

DEPARTMENT OF CHEMISTRY 2010 NEWSLETTER

Dear Friends and Colleagues

The year 2010 was an exciting time for students and staff alike. Some of our research students attended international and local conferences, received medals for academic achievements, and were co-authors in many of our research publications.

Through the hard work and efforts of staff, pass rates improved in all the undergraduate courses and modules. The number of research papers increased by 29%, and the involvement of the Department has increased considerably in the community by presentations to the general public, teachers and secondary school learners, and radio talks.

This newsletter summarizes some of the Department's activities in 2010. We are all looking forward to an exciting 2011, which is the *International Year of Chemistry*.

Prof. Thomas Gerber (HoD: Chemistry)

1. OPEN DAY ACTIVITIES

This was held on 7 and 8 May and again the chemistry stall in the Sport Centre received a lot of attention, with hundreds of students been shown interesting chemistry demonstrations and walking away with information about chemistry studies. The stall was once again well supported by staff from both campuses.



The Chemistry stall at open day

2. SUCCESSFUL SCIENCE DISCOVERY WEEK

About 60 Matric students from various schools spent a whole week (21-25 June) in the Science Faculty, as part of a project to advertize studies and careers in Science. The chemistry component consisted of a lecture by Prof P Loyson on : Chemistry at NMMU : qualifications, research and careers in chemistry; later students carried out interesting experiments in the laboratory. The following experiments were carried out by the students (in groups)

- Experimental determination of the heat capacity of a thermos flask
- Identification of metal ions from their flame colours
- Determination of the concentration of NaCl in a sample using conductivity
- Analysis of acetic acid in vinegar
- Measurement of pH : from litmus paper to a pH meter
- Separation of dyes in ball point ink using paper chromatography

The students were also given a chemical demonstration by Harold Marchand / Prof McClelland



Students watching Harold Marchand during the Chemistry demo during Science Discovery Week

3. HELPING MATRIC CHEMISTRY TEACHERS WITH SCHOOL SYLLABUS

In order to help Matric Science teachers with their Chemistry syllabus and trying to improve on the pass rates of Science in the region, meetings were held with selected school science teachers and Mavis Mize, representing the Department of Education in the region. This project was spearheaded by Prof Tommy Gerber and Prof Peter Loyson. A survey was carried out amongst all the schools in the region in order to determine the most difficult sections of the syllabus and a schedule was worked out where these topics could be taught and dates were selected for University staff to give lectures for Science teachers on these topics. The venue would be the old Algoa College Campus and every two weeks a lecture would be held. The program was started on 21 July, but after 3 lectures it ground to a halt due to the teachers strikes.

The following 3 lectures were held :

21 July	Chemical Industries	Prof Peter Loyson
4 August	Organic molecules	Mrs Marilyn Gibbs (Education)
18 August	Electrochemical reactions	Dr Ernst Ferg

It is hoped that we can carry on with this project in 2011.

4. Talk at Science Center Scibono in Johannesburg

On 15 June Prof Loyson was invited by the largest Science Centre in South Africa, Scibono in Johannesburg to give a lecture dealing with Mathematics. The title of his talk was : Ancient Egyptian Mathematics.

5. Participation in SciFest Africa, Grahamstown

The annual Science Festival in Grahamstown, sponsored by Sasol and other companies, was held from 24-30 March 2010, and two lectures were presented there by Prof Loyson, one dealing with Ancient Egyptian Mathematics and the other with Ancient Egyptian Technology. These lectures were attended by about 200 people, largely students.

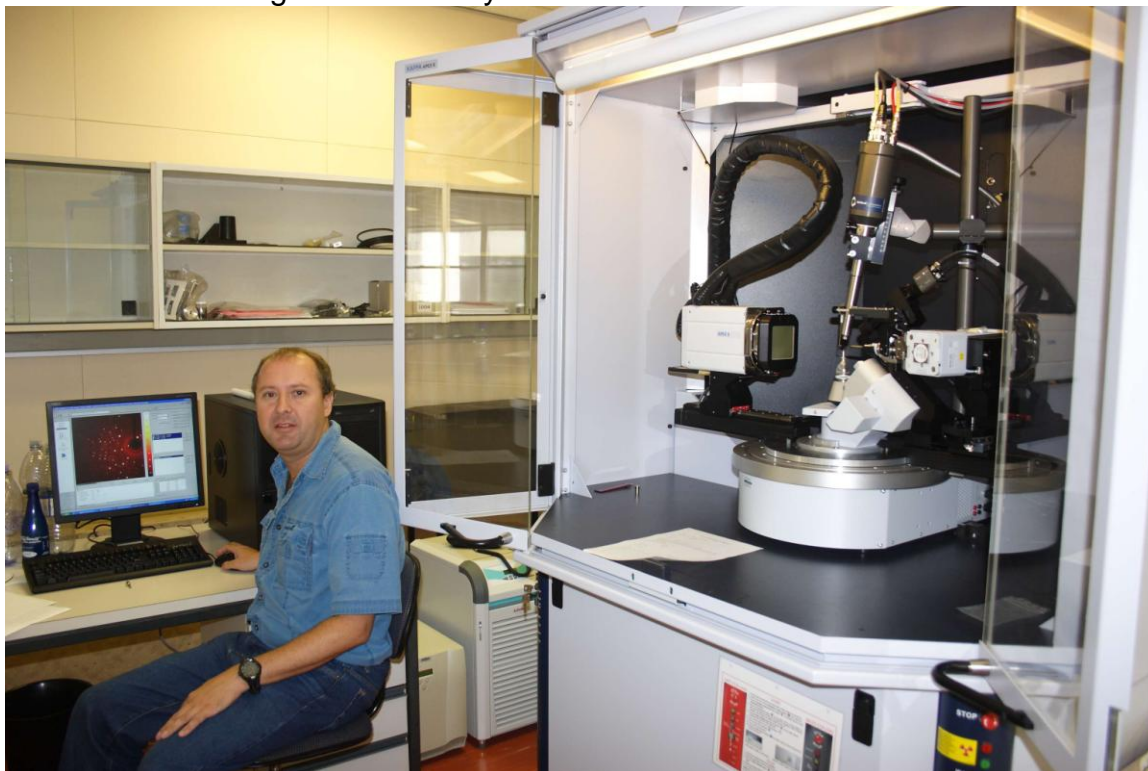
6. Science Festival, 23-25 September, University of Moi, Eldoret, Kenya

This was organized by AMSTREF (African Maths / Science / Technology Research and Education Foundation) and geared for secondary school pupils, concentrating on Mathematics and Science - Prof P Loyson was invited to present 3 lectures dealing with ancient Egyptian science: Maths, Technology , Pharmacy and Medicine (the last lecture was at the Medical Faculty for senior students).

7. **Various School visits** (Victoria Park, Walvis Bay, others) visited the Department and Innoventon during the year.

NEW EQUIPMENT

During 2011 a new X-Ray diffractometer from Bruker worth R 4.5m was installed in the Inorganic Chemistry section.



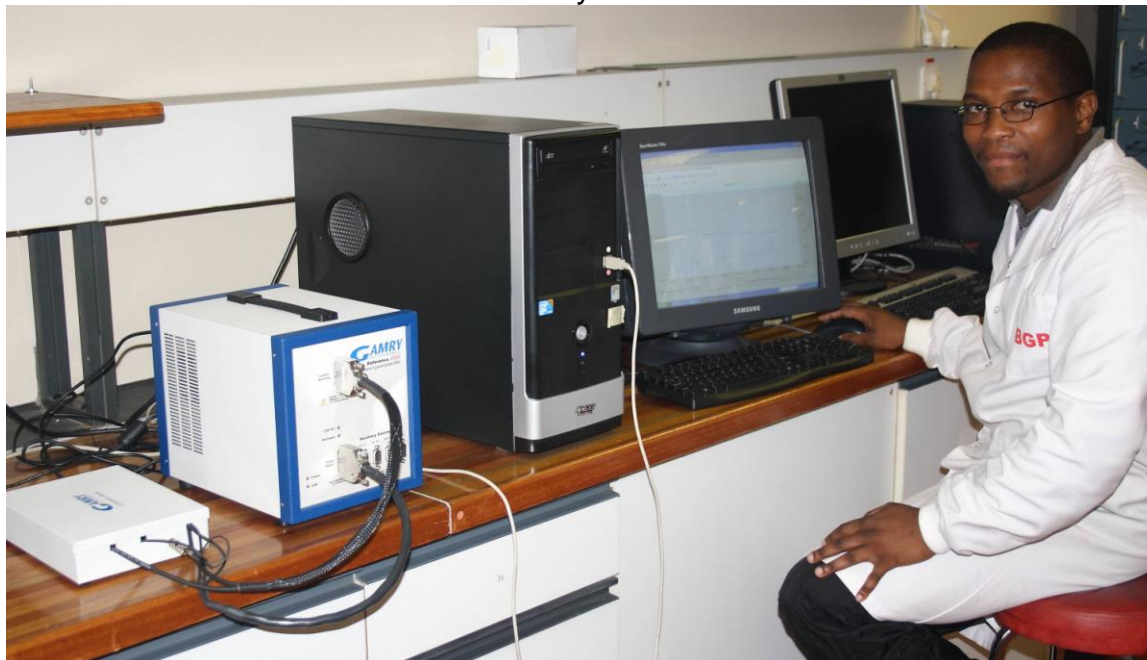
Dr Hosten with the new Bruker KAPPA APEX II diffractometer for single crystal X-ray diffraction.

The Organic Chemistry research section received approval for purchasing a range of instruments that were damaged during the fire in 2009. The new instruments bought are :

- a 400 MHz NMR (Bruker) spectrometer
- ESR (electron spin resonance) spectrometer (Bruker)
- Infra red spectrophotometer (Bruker)
- GS / MS (Agilent Technologies)
- HPLC (Agilent Technologies)

All these instruments will be delivered and installed during February 2011. In addition a gas delivery system has also been installed.

The battery research centre in the Physical Chemistry section took delivery of a Gamry Impedance Analyser, which is used extensively in battery research to evaluate the State of Health of the battery.



The Gamry Impedance Analyser being operated by MTech student Mr Thembelani Phangalala

OFFICIAL OPENING OF BATTERY RESEARCH CENTRE

The Willard Battery Research Centre, situated in the Physical Chemistry section on the South Campus was officially opened by the Dean of Science, Prof A Leitch on 4 June. Delegates from Willard Batteries were present as well as research students and relevant staff of the unit.

STRONG SUPPORT FROM INDUSTRIES FOR POLYMER TECHNOLOGY

During 2010 the Polymer Technology programme received strong support from industry in the form of student bursaries. This will encourage more students to enter this Diploma with several attractive career opportunities in the Paint, Rubber and Plastics fields.

The University was very fortunate to receive substantial contributions in the form of bursaries for students from Continental, a German international tyre manufacturer, Tega Beruc an Indian rubber goods manufacturer based in Gauteng and Freeworld Automotive coatings, part of the Freeworld group (formerly known as Plascon) based in Port Elizabeth.

Through this assistance several students received much needed financial assistance and student numbers have increased substantially above those of 2009. The fact that Freeworld has decided to continue their support into 2011 is particularly pleasing and bodes well for the future.

SHORT COURSE

A short course in Practical Rubber Technology was presented for the local rubber industry during the 2nd semester on a one day per week basis by the polymer technology group. There were 15 delegates from Goodyear, Veyance, Bridgestone, Continental and Evonic. Lectures were presented by Dr James Carson, with assistance from Fanus Gerber and Rekha Neglur.

The success of this course has caused more interest in the local industry such that bookings for another course in 2011 have already been received. Also companies in Durban – Pietermaritzburg are keen to get involved.

GRADUATION NEWS

The graduation ceremony for Science was held on Friday 16 April.

The following Chemistry Diplomas were presented :

- National Diploma : Analytical Chemistry (10)
Cum laude : Nomatshawe MAKU
- National Diploma : Polymer Technology (4)
Cum laude : Surene Botha

The following degrees were awarded :

- B Tech : Chemistry (5)
- B Sc with Chemistry as major : (9)
Cum laude : Natasha HOFFMANN
- B Sc Hons : (1)
- M Sc : (5) 2 cum laude (Davis and Potgieter)
- M Tech : Chem : (1)
- D Tech : Chem : (1)

M Sc degrees in Chemistry

Davis, John Christopher – CUM LAUDE

Title of dissertation : A speciation study of the chloro-hydroxo complexes of Pt(II)

Supervisor : Prof HE Rohwer

Potgieter, Kim Carey – CUM LAUDE

Title of dissertation : Complexes of the $(\text{ReO})^{3+}/\text{Re}(\text{CO})_3^+$ cores with multidentate N_2O donor chelates

Supervisor : Prof TIA Gerber

Van Aswegen, Werner

The kinetics and associated reactions of Ruthenium (VIII)

Supervisor : Prof HE Rohwer

Yumata, Nonzaliseko Christine

Title of dissertation : Reactivity of Rhenium(III) and Rhenium(IV) with multidentate N,N and N,O donor ligands

Supervisors : Prof TIA Gerber and Dr A Abrahams

Zheng, Sipeng

Title of dissertation : The reactions of Ruthenium (II) Polypyridyl complexes

Supervisor : Prof HE Rohwer

M Tech : Chem

Majavu, Avela

Title of dissertation : Modeling of arsenic removal from aqueous media using selected coagulants

Supervisors : Dr G Rubidge and Dr N Vorster

DOCTORAL DEGREES

There were 4 doctoral candidates, 1 D Tech and 3 Ph Ds.

D TECH : CHEMISTRY

Thomas, Maxwell Paul

Title of thesis :The selective dechlorination of poly-chlorophenols

Promoter : Prof B Zeelie



Dr Maxwell Thomas



Dr Irvin Booysen



Dr Douglas Onyancha

D Phil : CHEMISTRY

Booyesen, Irvin Noel

Title of thesis : Rhenium (V) imido complexes with potentially multidentate ligands containing the amino group

Promoter : Prof TIA Gerber

Makgwane, Peter Ramashadi

Title of thesis : Immobilization of catalysts in wall-coated micro-structured reactor for gas / liquid oxidation of *p*-cymene

Promoters : Prof B Zeelie, Dr E Ferg



Dr Peter Makgwane with the micro-structured reactor

Onyancha, Douglas Okerio

Title of thesis : Synthesis, characterization and reactions of ferrocenylimidazoles as donor ligands

Promoters : Prof CW McClelland, Prof TIA Gerber

STAFF RESEARCH ACHIEVEMENTS

One of our Physical Chemistry staff members, Driekus Grooff, obtained his doctorate through the University of the North West (previously Potchefstroom) with the title : *Characterization of thermally induced phase transformations of nifedipine polymorphs*. He did these studies part-time whilst being a full time lecturer.



Dr Driekus Grooff

POST-DOC INORGANIC EXPERT FROM GERMANY

Dr Richard Betz from Germany is spending some time with the Inorganic Chemistry Department on the South Campus. He is an expert on XRD and arrived in the country towards the end of July. He obtained his Doctorate from the Ludwig Maximilian University in Munich in 2009 and has 50 publications to his name. In only 3 weeks of work on the new XRD instrument, he has already had an extra 4 publications accepted, with several others in the pipeline.



Dr Richard Betz from Germany

CONFERENCES ATTENDED BY STAFF

Electrochem 2010, September 13-15, Ruhr University Bochum, Germany (Prof Peter Loyson)

International Symposium on Technetium and other Radiometals in Chemistry and Medicine, 8-11 Sept, Bressanone, Italy – Poster entitled : The Isolation of '3+3' and '4+0' Complexes of Rhenium (V) and (I) presented by Kim Potgieter, Thomas Gerber

Third European Chemistry Congress, 29 Aug-2 Sept, Nurnberg, Germany – Poster entitled : Rhenium complexes with Tetradentate (N_4) and Pentadentate (N_3O_2) donor ligands presented by Kim Potgieter, Thomas Gerber

CATSA (Catalytic Society of SA) Conference, 7-10 Nov, Bloemfontein : presentations by NMMU / Innoventon staff/ students :

- Physical and Electrochemical Characterization of Pt-based Catalysts for low temperature PEM Fuel Cells (poster) by R Mohamed, S Gouws, E Ferg
- Manufacturing and characterization of alternative materials for PEM electrolyser (poster) by N Gojela, S Gouws, E Ferg
- Hydrogen Economy : Electrocatalysis (poster) by S Gouws, N Gojela, R Mohamed
- Development of a zeolite wash coating technique for the synthesis of thymol in microstructured reactors (poster) by L Truter, J Fletcher, B Zeelie
- Comparison of Microstructured and Fixed Bed Reactors for the Oxidative Dehydrogenation of Cyclohexane to Cyclohexene and Benzene : oral presentation by B Mpuhlu

RESEARCH PAPERS PUBLISHED

Synthesis and Crystal Structure of an Unusual Mixed Crystal containing an Oxorhenium(V) and Imidorhenium(V) Complex. - P. Mayer, E. Hosten, T.I.A. Gerber*, I. Booyen
J. Iranian Chem. Soc., 2010, **7(3)**, 775-780.

Solvent-free Synthesis of Bisferrocenylimines and their Rhodium(I) Complexes - P.E. Kleyi, C.W. McClelland, T.I.A. Gerber
Polyhedron, 2010, **29**, 1095-1101.

2-(5-Benzo[d]thiazol-2-yl)thiophen-2-yl)benzo[d]thiazole - K. Potgieter, P. Mayer, E. Hosten, T.I.A. Gerber
Acta Cryst., 2010, **E66**, o531.

1-(4-Ferrocenylphenyl)-3-methyl-1H-imidazolium Iodide Hydrate - D. Onyanha, C. McClelland, T.I.A. Gerber, E. Hosten, P. Mayer
Acta Cryst., 2010, **E66**, m49

Coordination of 4-Aminoantipyrine to Rhenium(V) - P. Mayer, K.C. Potgieter, T.I.A. Gerber*
J. Chem. Cryst., 2010, **40**, 1146-1149

Rhenium(I), (III) and (V) Complexes of Tridentate ONX (X=O,N,S)-donor Schiff Bases - K.C. Potgieter, T.I.A. Gerber*, P. Mayer
Polyhedron, 2010, **29**, 1423-1430

The Reaction of Rhenium(V) Cores with a Tetradentate Schiff Base. The Isolation of '3+3' and '4+0' Complexes of Rhenium(V) - K.C. Potgieter, P. Mayer, T.I.A. Gerber*
Aust. J. Chem., 2010, **63**, 1382-1388

Reactions of the *fac*-[Re(CO)₃]⁺ and [ReO]³⁺ moieties with Substituted Benzothiazoles. - I.N. Booyen, T.I.A. Gerber*, P. Mayer
Inorg. Chim. Acta, 2010, **363**, 1292-1296.

The Oxidation of Rhenium(III) by Dioxygen in the Presence of Tri- and Tetradentate *N,O*-donor Ligands. - P. Mayer, N.C. Yumata, T.I.A. Gerber*, A. Abrahams
S.A. J. Chem., 2010, **63**, 40-44

Synthesis of a '4+1' Re(V) Complex from Re(III), and its disproportionation to Re(IV) and (VII) - P. Mayer, N.C. Yumata, T.I.A. Gerber*, A. Abrahams
Bull. Ethiopian Chem. Soc., 2010, **24(3)**, 411-413

The Isolation of Rhenium(V) 3+3 and 4+0 Complexes of Rhenium(V) - K.C. Potgieter, T.I.A. Gerber, P. Mayer
Tech. Radiomet. Chem. Med, 2010, 73-75

Coordination of the Bidentate Ligands 2,2'-Dipyridylamine, and 1-Phenyl-1,3-butadione and N'-(Propan-2-ylidene) benzohydrazide to Rhenium(III).
P. Mayer, N.C. Yumata, T.I.A. Gerber, A. Abrahams
S.A. J. Chem., 2010, **63**, 180-185.

Teaching kinetics using Excel - P Loyson , J. Chem. Educ. 2010, **87** (9), 998

Influences from Latin on chemical terminology - P Loyson, J. Chem. Educ., 2010, **87**(12), 1303-1307

Selective oxidation of *p*-cymene catalysed by VPO catalysts : process performance and kinetic studies – PR Makgwane, NI Harmse, E. Ferg, B Zeelie
Chem Eng Journal 162 (2010) 341-349

A new look at determining acid absorption of lead oxide used in the manufacture of Pb-acid batteries – E Ferg, T Phangalala, T van Dyl - J. Electrochem.(2010) 40 : 383-391.

Characterization and long term usage catalytic properties of $(\text{VO})_2\text{P}_2\text{O}_7/\gamma\text{Al}_2\text{O}_3$ stainless steel coated catalyst in *p*-cymene oxidation – PR Makgwane, E Ferg, B Zeelie – Applied Catalysis A : General 373 (2010) 132-139.

Liquid phase oxidation of *p*-cymene by $(\text{VO})_2\text{P}_2\text{O}_7$ and $\text{VO}(\text{PO}_3)_2$ catalysts – PR Makgwane, E Ferg, DG Billing, B Zeelie – Catal Lett (2010) 135 : 105-113.

Instability of highly concentrated emulsions with oversaturated dispersed phase. Role of surfactant – NN Tshilumba, E Ferg, I Masalova – Colloid Journal 2010, 72, 4, 560-564.

Papers accepted for publication but appearing in Journals in 2011

Chemistry in the Time of the Pharaohs – P Loyson, J. Chem. Educ. 2011, **88** (2), 146-150 (published on web 12 / 03/ 2010)

Characterization of base metal catalysts with platinum to replace PGM content in a PEM electrolyser cell – N Gojela, S Gouws , Analytical Letters (March issue)

Preparation and Transformation of True Nifedipine Polymorphs : Investigated with Differential Scanning Calorimetry and X-Ray Diffraction Pattern Fitting Methods – D Grooff, W. Liebenberg, M.M. De Villiers – Journal of Pharmaceutical Sciences, accepted 28 Oct 2010.

INNOVENTON NEWS

Plettenberg Bay Workshop, 11-15 January : meeting between Innoventon (Prof B Zeelie, Dr G Dugmore and Dr P Makgwane) and the UCT Catalysis Research Unit (Prof J Fletcher, Mr S Roberts, Mr K van der Merwe and Mr R Weber) to discuss and agree on collaborative research projects

Innoventon Analytical received SANAS Accreditation on 16 Feb 2010

Opening of the NMMU algae-to-energy project in February : the project uses micro-algae to convert harmful CO₂ from the atmosphere into crude oil, hydrogen gas and a water solution rich in sugars and proteins.

Visit by Prof Vladimir Linkov from the University of the Western Cape SAIAMC, HySA systems on 26 March : Electrical Energy Storage for Fuel Cell Vehicles of the Future : Combining Li-ion batteries with supercapacitor technologies

Training week at University of Western Cape HySA Systems : 12-16 April – Several post grad students and staff attended this training week. Topics discussed were : fuel cells, hydrogen storage and compression, H₂ purification and batteries, modeling of key components

Short course in April : Design and Analysis of experiments for the development of formulations, mixtures and blends, presented by Koos Bosma (8 students)

Farewell to Dr Nigel Harmse 28 June

SOUTH AFRICAN CHEMICAL INSTITUTE MATTERS

SACI / ASPEN PHARMACARE regional student Post-grad Chemistry seminar

The annual regional post-graduate chemistry seminar, sponsored by SACI and Aspen Pharmacare, took place on Friday 22 October at the Nelson Mandela Metropolitan University in Port Elizabeth. Post-graduate students and staff from the chemistry departments of the four universities in the Eastern Province gathered together to listen to the latest chemistry research being carried out at the various universities.

The participating universities were : Rhodes , Fort Hare, Walter Sisulu and the Nelson Mandela Metropolitan University (NMMU). It was encouraging to see so many people coming from far out to be part of this auspicious event : there was a large contingent from Walter Sisulu University in Umtata (6 hours by car) and from Fort Hare (4 hours by car) , as well as from Rhodes. All together there were 110 people present.

As usual we had two sections : a junior section incorporating BSc Hons / B Tech and 1st year M, and a senior section covering the higher studies : 2nd year M and PhD.

Professor Tommy Gerber, Head of the Department of Chemistry at NMMU briefly welcomed the delegates after which Prof Peter Loyson, chairman of SACI (EP), gave a brief introduction to SACI, its activities and the benefits of belonging to SACI and he presented the James Moir medal to Mr Clive Eley from Rhodes.

The 1st prize in the Junior category went to Matthew Coombes from Rhodes with the title : Synthesis, characterization, and computational analysis of a Cu(II) Metal Organic Framework, whilst the 2nd prize went to Claire Rossouw from NMMU with the title : The accelerated life cycle testing and modeling of Lithium-ion cells used in electric vehicle applications.

The 1st prize in the senior category went to Ryan Walmsley from Rhodes with the title : A catalytic exploration of vanadium; the 2nd prize went to Tavengwa Bunhu from Fort Hare with the title : Preparation of polymer-grafted lignocellulose / clay composites for the removal of heavy metals from aqueous solution.

The standard of each presentation was exceptionally high and the large number of post grad students present augurs well for the future of chemistry in the Eastern Cape.

After the academic programme was concluded, students and staff enjoyed refreshments sponsored by Aspen Pharmacare.



Photo 1 : The two junior prize winners : from left to right : Prof Loyson (chairman), Matthew Coombes from Rhodes (1st prize), Claire Rossouw from NMMU (2nd prize) and Dr Nigel Harmse from Aspen Pharmacare.



Photo 2 : senior prize winners. From left to right : Prof Loyson, Ryan Walmsley from Rhodes (1st prize), Tavengwa Bunhu (2nd prize), Dr Nigel Harmse (Aspen)