

KONFERENSIES / CONFERENCES - 2013 - RIMS

1. **Brink, A., Schutte-Smith, M., Visser, H.G., Roodt, A.** 2013. Expanding the Library of Bifunctional Chelator Systems: The Reactivity of N,O-Rhenium Tricarbonyl Complexes, p 37. (Oral). Rhemantec II International Symposium, Saas-Grund, Switzerland, 24 Feb-2 March 2013.
2. **Visser, H.G., Roodt, A., Schutte-Smith, M., Brink, A** The Role of Chemical Kinetics in Radiopharmaceutical Design: Focus in $[\text{Re}(\text{CO})_3]^+$, p 39. (Oral). Rhemantec II International Symposium, Saas-Grund, Switzerland, 24 Feb-2 March 2013.
3. **Schutte-Smith, M., Brink, A., Visser, H.G., Roodt, A.** 2013. Aqua substitution kinetics in a *fac*-Re(I) tricarbonyl tropolonato complex, , p. 5. (Oral). Second EuCheMS Inorganic Chemistry Conference, Jerusalem, Israel, 7–11 July 2013.
4. **Engelbrecht, I., Roodt, .A and Visser, H.G.** 2013. Crystallographic Investigation of Platinum(II) Phosphine Based Complexes for use in Cancer Treatment. International Symposium on the Mn-triad. (Oral). (RheManTec-II) Symposium, Saas-Grund, Switzerland, 24 Feb–2 March.
5. **Tsai, C. and Langner, E.H.G.** 2013. Synthesis of nano-sized ZIF-8 with applications in heterogeneous catalysis. (Poster). INORG 2013 Conference, Durban, South Africa, 30 June-4 July 2013.
6. **Peens, F.H. and Langner, E.H.G.** Amino-MIL-53(Al) and Its Post-Synthetic Modification with Ferrocenecarboxylic Acid. (Poster). INORG 2013 Conference, 30 June 2013-4 July 2013, Durban.
7. **Ferreira, H., Conradie, M.M. and Conradie, J.,** An Electrochemical and Computational Study of Thenoyl-containing Rh(I) β -diketonato Complexes. (Poster). INORG 2013, Durban, South Africa, 30 June-4th July 2013.
8. **Freitag, R. and Conradie, J.** 2013. Crystal and electronic structure of the redox stable Mn(dibenzoylmethanato)₃ complex. (Poster). INORG 2013 Conference, Durban, South Africa, 30 June 2013-4 July 2013.
9. **Govender, M., Swarts P.J. , Claus R., Fourie E. and Swarts J.C.** 2013. Synthesis and electrochemical studies of ferrocene-containing polyphosphazenes. (Poster). INORG2013. Durban, South Africa. 30 Jun-4 Jul 2013.
10. **Fourie, E. and Swarts, J.C.** 2013. Modified porphyrins containing β -diketone substituents. (Poster). 16th Biennial SACI Inorganic Chemistry Conference, Durban, South Africa, 30 June-4 July 2013.

11. **Oosthuizen, D.N., Swarts, P.J., Buitendach, B.E., Fourie, E., Claus, R. and Swarts, J.C.** 2013. Synthesis and electrochemical studies of phthalocyanine- and ferrocene- containing polysiloxanes. (Poster). 16th Biennial SACI Inorganic Chemistry Conference, Durban, South Africa, 30 June-4 July 2013.
12. **Liu, R. and Conradie, J.** 2013. Synthesis, Crystal structure and Cyclic Voltammetry (CV) of tris(β -diketonato)chromium(III) and tris(β -diketonato)cobalt(III) complexes. (Poster). INORG2013 Conference, Durban, South Africa, 30 June-4 July 2013.
13. **Langner, E.H.G.** 2013. Metal Organic Frameworks in Heterogeneous Catalysis. (Oral). 16th Biennial SACI Inorganic Chemistry Conference, Durban, South Africa, 30 June-4 July 2013.
14. **Sebitlo, M.R., Erasmus, E. and Swarts J.C,** 2013. Synthesis of rhodium complexes immobilized on different solid supports for catalytic use. (Poster). INORG2013 Conference, Southern Sun Elangeni Hotel, Durban, South Africa, 30 June-4 July 2013.
15. **Nkosi, G., Purcell, W. and Nel, J.** 2013. Analysis of four high-temperature oxidized zirconium alloys by glow discharge optical emission spectroscopy. (Poster). Precious Metals 2013 Conference, Cape Town, 14-16 October 2013.
16. **Nete, M., Purcell, W and Nel, J.T.** 2013. Evaluation of ammonium bifluoride dissolution on different tantalum and niobium mineral samples. (Poster). Precious Metals 2013 Conference, Cape Town, 14-16 October 2013.
17. **Steyn, M., Visser, H.G. and Roodt, A.** 2013. Synthesis and crystal structure of tetrakis(1,3-diphenyl-1,3-propanedionato) zirconium(iv). (Poster). Precious Metals 2013 Conference, Cape Town, 14-16 October 2013.
18. **Lötter, S.,_Purcell, W. And Nel, J.T.** 2013. GD-OES analysis of zirconium carbide. (Poster) Precious Metals 2013 Conference, Cape Town, 14-16 October 2013.
19. **Viljoen, J.A., Visser, H.G. and Roodt, A.** 2013. The chelation behaviour of hafnium(IV) with 8-hydroxyquinoline. (Poster). Precious Metals 2013 Conference, Cape Town, 14-16 October 2013.
20. **Chiweshe, T.T., Purcell, W. And Venter, J.A.** 2013. Determination of rhodium and the crystal waters in $\text{RhCl}_3 \cdot x\text{H}_2\text{O}$. (Poster) Precious Metals 2013 Conference, Cape Town, 14-16 October 2013.
21. **Koen, R., Roodt, A. And Visser, H.G.** 2013. The coordination of acetylacetone to tantalum(V) chloride: a kinetic study. (Poster). Precious Metals 2013 Conference, Cape Town, 14-16 October 2013.
22. **Herbst, L., Visser, H.G. and Roodt, A.** 2013. Formation kinetics of (acetylacetonato- $\kappa^2\text{O},\text{O}'$)chloridotrimethoxidoniobium(V). (Poster). Precious Metals 2013 Conference, Cape Town, 14-16 October 2013.
23. **Roodt, A., Venter, G.J.S. and Twigge, L.** 2013. Magnetization Transfer Study on the Exchange Reaction of $[\text{Rh}(\text{N},\text{O-Bid})(\text{CO})(\text{PPh}_3)]$ Complexes with PPh_3 . (Poster). Small Molecule NMR Conference, Santiago de Compostela, Spain, 22-25 September 2013.

24. **Swarts, J.C.** 2013. Polysiloxanes as soluble supports for drug delivery and catalysis of rhodium and ferrocene systems. (Invited lecture). INORG 2013, Durban, South Africa, 30 June-4 July 2013.
25. **Magqi, N., Erasmus, E., Swarts, J.C.** 2013. Preparation of model platinum catalysts supported on modified silicon wafers and applications under solvent-free aerobic oxidations. (Poster). INORG 2013, Durban, South Africa, 30 June-4 July 2013.
26. **Lewtak, J.P., Swarts, J.C.** 2013. Simplified synthesis and electrochemical studies of Ferrocenyl-alkanethiols. (Poster). INORG 2013, Durban, South Africa, 30 June-4 July 2013.
27. **Joubert, C.C., Swarts, J.C.** 2013. Immobilization of copper and iron on silicon wafers as model catalysts. INORG 2013, Durban, South Africa, 30 June-4 July 2013.
28. **Buitendach, B.E., Swarts, J.C.** 2013. Synthesis, electrochemistry and kinetic studies of metallocene-containing betadiketones possessing an $(CH_2)_nOH$ side chain. INORG 2013, Durban, South Africa, 30 June-4 July 2013.
29. **Venter, J.A.** 2013. Towards a ligand knowledge base: An attempt to predict ligand effects. (Oral), RheManTec 2 International Symposium, Saas Grund, Switzerland, 24 February-1 March 2013.
30. **Van der Merwe, K.A., Roodt, A., Steyl, G., Visser, H.G., Venter, J.A.** 2013. Structural investigation of bidentate phosphonate ligands coordinated to middle/late transition metal centres. (Oral), RheManTec 2 International Symposium, Saas Grund, Switzerland, 24 February-1 March 2013.
31. **Venter, J.A., Purcell, W., Warsink, S.** 2013. Adjacent phosphines used to probe bidentate cupferrate ligands. (Poster), 20th EuCheMS International Conference on Organometallic Chemistry, St. Andrews, Scotland, 30 June-4 July 2013.
32. **Purcell, W., Venter, J.A., Conradie, J., Chiweshe, T.T.** 2013. Oxidative addition of CH_3I to $[Rh(cupf)(CO)(DPP)]$: Kinetics and DFT calculations. (Poster), 20th EuCheMS International Conference on Organometallic Chemistry, St. Andrews, Scotland, 30 June-4 July 2013.
33. **Gohain, M., du Plessis, M. and Bezuidenhoudt, BCB.** 2013. $Al(OTf)_3$: A Versatile Catalyst for Chemical Transformations. (Invited Oral presentation). 2nd Binational South African - German Organic Chemistry Conference (BOCC-2013), Tutzing, Germany, 29 September-4 October 2013.
34. **van Tonder, J.H. and Bezuidenhoudt, BCB.** 2013. Synthesis of alkyl and alkoxy substituted ruthenium phthalocyanines as epoxidation catalysts. (Poster). 2nd Binational South African - German Organic Chemistry Conference (BOCC-2013), Tutzing, Germany, 29 September – 4 October 2013.
35. **du Plessis, M. and Bezuidenhoudt, BCB.** 2013. Parameters influencing regioselectivity in the palladium catalyzed hydroesterification of aromatically substituted alkenes. (Poster). 2nd Binational South African - German Organic Chemistry Conference (BOCC-2013), Tutzing, Germany, 29 September-4 October 2013.

36. **Pieterse, T. and Bezuidenhout, BCB.** 2013. Ring closing metathesis as new methodology for the synthesis of monomeric flavonoids. (Poster). 2nd Binational South African - German Organic Chemistry Conference (BOCC-2013), Tutzing, Germany, 29 September–4 October 2013.
37. **Conradie, J.** 2013. Frontier orbital energies and the reactivity of square planar β -diketonato-containing rhodium(I) complexes: Virtual lab makes chemistry 'greener'. (Invited Keynote lecture). 41st National Convention of the South African Chemical Institute, River Park Convention Centre, East London 1–6 December 2013.
38. **Conradie, J.** 2013. Density Functional Theory calculations with High Performance Computing predicts chemical reactivity. (Oral) Centre for High Performance Computing (CHPC) National Meeting, Cape Town International Convention Centre, Cape Town, South Africa, 2–6 December 2013.
39. **Freitag, R., Liu, R., Conradie, M.M. and Conradie, J.** 2013. Frontier orbital energies and the redox potentials of $M(\beta\text{-Diketonato})_3$ complexes. (Poster). 41st National Convention of the South African Chemical Institute, River Park Convention Centre, East London 1–6 December 2013.
40. **Freitag, R. and Conradie, J.** 2013. Ondersoek van die Jahn-Teller distorsie wat waargeneem word in die $Mn(\text{dibensoïelmetanato})_3$ kompleks deur middel van berekeningschemie en X-straalkristallografie. (Oral in Afr). Natural Science Symposium for Postgraduate Students, University of Pretoria, Pretoria, RSA 7–8 November 2013.
41. **Ferreira, H., Conradie, J. and Conradie, M.M.** 2013. An Electrochemical and Computational Study of Thenoyl-containing Rh(I) β -diketonato Complexes. (Oral in Afr). Natural Science Symposium for Postgraduate Students, University of Pretoria, Pretoria, RSA 7–8 November 2013.
42. **Berg, S., Conradie, J. and Ghosh, A.** 2013. DFT calculations as a teaching aid in introductory inorganic chemistry: Main group oxo transfer mechanisms as illustrative examples. (Oral) 45th American Chemical Society National Meeting & Exposition New Orleans, LA 7-11 April 2013.
43. **Langner, E.H.G. and Tsai, C.** 2013. The Effect of Synthesis Temperature on the Size of ZIF-8 Nanoparticles. (Poster). The Third International Conference on Multifunctional, Hybrid and Nanomaterials (Hybrid Materials 2013), Sorrento, Italy, 3 - 7 March 2013.
44. **Conradie, M. and Conradie, J.** Theoretical and Experimental Study of $Rh(\text{acac})(CO)(PPh_3)$ - what happens during and after CH_3I addition? INORG2013, Southern Sun Elangeni Hotel, Durban, RSA, 30 June – 4 July 2013.
45. **Phungula K., van Vuuren S., Bonnet S.L, Marston A.** *Combretum apiculatum* (Combretaceae): Antimicrobial activity of extracts from the leaves and seeds. (Poster). 61st international Congress and Annual meeting of the Society of Medicinal plants and Natural Products research (GA), Munster, Germany. 1 – 5 September 2013.
46. **Ngarivhume, T. van der Westhuizen, J.H., Marston, A. and van Zyl, R.** Bioactivities of some herbal medicines from Zimbabwe. (Poster) 61st international Congress and Annual meeting of the Society of Medicinal plants and Natural Products research (GA) Munster, Germany 1 – 5 September 2013.

47. **Phungula K., Khamane M. and Marston A.** Ethnobotanical survey of medicinal plants used by traditional healers for the management of tuberculosis in the Free State province, South Africa. (Oral) MUTHI workshop, Makerere University, Uganda 1 - 6 February 2013, Makerere University, Uganda.
48. **Phungula K., Khamane M., Bonnet S.L.** Protocol: Retrospective treatment outcome of medicinal plants used for the treatment of headaches using Traditional healers and their families as patients. (Oral) MUTHI workshop, MRC Durban, South Africa, 2 – 6 October 2013.
49. **Nel, E.** Protocol: Survey of medicinal plants used for the treatment of diarrhoea in children around Bloemfontein. (oral) MUTHI workshop, MRC Durban, South Africa. 2 – 6 October 2013.
50. **Wilhelm-Mouton, A.** Protocol: A randomized double-blind, placebo-controlled trial of plant X against cardiovascular risks in abdominally obese male patients. (oral), MUTHI workshop 2 – 6 October 2013, MRC Durban, South Africa
51. **Bonnet, S.L.** Protocol: Does Diminish cause weight loss in adult obese women in urban areas?, MUTHI workshop, MRC Durban, South Africa 2–6 October 2013.
52. **Reid, D.G., Bonnet, S.L., Kemp, G. and van der Westhuizen, J.H.**, Solid state ¹³C NMR as a tool for in situ analysis of proanthocyanidin tannins, in heartwood and bark of quebracho and acacia, and related species. (oral) Bruker Conference, Gariepdam, South Africa, 23–25 January 2013.
53. **Van der Westhuizen, J.H, Davis, H.J, Taylor G.J.** Composition and methods for Treating Wounds, ZA Provisional **Patent** Applications 2013/08959, November 28 2013.
54. **Achilonu, M.C., Bonnet, S.L., Van der Westhuizen, J.H.**. Method for the Preparation of C-4 Coupled Flavonoids, Proanthocyanidins and Analogues thereof. US **patent**, US 8,501,970 B2, Aug. 6, 2013.
55. **Brink, A., Schutte-Smith, M., Visser, H.G., Roodt, A.** Coordinated Ligand Manipulation of Rhenium Tricarbonyl Reactivity. (Oral). 28th European Crystallographic Meeting, ECM 28, Warwick, United Kingdom. 25-29 August 2013.
56. **Schutte-Smith, M., Brink, A., Visser, H.G., Roodt, A.** Aqua substitution kinetics in a *fac*-Re(I) tricarbonyl tropolonato complex. (Oral), Second EuCheMS Inorganic Chemistry Conference, Jerusalem, Israel 7–11 July 2013.
57. **Visser, H.G., Roodt, A., Engelbrecht, I., Cloete, N., Overett, M.J. and Gabrielli, F.** X-ray Crystallography meets Catalysis: Ethylene Polymerisation with PNP ligands. (Poster). 20th EuCHEMS Conference on Organometallic Chemistry, St Andrews, Scotland 30 June-4 July 2013.
58. **A. Roodt, A., Visser, H.G., Brink, A., Schutte, M. & Hill, T.** Kinetics and other systematic probing of electron density at transition metal centres for application in chemical processes. (Invited Keynote Lecture). The twenty-second Croatian-Slovenian crystallographic meeting - CSCM22. Biograd, Croatia, June 12 - 16, 2013.

59. **Roodt, A.** (Small) Molecular Materials for Radiopharmaceutical Applications (Invited Lecture). 7th International Conference of the Africa Materials Research Society, Addis Ababa, Ethiopia, 8-13 December 2013.
60. **Roodt, A., Brink, A., Koen, R. and Pretorius, C.** Strategies for the Refinement of Small Molecular Materials in X-Ray Crystallography. (Invited oral presentations) Satellite Workshop on Crystallography. 7th International Conference of the Africa Materials Research Society, Addis Ababa, Ethiopia, 8-13 December 2013.
61. **Roodt, A.** 2012. Systematic probing of electron density at transition metal centres for application in chemical processes: role of kinetics? (Lecture KS5). The 16th South African Chemical Institute (SACI) inorganic chemistry conference (INORG2013), Durban, South Africa, 30 June - 4 July 2013.
62. **Steyn, M., Roodt, A. and Visser, H.G.** Comparative Evaluation of Oxine-type Ligand Chelation with Zirconium(IV). (Poster P47). The 16th South African Chemical Institute (SACI) inorganic chemistry conference (INORG2013), Durban, South Africa, 30 June - 4 July 2013.
63. **Viljoen, J.A., Visser, H.G. and Roodt, A.** A Coordinative Investigation of Novel Hafnium(IV) Complexes Containing Oxinato-type Ligand Systems. (Poster P94). The 16th South African Chemical Institute (SACI) inorganic chemistry conference (INORG2013), Durban, South Africa, 30 June - 4 July 2013.
64. **Herbst, L., Visser, H.G. and Roodt, A.** Crystallographic study of various O,O'-bidentate complexes of niobium(V) and tantalum(V). (Poster P35). The 16th South African Chemical Institute (SACI) inorganic chemistry conference (INORG2013), Durban, South Africa, 30 June - 4 July 2013.
65. **Koen, R., Roodt, A. and Visser, H.G.** An in-depth study into the separation of Tantalum(V) and Niobium(V) complexes utilizing various mono- and bidentate ligands. (Poster P60). The 16th South African Chemical Institute (SACI) inorganic chemistry conference (INORG2013), Durban, South Africa, 30 June - 4 July 2013.
66. **Van der Berg, P.C.W., Visser, H.G. and Roodt, A.** Development and Assessment of Metal Complexes as Model Radiopharmaceuticals for Cancer Treatment. (Poster P95). The 16th South African Chemical Institute (SACI) inorganic chemistry conference (INORG2013), Durban, South Africa, 30 June - 4 July 2013.
67. **Van der Merwe, K.A., Roodt, A. and Steyl, G.** Copper Bis-O,O'-Bidentate Complexes used in Oxidation Catalysis of Phenolic Compounds. (Poster P82). The 16th South African Chemical Institute (SACI) inorganic chemistry conference (INORG2013), Durban, South Africa, 30 June - 4 July 2013.
68. **Loganathan, N., Chandrasekhar, V. and Roodt, A.** Butterfly Cored Deca- and Hexadecanuclear Copper(II) Phosphonate Cages Containing 3-Substituent Pyrazole Ligands. (Poster P19). The 16th South African Chemical Institute (SACI) inorganic chemistry conference (INORG2013), Durban, South Africa, 30 June - 4 July 2013.

69. **Loganathan, N., Chandrasekhar, V. and Roodt, A.** Multinuclear Copper(II) Phosphonate Cages Containing Substituted Pyrazole Ligands. (Lecture O10). The 16th South African Chemical Institute (SACI) inorganic chemistry conference (INORG2013), Durban, South Africa, 30 June - 4 July 2013.
70. **Bungu, P.** The Solid and Solution States Mysteries in Functionalized Tropolonato Complexes Rhodium(I). (Poster) European Crystallographic Meeting (ECM 28) in Warwick, UK. 24-29 August 2013.
71. **Volmink, A., Visser, H.G., Roodt, A.** 2013. Re(I)-acac based complexes as models for radiopharmaceuticals, p 9. (Oral). Rhemantec II International Symposium, Saas-Grund, Switzerland, 24 Feb – 2 March 2013.
72. **Twala, T.N., Visser, H.G., Roodt, A.** 2013. The Synthesis and Characterization of *fac*-Tricarbonyl Aqua Manganese(I) Complexes, p 10. (Oral). Rhemantec II International Symposium, Saas-Grund, Switzerland, 24 Feb – 2 March 2013.
73. **Viljoen, J.A., Visser, H.G., Roodt, A.** 2013. An in-depth coordination study of Hafnium(IV) complexes containing well known tumor-inhibiting ligand systems, p 13. (Oral). Rhemantec II International Symposium, Saas-Grund, Switzerland, 24 Feb – 2 March 2013.
74. **Van der Berg, P.C.W., Visser, H.G., Roodt, A.** 2013. Development and Assessment of Gallium(III) and Gold(III) complexes as Model Radiopharmaceuticals for Cancer Treatment, p 14. (Oral). Rhemantec II International Symposium, Saas-Grund, Switzerland, 24 Feb – 2 March 2013.
75. **Pretorius, C., Brink, A., Venter, J.A., Roodt, A.** 2013. A Solution and Solid Study of Vanadium Complexes as Models to Catalytical and Future Pharmaceutical Behaviour, p 19. (Oral). Rhemantec II International Symposium, Saas-Grund, Switzerland, 24 Feb – 2 March 2013.
76. **Van der Merwe, K.A., Venter, J.A., Visser, H.G., Steyl, G., Roodt, A.** 2013. Structural Investigation of Bidentate Phosphonate Ligands Coordinated to Middle/Late Transition Metal Centres, p 32. (Oral). Rhemantec II International Symposium, Saas-Grund, Switzerland, 24 Feb – 2 March 2013.
77. **Suthiram, J., Visser, H.G., Steyl, G., Kemp, G., Zeevart, J.R., Roodt, A.** 2013. The synthesis & bio-evaluation of Tc and Re complexes labelled with biologically active moieties, p 33. (Oral). Rhemantec II International Symposium, Saas-Grund, Switzerland, 24 Feb – 2 March 2013.
78. **Roodt, A.** 2013. Applied Systems Analysis Approach to Predicting Radiopharmaceutical Behaviour, p 35. (Oral). Rhemantec II International Symposium, Saas-Grund, Switzerland, 24 Feb – 2 March 2013.
79. **Venter, J.** 2013. Towards a Ligand Knowledge Base: an Attempt to Predict Ligand Effects, p 51. (Oral). Rhemantec II International Symposium, Saas-Grund, Switzerland, 24 Feb – 2 March 2013.

80. **Pretorius, C., Venter, J.A. and Roodt A.** Crystallographic and Kinetic Study of O,O' Bidentate Vanadium Complexes. (oral YC1-01) European Young Crystallographers Satellite Meeting a part of ECM 28. 25–29 Aug 2013, University of Warwick, United Kingdom.
81. **Loganathan, N., Chandrasekhar, V. and Roodt, A.** Multi Nuclear Copper(II) Phosphonate Cages: (oral YC2-05) An Ancillary Ligand Approach. European Young Crystallographers Satellite Meeting a part of ECM 28. 25–29 Aug 2013, University of Warwick, United Kingdom.
82. **Brink, A., Visser, H.G. and Roodt, A.** Coordinated ligand manipulation of rhenium tricarbonyl reactivity. (oral YC2-05) European Crystallographic Meeting 28 (ECM 28), 25–29 Aug 2013, University of Warwick, United Kingdom.
83. **Loganathan, N., Chandrasekhar, V. and Roodt, A.** Butterfly cored deca- and hexadecacopper(II) phosphonates. (poster) European Crystallographic Meeting 28 (ECM 28), 25–29 Aug 2013, University of Warwick, United Kingdom.
84. **Pretorius, C., Venter, J.A. and Roodt, A.** A crystallographic and kinetic study of O,O'-bidentate vanadium complexes. (poster) European Crystallographic Meeting 28 (ECM 28), 25–29 Aug 2013, University of Warwick, United Kingdom.
85. **Koen, R., Visser, H.G. and Roodt, A.** An in-depth crystallographic study of tantalum(V) and niobium(V) complexes utilizing various mono- and bidentate ligands in European Crystallographic Meeting 28 (ECM 28), 25–29 Aug 2013, Warwick, United Kingdom.