bridge and may be responsible for misconceptions 2a or 2e.

The results of this analysis should prompt textbook authors to carefully examine and reconsider the language used in their chemistry textbook. The use of detailed diagrams and animations about current flow through electrolyte solutions and the salt bridge should be included in a multimedia presentation to help students to visualize these concepts.

**Methods for preventing Misconceptions:**

We have become increasingly interested in the use of video (or computer) animations as a lecture tool to enhance students’ ability to visualize and understand chemical concepts on the molecular level. In a typical lecture, the instructor performs a live chemical demonstration, writes the relevant balanced chemical equations on the board, and shows and explains a computer animation depicting the reaction on the molecular level. In this way, the lecturer attempts to facilitate students’ connection of the macroscopic, symbolic, and microscopic representations of chemical processes (14, 15). Examples of electrochemistry animations used in these lectures have been reported by Greenbowe (16). Preliminary studies to determine whether we can reduce the number of students holding the misconception that electrons flow in the salt bridge by teaching to actively confront, and therefore prevent or dispel, this misconception are encouraging.

After receiving instruction on electrochemistry, students in the first semester of introductory chemistry for non-science majors answered three conceptual questions about the flow of electrons in electrolyte solutions and the salt bridge (Appendix 1) (17). The instructor had explicitly emphasized that electrons do not flow in electrolyte solutions or the salt bridge and showed several video (or computer) animations that modeled the correct flow of current in galvanic and electrolytic cell. Table 2 contains a description and an approximate running time of the video (or computer) animations employed. Each one was displayed three times in succession while the instructor provided a narration of events. Presenting visual and verbal (written and oral) information simultaneously is consistent with Mayer and Anderson’s contiguity principle (18).

**Table 2: Animations Used in Electrochemistry Lesson**

<table>
<thead>
<tr>
<th>Animation</th>
<th>Focal Point</th>
<th>Time(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>I. Zn and Cd electrochemical cell.</td>
<td>Ion migration in electrolyte solutions and the salt bridge movement of electrons in the wire;</td>
<td>50</td>
</tr>
<tr>
<td>II. Salt bridge</td>
<td>Cation and anion migration out of the salt bridge; balance in each half-cell.</td>
<td>35</td>
</tr>
<tr>
<td>III. Electroplating silver onto iron.</td>
<td>Electron movement in the wires; ion migration in the aqueous solution; oxidation process at anode; reduction process at cathode.</td>
<td>50</td>
</tr>
</tbody>
</table>

The animations of the salt bridge included an overall animation that focused on the dynamics of the entire zinc and cadmium electrochemical cell, and a (close-up) of cation and anion migration out of the salt bridge (Figure 1). The animation clearly shows only ions migrating in solution. This (close-up) view allows students to focus their attention on the critical concept being illustrated.
Aust. J. Ed. Chem., 2005, 65,

Figure 1. Cation and anion migration in the salt bridge of zinc – cadmium electrochemical cell.

Video animation of the electrolytic cell illustrates the plating of silver metal on an iron spoon tea (Figure 2). The animation clearly shows electrons being released at the anode, bumping up from the anode through the wire and the battery to the cathode. Silver ions in solution migrate toward the iron cathode (spoon tea) where they capture electrons at the solution-metal interface, plating out on the electrode as silver metal. The animation clearly shows that only ions migrate in solution.

Figure 2.
The electrolytic plating of silver metal onto an iron spoon.

The distracters in each question were classified as being consistent or inconsistent with the misconception that electrons flow in electrolyte solutions. Responses to the three conceptual questions (Appendix 1) were analyzed to determine whether students consistently demonstrated or failed to demonstrate this misconception. Of the 40 students who took the final exam, five (12.5%) consistently chose responses suggesting that electrons are present in solution, ten (25%) consistently chose responses not suggesting that electrons exist in solution, and 25 (62.5%) chose responses inconsistent with regard to the presence of electrons in electrolyte solutions.

These results can be compared to those reported by Ogude and Bradley (1994), in which 40 first-year college students answered five conceptual questions concerning the flow of electrons in electrolyte solutions. In their study, 11 (28%) consistently demonstrated the misconception; 12 (30%) consistently did not demonstrate the misconception; and 17 (42%) were inconsistent. These numbers are complicated by the fact that Ogude and Bradley also used question 2 in Figure 1, but they included only response 5 as being consistent with the misconception; we included responses 1, 2 and 5 because all of them suggest that electrons exist in solution. Since eight of the forty students in Ogude and Bradley’s study chose responses 1 and 2 for this question, it is likely that more than 28% consistently demonstrated and less than 30% consistently did not demonstrate this misconception.

The chi-square test of independence was performed on the number of students in each study. The results of this test \(X^2 (2) = 21.80, p<0.0001\) support the assumption that our teaching method had an effect on the majority of students consistently demonstrating this misconception.

This study suggests that active teaching to confront the misconception that electrons flow in electrolyte solutions and the salt bridge, using video (or computer) animations to help students visualize chemical reactions at the molecular level, decreased the proportion of students consistently demonstrating this misconception. The effect of viewing animations that focus attention on the molecular level can be seen also in Williamson and Abraham’s study (15) in which students who viewed animations based on the states of matter and reactions in solution were better able to visualize particulate behavior in chemical reactions.

The test of independence does not suggest a difference in the proportion of students inconsistently demonstrating the misconception, these numbers should be scrutinized. Since Ogude and Bradley’s students answered five questions while ours answered only three, it is not unreasonable to expect a larger inconsistent group in their study due to random effects; however, this study shows a large proportion of students who were inconsistent in their responses. Even though our students received instruction in electrochemistry that emphasized the correct model of current flow in electrolyte solutions and the salt bridge and were directed to readings about this topic in their textbook, previous experience suggests that this misconception resists change. Perhaps the animations shown in the lecture were not shown long enough for students to process the information. Research is needed to determine whether these animations adequately explained the students’ experiences and observations and appeared logical to the students.

Results

In the result, the difficulties that some students were facing in understanding electrochemistry events are arising from the use of some misconceptions. Although the students had some misconceptions in electrochemistry, they were able to calculate a cell potential by using known equations at memorization base. However, this may not indicate that the subject is understood correctly by students. Therefore, to be able to identify misconceptions, quantitative studies
should be conducted. One way of this may be that a good dialogue should be established between instructors and students. This dialogue may lead to develop a new improved education method. Abstract and concrete phenomenons are presented through animations. It was found that there was a significant decrease in the number of misconceptions, as the animations helped students to make clear the relationship between the concepts, to see the cause-effect relationship and manipulate the concrete phenomenons.

References

Appendix 1

1. Electrons in the cell flow through the --- toward the --.
   a) wire, silver electrode
   b) wire, electrode
   c) cadmium electrode, salt bridge
   d) silver electrode, salt bridge

2. In an electrochemical cell, conduction through the electrolyte is due to,
   a) electrons moving through the solution attached to the ions
   b) electrons moving from ion to ion through the solution
   c) the movement of both negative and positive ions
   d) the movement of water molecules
   e) electrons moving through the solution from one electrode to the other.

3. The electrochemical cell shown below has 1.16 volts for its EMF.
   There is an oxidation reaction and a reduction reaction.

Which one(s) of the diagrams below depict each half-cell as the reactions proceed?
New light from an old reagent: Chemiluminescence from the reaction of potassium permanganate with sodium borohydride.


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Abstract
When aqueous sodium borohydride (50 mM) is added to a solution of potassium permanganate (1mM, in sodium hexametaphosphate) at acidic pH, bright red-orange emission is easily visible in a darkened room. This chemiluminescence emission is due to an excited state of manganese (II) that undergoes solution phase phosphorescence and provides an excellent opportunity for students to explore the relationship between the initial oxidation state of the manganese and the likelihood of luminescence. Not surprisingly Mn(VII), Mn(IV) and Mn(III) all give rise to chemiluminescence whereas Mn(II) fails to react.

Introduction
Since its first observation by Glauber (1659), and subsequent characterisation by Forchhammer (1820) and Mitscherlich (1832) the deep violet colour of potassium permanganate has held a fascination for most chemists (1). Now established as an oxidant, especially in volumetric analysis (2), potassium permanganate is well known to most high school students. Surprisingly in Harvey’s (3) detailed account of the history of luminescence prior to 1900 there is no mention of this common oxidant being used as a chemiluminescence reagent. Although largely ignored in the classroom demonstrations, (the oxidation of siloxene (4, 5) is the only well-known demonstration of chemiluminescence involving the permanganate ion), potassium permanganate has a history as a chemiluminescent reagent in analytical chemistry (6). Under certain circumstances, higher oxidation states of manganese can be reduced to form an excited state Mn(II) species which undergoes solution phase phosphorescence to emit red chemiluminescence (7).

In this paper we describe what is undoubtedly one of the simplest of all chemiluminescent reactions, namely the reaction of potassium permanganate with sodium borohydride in aqueous solution. The demonstration provides an excellent opportunity for students to explore the relationship between the initial oxidation state of the manganese and the emission of light. Not surprisingly Mn(VII), Mn(IV) and Mn(III) all give rise to chemiluminescence whereas Mn(II) fails to emit. This demonstration has the potential to be further developed as a high school experiment where students can not only explore the oxidation state of the manganese but also the effect of variables such as reagent concentration and pH on the intensity of the light emitted. Furthermore all of the chemicals and equipment required are readily available in a high school laboratory and the only other thing required is the human eye, a most sensitive detector.

Experimental Procedure
Materials and Equipment
Potassium permanganate
Manganese sulfate
Sodium borohydride
Sodium hexametaphosphate (Calgon)
Sodium hydroxide (0.001 M)
Sulfuric acid (2 M)
Phosphoric acid (3 M)
Ultrasonication bath
Deionised Water
1 × 500 mL beakers
3 × 200 mL beakers
several extra 500 mL beakers to pour solutions into

Preparation of solutions
Manganese(VII): Dissolve 0.079 g (0.5 mmol) of potassium permanganate and 10 g of sodium hexametaphosphate in 1.0 L of deionised water. Adjust the pH of the solution to 2.0 with 2 M sulfuric acid. This solution is stable for more than 24 hours.

Sodium borohydride: Dissolve 0.2 g (ca. 11 mmol) of sodium borohydride in 500 mL of aqueous sodium hydroxide (0.2 g in 5.0 L).

Manganese(II): Dissolve 0.5 g (3.3 mmol) of manganese(II) sulfate and 1.0 g of sodium hexametaphosphate in 100 mL of deionised water.

Manganese(IV): Dissolve 0.5 g (3.3 mmol) of manganese(IV) sulfate and 2.5 g of sodium hexametaphosphate in 250 mL of deionised water. Adjust the pH to 2.0 with 2M sulfuric acid. Add 0.025 g (0.158 mmol) potassium permanganate to this solution and allow to react for thirty minutes. This resulting solution contains approximately 0.05 M Mn(III).

Manganese(III): Solutions of manganese(III) can be prepared from manganese dioxide synthesised by the method of Jáky and Zriniyi (8). Wet manganese dioxide
(0.04 g) is dissolved in 100 mL of phosphoric acid (3 M) assisted by ultrasonication.

**Demonstration**
When you wish to begin the demonstration turn out the room lights. Slowly pour some of the sodium borohydride solution into a 500 mL beaker containing some of the potassium permanganate solution. An intense and rapid red-orange chemiluminescence emission that fills the entire beaker is observed.

The potassium permanganate can be replaced with solutions of manganese(II), (III) or (IV) to demonstrate the effect of manganese oxidation state on the reaction. The light emission from the manganese(IV) reaction is low and therefore not recommended unless the room is entirely darkened, and not surprisingly the manganese(II) fails to emit chemiluminescence.

**Hazards**
Potassium permanganate is a strong oxidant whilst sodium borohydride is a powerful reductant and the reaction is a potential source of hydrogen gas. Therefore goggles, gloves and a laboratory coat should be worn whilst preparing the solutions and performing the demonstration. Care must be taken to exclude all sources of ignition, and the reaction should be conducted in a well-ventilated space.

**Discussion**
Chemiluminescence, or the emission of light as a result of a chemical reaction, has fascinated and enchanted young and old alike for centuries (3). No-longer a laboratory curiosity, the number of applications of chemiluminescence in analytical chemistry has increased in recent years (6, 9, 10) whilst the novelty industry has marketed the phenomenon in the form of Cyalume® lightsticks.

In this demonstration the chemical reaction that produces the chemiluminescence involves the reduction of potassium permanganate by sodium borohydride. An electronically excited species of manganese (II) is formed, which de-excites to the ground state to yield light around 690nm (see equation 1).

\[
\text{NaBH}_4 + \text{Mn(III, IV or VIII)/H}^+ \rightarrow \text{products} + \text{Mn(II)*} \rightarrow \text{Mn(II) + light (~690nm)}
\]

**Equation 1**
It can be seen by the naked eye that all three manganese oxidation states result in chemiluminescence of the same colour (and therefore wavelength), these observations have been confirmed spectrophotometrically (See Figure 1.). Comparison of the chemiluminescence emission spectra with the phosphorescence spectra of manganese (II) at 77K confirms the formation of an excited state manganese (II) species (See Figure 2). It is not surprising that manganese (II) does not emit as it is in the ground 2+ oxidation state and consequently unable to form the excited state species upon reaction with sodium borohydride.

**Table 1.** Effect of pH on the chemiluminescence reaction of manganese(II) with sodium borohydride

<table>
<thead>
<tr>
<th>pH</th>
<th>Observations</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.0</td>
<td>Brightest and fastest</td>
</tr>
<tr>
<td>2.5</td>
<td>Slightly weaker and slower</td>
</tr>
<tr>
<td>3.0</td>
<td>Weakest and slowest</td>
</tr>
</tbody>
</table>
Conclusions

The reactions of manganese(III), (IV) or (VII) with sodium borohydride are some of a small group of purely inorganic chemiluminescent reactions. Whilst not as spectacular in intensity as the oxidation of white phosphorus or the combustion of carbon disulfide in nitrous or nitric oxides, it is our opinion that this simple demonstration is considerably superior to the oxidation of siloxane. As a demonstration it is devoid of toxic or corrosive by-products and sufficiently cheap to make it readily accessible to high school classrooms.

References


Table 2.

<table>
<thead>
<tr>
<th>NaBH</th>
<th>Manganese(VII)/M</th>
<th>0.0001</th>
<th>0.0005</th>
<th>0.001</th>
<th>0.005</th>
</tr>
</thead>
<tbody>
<tr>
<td>4/M</td>
<td>Dull</td>
<td>Dull</td>
<td>Not Obs.</td>
<td>Not Obs.</td>
<td></td>
</tr>
<tr>
<td>0.001</td>
<td>Dull</td>
<td>Dull</td>
<td>Not Obs.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.005</td>
<td>Brighter</td>
<td>Brighter</td>
<td>Not Obs.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.01</td>
<td>Brightest</td>
<td>Bright</td>
<td>V. Dull</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.05</td>
<td>Brightest</td>
<td>Bright</td>
<td>V. Dull</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.1</td>
<td>Dull</td>
<td>Brightest</td>
<td>Bright</td>
<td>Not Obs.</td>
<td></td>
</tr>
</tbody>
</table>

Table 3. Effect of pH on the chemiluminescence reaction of manganese(III) with sodium borohydride (0.05M)

<table>
<thead>
<tr>
<th>Manganese(III)/M</th>
<th>Observations</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0001</td>
<td>V. Dull</td>
</tr>
<tr>
<td>0.0005</td>
<td>Bright</td>
</tr>
<tr>
<td>0.001</td>
<td>Brightest</td>
</tr>
<tr>
<td>0.005</td>
<td>Brightest</td>
</tr>
<tr>
<td>0.01</td>
<td>Bright</td>
</tr>
</tbody>
</table>

Table 4. Effect of pH on the chemiluminescence reaction of manganese(IV) with sodium borohydride (0.05M)

<table>
<thead>
<tr>
<th>Manganese(IV)/M</th>
<th>Observations</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.001</td>
<td>Not Obs.</td>
</tr>
<tr>
<td>0.005</td>
<td>Very Dull</td>
</tr>
<tr>
<td>0.001</td>
<td>Dull</td>
</tr>
</tbody>
</table>

Table 2.

<table>
<thead>
<tr>
<th>NaBH</th>
<th>Manganese(VII)/M</th>
<th>0.0001</th>
<th>0.0005</th>
<th>0.001</th>
<th>0.005</th>
<th>0.001</th>
<th>0.005</th>
<th>0.001</th>
<th>0.005</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.001</td>
<td>Dull</td>
<td>Dull</td>
<td>Not Obs.</td>
<td>Brighter</td>
<td>Not Obs.</td>
<td>Dull</td>
<td>Not Obs.</td>
<td>Brightest</td>
<td>Bright</td>
</tr>
<tr>
<td>0.005</td>
<td>Brighter</td>
<td>Brighter</td>
<td>Not Obs.</td>
<td>Brighter</td>
<td>Not Obs.</td>
<td>Dull</td>
<td>Not Obs.</td>
<td>Brightest</td>
<td>Bright</td>
</tr>
<tr>
<td>0.01</td>
<td>Brightest</td>
<td>Bright</td>
<td>V. Dull</td>
<td>Brightest</td>
<td>Bright</td>
<td>V. Dull</td>
<td>Brightest</td>
<td>Bright</td>
<td>Brightest</td>
</tr>
<tr>
<td>0.1</td>
<td>Dull</td>
<td>Brightest</td>
<td>Bright</td>
<td>Not Obs.</td>
<td>Brightest</td>
<td>Bright</td>
<td>Not Obs.</td>
<td>Brightest</td>
<td>Bright</td>
</tr>
</tbody>
</table>

The determination of the best separation conditions for a mixture of preservatives of varying polarity using HPLC: An ACELL experiment.

3.9 Are there any other features of this experiment that made it a particularly good or bad learning experience for you?

S1: I am easily distracted, so I found the small amount of “hands on” work to be not engaging enough. This may just be me, however.
S2: Like practicing, injecting, purging, conditioning column.
S3: This kind of experiment is one where I would need to take my own time to work on the machine etc. In this way, group work is quite frustrating – I wanted to go slowly at one point, and they rushed ahead.
S4: Nice clear demonstration – can see on paper that peaks separate.
S5: No time to comment.
S6:

3.10 What improvements could be made to this experiment?

S1: No real comments/suggestions
S2: Actually using real life samples eg. cosmetic or food.
S3: Don’t know.
S4: None.
S5:
S6:

3.11 Other Comments

Demonstrator was v.good and explained things clearly and concisely.

Not sure if the design of the experiment is meant to be so demonstrator-centred. As a student, that would drive me nuts!

References

Chemistry vocabulary: Part 1, Terms concerning processes.

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Abstract
Although chemistry impacts largely on society and civilization, the subject is still viewed with awe. This is because the language of chemistry of which the technical terms are an important component, is not easily comprehensible even for the practicing scientists; let alone the layman. However, many of these terms, in English, can be noted as derived from a few root words, e.g., ortho, tropo, mer, meta, iso, para, hetero, syn, homo, topo, dia and pseudo, etc. Identifying the roots from which a word is formed can help understand it better, or even predict what a new term to be encountered stands for. The meanings and significance of various root words occurring in technical terms as also several unique words of chemistry are explained in the present article and its companion article in the next issue of this Journal.

Introduction
Alchemy (al=the; chyma=fluid in Arabic) was the Egyptian art of ‘pouring’ to convert other metals into gold and in the preparation of the elixir of life. Xenobiotics (Greek: xenos=guest/stranger; bios=life) are man-made chemicals foreign to the Earth’s ecosystem. From alchemy to the xenobiotics, the journey of chemistry was in intimate involvement with the progress of civilization. Several common terms of the day got into the chemical vocabulary and in the course of time, the vice versa also happened, enriching the language. Over the years, chemists have enjoyed exclusivity – social as well as scientific. This is not only a tribute to them for their achievements, but also a reminder of their inaccessibility and treating good chemistry as their preserve. In the present chemical age, more than ever before, chemistry needs to be taken aggressively to the masses, and particularly to the non-specialists, i.e., specialists of other branches working on the borders of chemistry. This can probably be promoted by explaining the language of chemistry in simpler terms. Chemistry language consists of (i) the symbols, formulae and chemical equations, on which several reviews/monographs are available, and (ii) the vocabulary of chemical terms, on which the available information is extremely limited. Dictionaries1,2 or glossaries,3 and standard text books of chemistry4-7 do serve as reference material, but do not exactly provide the root-based vocabulary learning that can help understand the concepts. Even with the more serious learner, he/she is like a pedestrian trying to scale the mountain of chemistry knowledge and reach the peak from where a panoramic view of the cosmopolitan landscape down below, i.e., science in general, is available. A rudimentary understanding of the language and vocabulary of chemistry is essential for him to negotiate the wilderness. It is the common experience that although many terms are understood per se, their origins are not known so well. This acts as a limiting factor as one advances. For in all phenomena, including the learning process, the law of diminishing returns applies restricting the continued ability of the learner. On the other hand, acquiring new knowledge can become child’s play if the structure and the organization of the chemical terms are known well.

The word English itself is from ‘Angleish’, the Germanic language of the immigrant Anglo Saxons (AD 450-550) of the British Isles. Hence, it is no wonder that upon the Norman conquest (AD 1066) of England, and the consequent influence of scientific scholars and their scholarly languages of Latin and Greek that followed, classical Greek and Latin terms were adopted for the new scientific concepts that developed. As these classical languages are not spoken now having been replaced by the modern Greek and Italian, the meanings of the classical Latin and Greek roots have not changed, unlike what could have happened if the languages were in common use. Hence, from the language point of view, the terms have a sort of permanence. But from the (dynamic) science point of view, the terms can at best indicate the level of knowledge that existed. For, as the concepts get more and more refined due to advancement of science, the terms coined originally may not fully explain and may mislead occasionally. In such a situation, stretching the etymology approach beyond a point may prove counter-productive. The IUPAC have done yeomen service by standardizing the chemistry terms, defining them precisely and in quite a few cases, recommending the use of new terms in place of old confusing ones.3 However, in the case of most chemistry terms in use, the etymology approach can be extremely useful to a new starter, and perhaps educators.

Methodology
An extensive list of technical terms in current popular usage was initially prepared from the IUPAC Compendium1 of standard text books of all branches of chemistry.4-7 From this list, such terms involving not-so-obvious etymology were sifted out. The origin of each term, and in a few cases their historical background were probed from available literature.3-7 The chemistry terms for which the information is thus available in a piecemeal fashion, were subjected to classification. A classification was developed by which substantive topics with minimum possible overlap are identified. While sequencing the topics, and in each topic the terms, care was taken so that the descriptive account can steer clear cumulatively, and does not suffer from redundancy. Instances of the necessity of a term being explained in a later section for understanding the present concept (term) are rare. The inclusion of a term in a particular topic and sequence was
based on personal discretion, and a refinement is possible. Due to the space constraint, illustrations of chemical structures are avoided, even though it could have added to the clarity of the terms (concepts) being described.

In a stand alone article, I have recently presented a few foreign (Greek, Latin, French and German) roots from which many organic chemistry terms are formed. In the twin articles now, I have concentrated on the generic origin and significance of various general chemistry terms in popular usage, broadly classified as chemistry at the macro level (processes; Part 1, this article) and chemistry at the micro level (structure; Part 2). As an illustration of the approach, let us examine the Greek root *kata* (or *cata*). It has different related meanings: down/ back/in order. Catalyst (*lein* = to loosen), cataphoresis (*phorein* = to bear), catabolism and katamorphism are words in the first sense. A catalyst helps break bond(s). In cataphoresis (which is the same as electrophoresis), migration (of the charge-bearing suspended particles, e.g., protein macromolecules) takes place under the influence of an electric field. Catabolism is the breakdown of complex organic molecules by living organisms (resulting in the liberation of energy). Katamorphism (*morphe* = shape), in the field of geology, is the breaking-down process of metamorphism, as opposed to the building-up process of anamorphism (*ana* = up). In the sense of ‘back’, *cata/kata* is present in cataacoustics/cataphonics — the branch of acoustics that deals with echoes. In the third sense of ‘in order’, the catalogues (*legein* = to reckon) of books, chemicals etc. are well known.

**Lighting up**

Lumen is light in Latin. Luminescence is emission of light other than by incandescence (and so at a relatively cool temperature); its mechanism is chemical in chemiluminescence and biochemical in bioluminescence (Greek: *bios* = life). Bioluminescence is exhibited by several organisms e.g., glow-worms, some marine mollusks, fish, bacteria and fungi. In triboluminescence (Greek: *tribein* = to rub), light results from the rubbing together of the surface of certain solids. Piezoluminescence (Greek: *piezein* = to press; piezochemistry is the study of the effect of high pressures on chemical reactions; piezoelectricity is the electric polarization of some anisotropic stress-deformed crystals) is the luminescence observed when certain solids are subjected to a change in pressure. Sonoluminescence (Latin: *sonare* = to sound) is induced by sound waves.

The suffix escence of these terms, of Latin origin, indicates an inchoative meaning,¹ and is present in terms e.g., iridescence, opalescence, fluorescence, effervescence, etc. In iridescence (Greek: *iris* = rain bow), a play of colours is caused by interference as on bubbles. Opalescence is milky iridescence. Fluorescence of substances such as fluor (spar) is the emission of light of larger wavelength than that to which the substance is exposed. On removal of the source, the fluorescence disappears. But in phosphorescence of substances such as phosphor, the luminescence persists for more than 0.1 nano seconds after excitation. The action of acid on carbonates causes effervescence (Latin: *fervere* = to boil) of carbon dioxide.

**Principle Bound**

Colligative (Greek: *col* = together; *ligare* = to bind) properties are the properties coming under a general principle. In a solution, these properties are dependent on the concentration of solute, and not on its nature. The solutions exert pressure, called osmotic pressure (Greek: *osmos* = impulse, to push). (As a side note, *osme*, in Greek means odour, a reason why the element osmium was called so). The osmotic pressure depends on the tone differential (Greek: *tonos* = pitch, tension; Latin: *tonus*) of two solutions across a semi-permeable membrane. Osmolality and osmolality (now replaced with osmotic concentration) are quantitative expressions based on the rational activity of water.³

**Kinds of Sorption**

Sorption (Lat: *sorbere* = to suck in) is of different types — absorption (*ab* = from), adsorption (*ad* = to), physisorption, chemisorption and perisorption. The *ab/ad* duo is illustrated with the Latin phrases *ab initio* (from the beginning, i.e., from scratch) models, and *ad infinitum* (to a limitless end, i.e., infinite) dilution. In absorption, the whole of the absorbing medium (solid or liquid) is engaged, e.g., (photometric) absorption coefficient. In adsorption, the surface layer only is involved, e.g., adsorption chromatography, adsorption hysteresis, adsorption isostere, adsorption isotherm, and adsorption potential. In hysteresis, the effect lags behind its cause; adsorption hysteresis (Greek: *hysteros* = later) occurs when adsorption and desorption values deviate from one another. *Stereos* is solid in Greek. Adsorption isostere (Greek: *isos* = equal) is for a given (the same) amount of solid — its capacity of adsorbing a constant (or constant excess) amount of substance under different pressure-temperature conditions.

Physisorption is the abbreviation of physical adsorption. It involves weak van der Waal’s interaction between the adsorbate and the substrate. Chemisorption is the abbreviation of chemical adsorption. It involves irreversible adsorption, often by chemical (usually covalent) bond formation. Perisorption (Greek: *peri* = thorough) is an extremely effective adsorption of a gas by a solid with the formation of an almost molecular mixture of the two substances.

**Placing Together**

The prefix *syn* (Greek: *syn* = together) is associated with synchronous (Greek: *chronos* = time), synopsis/synoptic (*opsis* = view), synthesis (*thesis* = a placing; if the placing is only an assumption that is yet to be tested, it becomes hypothesis; biosynthesis and photosynthesis are mediated through the action of *bios* and *photos*, i.e., life and light respectively), etc. *Sym* is an identical prefix, as in symbiosis and symposium (*posis* = drinking). Perhaps, the symposia were meant to celebrate the scientific successes than for deliberations!
Equal in one way

Iso in Greek is for equal (see above). With iso as prefix, several terms occur, e.g., isobar (Greek: baros=weight), isoelectric point, isohydric solutions, isenthalpic reactions, isomerism (meros=part), isomorphism (morphè=shape), isopleth (plethos=great number), isotonic (tonos=pitch), isotactic/isotaxy (taktos=order), isothermal (therme=heat; read temperature!), etc.

In atmospheric chemistry, charts are prepared of property isolines. Isochrome (Greek: chorè=space) is a curve relating quantities measured under conditions in which the volume remains constant. Isohaline (Greek: halos=salt) is a line drawn on a map through points of equal salinity in the sea. Isohyet (Greek: hyetos=rain) is a contour line of equal rainfall. Isopycnic (or isopycnal) (Greek: pyknos=dense) is a line on a chart joining points of the same atmospheric (or ocean water) density. Isotach (Greek: tachys=swift) is a line on a chart joining points of equal wind speed.

Antagonism – but not always

De (Latin: off/from) is usually a prefix used when an opposite meaning is to be conveyed, e.g., decoupling, degenerate (=fallen from a noble state; degenerate orbitals have about the same energy), dehydration, denatured (spirit), demulsification, descending (order) etc. However, in desiccation (Latin: sicca=dry) and deliquescent de is used as an affirmative prefix.

Il, im and in are similar-meaning prefixes, often in the negative sense like un, e.g., imbalance, immiscible, impermeable, inactive, incongruent (Latin: conguere=to run together, e.g., incongruent melting), indistinguishable, indivisible, inelastic, inert, insignificant etc. But in quite a few cases, they are also used in the positive sense, e.g., illuminate, illustrate, implant, incandescent (Latin: candere=to glow), incinerate (Latin: cineris=ashes), incline (Latin: clinate=to lean), inflammable, innoculate, inseminate, insect (Latin: secare=to cut), etc.

Turning Related

Tropos, in Greek means a turn. This root word is one of the largest contributors of scientific terms, particularly of chemistry and biology. Allotropy (allos=different) is the existence of an element in two or more solid, liquid or gaseous forms, in one phase of matter. Allotropy owes its origin to differing bond angles. For example in white P, the P-P-P bond angle is 60° (tetrahedral), while in black P, the angle is 90-100°. Sulfur has a profusion of allotropes; the thermodynamically most stable form is the orthorhombic form with S8 rings. Polytropic processes are those that satisfy the condition PV=C, where C is a constant. Isotropic (opposite: anisotropic) medium is one for which the physical properties e.g., magnetic susceptibility or elastic constants do not vary with direction. Thixotropy (Greek: thrixis=action of touching) is the property of showing a temporary reduction in viscosity when shaken or stirred, e.g., paints.

Liquid crystals exhibiting thermotropy or lyotropy, do so when the transition to liquid crystalline phase is resulting as the temperature is changed, or as the composition of the liquid is changed. More terms derived from tropos are described in part 2.

Off a normal phenomenon (Ortho, Para, Meta and Dia as prefixes)

In Greek, orthos means straight, upright and correct, para means beside, meta means after or beyond, and dia through. They are used as prefixes for terms denoting the extent to which the true phenomenon is away. The usage of ortho, meta and para is also mentioned in the following article.

i) Ortho: The prefix ortho is used for an observed phenomenon closest to the normal phenomenon. In orthogonal arrangement, right angles (90°) are involved. In colloids, orthokinetic aggregation implies collisions (between atomic/molecular entities) caused by hydrodynamic motions (and perikinetic aggregation implies collisions caused by Brownian motion).

ii) Para: Paramagnetism is another (i.e., other than ferro) magnetism, as in the O2 molecule. When placed between the poles of a magnet, the molecules align themselves with the lines of (magnetic) force.

iii) Meta: Metastable phases are thermodynamically unstable phases (but they do persist because the transition is kinetically hindered). Diamond is a metastable phase of carbon, the stable phase being graphite. Metatectoid (also called peritectoid; Greek: tekton=craftsman of a building/construction) reaction is a solid state (isothermal, reversible) reaction of different phases producing a decreased (by one at a time) number of new solid phases.

iv) Dia: In diamagnetism, the molecules (mostly) allow the magnetic lines of force through them without realigning themselves (at the finer level however, they experience weak repulsive forces and are realigned in the opposite direction).

Adiabatic (Greek: batos=passable) is when no heat flow takes place during a change in state. As opposed to adiabatic boundary, the diathermic boundary permits energy transfer as heat. Dialysis is used to study the binding of small molecules to macromolecules. It is very slow and is accelerated by applying electricity, when it is called electrodialysis.

Work is done anyway

Ergon, in Greek is work. In an exergonic (exo=outside) reaction (ΔG<0), energy is released that may be transferred as work or heat. Work and heat may have equivalence but they are not the same. If the transferred energy is in the form of heat, it is exothermic. In an endergonic (endo=within) reaction (ΔG>0), work is done on the system or heat consumed from the surroundings. If it is the heat that is consumed, it is endothermic. Heat and work are forms of energy transfer, and exist only at the time they are transferred.
Enabling

The prefix en is an enabling prefix used for words of Latin/French origin in the sense of in/into/upon or words of Greek origin in the sense of in. Enthalpy (Greek: enthalpein = to warm in), entropy (Greek: trope = turning, following article 9). Enthalpy is a thermodynamic property or state function. Trope of entropy is intended to mean that useful energy is turned to less useful energy. Thus, entropy is a measure of the energy that is unavailable for doing work since it exists as the internal motion of molecules. It is thus a measure of the disorder of a system.

It's about fleeing away

The term centrifugal (Latin: fugere = flee) is associated with a tendency to flee away from the centre (the opposite of centrifugal is centripetal; Latin: petere = to seek). Fugacity is the tendency of a gas to expand or escape. Fugacity is a specific thermodynamic function related to pressure, by a fugacity coefficient, in the same way that activity is related to concentration by an activity coefficient. Like many terms of thermodynamics, fugacity, notwithstanding its literal meaning, is a word now meant to express a specific concept.

Leaving groups are termed fuges; one that carries away the bonding electron pair (e.g., Cl\(^{-}\) in the hydrolysis of RCl) is called a nucleofuge, and one (e.g., H\(^{+}\) in the nitration of benzene) that carries away the positive charge is called an electrophuge.\(^{3}\) The reagents' OH\(^{-}\) of the former reaction is a nucleophile (Greek: phi = friend), and the Cl\(^{-}\) of the latter reaction, an electrophile. The tendency to depart as the charged species is termed nucleofugality and electrofugality respectively.\(^{3}\)

Piecing Together

The word canon (Greek: kanon = a straight rod), in music, is to piece with different parts, taking up the same theme successively. Canonical rate constant is the rate constant for a system in which the reactants are in thermal equilibrium at a given temperature. Ensemble (Latin: together) basically means collection. The thermodynamic systems of canonical ensemble and microcanonical ensemble are characterised, in addition to constant volume, and constant compositions, with common temperature and common energy respectively. In grand canonical ensemble, in addition to volume, temperature and chemical potential are also common.

Not a critic though

Critical routinely means dangerous. In chemistry, it means transitional, c.f., critical constants, and critical solution temperature. Criticality is the state in a nuclear reactor when the multiplication factor for neutron flux reaches unity and the external neutron supply is no longer required to maintain the power level.

Cloudiness application

Talking of cloud to a chemist instantly brings the classical Wilson's cloud chamber, a simply named term to his attention. Cloud is nephele in Greek; nephelometry is the measurement of concentration by the principle of scattering of light by the colloidal suspensions. Nephelauxetic effect (Greek: auxein = to increase, cf., auxins, auxochrome etc.) is in particular reference to electron cloud. Smaller the electron-electron repulsions, greater is the nephelauxetic effect.

Roots of Biological Terms Common to Chemistry

The exo-endo pair of prefixes (cf., exothermic and endothermic above) is used extensively in biology. Endocytosis (Greek: kytos = vessel, case) is the uptake by a cell of particles that are too large to diffuse through the cell wall. It includes both phagocytosis (phagos = mouth; phag = to eat) and pinocytosis. Exocytosis is the discharge from a cell of particles too large to diffuse through the cell wall.

Taxis (Greek: arrangement) is the noun form of tactic (Greek: taktos = order), e.g., phototaxis, chemotaxis etc. Phototaxis is moving towards light. The opposite phenomenon of moving away from light is by negative phototactic response. In polymer nomenclature, atactic, syndiotactic, etc. indicate the tacticity. In epityps, a unified crystal growth or deposition of one crystal layer on another is effected.

Some Left-outs

Gravis is heavy in Latin, as in specific gravity and gravimetric (metron = measurement). Gyros, also of Latin is a circle. Magnetogyratic ratio is the ratio of magnetic moment to angular (gyric) moment.

The term valency is from valere (Latin) that means to be strong. Stoichiometry (Greek: stoicheion = an element) is the determination of exact proportion of elements to make pure compounds, complexes, etc.

Vulcanus in Latin is the God of fire. Vulcanisation is the heat-treatment of rubber with sulfur to increase the strength. Galvanic is from Luigi Galvani, the discoverer of galvanic action.

Conclusion

In this first of two articles relating to the vocabulary of chemical terms, I have explained the meanings of several terms relating to chemistry at the macro level that have their origins mainly in Greek or Latin. From the examples that I have discussed, whether the concept is physical, chemical or biological, the etymology approach is applicable and can help in understanding more easily the language and philosophy of chemistry.

References

A Simple Method for Determining the Number of Rings in Polycyclic Compounds

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Abstract

One of the main problems for B.S. students of chemistry is determining the number of rings in polycyclic compounds. Here, for solving this fundamental problem, a simple, fast and high accuracy method is explained. Application of this method in a course of organic chemistry (I. A. U.) showed very good results.

Introduction

Polycyclic compounds in an attractive variation of structures and wonderful forms have been synthesized.\textsuperscript{1} These structures have two or more rings that share a number of carbons. For the students, the system could be illustrated with bicyclo compound (I). The systematic name of I is “bicyclo[2.2.2]octane”: (a) Octane, since compound (I) contains eight carbon atoms; (b) bicyclo, because it has two rings, that is converted into an open-chain when we break two C-C bonds; (c) [2.2.2], since the number of carbons on the bridge (shared carbons) are two carbon atoms (C2 & C3), two carbons (C5 & C6), and two atoms of carbon (C7 & C8).\textsuperscript{5} See note-1.

Figure 1a

The calculation of the number of rings in complex polycyclic compounds can be difficult. The molecular formula of compound II (nortricyclene) is C\textsubscript{7}H\textsubscript{10}. Visualizing the number of rings in this compound, however, is difficult. This system is a tricyclo alicyclic compound.

Figure 1b

In identifying the rings in a structure such as compound II (nortricyclene), a student should begin by tracing any ring of carbons in the polycyclic ring structure (generally the largest ring, but this is not required); this is the parent ring (ring number =1). Next connect remaining atoms to the parent ring, by any path, but being careful not to retrace any paths previously used. Finally, connect remaining segments by the longest path available, again being careful not to retrace (Young’s method).\textsuperscript{5} The possible sequences for II (tricyclo[2.2.1.0\textsuperscript{2,6}]heptane ) followed in Figure 2.\textsuperscript{5} See note-2.

Figure 2.

The possible sequences for nortricyclene (II)

Simple Method

One of the main problems in acyclic compounds (a chapter of organic chemistry course) for students of chemistry is determining the number of rings in a polycyclic compound. According the mentioned rules in the above phrases for determining the number of rings in polycyclics, the students must break some of the bonds and convert it to an open-chain compound. But, there are two important questions: 1) Which bonds? and, 2) How could we break the bonds to receipt the open-chain compounds?
For students, answer to these main questions in the great number of polycyclics is very difficult. The lecturers for teaching these points have partially some difficulties.

Here, a simple method is tried to explain for students: “How we can determine the number of rings in polycyclic compounds?” This method was examined in the course of organic chemistry(I) for B.S. chemistry students of I.A.University. The results were very good. The students mentioned that: “This is a simple method in comparison with other methods and we can determine the number of rings in complex polycyclic compounds readily and very fast by this manner”. The foundation of this method is located on determination “the degrees of unsaturation” (D.U.). The stages for determining this in polycyclics are:

1. Recognition of skeletal structure of the polycyclic compound.
2. Remove all of side chains, with H-atoms.
3. Remove multiple bonds (double & triple bonds) with simple C-C bonds (in the main cyclic system).
4. Counting the carbon and hydrogen atoms and write the molecular formula. The number of hydrogen atoms are shown by "\( \alpha \)" symbol.
5. Write the molecular formula of an alkane according to the number of carbons that were counted in stage-4. The number of hydrogen atoms in the molecular formula are shown by "\( \beta \)" symbol.
6. Calculate the “degrees of unsaturation”, by comparison with the number of H-atoms between stages – 4 & 5. (D.U. = (\( \beta \) - \( \alpha \))/2).

This is the number of rings in a polycyclic compound. For example, the number of rings in Nortricyclene II (tricyclo[2.2.1.0^2,6]heptane) by using the above method is three (according to the name of this molecule, that was given from previous methods). It would be possible to simply determine the double bond equivalents (DBE) and then subtract the number of degrees of unsaturation (number of \( \pi \)-bonds).

As you see in Figures 3 & 4, the number of rings in some of the polycyclic compounds are calculated by this method.

### Results

Comparison of this method with other methods for recognition the number of rings in acyclic compounds shows that this manner is simple for application, fast in illustration and high accuracy for counting the number of rings in polycyclic compounds. All the concern evidence about using this method emphasized that the students and the lecturers confirmed the facility, rapidity and high accuracy of this method for teaching and learning.

### References

FUTURE OF CHEMISTRY STUDY:  
Supply and Demand of Chemists  
- Educational aspects

The Royal Australian Chemical Institute has recently commissioned a review of the state of Chemistry in Australia, and published a report entitled Future of Chemistry Study: Supply and Demand of Chemists, which can be accessed from the RACI website http://www.raci.org.au/

Extracts from the Executive Summary which are directly relevant to education are reproduced here. We urge you to read the report to understand the full context of these excerpts.

The state of chemistry in Australian schools

Within Australian schools, the teaching of science, including chemistry, has two broad aims. One is to create a scientifically literate society and the other is to prepare school students for university level chemistry courses. These aims can only be achieved if our primary and secondary school teachers are inspired and capable of teaching the science. In Australia, we have a population of extremely dedicated teachers, but, many are working under difficult conditions and, as the modal age of chemistry teachers at secondary schools continues to increase, there is a great risk that when they retire they may not be adequately replaced.

Inspiring teachers open up a world of possibilities to enquiring minds and have a great impact on the future trajectories of their students.

Recommendation 1: That recognition is given to science teachers for their additional training by adjusting starting salaries accordingly

Recommendation 2: That mechanisms are explored for university students undertaking chemistry to receive incentives to undertake teacher training

Recommendation 3: That teachers of chemistry are provided with links to industry through placements in industry

Recommendation 4: That evaluations are undertaken to assess the impact of State and Commonwealth programmes, including careers advice, on improving scientific literacy and increasing the number of chemists

The state of chemistry in Australian universities

Within the Australian tertiary sector, the number of university students studying chemistry has fallen over the last ten years. This has placed a strain on departments, some of which have been subsumed by larger schools and study areas, and many of whom have lost staff and funding. In a response to this, some universities have diversified their teaching areas to encompass subject areas more appealing to students. This, in turn, has created a wide variety of chemistry courses to appeal to many different students. Within many departments, there has also been a concerted effort to create strong links to industry in order to promote careers for students as well as create an atmosphere in which industry and universities can conduct collaborative research.

If the decline in chemistry student numbers is to be stemmed then students need to understand the career pathways for chemists as well as being supported through their studies by highly qualified staff. They also need access to quality materials, equipment and physical facilities that will allow them to become highly skilled graduates. The current chemistry curriculum also posed its own unique challenges with many industry voices requesting ‘work ready’ students. Achieving a balance between academic and work skills without impinging on the teaching of core skills in chemistry is no easy task: it is one which many universities are working towards.

There are several implications for the reduction in the number of students studying chemistry, the most obvious of which is a decline in the number of chemistry graduates available to work within the Australian chemical and related industries, which in turn will have costly consequences for the industry. The scientific and Research and Development (R&D) capacity of Australia will also be severely compromised if the numbers of chemistry graduates, and specifically PhD graduates is reduced. As many chemistry graduates are desired by employers for their strong analytical skills, a continued decrease in the number of students studying chemistry will impact on many other sectors, as well as stifling the scientific literacy levels of Australia. In order to ensure that chemistry remains a vibrant science at university level, the RACI recommends the following:

Recommendation 5: That there is access to quality materials, equipment and physical facilities for students and university staff

Recommendation 6: That every second year there is an accreditation of university chemistry courses with a focus on international best practice

Recommendation 7: That more formal linkages are created between universities and industry

Recommendation 8: That students undertaking chemistry have access to adequate information pertaining to potential careers in chemistry
EXCELLENT RESOURCES FOR SENIOR SECONDARY SCIENCE COURSES AVAILABLE WITHIN AUSTRALIA

The Chemical Education Group of the RACI (SA Branch) has exclusive distribution arrangements within Australia for a number of high quality science magazines, predominantly in Chemistry. The magazines are available on a subscription basis. A few selected books and CD ROMs are also available for purchase.

All of the materials are suitable for teacher and student use. The resources available are:

Magazines

- ChemMatters: Published 4 times per year by the American Chemical Society
- Chemistry Review: Published 4 times per year for the Chemistry Dept, University of York (UK)
- CHEM 13 NEWS: Published 9 times per year by the Chemistry Department, University of Waterloo (Canada)
- Physics Review: Published 4 times per year for the Physics, Electronics and Education Departments, University of York (UK)
- Biological Sciences Review: Published 4 times per year for the School of Biological Sciences, University of Manchester (UK)

CDROMs

- ChemMatters CD ROM (version 2.0): Contains all issues of the magazine from Feb ’83 to Apr ’98

Books

- Ben Selinger: Chemistry in the Marketplace (5th Ed.)
- Ben Selinger: Why the Watermelon won’t Ripen in your Armpit

By ordering/subscribing through the Chem Ed Group of RACI (SA) rather than through the overseas publishers of the magazines the hassle and expense of bank drafts in foreign currencies is avoided. Our magazine prices are cheaper than direct subscription prices from the publishers.

For prices, catalogues and order forms or further information please contact Bob Morton, Publications Coordinator:

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Cover photographs: Courtesy of Kieran F. Lim (林百君) and Jeanne Lee (李静宁).