# NMMU CHEMISTRY 2008 NEWSLETTER

# A note from the Head of Department

The Department of Chemistry functions over three campuses (Summerstrand South and North, and Missionvale), offering programmes ranging from diplomas in Analytical Chemistry and Polymer Technology to research degrees up to doctoral level. Further chemistry activity is centered in InnoVenton, a research institute whose purpose is to provide chemical R&D expertise, technology support, technology transfer and professional teaching services to industry. The staff of the Department and InnoVenton comprise over twenty academics and about forty support personnel. A wide variety of resources and specialist equipment is available to support both pure and applied research projects.

The merger that led to the formation of the NMMU brought with it many challenges, not least those for the Chemistry nexus as we have sought ways to optimise our various activities. These are on-going and it is a tribute to the commitment of the staff that they have continued to provide high quality teaching and training and research, often under demanding circumstances.

The students are the lifeline of our activities and it is gratifying to observe their progress through the years, with many developing into excellent scientists and technologists. We trust that Chemistry will continue to inspire all who are fortunate to enter its portals.



Prof B Zeelie (Director of School of Biomolecular and Chemical Sciences; Director of Inno Venton) Prof CW McCleland (Head: Department of Chemistry)

Front row : H Marchand, Dr B van Brecht, Prof H Rohwer, Prof JGH du Preez, E. Wagenaar, V Magoko, N Mama, D Funkuza

Middle row : Prof C McCleland, Dr N Vorster, Prof T Gerber, Prof P Loyson, M Vosloo, P Wallis, M Yose, H Jaggers, V Xokozela, D Mabulu

Last row : P Hlangothi, Dr E Hosten, A Abrahams, H Schalekamp, F Gerber, Prof B Zeelie, D Grooff Absent : R Neglur, Dr E Ferg, L Ingram, R Venter, G Rubidge, A Noah, F Olivier, M Ghenne, Dr L Goosen, S Bosman

### for tomorrow

Nelson Mandela

Metropolitan

University

#### Prof du Preez' final farewell



In September we said a final farewell to Prof JGH du Preez after 41 years of service at the University. Prof du Preez started as a founding Professor of Inorganic Chemistry at the then University of Port Elizabeth in January 1967, and has played a leading role in the Department ever since.

He was Director of the Uranium Chemistry Unit, later re-named as the Research Unit for Metal Ion Separation, and from 2005 the Research Unit for Platinum Group Chemistry.

He was awarded two gold metals in his long research career : the AECI Gold Medal in 1971, and the SACI Gold Medal in 1990. He was rated as a B1 Scientist by the FRD in 1995.

He has published 184 research papers in international Journals as well as 11 patents, of which 8 are international.

His research contributions has included all aspects of f-transition metal chemistry and basic and applied aspects of the hydrometallurgy of d- and f- transition metals, for example metal extraction, separation, equilibria in aqueous and non-aqueous media. Since 1992 he has concentrated on the hydrometallurgy and coordination properties of Platinum Group Metals, using their co-ordination to design new separating agents. Since 2002 he has carried out fundamental research on the development of anti-tumour agents based on platinum.

He has retired to Stilbaai, but will still be acting as a consultant for Shimoda Laboratories, a pharmaceutical company in George.



Prof du Preez and members of his research group

# 6<sup>th</sup> International Symposium on Technetium and Rhenium (7-10 October 2008)

This was held in the North Campus Conference Centre of NMMU. It was organized by Prof Tommy Gerber from NMMU, an internationally known expert in the field of technetium and rhenium. It was attended by 21 international delegates, many of them world authorities, and 13 local delegates. Below is a photo of Prof Gerber with some of the important international speakers. There were 25 oral presentations and 11 posters.



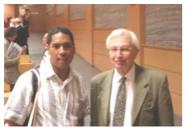
Some of the important speakers at the International Conference on Technetium and Rhenium From left to right : Dr Ozawa (Japanese Atomic Energy Agengy), Prof Maes (Katolieke Universiteit Leuven, Belgium), Prof Sekine (Tohoku University, Japan), Prof Gerber (NMMU), Prof German (Russian Academy of Sciences, Moscow).

# **Outstanding student performance**



Mr Robert Bosch, a chemistry Ph D student, achieved top honours and R 300 000 in prize money, when he was voted the winner of the INNOVATION FUND's National Competition at an awards function at Spier Wine Estate near Stellenbosch. His research project deals with the replacement of zinc oxide in vulcanized rubber by a rubber nano product liquid activation system. This innovative project has application in any industry that uses rubber products, and will have a substantial beneficial impact on industries such as the tyre and conveyor belt industry.

#### Post graduate research student news



Our research students continue to be involved in top-class research projects and to be exposed to world leaders. In the photo Mr A Abrahams, a doctoral student staff member is pictured together with Prof Jean- Marie Lehn, the 1987 Nobel Prize winner in Chemistry. Prof Lehn is from the Collège de France, in Paris, and is an authority on supramolecular chemistry, nanoscience, molecular recognition and other fields.

The photo was taken at a recent conference in Budapest, where 5 Nobel Prize winners addressed young chemists.

#### Mr A Abrahams with Prof Lehn, the 1987 Nobel Prize winner in Chemistry

The photo below shows staff and post graduate students



Staff and research students

#### Staff research achievements

Prof T Gerber was elected the top researcher in the faculty of Science of NMMU.

Dr E Ferg was rated as a C3 researcher by the NRF.

### New research instrument



During the year a new, highly sensitive rheometer was delivered to the Physical Chemistry laboratories. This instrument will study the viscosity of solid rubber samples at different temperatures and determines their curing times. Mr Percy Hlangothi, a lecturer in the Department, who is using the instrument in his doctoral research, and Mrs Rekha Neglur, the polymer technician, are shown at the highly sophisticated new instrument.

Mr P Hlangothi and Mrs R Neglur at the new rheometer

#### Research into battery electrochemistry



Dr Ernst Ferg

In November 2008 a meeting took place between the head of the Altron Group of Companies, Robbie Venter, and the University. Amongst other things agreed upon was the commitment towards long-term ongoing research support in the field of energy storage such as lead-acid battery technology.

Dr Ernst Ferg has been involved for many years with research work for Willard Batteries, one of companies belonging to the Altron Group.

The company will be funding new battery testing equipment, which will be located in the physical chemistry laboratories on the South Campus. This equipment will be the only one of its kind to be found at a university

in South Africa. New research projects to be undertaken will concentrate on modifying the battery electrode material to withstand the harsh conditions of electric vehicle applications. Other research fields will include the study of fuel cells.

# Visit by an International Rubber Company

During the year we had a high-profile visit by Apollo Tyres from India looking at possible training cooperation. Dr PK Mohamed, the Technical Director of Apollo Tyres, together with Kaushik Roy, the Head of Purchasing, and Mr Danie Langner, the Technical Director of Dunlop Tyres, had discussions with the relevant staff regarding training needs.

#### **Donation from Industry**

The Polymer Technology section of the Department received a donation of R 20 000 from Free World Automotive Coatings (Plascon), for which the Department is grateful. The same company has also decided to institute a bursary scheme for students to be trained in polymer technology.

# **Graduation news**

The Science faculty graduation ceremony was held on 22 April 2008. The following Diplomas in Chemistry were presented :

- > National Diploma in Analytical Chemistry : 39 students, with one cum laude : Anke De Wit.
- National Diploma in Polymer Technology : 12 students

The following degrees were awarded :

- B Tech : Chemistry : 2
- B Tech : Polymer Technology : 1
- > B Sc with Chemistry as major : 9 (*cum laude* : Kim Potgieter)
- ➢ B Sc Hons : 4

# Masters degrees :

# **MTech : Chemistry**

Ndavheleseni David SATHIKGE – Title of dissertation : Process for the preparation of cis- and trans- 3,7dimethyl-2,6-octadiene-1-ol from crude sulphated turpentine stream. Promoter Prof B Zeelie

Maria Isabel TORAL DEL RIO – Title of dissertation : An analysis of the influence of phosphorus poisoning on the exhaust emission after treatment systems of light-duty diesel vehicles. Promoter Dr M Auphan de Tessan, co-supervisors : Dr E Ferg, Mr F Haack

# MSc : Chemistry

Heine JONCK – *cum laude* – Title : Development of Platinum Metal Specific Separating Agents. Promoter : Prof JGH Du Preez.

Duduetsang SAKU – cum laude – Title : Synthesis and characterization of symmetrical and unsymmetrical ferrocenyl ligands for use in the preparation of redox-active Ruthenium Alkylidene Complexes. Promoter Prof Christopher Imrie (passed away December 2007)

Jason Leigh VAN ROOYEN – Title : A comparison of the vulcanization of polyisoprene by a range of thiuram disuphides. Promoter : Dr C D Woolard.

# **Doctoral degrees** :

Six candidates were awarded Doctoral degrees in Chemistry : two with a D Tech : Chemistry, and four with Ph D in Chemistry.



The two recipients of doctoral degrees in Technology (Chemistry):

Jayant Indurkar and Melissa Gouws

Jayant Ravichandra INDURKAR – Title of thesis : Selective para-functionalization of phenol – Promoter Prof B Zeelie, co-promoter Dr B Barton

Melissa Claire GOUWS – Title of thesis : Practical and scalable synthesis of N-Alkyl-N, N'-Diacylhydrazine – Promoter Prof B Zeelie, co-promoter Dr G M Dugmore

The four PhD candidates were :



Elago Robinson Tangeni ELAGO – Title of thesis : The solvent-free approach versus the use of ionic liquids in the synthesis of ferrocenes. Promoter Prof Christopher Imrie, co-promoter Prof C McCleland

Talana LOUW – Title of thesis : The separation of Platinum and Gold from an industrial feed solution. Promoter Prof JGH Du Preez

Belinda Julie MCFADZEAN – Title of thesis : The kinetics and associated equilibria of high oxidation state Osmium complexes. Promoter Prof HE Rohwer

Mauritz WENTZEL – Title of thesis : Identification and characterization of novel oncology-related Platinum complexes using chromatographic and mass spectrometric techniques. Promoter Prof JGH Du Preez

# **INNOVENTON NEWS**

#### > New biodiesel research and testing facility

NMMU's Institute for Chemical Technology and its Downstream Chemicals Technology Station, known as Innoventon, is taking the lead by upgrading its facilities with R 7 million to research and test biodiesel and associated products. Deputy Minister of Science and Technology Derek Hanekom, whose Department will be funding R 1 million worth of equipment for the upgrade, recently visited the facilities and announced them to be among the best in the country. NMMU and Industry would each fund R 3 million towards the initial upgrade. Prof Ben Zeelie, the Institute's Director, anticipates the facility to be completed by the end of 2008.

In the first phase a biodiesel analytical laboratory will be completed. This facility will be extended to include the testing of all principal transport fuels.

Plans for the next two years for the Institute include a further R 13 million extension to increase its research and development capability to serve the chemical industry, both locally and nationally.



Deputy-Minister of Science and Technology Derek Hanekom (centre) during his visit to Innoventon, the Institute of Chemical Technology. With him are from left Prof Mohammed Jeenah, DVC Research, Technology and Innovation, Nurunessa Moolla, Chief of Staff in the Deputy Minister's Office, Dr Gary Dugmore, Deputy Director, Technology Demonstration, Prof Ben Zeelie, Director Innoventon and Dr Nawaz Mahomed, Manager Innovation DST.

# > Commercialization agreement for insect repellent products

NMMU announced on 24 June 2008 that it has reached an agreement with an investment partner, Afrepell Manufacturing Pty (Ltd), for the commercialisation of a range of insect repellent products developed by NMMU's Institute of Chemical Technology, InnoVenton.

NMMU has developed a new insect repellent formulation that is more effective at lower concentrations of active compounds than existing products. Most insect repellent products depend on a single active substance at high concentration to repel insects.



Researchers at NMMU, among whom Dr Ilse Asquith, discovered that by combining several different types of chemicals, which differ in their mode of action into a single mixture, the resulting mixture is more effective than the compounds acting alone, and at lower concentrations.

Dr Ilse Asquith

The formulation, RepelloX, developed by NMMU, has many potential advantages, including improved efficacy, improved safety (using "safe" ingredients and using significantly less material), and improved consumer acceptance (smell and skin-feel).

NMMU and Afrepell Manufacturing have agreed to enter into a joint venture to manufacture, sell and license RepelloX. Afrepell Manufacturing have already entered agreements with KORAM Ltd in the

United Kingdom and KORAM USA Inc in the United States to market RepelloX products and technology internationally.

#### > New B Sc Honours in Formulation Science offered by Innoventon

In June 2008 a new B Sc Honours programme was started, specializing in Formulation Science. It's the first such programme in South Africa. The programme teaches the basic principles of the science and technology involved in formulations and this can be applied in a number of different formulation industries, such as cosmetics, paints, household / industrial cleaning products and agricultural / pharmaceutical products. Graduates will acquire the skills to produce new consumer products as part of their research project. This product may then be commercialised and could lead to commercial benefits for the student and the Institute. The photo below shows some of the students with the course co-ordinator, Dr Nicolle Vorster, and some of the lecturing staff.



From left : Dr Shawn Gouws, Riekie Slabbert, Coos Bosma, Tutu Maseko, Dr Nicole Vorster, Prof Ben Zeelie, Somikazi Konkwane, and Humbulani Shekhobe.

# **Conferences attended in 2008**

The following conferences were attended by staff members and research students during the year, with details of the presentations :

1<sup>st</sup> International Symposium on Electrochemistry, 9-11 July, University of Western Cape, Bellville, South Africa (2 lectures)

Prof P Loyson : keynote speaker : Bmim ionic liquids as media for the electrochemical oxidation of 2,6-di-*t*-butylphenol

Dr S Gouws : A new mechanistic approach to the electrochemical production of alkoxy-substituted phenol ethers

Euchem 2008 Conference on molten salts and ionic liquids : 24 – 29 August, Copenhagen, Denmark ( Prof P Loyson )

# **10<sup>th</sup> Annual Unesco / IUPAC Conference on macromolecules & materials** : 8-11 Sept, Kruger National Park

Mr P Hlangothi ( poster ) : Influence of cyclic disulfide vulcanization systems on iso-grip(3,4-polyisoprene )

#### 2<sup>nd</sup> Euchem Chemistry Congress, 16-20 Sept 2008, Torino, Italy

Mr I Booysen ( poster ) : Imido, amido and Oxofree complexes of Re (V) with multidentate aromatic amines

# **IST 2008 : 6<sup>th</sup> International Symposium on Technetium and Rhenium**, 7-10 Oct, NMMU, Port Elizabeth

Mr A Abrahams ( doctoral student, lecture ) : Rhenium(V)-mediated Syntheses and Structures of Oxypyridinium-ammonium zwitterions

Mr I Booysen ( doctoral student, lecture ) : Imido, amido and amino complexes of  $Re(V)\;$  with multidentate aromatic amines

#### CATSA 2008, 9-12 November Parys, Sasolburg

Mr P Makgwane (doctoral student, poster): Comparison of the liquid-phase oxidation of *p*-cymene in a well-stirred batch reactor and a falling film micro-structured reactor

**39<sup>th</sup> SACI National Convention,** 30 Nov-5 Dec , Stellenbosch University : Several presentations were made here : 5 lectures, 6 posters

#### Lectures presented (5)

Dr Ernst Ferg : Determining the crystallization of highly concentrated emulsions of ammonium nitrate using powder X-ray diffraction

Prof Peter Loyson : Chemistry in ancient Egypt

Dr N Vorster : New training opportunity in Formulation Science : Overview and Discussion

N Rust ( D Tech student ) : The synthesis of fine chemicals using micro-structured reactors

PR Makgwane ( D Tech student ) : Comparison of the liquid phase oxidation of p-cymene in a well-stirred batch reactor and a falling film micro-structured reactor

#### Posters presented (6) :

T E Geswindt : The use of computational / geometrical methods for the analysis of the reduction of  $OsO_4$  in aqueous basic media ( Prof H Rohwer, W Gerber, E Hosten )

TE Geswindt : Spectrophotometric investigation of the interaction between  $[OsO_4(OH)_2]^{2^-}$  and  $[OsO_2(OH)_4]^{2^-}$  in aqueous hydroxide medium ( Prof H Rohwer, W Gerber, E Hosten)

JC Davis : Speciation of PGMs by ion-pair chromatography ( Prof H Rohwer, E Hosten )

T Phangalala : A look at the technique of determining acid absorption of PbO used in the manufacture of Pb / acid batteries ( E Ferg,T van Dyl )

Sipeng Zheng : The investigation of kinetic and electrochemical properties of Ruthenium (II) polypyridyl complexes ( Prof H Rohwer, E Hosten )

D Onyancha : Reactions of 4-ferrocenylbenzyl-1 H-imidazole-1-carboxylate with  $K_2PtCl_4$ ,  $K_2PdCl_4$  and alcohol ( Prof C McCleland, VO Nyamori )

#### Papers published in 2008 :

The following research papers were published by staff in peer-reviewed Journals

Synthesis and Structure of a Rhenium(V) Complex containing a Tridentate Imido-coordinated Schiff base : I. Booysen, T.I.A. Gerber\*, E. Hosten, P. Mayer Bull. Chem Soc. Ethiop., 2008, **22**, 101-105.

A Trigonal-bipyramidal Oxorhenium(V) Complex with a Bidentate Nitrogen-donor Ligand I. Booysen, T.I.A. Gerber<sup>\*</sup>, P. Mayer, J. Coord. Chem., 2008, **61(10)**, 1525-1531.

Oxidation of 5,6-Diamino-1,3-dimethyl-2,4-dioxopyrimidine by Perrhenate I. Booysen, T.I.A. Gerber<sup>\*</sup>, P. Mayer - J. Braz. Chem. Soc., 2008, **19(1)**, 199-202.

A *cis*-Dibromorhenium(V) Iminophenolato Complex A. Abrahams, I. Booysen, T.I.A. Gerber<sup>\*</sup>, P. Mayer - Bull. Chem. Soc. Ethiop., 2008, **22**, 247-252.

Synthesis and Crystal Structure of the First Oxofree `3+3` Rhenium(V) Complex I. Booysen, T.I.A. Gerber<sup>\*</sup>, E. Hosten, P. Mayer - Inorg. Chem. Commun., 2008, **11(1)**, 33-35.

Imidazole-based Bifunctional Chelates for the "*fac*-[Re(CO)<sub>3</sub>]<sup>+</sup>" Core Z. Tshentu<sup>\*</sup>, T.I.A. Gerber, R. Walmsley, P. Mayer - Polyhedron, 2008, **27(1)**, 406-410.

Unexpected Formation of a new Nitrosylrhenium(II) Complex from Oxorhenium(V) I. Booysen, T.I.A. Gerber<sup>\*</sup>, P. Mayer - Inorg. Chem. Commun., 2008, **11**, 461-464.

Formation of a Six-coordinate fac-[Re(CO)<sub>3</sub>]<sup>+</sup> Complex by the N-C Bond Cleavage of a Potential Tetradentate Ligand.- I. Booysen, T.I.A. Gerber, E. Hosten, P. Mayer - J. Iran Chem. Soc., 2008, **5(4)**, 689-693.

The influence of particle size and composition on the quantification of airborne quartz analysis on filter paper EE Ferg, P Loyson, G Gromer - Industrial Health, 46 (2008) 144-151

Electrochemical production of alkoxy-substituted phenols S Gouws, B Barton, P Loyson, B Zeelie - Electrochimica Acta, 53 (2008) 4544-4549

#### Patent

Internal temperature monitor for lead acid batteries : Dr E Ferg, N Rust, SA Patent

#### **SACI NEWS**

A number of functions were held in the Chemistry Department under the auspices of the South African Chemical Institute. These were mainly lectures by academics and industrial speakers. The annual post-graduate SACI / Aspen-Pharmacare Seminar was held in 2008, for the first time at the Walter Sisulu University Campus in East London on 17 October. Three of our research students presented lectures on their work :

Charmelle Snyders (BTech): The influence of different vulcanization systems on Iso-Grip rubber

Ntombekaya Gojela (BTech ): Hydrogen economy - water electrolysis

Nadia Adams : (PhD) Solvent- Free Synthesis of Substituted (1-Ferrocenylethylidene)benzamines

#### Science School Teachers Workshops

Two workshops aimed at helping Science school teachers with the new syllabus were presented by Dr L Goosen at Victoria Girls High School in Grahamstown. The first one dealt with Polymers (18 Feb) whilst the 2<sup>nd</sup> one covered Electrolysis and the Chlor-Alkali Industry (19 May).