

## **Publications: Conference contributions 2010**

1. **Ahmad, E.E.M. & Luyt, A.S.** *The influence of peroxide initiated crosslinking on the morphology and physical properties of OEsisal fibre micro- and nanocomposites* (Oral). The Polymer Processing Society 26<sup>th</sup> Annual Meeting, Banff, Canada, 4-8 July 2010.
2. **Barnard, N.I. & Swarts, J.C.** *The influence of ligand chain length and central metal on the thermal and structural properties of metal carboxylates* (Poster). Annual Conference of the Catalysis Society of South Africa (CATSA 2010), Bloemfontein, South Africa, 7-10 November 2010.
3. **Bezuidenhoudt, B.C.B., Sunil, A.C., Marais, C. & Langner, E.H.G.** *Mechanism of the copper catalysed rearrangement of o-toluic acid to meta-cresol* (Poster). 39<sup>th</sup> International Conference on Coordination Chemistry, Adelaide, Australia, 25-30 July 2010.
4. **Brink, A., Roodt, A. & Visser, H.G.** *Crystallographic Study of N-O Schiff Bidentate Rhenium and Copper Complexes* (Poster). 26<sup>th</sup> European Crystallographic Meeting, Darmstadt, Germany, 29 August-2 September 2010.
5. **Brink, A., Visser, H.G. & Roodt, A.** *Anomalies observed from iodomethane oxidative addition to rhodium(I) acetylacetonato complexes* (Poster). Annual Conference of the Catalysis Society of South Africa (CATSA2010), Bloemfontein, South Africa, 7-10 November 2010.
6. **Buitendach, B.E. & Swarts, J.C.** *Syntheses and electrochemistry of Zr(IV) and Hf(IV) phthalocyanines with ferrocene-containing betadiketones as axial ligands* (Poster). Annual Conference of the Catalysis Society of South Africa (CATSA 2010), Bloemfontein, South Africa, 7-10 November 2010.
7. **Cawood, M., Marston, A., Van der Westhuizen, J.H. & Zietsman, P.** *High-performance countercurrent chromatography for the efficient isolation of alkaloid acetylcholinesterase inhibitors for Nerine species (Amaryllidaceae)* (Poster). National Postdoctoral Research Forum, Somerset West, South Africa, 6-9 December 2010.
8. **Chiweshe, T.T., Purcell, W., Venter, J.A. & Mtshali, T.** *Quantification of rhodium in inorganic and organometallic compounds* (Poster). Analitika2010, Stellenbosch University, South Africa, 5-10 December 2010.
9. **Conradie, J, Gracia J. & Niemantsverdriet, J.W.** *H-spillover between rutile and rhodium - is it possible? A DFT view* (Lecture). Annual Conference of the Catalysis Society of South Africa (CATSA2010), Bloemfontein, South Africa, 7-10 November 2010.
10. **Conradie, J. & Ghosh, A.**  *$\pi$ -Acceptors to the rescue: Designing iron-group imido transfer reagents* (Poster). 239<sup>th</sup> ACS National Meeting & Exposition, San Francisco, California, 21-25 March 2010.

11. **Conradie, J.** 2010 *Once upon a time there were no Super Computers* (Lecture). Centre for High Performance Computing (CHPC) National Conference, Cape Town, South Africa, 7-9 December 2010.
12. **Conradie, M.M. & Conradie, J.** *A DFT study of the Oxidative Addition of Methyl Iodide to acetylacetona**tobis(triphenylphosphite)rhodium(I)*** (Poster). First Principles Quantum Chemistry, Bad Herrenalb, Germany, 14-17 April 2010.
13. **Conradie, M.M. & Conradie, J.** *DFT mechanistic investigation of the oxidative addition and methyl migration steps in the reaction [Rh(acac)(CO)(PPh)<sub>3</sub>] + CH<sub>3</sub>I* (Poster). Annual Conference of the Catalysis Society of South Africa (CATSA2010), Bloemfontein, South Africa, 7-10 November 2010.
14. **Conradie, M.M. & Conradie, J.** *DFT modeling of simplified and full experimental molecular systems - a case study* (Lecture). Centre for High Performance Computing (CHPC) National Conference, Cape Town, South Africa, 7-9 December 2010.
15. **Engelbrecht, I., Roodt, A. & Visser, H.G.** *Kinetic and Crystallographic Investigation of Model Iridium(Carbonyl)(Acetylacetonato) Complexes in Olefin Hydroformylation-/Transformations* (Poster). 39<sup>th</sup> International Conference on Coordination Chemistry, Adelaide, South Australia, 25-30 July 2010.
16. **Engelbrecht, I., Visser, H.G. & Roodt, A.** *Structural/Kinetic study of phosphine-based model iridium compounds for application in olefin hydroformylation* (Poster). Annual Conference of the Catalysis Society of South Africa (CATSA2010), Bloemfontein, South Africa, 7-10 November 2010.
17. **Erasmus, E., & Niemantsverdriet, J.W.** 2010 *Single-source precursor for Pd-Co/SiO<sub>2</sub> heterogeneous bimetallic catalysts*. (Poster). Annual Conference of the Catalysis Society of South Africa (CATSA 2010), Bloemfontein, South Africa, 7-10 November 2010.
18. **Grove, J.J.C., Bezuidenhoudt, B.C.B. & Ferreira, D.** *Conversion of Pravastatin into an advanced Intermediate in the Synthesis of the HMG-CoA Reductase Inhibitor BB-476* (Oral). South African Chemical Institute - Frank Warren Conference, Pietermaritzburg, South Africa, 17-24 January 2010.
19. **Hansson, C., Kirsten, L., Oskarsson, Å. & Roodt, A.** *[Pt(tht)<sub>4</sub>](CF<sub>3</sub>SO<sub>3</sub>)<sub>2</sub> in the Temperature Range 202-295K* (Poster). 26<sup>th</sup> European Crystallographic Meeting, Darmstadt, Germany, 29 August-2 September 2010.
20. **Herbst, L., Visser, H.G. & Roodt, A.** *Identification of Niobium(V) Complexes for the possible Separation of Niobium and Tantalum* (Poster). 39<sup>th</sup> International Conference on Coordination Chemistry, Adelaide, South Australia, 25-30 July 2010.
21. **Herbst, L., Visser, H.G. & Roodt, A.** *Investigation into the catalytic activities of niobium pentachloride and its derivatives* (Poster). Annual Conference of the

Catalysis Society of South Africa (CATSA2010), Bloemfontein, South Africa, 7-10 November 2010.

22. **Hill, T., Roodt, A. & Steyl, G.** *Crystallographic and computational aspects of  $\beta$ -diketonate palladium systems* (Poster). Annual Conference of the Catalysis Society of South Africa (CATSA2010), Bloemfontein, South Africa, 7-10 November 2010.
23. **Joubert, C.C. & Swarts, J.C.** *The synthesis and characterization of ruthenocene-containing poly(aminoacid) derivatives as possible catalysts* (Poster). Annual Conference of the Catalysis Society of South Africa (CATSA 2010), Bloemfontein, South Africa, 7-10 November 2010.
24. **Koen, R., Visser, H.G. & Roodt, A.** *Synthesis of Model Tantalum(V) Complexes for the Separation of Niobium and Tantalum* (Poster). 26<sup>th</sup> European Crystallographic Meeting, Darmstadt, Germany, 29 August-2 September 2010.
25. **Koen, R., Visser, H.G. & Roodt, A.** *Synthesis of model tantalum(V) multidentate complexes for use in industrial catalysis* (Poster). Annual Conference of the Catalysis Society of South Africa (CATSA2010), Bloemfontein, South Africa, 7-10 November 2010.
26. **Kuo, C-M. & Bezuidenhoudt, B.C.B.** *Studies towards the Synthesis of a naturally occurring novel Homoisoflavanone* (Poster). South African Chemical Institute - Frank Warren Conference, Pietermaritzburg, South Africa, 17-24 January 2010.
27. **Langner, E.H.G., Cheruvathur, A.V., Niemantsverdriet, J.W. & Thúne, P.C.** *Surface Chemistry of MgC<sub>12</sub> thin films used as support for model Ziegler-Natta catalysts* (Poster). Annual Conference of the Catalysis Society of South Africa (CATSA), Bloemfontein, South Africa, 7-10 November 2010.
28. **Lötter, S., Nkabiti, L., Purcell, W. & Nel, J.T.** *Rapid quantification of major and trace components of high purity zirconium metal by ICP-OES* (Oral). Light Metals 2010, Misty Hills, Muldersdrift, South Africa, 27-29 October 2010.
29. **Luyt, A.S.** *Polymer/wax blends as phase change materials for energy storage: Benefits and challenges* (Oral). International Conference on Recent Trends in Materials Science and Technology, Thiruvananthapuram, Kerale, India, 29-31 October 2010.
30. **Marston, A.** *Application of centrifugal countercurrent chromatography in the separation of natural products* (Lecture). Analitika, Stellenbosch University, South Africa, 5-9 December 2010.
31. **Marston, A.** *High-Speed Countercurrent Chromatography - New Applications* (Lecture). 7<sup>th</sup> International Symposium on the Chromatography of Natural Products, Lublin, Poland, 14-17 June 2010.

32. **Marston, A.** *High-Speed Countercurrent Chromatography in the Separation of Polyphenols* (Lecture). 25<sup>th</sup> International Conference on Polyphenols, Montpellier, France, 23-27 August 2010.
33. **Marston, A.** *Isolation of acetylcholinesterase inhibitors from the Amaryllidaceae by high-speed countercurrent chromatography* (Lecture). 11<sup>th</sup> Frank Warren Conference, University of KwaZulu-Natal, Pietermaritzburg, South Africa, 17-21 January 2010.
34. **Marston, A.** *LC/NMR in the study of unstable compounds from Jamesbrittenia fodina (Scrophulariaceae)* (Lecture). Bruker NMR Meeting, Hermanus, South Africa, 28-29 January 2010.
35. **Marston, A.** *What exactly is there in a cup of Rooibos?* Annual General Meeting and Research Day of the South African Rooibos Council, Clanwilliam, South Africa, 5 May 2010.
36. **Marston, A., Cawood, M., Van der Westhuizen, J.H. & Zietsman, P.** *The isolation of inhibitors of acetylcholinesterase inhibitors from Nerine species (Amaryllidaceae)* (Poster). Indigenous Plant Use Forum, Keimoes, South Africa, 28 June-1 July 2010.
37. **Marston, A., Cawood, M., Van der Westhuizen, J.H. & Zietsman, P.** *High-performance countercurrent chromatography for the efficient isolation of alkaloid acetylcholinesterase inhibitors from Nerine species (Amaryllidaceae)* (Poster). 58<sup>th</sup> International Congress and Annual Meeting of the Society for Medicinal Plant and Natural Product Research, Berlin, Germany, 29 Augustus - 2 September 2010.
38. **Miller, B.J. & Bezuidenhoudt, B.C.B.** *Ring-closing metathesis for the Synthesis of Phenyl Substituted 4H-Chromes* (Poster). South African Chemical Institute - Frank Warren Conference, Pietermaritzburg, South Africa, 17-24 January 2010.
39. **Mngomezulu, M.E., Luyt, A.S. & Krupa, I.** *Phase change materials based on polyethylene, paraffin wax and wood flour* (Poster). MACRO2010 43<sup>rd</sup> IUPAC World Polymer Congress, Glasgow, Scotland, 11-16 July 2010.
40. **Msutu, A., Hunter, R., Bezuidenhoudt, B.C.B. & Young, D.A.** *New Chemistry of CO<sub>2</sub>* (Poster). South African Chemical Institute - Frank Warren Conference, Pietermaritzburg, South Africa, 17-24 January 2010.
41. **Muller, T.J., Steyl, G. & Roodt, A.** *Copper Based Oxidation Catalysis* (Oral). 26<sup>th</sup> European Crystallographic Meeting, Darmstadt, Germany, 29 August-2 September 2010.
42. **Muller, T.J., Steyl, G. & Roodt, A.** *Copper based oxidation catalysis* (Oral). Annual Conference of the Catalysis Society of South Africa (CATSA2010), Bloemfontein, South Africa, 7-10 November 2010.

43. **Nete, M., Purcell, W., Snyders, E & Nel, J.T.** *Alternative dissolution methods for analysis of niobium containing samples* (Poster). Analitika2010, Stellenbosch University, South Africa, 5-10 December 2010.
44. **Nete, M., Purcell, W., Snyders, E. & Nel, J.T.** *Dissolution and analytical characterization of tantalite ore* (Oral). Light Metals 2010, Misty Hills, Muldersdrift, South Africa, 27-29 October 2010.
45. **Oyourou, J.-N., Combrinck, S., Regnier, T. & Marston A.** *Purification of verbascoside from plant extracts using column and countercurrent chromatography* (Poster). Analitika, Stellenbosch University, South Africa, 5-9 December 2010.
46. **Pretorius, C., Roodt, A. & Venter, J.A.** *Synthesis of novel vanadium(III) and vanadium(IV) complexes with O,O' bidentate ligands for catalytic application* (Poster). Annual Conference of the Catalysis Society of South Africa (CATSA2010), Bloemfontein, South Africa, 7-10 November 2010.
47. **Pretorius, C., Roodt, A. & Venter, J.A.** *Vanadium(III) and Vanadium(IV) Complexes with O, O- Bidentate Ligands* (Poster). 39<sup>th</sup> International Conference on Coordination Chemistry, Adelaide, South Australia, 25-30 July 2010.
48. **Roodt, A.** *Relevance of X-ray Structure Data to Kinetic Studies.* (Keynote Lecture). 26<sup>th</sup> European Crystallographic Meeting, Darmstadt, Germany, 29 August-2 September 2010.
49. **Roodt, A., Visser, H.G. & Cloete, N.** *Ethylene Tetramerisation: Diphosphinoamine Ligand Evaluation in Metal-Based Catalyst Precursor Models* (Oral). 39<sup>th</sup> International Conference on Coordination Chemistry, Adelaide, South Australia, 25-30 July 2010.
50. **Schutte, M., Visser, H.G. & Roodt, A.** *Interesting Observations between Kinetic and Crystallographic data of [Re(CO)<sub>3</sub>(L,L')(H<sub>2</sub>O)] Compounds* (Oral). 39<sup>th</sup> International Conference on Coordination Chemistry, Adelaide, South Australia, 25-30 July 2010.
51. **Schwoerer, H., Von Eschwege, K.G., Bosman, G., Krok, P. & Conradie, J.** *Ultrafast photochemistry of dithizonatophenylmercury(II): Isomerisation around a C=N double bond* (Poster). Ultrafast Phenomena Conference, Colorado, USA, 18-23 July 2010.
52. **Sebitlo, M.R., Erasmus, E. & Swarts, J.C.** *Synthesis and Characterisation of Rh(I) polysiloxane catalyst derivatives* (Poster). Annual Conference of the Catalysis Society of South Africa (CATSA 2010), Bloemfontein, South Africa, 7-10 November 2010.
53. **Steyn, M., Roodt, A. & Visser, H.G.** *A coordinative and behavioral study of mixed halido and N,O-donor multidentate ligand complexes of zirconium(IV)*

(Oral). International Light Metals Conference 2010, Misty Hills, Muldersdrift, South Africa, 27-29 October 2010.

54. **Steyn, M., Visser, H.G. & Roodt, A.** *Formation Kinetics of Mixed Halido and N-O-donor Multidentate Ligand Complexes of Zirconium* (Poster). 39<sup>th</sup> International Conference on Coordination Chemistry, Adelaide, South Australia, 25-30 July 2010.
55. **Stuurman, N.F., Hopmann, K.H., Muller, A. & Conradie, J.** *CO substitution in the catalytic precursor [Rh( $\square$ -diketonato) (CO)<sub>2</sub>]* (Poster). Annual Conference of the Catalysis Society of South Africa (CATSA2010), Bloemfontein, South Africa, 7-10 November 2010.
56. **Sunil, C.A., Marais, C. & Bezuidenhoudt, B.C.B.** *Probing the application of the Diels-Alder Reaction in the Synthesis of Resorcinol* (Poster). South African Chemical Institute - Frank Warren Conference, Pietermaritzburg, South Africa, 17-24 January 2010.
57. **Swarts, J.C.** *Catalysts in Rockets, Fine Chemicals and Biology* (Oral). Annual Conference of the Catalysis Society of South Africa (CATSA 2010), Bloemfontein, South Africa, 7-10 November 2010.
58. **Swarts, J.C.** *Syntheses and Characterisation of Water-Soluble Polymer-Bound Lipophylic Phthalocyanines and Porphyrins* (Oral). The 6<sup>th</sup> International Conference on Porphyrins and Phthalocyanines, ICPP6, Albuquerque, USA, 4-9 July 2010.
59. **Trzebiatowska-Gusowska, M., Erasmus, E. & Swarts, J.C.** *Preparation of 2D iron catalysts based on silicon wafers* (Poster). Annual Conference of the Catalysis Society of South Africa (CATSA 2010), Bloemfontein, South Africa, 7-10 November 2010.
60. **Van der Merwe, K., Visser, H.G. & Venter, J.A.** *Investigation of the catalytic behavior of cobalt- and chromium-diphosphonate complexes* (Poster). Annual Conference of the Catalysis Society of South Africa (CATSA2010), Bloemfontein, South Africa, 7-10 November 2010.
61. **Van der Westhuizen, J.H.** *Photochemistry Synthesis of Flavonoids and Related Compounds* (Lecture). 11<sup>th</sup> Frank Warren Conference, Pietermaritzburg, South Africa, 17-21 January 2010.
62. **Van der Westhuizen, J.H.** *Solid state NMR and MALDI-TOF investigation of Acacia mearnsii (Black Wattle) Tannin Extracts* (Lecture). Bruker User Meeting, Hermanus, South Africa, 27-29 January 2010.
63. **Van der Westhuizen, J.H., Bonnet, S.L. & Achilonu, M.C.** *A Novel Approach towards the Syntheses of Proanthocyanidins and Biflavonoids* (Lecture). 7<sup>th</sup> Tannin Conference, Berlin, Germany, 29 August-2 September 2010.

64. **Van Tonder, B., Chiweshe, T.T. & Bezuidenhoudt, B.C.B.** *Synthesis of Phenolic Dimethyl acetals* (Poster). South African Chemical Institute - Frank Warren Conference, Pietermaritzburg, South Africa, 17-24 January 2010.
65. **Van Tonder, J.H. & Bezuidenhoudt, B.C.B.** *Studies toward the Regioselective Formation of Flavonoid Chromium(O)tricarbonyl complexes* (Poster). South African Chemical Institute - Frank Warren Conference, Pietermaritzburg, South Africa, 17-24 January 2010.
66. **Venter, G.J.S., Steyl, G. & Roodt, A.** *Influence of Substituents on PhonyH and its Associated Rh(I) Carbonyl Complexes* (Oral). 26<sup>th</sup> European Crystallographic Meeting, Darmstadt, Germany, 29 August-2 September 2010.
67. **Venter, G.J.S., Steyl, G. & Roodt, A.** *Influencing 4-(phenylamino)pent-3-en-2-one and its associated Rh(I) dicarbonyl complexes through halide substitution* (Poster). Annual Conference of the Catalysis Society of South Africa (CATSA2010), Bloemfontein, South Africa, 7-10 November 2010.
68. **Venter, J.A. & Purcell, W.** *Modelling of the separation of steric and electronic effects of phosphine ligands in rhodium complexes of N-aryl-N-nitrosohydroxylamines* (Oral). 24<sup>th</sup> International Conference on Organometallic Chemistry, Taipei, Taiwan, 18-23 July 2010.
69. **Viljoen, J.A., Roodt, A. & Visser, H.G.** *Complex Formation of Hf(IV) with O,O'- and N,O-Bidendate Ligands* (Oral). International Light Metals Conference 2010, Misty Hills, Muldersdrift, South Africa, 27-29 October 2010.
70. **Viljoen, J.A., Visser, H.G. & Roodt, A.** *Multistep Bidentate Ligand Coordination at Hafnium(IV)* (Oral). 26<sup>th</sup> European Crystallographic Meeting, Darmstadt, Germany, 29 August-2 September 2010.
71. **Visser, H.G., Roodt, A., Brink, A., Kemp, G. & Schutte, M.** *When Crystallography meets Kinetics. A study of Rhenium(I) tricarbonyls* (Oral). 26<sup>th</sup> European Crystallographic Meeting, Darmstadt, Germany, 29 August-2 September 2010.
72. **Visser, H.G., Roodt, A., Schutte, M., Brink, A. & Kemp, G.** *Coordinated Ligand Effects in the Substitution Kinetics of Re(I) Tricarbonyls: Application in Radiopharmaceutical Design* (Oral). XV Brazilian Meeting on Inorganic Chemistry, Angra dos Reis, Brazil, 16-20 August 2010.
73. **Visser, H.G., Roodt, A., Schutte, M., Brink, A. & Kemp, G.** *When basic Chemistry meets Radiopharmaceutical Design: Coordinated Ligand Effects in the Substitution Kinetics of  $[Re(CO)_3(L,L')(H_2O)]^n$*  (Oral). 39<sup>th</sup> International Conference on Coordination Chemistry, Adelaide, South Australia, 25-30 July 2010.

74. **Von Eschwege, K.G., Schwoerer, H., Swarts, J.C. & Conradie, J.** *Photochromic dithizonatophenylmercury(II)* (Poster). XXIII<sup>rd</sup> IUPAC Photochemistry Symposium, Ferrara, Italy, 11-16 July 2010.
75. **Wilhelm-Mouton, A.** *Syntheses of Biflavonoids* (Lecture). 11<sup>th</sup> Frank Warren Conference, Pietermaritzburg, South Africa, 17-21 January 2010.
76. **Young, C., Bezuidenhoudt, B.C.B. & Roodt, A.** *Bipyridine type Ligand Bridged Complexes of Palladium(II) and Gold(III) as Carbon-Carbon Bond Formation Catalysts* (Poster). 39<sup>th</sup> International Conference on Coordination Chemistry, Adelaide, South Australia, 25-30 July 2010.
77. **Young, C.A., Roodt, A. & Bezuidenhoudt, B.C.B.** *Bipyridine based bridging ligands as building blocks for square planar Palladium(II) catalysts* (Poster). Annual Conference of the Catalysis Society of South Africa (CATSA2010), Bloemfontein, South Africa, 7-10 November 2010.