



## Departments in *the Natural Sciences*



Prof. André Roodt

# Department of Chemistry

## Overview

In pursuit of the strategic priorities of the UFS and the faculty, the Department of Chemistry experienced a further revival in quality and excellence.

Three postdoctoral associates, 20 M.Sc. and 25 Ph.D. students in different sub-disciplines led to a significant sustained research output for 2007. More than 60 research articles were published in international accredited journals and numerous local and international congress presentations were made.

Several prominent scientists visited the department, such as Profs Roger Alberto (Zurich, Switzerland), Ola Wendt (Lund University, Sweden), Rui Carvalho (University of Coimbra, Portugal), Daneel Ferreira (University of Mississippi, United States of America (USA)), Alexander Vinkelstein and Sasha Efimov (both from the Moscow State University, Puschino Campus, Russia), Dr Ettiene Snyders (South African Nuclear Energy Corporation (NECSA)), Prof. Mikhail Kritskey (Aleksey Nikolaevich Bach Institute of Biochemistry, Russian Academy of Sciences, Moscow State University, Russia), Dr Johann Nel (NECSA), Dr Willem van Otterloo (University of the Witwatersrand (Wits)), Dr Cassie Carstens (NECSA), Prof. Åke Oskarsson (Lund University, Sweden), Dr Marco Zappa (Mettler Toledo, Zurich, Switzerland), and Dr Andy Cammidge (University of East Anglia, Norwich, United Kingdom (UK)).

These scientists presented lectures and held research discussions with the department's researchers and postgraduate students in the departmental research seminar programme, which continued very successfully with around forty research presentations during 2007.

The upgrading of the Moerdyk and associated annexed building, which house the department continued. The project, to the value of R40 million, will be completed over a three-year period. This unprecedented investment in Chemistry by university management and the commitment to create a highly competitive teaching and research unit, made good progress during 2007, in spite of several unfortunate delays.

Furthermore, the further upgrading of the department's chemistry equipment contributed to a sustained high research output. This new equipment strategy forms part of the faculty's vision to be internationally visible with quality research outputs in niche areas, to provide leadership in advanced training to the

African continent student corps and to establish the UFS as an important player amongst South African universities as well as a competitor internationally.

During August 2007, a fire destroyed four laboratories in the department, causing damage of tens of millions of rand to the building structure and research infrastructure. Moreover, it caused significant emotional trauma and research result losses to a number of postgraduate researchers. This, together with the interruptions due to the renovation of the complete building, posed a range of unique problems in terms of practical classes, theory and research, and placed significant stress on the department. In spite of this setback, the enthusiasm of Chemistry personnel was illustrated by the fact that most activities were back on track within a month after the incident.

The way the staff of the department responded after the fire was simply remarkable and all inputs are highly appreciated and applauded. The support of senior management, particularly from faculty level in the person of Prof. Herman van Schalkwyk, Dean of Natural and Agricultural Sciences, as well as faculty colleagues, in providing office and laboratory space and other support for Chemistry under- and postgraduate students, is again gratefully acknowledged.

The three-year agreement between the UFS and SASOL, worth R9 million, according to which process technology and research development catalysis reside in the department, was continued and supported by the continued seconding of Prof. Ben Bezuidenhout to the department.

Teaching aspects on undergraduate level have been a focus of the department. The content of first-year modules was further upgraded and packaged differently in order to improve the success rates of distance learning, extended learning and main stream students. The continued teaching in parallel medium on the Main Campus was quite demanding on individuals; this challenges the lecturers to improve constantly, also with respect to using more sophisticated teaching methods and computers during class. The enthusiasm in terms of lecturing in Chemistry theory and practical classes on both the Main and QwaQwa Campuses is noted and gratefully acknowledged.

A special course focusing on computer skills specifically for disadvantaged students was presented by Dr Jeanet Conradie.

Web-based tutoring and expansion of teaching methods via WebCT were significantly expanded in 2007, specifically in Physical Chemistry, where many learners struggle with primary chemical knowledge due to backlogs and disadvantaged school teaching environments.

Advanced topics in a number of courses in the B.Sc. honours programme were further introduced and refined by outside scholars, exposing the department's students to international teachers. These included lectures on nuclear magnetic resonance (NMR) by Prof. Carvalho, natural product chemistry by Prof. Ferreira, industrial and organometallic chemistry by Prof. Bezuidenhout, and computational chemistry by Drs Petrie Steynberg from SASOL and Gideon Steyl from the UFS in the standard honours courses in Organic and Inorganic Chemistry. The special honours course saw the refining of advanced topics in bioanalytical chemistry by Profs Ken Swart and Thinus van der Merwe of FARMOVS-PAREXEL, and in Crystallography by Prof. Oskarsson. Furthermore, courses on heterogeneous catalysis by Dr Thys Botha from SASOL, protein physics and chemistry by Profs. Vinkelstein and Efimov, and thermal analysis by Dr Zappa were included.

The 13th successive science quiz competition, MINQUIZ, one of the faculty's community service flagships and jointly sponsored by the UFS and MINTEK, was successfully presented by Mrs Ina du Plessis and Prof. Jannie Swarts. A group of 200 pupils, comprising the three top physical science learners of each secondary school in the Free State province, visited the Main Campus during March 2007 where they were exposed to information on career opportunities in Chemistry, Physics and Geology. Prizes were awarded to the six winning schools in order to improve their science laboratory facilities.

Many colleagues in the department were involved in different committees, notably Prof. Swarts, who continued to contribute significantly in planning and negotiations to expand the equipment infrastructure of the Faculty of Natural and Agricultural Sciences. Others served on faculty and UFS committees, acted as external reviewers for the National Research Foundation (NRF) and for various international chemistry journals. Still others made their contributions as external examiners for a number of universities on undergraduate and graduate level and represented the UFS on international



*The department bade farewell to Prof. Steve Basson after 49 years at the UFS: From the left are: Profs André Roodt, Departmental Chairperson, Ben Bezuidenhout, Steve Basson, Walter Purcell, Jan van der Westhuizen, and Robbie Dennis.*

research councils (Profs. Swarts: Irish Health Council, and André Roodt, Departmental Chairperson: Swiss National Science Foundation). Most lecturers were involved in continuous career guidance and laboratory demonstration sessions to individual and groups of school learners, and colleagues at both the campuses contributed to UFS open and Expo days.

Prof. Steve Basson, head of the Analytical division and former Chair of the department, retired at the end of 2007 after a career of 49 years at the UFS.

Fifteen oral presentations were made on invitation at international conferences and venues as well as eighteen poster presentations at local and international venues, with more than 60 research papers published.

The NRF's Thrust for Industrially Related Projects (THRIP) application in Applied Process Chemistry from combined inputs of Inorganic, Physical and Organic Chemistry (Profs. Roodt, Swarts, and Bezuidenhout) was successful and sourced an additional R2.37 million for the upgrade of equipment and extended capacity building.

The **Physical Chemistry** division has two research groups, one headed by Prof. Swarts, and the other by Dr Conradie, both of whom are rated researchers with the NRF. Mr Ernie Langner is in the final stages of his Ph.D. studies, and while both NRF-rated researchers hold NRF research grants, Mr Langner is the holder of a Thuthuka NRF grant. The Swarts group is also funded by the Cancer As-

sociation of South Africa (CANSAs), the NRF's THRIP, and industrially by research grants from SASOL.

During 2007 the Physical Chemistry division supervised eight Ph.D. and two M.Sc. students, who are at various stages of their studies.

The main research question of the research group of Prof. Swarts concerns synthetic and physical chemistry aspects of multinuclear metallocenes. The group currently focuses on six projects:

- Porphyrin and phthalocyanine compounds bearing metallocene substituents
- Titanocene, zirconocene, hafnocene, ferrocene, ruthenocene and osmocene derivatives especially in association with rhodium, iridium, silver, gold and copper
- Electrochemical, kinetic and thermal analyses of these complexes
- Medicinal aspects of these complexes
- Polymer and protein chemistry in association with metallocenes
- Industrial studies on carboxylato complexes in collaboration with SASOL.

A research highlight from the Swarts group included results from an electrochemistry study on porphyrin-ferrocene conjugates with implications for structure and reactivity. This research received much international acclaim in that it reached the cover page of *Dalton Transactions* – (Auger, A., Muller, A.J. & Swarts, J.C. 2007.



Remarkable isolation, structural characterization and electrochemistry of unexpected scrambling analogues of 5-ferrocenyl-10,20-diphenyl porphyrin, *Dalton Transactions*, 3623-3633).

The Swarts group has international collaboration with Prof. Mike Cook at the University of East Anglia, Norwich, UK on phthalocyanine chemistry, Prof. Manuel Aquino at the St. Francis Xavier University, Antigonish, Canada on metal carboxylates, and Prof. William (Bill) Geiger at the University of Vermont, USA, on electrochemistry.

During 2007, Prof. Swarts paid research visits to Profs Cook, Geiger and Aquino as well as to Prof. Van Lier at Sherbrooke University, Canada (medicinal chemistry). Mr Langner visited Prof. Cook and purchased a Cyclograph capable of separating and purifying newly-synthesised compounds with much greater ease and speed.

The Swarts research group hosted international scholars from Russia (Prof. Alexander Vinkelstein from Moscow University, Moscow, a protein physicist), Switzerland (Dr Marco Zappa from Mettler Toledo, Zurich, a thermodynamic materials chemist), and the UK (Dr Andy Cammidge, University of East Anglia, Norwich, UK a porphyrin and phthalocyanine chemist).

The industrial research collaboration of the Swarts group led to visits by Dr Thys Botha (heterogeneous catalysis), Dr Reinier Nel (carboxylate chemistry) and Dr Frans Prinsloo (aluminium chemistry), all from SASOL on various industrial research issues.

The research group of Dr Conradie focuses on the characterisation of known and unknown transition metal complexes and intermediates by means of synthetic and computational chemistry. The following classes of compounds are presently investigated: Transition metal porphyrin and related compounds; O,O'-Chelated titanocene and titanium complexes; Beta-diketonato-carbonyl complexes of rhodium(I) and rhodium(III) and Dithizonato compounds of transition metal complexes.

The Conradie group has international collaboration with Prof. Abhik Ghosh (Department of Chemistry and Centre for Theoretical and Computational Chemistry, University of Tromsø, Tromsø, Norway), Prof. Mark Gladwin (Chief, Vascular Medicine Branch National Heart Lung and Blood Institute, Critical Care Medicine Department Clinical Centre, Maryland, USA), Prof. Daniel Kim-Shapiro (Physics, Wake Forest University, Winston-Salem, North Carolina, USA), Prof. Stephen Lippard (Massachusetts Institute of Technology, Cambridge,

Massachusetts), Prof. Stephen Koch (State University of New York at Stony Brook, New York, USA) and Prof. Penny Brothers (Auckland, New Zealand).

A highlight of the research activities of the Conradie group included a publication in the high impact factor science journal (12.4), *Nature*. (Basu, S., Grubina, R., Huang, J., Conradie, J., Huang, Z., Jeffers, A., Jiang, A., He, X., Azarov, I., Seibert, R., Mehta, A., Patel, R., King, S. B., Ghosh, A., Gladwin, M. T. & Kim-Shapiro D. B. 2007. Catalytic Generation of  $N_2O_3$  by the Concerted Nitrite Reductase and Anhydrase Activity of Hemoglobin, *Nature Chemical Biology*, 3, 785-794).

Another key research result was published in the *Journal of the American Chemical Society*, a flagship of the American Chemical society (Jeanet Conradie, Duncan A. Quarless, Jr., Hua-Fen Hsu, Todd C. Harrop, Stephen J. Lippard, Stephen A. Koch & Abhik Ghosh. 2007. Electronic structure and FeNO conformation of nonheme iron-thiolate-NO complexes: A combined experimental and DFT study, *J. Am. Chem. Soc.* 129, 10446-10456).

Dr Conradie was invited to visit the Scientific Computing & Modelling offices in Amsterdam, the Netherlands in May 2007. During this visit, she identified three 'bugs' in the Amsterdam Density Functional (ADF) programme that led to the improvement thereof. She also paid a research visit to Prof. Ghosh at the University of Tromsø, Tromsø, Norway.

Research in **Inorganic Chemistry** concentrates on Coordination Chemistry with the primary focus on an integrated investigation of reaction mechanisms through the use of crystallography, spectroscopy, computational chemistry and reaction kinetics. Two research thrusts focus on industrial reactions/homogeneous catalysis and applications to medicine (radiopharmaceutical and chemotherapeutic agents). This research in the group of Prof. Roodt continued and the infrastructure was expanded, supported by Dr Deon Visser, three contracted researchers at senior lecturer level, namely Drs Alfred Muller (Crystallography), Reinout Meijboom (synthesis) and Gideon Steyl (Computational Chemistry), as well as Drs Thato Mtshali, Johan Venter and 11 postgraduate students. Over 30 research articles and more than 20 conference contributions, of which ten were invited oral presentations, were produced.



Renowned guest speakers in the department are, from the left: Prof. Alexei Vinkelstein, Russia, Dr Marco Zappa, Mettler, Switzerland, Prof. Jannie Swarts, Professor at the department, and Dr Thys Botha, SASOL.

Dr Meijboom obtained a 'promising young scientist' rating from the NRF, while Dr Mtshali was successfully evaluated under the Thuthuka programme and obtained good funding for the next two years. Prof. Roodt as principal applicant successfully obtained funding of R700 000 under the NRF's Economic Growth and International Competitiveness (EGIC) programme for the next three years.

The homogeneous catalysis research is driven in close collaboration with SASOL and the Department of Science and Technology at the University of Cape Town's Centre for Excellence in Catalysis, c\*change. The research focus is on the conversion of simple feedstock molecules into value-added products and includes studies of classical reaction types such as carbonylation (synthesis of acetic acid and other products from methanol and carbon monoxide), hydroformylation (aldehydes and alcohols from olefins and synthesis gas) and oligomerisation (ethene). Collaboration with SASOL, the North-West University, the Universities of Johannesburg, Cape Town, Western Cape, and Lund (Sweden) forms part of this thrust. A highlight of this research was a paper published in the high impact factor science journal (10.2), *Angewandte Chemie, International Edition* (Ferreira, A.C., Crous, R., Bennie, L., Meij, A.M.M., Blann, K., Bezuidenhout, B.C.B., Young, D.A., Green, M.J. & Roodt, A. 2007. Borate esters as alternative acid promoters in the palladium-catalyzed methoxycarbonylation of ethylene. *Angewandte Chemie, International Edition* 46: 2273-2275.)

Similarly, the medical research focus, in collaboration with the Universities of Missouri, USA (Dr Hendrik Engelbrecht), Lund, Sweden (Profs. Ola Wendt and Ake Oskarsson), Zurich, Switzerland (Prof. Roger Alberto), CANSA (Prof. Connie Medlen, Pharmacology, UP) and PETLabs Pharmaceuticals (Dr Gerdus Kemp) showed good progress and several research reports and articles in international accredited journals were published. A spin-off of this research was the synthesis of model chemotherapeutic compounds which again yielded very positive results for future application.

The equipment in the group was further expanded by the acquisition of spectroscopy units with funding obtained from SASOL (Drs Chris Reinecke and Desmond Young) and PETLabs Pharmaceuticals (Dr Kemp), while funding under the THRIP programme, CANSA and the NRF was sourced.



A visit of the RheManTec International symposium delegates from Switzerland to PETLabs Pharmaceuticals, Pretoria. Here are: Dr Gerdus Kemp, Operations Manager: PETLabs, in the white coat, and Prof. Roger Alberto, University of Zurich, Switzerland in the grey shirt.



Mr Ernie Langner, Lecturer in Physical Chemistry, demonstrates experiments to MINQUIZ delegates.

The Computational Chemistry infrastructure was significantly expanded by financial inputs from UFS senior management, the Dean of Natural and Agricultural Sciences and the Inorganic Section, to establish a computing cluster of more than 130 central processing units (CPUs). Software was obtained by support from SASOL (Dr Petrie Steynberg and Prof. Bezuidenhout). The inputs of Dr Steyl and Messrs Sakkie van Rensburg and

Albert van Eck of the UFS Computer Services Division were invaluable in this regard to establish one of the best computer clusters in South Africa.

A high-pressure stop flow unit of more than R1 million was donated to the Roodt group by Prof. Lars Ivar Elding from the University of Lund, Sweden. This system is extremely important for the determination of intimate reaction





Students busy at a glove box for super-pure experiments. From the left are: Messrs Wade Davis, Chris Joubert, Ms Nicola Barnard, and Mr Henno Gericke.

mechanisms, and makes the department the only one in South Africa with this equipment, and one of only two in the Southern Hemisphere.

Funding under the STAC/STAFF programme allowed students from the UFS and the University of Lund, Sweden, to visit each other's research facilities. Ms Alice Brink, Truidie Venter, Messrs Leo Kirsten and Inus Janse van Rensburg visited Lund during 2007. Prof. Roodt, in partnership with Prof. Ola Wendt from the Lund University, sourced R900 000 under the Swedish International Development and Co-operation Programme (SIDA) for the next three years to continue this collaboration. Ms Alice Brink attended a course on High Pressure Gas Chromatography and was the only delegate in a class of 30 (from different industries) to complete the course 'cum laude'. Mr Inus Janse van Rensburg visited High-Tech Scientific in Manchester, UK, to obtain experience in high pressure stopped flow. Later in 2007 he won the third prize for best poster presentation at the Annual Conference of the Catalytic Society of South Africa in Richards Bay. Ms Marietjie Schutte visited the group of Prof. Alberto in Zurich, Switzerland for a month early in 2007 to gain experience in nuclear medicine. Her visit was partly sponsored by the Swiss National Science Foundation.

In collaboration with Prof. Roger Alberto (University of Zurich, Switzer-

land), Prof. Roodt successfully obtained funding from the NRF and the Swiss National Science Foundation to host the first International Symposium on the chemistry of the Mn triad of elements (Rhenium, Manganese and Technetium), RheManTec, at the UFS during November 2007. More than 50 delegates from nine countries attended this very successful meeting. Ms Marietjie Schutte visited the group of Prof. Alberto for a month early in 2007, partly sponsored by the Swiss National Science Foundation.

The **Organic Chemistry** division is headed by Profs Jan van der Westhuizen, Ben Bezuidenhout and Dr Susan Bonnet. One postdoctoral associate, Dr Ivana Jarak, and 19 students supported the research during 2007. Three M.Sc. dissertations and one Ph.D. thesis were completed by the end of 2007.

A counter-current chromatographic system was purchased in 2007, making the department the only laboratory in South Africa currently to boast such equipment. Collaboration with the Agricultural Research Council (ARC) on the synthesis and purification of water soluble organic compounds depends critically on this modern system.

Three different research thrusts were identified in the Organic Chemistry group, the first being the synthesis of internal standards for pharmaceutical com-

pounds in collaboration with FARMOVS-PAREXEL (M.Sc. programme and THRIP project).

The second project involves bio-analytical chemistry in collaboration with FARMOVS-PAREXEL and Applied Biosystems (Canada) (Ph.D. programme in the identification of potentially bioactive compound from South African plants). This project is part of the Advanced Biomolecular Research Cluster of the UFS and the NRF Institutional Research Development Programme. Under this programme, the Organic section synthesised and delivered eight internal standards to FARMOVS-PAREXEL that were used to develop novel bio-analytical procedures. They also documented the synthetic procedures as standard operating procedures and supplied FARMOVS-PAREXEL with a certificate of analysis for each internal standard.

The third thrust includes flavonoid chemistry, since the UFS has a long tradition of excellence therein, which is partly funded by the wattle industry. Mr Benji Elfaki, Lecturer in Organic Chemistry at the University of Khartoum, Sudan, visited Bloemfontein for eight months in 2007 to study structure elucidation of natural products with NMR and to work on his Ph.D. thesis.

Ms Anette Allemann attended the Chemical Research Applied to World Needs (Chemrawn) XII Conference in Stellenbosch. Prof. Van der Westhuizen attended the Eighth Tetrahedron Symposium in Berlin, Germany, and Prof. Van der Westhuizen and Dr Bonnet attended the International Symposium on Advances in Synthetic and Medicinal Chemistry, in St. Petersburg, Russia.

The **Process Chemistry** thrust, which was established in early 2006, is headed by Prof. Ben Bezuidenhout, SASOL-seconded Chair in Organic Chemistry. In 2007, the group already consisted of six M.Sc. and two Ph.D. students, which includes a full-time employee of SASOL, working on a collaborative project. Apart from these, two students are shared with the Physical Chemistry division.

The focus of the Bezuidenhout group includes a sub-thrust on organo-metallic synthetic procedures, while other research concentrates on the production of oxygenated compounds from olefins via epoxidation utilising phthalocyanine-based catalysts, the development of improved technology for the synthesis of m-cresol from xylene, utilisation of borosaliclic

acid in organic synthesis and hydrogenation of alpha-beta unsaturated ketones.

A collaborative agreement was negotiated with HE Essential Oils, who will sponsor two student bursaries at B.Sc. honours and M.Sc. level.

Several large pieces of equipment were acquired during 2007, which include a Premix autoclave reactor to the value of R350 000, a Gas Chromatograph from SASOL to the value of R120 000, and a MALDI-TOFF spectrometer to the value of R1.8 million. The latter will assist in evaluating catalysts in their active form, and will be the second facility in the world, complemented by the utilisation of X-ray crystallography, for the characterisation of reactive organometallic catalysts.

Prof. Bezuidenhout visited Profs Cathy Cutler, Delbert Day and Dr Hendrik Engelbrecht at the University of Missouri in the USA, Prof. Deryn Fogg at the University of Ottawa, Canada, Prof. David Cole-Hamilton, University of St Andrews, Scotland and Bruker Daltonics in Bremen, Germany, and discussed mutual research collaboration, which is anticipated to commence during 2008.

The **Polymer Science** research area is headed by Prof. Riaan Luyt in Chemistry at the Qwaqwa Campus. His group comprises nine students, and the research focuses on physical properties of polymer/wax mixtures, polymer/natural fibre composites and polymer nanocomposites. Chemistry at the Qwaqwa Campus again did exceptionally well in terms of research, given the infrastructure shortage and relatively high work load.

The Luyt group has national research collaboration with Prof Walter Focke, Institute for Applied Materials, University of Pretoria (UP) which culminated in combined student research seminars held at Qwaqwa (May 2007) and the UP (September 2007), as well as with Dr Suprakas Sinha Ray, Nanotechnology Research Group, Council for Scientific and Industrial Research (CSIR). Prof. Luyt is co-supervisor of three Ph.D. students working under the supervision of Dr Ray.

Furthermore, Prof. Luyt has research collaboration under the Formal South Africa-India bilateral project on latex-based nanocomposites with Prof Sanra Thomas, Institute for Macromolecular Science and Engineering, Mahatma Gandhi University, Kottayam, India, as well as a project on polymer phase



Here are Ph.D. students Mss Nicolene Cloete (left) and Tania Hill at the microscopes, probing for high quality single crystals.

change materials with Dr Igor Krupa, Polymer Institute, Slovak Academy of Sciences, Bratislava, Slovak Republic.

Another two formal collaborations were approved by the NRF during 2007, the first being a project on nanoparticles for polymer reinforcement with Prof M. Messori, University of Modena and Reggio Emilia, Modena, Italy, and the second on the development and investigation of injection moulded, natural fibre-reinforced composites using biodegradable matrixes, with Prof. Tibor Czigany, Department of Polymer Engineering, Budapest University of Technology and Economics Budapest, Hungary.

The Luyt group hosted international visitors Prof. Bert Klumperman, Professor at the Eindhoven University of Technology, the Netherlands and Department of Science and Technology Research Professor at the Polymer Institute, University of Stellenbosch, South Africa, as well as Prof. Azman Hassan, Head of the Polymer Engineering Department, Technology University of Malaysia, Malaysia.

The **Analytical** division currently consists of Prof. Walter Purcell, Dr Karel von Eschwege and Ms Rebotsamang Shago and is supported by five M.Sc. students.

Prof. Purcell is currently involved in the establishment and evaluation of different digestion methods (microwave and fluxes) of plasma dissociated and natural occurring zircon as well as the quantification of the different elements in these minerals. Inductively Coupled Plasma Emission Spectroscopy (ICP-OES), Atomic Absorption (AA) and ultraviolet (UV)/visible spectroscopy are mainly employed in the research. Preliminary investigations, in collaboration with Soil Sciences, are also involved in determining the possible pollution of irrigation water by agricultural activities in the Vaalharts Irrigation system. Another study involves the investigation of photochromic reactions in different transition metal complexes, with potential applications in high density optical molecular switching mechanisms. Instrumental techniques such UV/visible, Infrared (IR), Nuclear Magnetic

## Staff

### Main Campus:

**Professors:** Profs Steve Basson, André Roodt, Jannie Swarts, Ben Bezuidenhout

**Affiliated Professors:** Profs Daneel Ferreira, Rui Carvalho, Tinus van der Merwe, Ken Swart

**Associate Professors:** Profs Walter Purcell, Robbie Dennis, Jan van der Westhuizen

**Affiliated Associate Professor:** Prof. Fanie Otto

**Senior Lecturers:** Drs Jeanet Conradie, Deon Visser, Fanie Muller, Reinout Meijboom, Gideon Steyl

**Lecturers:** Drs Susan Bonnet, Karel von Eschwege, Johan Venter, Mr Ernie Langner

**Junior Lecturer:** Dr Thato Mtshali, Ms Rebotsamang Shago

**Subject Co-ordinators:** Dr Marietjie Versteeg, Ms Rina Meintjes

**Senior Professional Officers:** Dr Gabre Kemp, Mr Wade Davis, Ms Ina du Plessis

**Professional Officers:** Mss Magda van Tonder, Annette Alleman, Anke Wilhelm

**Assistant Professional Officers:** Mr Michael Coetzee, Ms Nicoline Cloete

**Supervisory Technician:** Mr Charles Smith

**Senior Administrative Officer:** Ms Tessa Swarts

**Administrative Officers:** Mss Marietjie Havenga, Alet van Rooyen, Alice Stander

**Technical Assistants:** Messrs Jafta Masedi, Solly Leroala, Daniel Fish, Henry Ramokone, Ms Jeanette Mmope

**Messenger:** Ms Maria Seithisho

### Qwaqwa Campus:

**Professor:** Prof. Riaan Luyt

**Lecturers:** Mss Moipone Mokoena, Buyiswy Jacobs, Messrs Tsietsi Tsoetsi, Percy Hlangothi

**Junior Lecturers:** Mss Dorine Dikobe, Mpondi Stuurman, Mr Rantooa Moji

**Professional Officers:** Messrs Tshwafo Motaung, Mfiso Mngomezulu

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Resonance (NMR), Cyclic-Voltammetry, Quantum Computational Chemistry (ADF & Gaussian) and X-ray Crystallography are employed in these studies.

Co-operation with NECSA was established and they are currently funding an M.Sc. student research project on the establishment of digestion methods and element quantification in plasma dissociated and natural zircon. NECSA further funded a new hydrogen fluoride (HF)-resistant plasma burner for the ICP which will allow the Analytical section to become the preferred Zr-F analytical facility for the Advanced Metals Initiative (AMI) of the South African Department of Science and Technology (DST). New ICP-OES and AA spectrophotometers were introduced into the Analytical section and two students are currently doing their research, mainly using these pieces of equipment. Mr Steven Lötter, M.Sc. student, attended a week-long course on the practical aspects of ICP in Pretoria in August 2007.

Dr Von Eschwege, a Thuthuka grant holder, was successful in his application for

the NRF's Institutional Research Development Programme (IRDP) funding under the Nanotechnology focus area. He was also awarded the Bruker prize for best Ph.D. student in 2007, and attended the "Summer School on Quantum Computing and Information" held in Durban during January 2007 and the Bruker NMR Seminar thereafter. Dr Von Eschwege also hosted Prof. Andrew Crouch of the University of Stellenbosch, who explored cooperation possibilities in his research field involving new dithizonato ligands.

## Additional research related outputs:

Prof. Roodt, as member of the Executive Committee of the European Crystallographic Association (ECA), attended the Executive Meetings in Manchester, UK (February 2007) and Marrakech, Morocco in August 2007, as member of the International Scientific Committee of 24th European Crystallographic Meeting. He served as Chairperson of the committee awarding the

prestigious Max Perutz Prize of the ECA, which was presented to Prof. Dave Stuart of Oxford University, UK. Prof. Roodt further served on the THRIP panel for 'Process Manufacturing' of the South African NRF, and also acted as Inorganic Editor for the South African Journal of Chemistry, as Co-Editor for the International Union of Crystallography (IUCr) journal, *Acta Crystallographica E* and was on the editorial board of the *Journal of Coordination Chemistry*.

Dr Bonnet visited the University of Mississippi in the USA (Prof. Daneel Ferreira) for a month in April 2007 and studied synthetic techniques and the synthesis flavonoids, while Prof. Van der Westhuizen visited Prof. Herbert Kolodziej in Münster, Germany to discuss pharmaceutical collaboration.

Prof. Purcell was invited to serve as a member of the local scientific committee of the 6th International Symposium on Technetium and Rhenium to be hosted in Port Elizabeth from 7-10 October 2008.



## Research articles

- Achilonu, M.C., Janse van Rensburg, J.M., Van der Westhuizen, J.H. & Roodt, A.** 2007. 1-(4-Methoxybenzyl)pyridinium *p*-toluenesulfonate. *Crystallographica Section E* E63: o4326.
- Auger, A., Muller, A.J. & Swarts, J.C.** 2007. Remarkable isolation, structural characterisation and electrochemistry of unexpected scrambling analogues of 5-ferrocenyl-10,20-diphenylporphyrin. *Dalton Transactions*: 3623-3633.
- Auger, A. & Swarts, J.C.** 2007. Synthesis and group electronegativity implications on the electrochemical and spectroscopic properties of diferrocenyl meso-substituted porphyrins. *Organometallics* 26: 102-109.
- Basu, S., Grubina, R., Huang, J., Conradie, J., Huang, Z., Jeffers, A., Jiang, A., He, X., Azarov, I., Seibert, R., Mehta, A., Patel, R., King, S.B., Hogg, N., Ghosh, A., Gladwin, M.T. & Kim-Shapiro, D.B.** 2007. Catalytic generation of  $N_2O_3$  by the concerted nitrite reductase and anhydrase activity of hemoglobin. *Nature Chemical Biology* 3: 785-794.
- Bertolasi, V., Hradil, P., Spáčilová, L., Muller, A. & Hlaváč, J.** 2007. 5-Phenyluridine trihydrate. *Acta Crystallographica Section E* E63: o3805.
- Booyens, S., Roodt, A. & Wendt, O.G.** 2007. Kinetic investigation of a ruthenium metathesis catalyst. *Journal of Organometallic Chemistry* 692: 5508-5512.
- Brandt, D.J., Steenkamp, J.A., Brandt, E.V. & Takeuchi, Y.** 2007. Conformational studies of (-)-epicatechin-Mosher ester. *Tetrahedron Letters* 48: 2769-2773.
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## Conference contributions

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**Brink, A., Cloete, N., Roodt, A. & Visser, H.G.** 2007. *Ring a ring of roses, a pocket full of phosphines*. Oral presentation at the RheManTec International Symposium on the Mn-triad in Life Sciences and Catalysis, Bloemfontein, South Africa. 19-24 November.

**Brink, A., Roodt, A. & Visser, H.G.** 2007. *The effect of group 15 ligands on selective rhodium(I) model complexes*. Poster presented at the Conference of the Catalysis Society of South Africa (CATSA), Richards Bay, South Africa. 11-14 November.

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**Dikobe, D.G. & Luyt, A.S.** 2007. *Thermal and mechanical properties of PP/EVA-WF and MAPP/EVA-WF polymer blend composites*. Poster presented at the International Conference on Natural Polymers, Bio-Polymers, Bio-Materials, their Composites, Blends, IPNS and Gels: Macro to Nano Scale, Mahatma Gandhi University, Kottayam, India. 19-22 November.

**Han, Z., Bonnet, S.L. & Van der Westhuizen, J.H.** 2007. *Synthesis of xanthine derivatives by photochemical transformations of pentoxifylline: A bidentate chromophore*. Poster presented at the International Symposium on Advances in Synthetic and Medicinal Chemistry of the European Federation for Medicinal Chemistry (EFMC), St Petersburg, Russia. 27-31 August.

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**Luyt, A.S. & Mngomezulu, M.E.** 2007. *Phase change materials based on polyethylene, paraffin*

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**Mogudi, B.M., Meijboom, R. & Roodt, A.** 2007. *Phosphite modified cobalt catalysts for 1-alkene hydroformylation.* Poster presented at the Conference of the Catalysis Society of South Africa (CATSA), Richards Bay, South Africa. 11-14 November.

**Montsho, R.M., Bonnet, S.L. & Van der Westhuizen, J.H.** 2007. *The reaction between  $\alpha$ -keto acids and phloroglucinol.* Poster presented at the International Symposium on Advances in Synthetic and Medicinal Chemistry of the European Federation for Medicinal Chemistry (EFMC), St Petersburg, Russia. 27-31 August.

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**Roodt, A.** 2007. *Implications for nuclear medicine from mechanistic studies on substitution reactions in complexes of the manganese triad.* Keynote lecture presented at the RheManTec International Symposium on the Mn-triad in Life Sciences and Catalysis, Bloemfontein, South Africa. 19-24 November.

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**Roodt, A. & Botha, J.M.** 2007. *Implications for nuclear medicine from a kinetic and high-pressure mechanistic study on substitution in  $\text{Re(V)}$  and  $\text{Tc(V)}$  complexes.* Invited oral presentation at the 4th Cancer Association of South Africa (CANSA) Colloquium, Pretoria, South Africa. 2-4 September.

**Roodt, A., Meijboom, R. & Venter, G.J.S.** 2007. *Supramolecular coordination chemistry of silver phosphine complexes.* Invited oral presentation at the Inorganic Chemistry Conference INORG 007, Conference of the South African Chemical Institute, Club Mykonos, Langebaan, South Africa. 8-12 July.

**Schutte, M., Roodt, A. & Visser, H.G.** 2007. *Rhenium(I) compounds in nuclear medicine: Crystallographic and kinetic investigation of different  $[\text{Re}(\text{CO})_3(\text{L1})(\text{L2})]^+$  complexes.* Oral presentation at the RheManTec International Symposium on the Mn-triad in Life Sciences and Catalysis, Bloemfontein, South Africa. 19-24 November.

**Steyl, G.** 2007. *UFS-HPC and chemistry: A review.* Invited oral presentation at the National Super Computing Congress (CHPC), Cape Town, South Africa. 3-5 December.

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RheManTec International Symposium, Bloemfontein, South Africa. 19-24 November.

**Steyn, M., Steyl, G. & Roodt, A.** 2007. *Speciation and interconversion mechanism of mixed fluoro and O,O- and O,N-bidentate ligand complexes of Zirconium.* Oral presentation at the RheManTec International Symposium on the Mn-triad in Life Sciences and Catalysis, Bloemfontein, South Africa. 19-24 November.

**Swarts, J.C.** 2007. *An overview of metallocene-containing anticancer drugs.* Invited oral presentation at the 4th Cancer Association of South Africa (CANSA) Colloquium, Pretoria, South Africa. 2-4 September.

**Venter, G.J.S., Meijboom, R. & Roodt, A.** 2007. *Silver(I) coordination with group 15 ligands and the ligand exchange mechanism.* Oral presentation at the RheManTec International Symposium on the Mn-triad in Life Sciences and Catalysis, Bloemfontein, South Africa. 19-24 November.

**Venter, G.J.S., Roodt, A. & Meijboom, R.** 2007. *Coordination of selective coin metals by group 15 ligands and the ligand exchange mechanism.* Oral presentation at the DST-NRF c\*change Symposium, Richards Bay, South Africa. 9-10 November.

**Venter, G.J.S., Roodt, A. & Meijboom, R.** 2007. *Silver(I) complexes with group 15 ligands: Model hydroformylation catalysts?* Poster presented at the Conference of the Catalysis Society of South Africa (CATSA), Richards Bay, South Africa. 11-14 November.

**Venter, J.A., Basson, S.S. & Purcell, W.** 2007. *Evaluation of ligand and solvent effects on a potential catalyst using a rhodium cupferrate system as model.* Oral presentation at the RheManTec International Symposium on the Mn-triad in Life Sciences and Catalysis, Bloemfontein, South Africa. 19-24 November.

**Visser, H.G., Kemp, G., Schutte, M. & Roodt, A.** 2007. *Rhenium(I) carbonyl complexes as model radiopharmaceuticals.* Oral presentation at the RheManTec International Symposium on the Mn-triad in Life Sciences and Catalysis, Bloemfontein, South Africa. 19-24 November.