



NATURAL AND
AGRICULTURAL SCIENCES
NATUUR- EN
LANDBOUWETENSKAPPE

UFS·UV

KONFERENSIES /CONFERENCES - 2015 - RIMS

1. **Landman, M., Buitendach, B.E., Liu, R., Pretorius, R., Fraser, R., Freitag, R., Conradie, M.M., van Rooyen, P.H. and Conradie, J.** 2015. Electrochemical Behaviour of Cr and W Fischer carbenes: a comparative study. (poster) 3rd International Symposium on Electrochemistry, University of the Western Cape, Bellville, South Africa, 26-28 May 2015.**ufs-022888**
2. **Visser, H.G., Roodt, A., Schutte-Smith, M. Brink, A., Twala, T.N., Kemp, G. and Zobi, F.** 2015 Reactivity and structure relations in Mn(I), Re(I) and Tc(I)-tricarbonyl complexes – impact on drug design (Poster). 21st International Symposium on Radiopharmaceutical Sciences, ISRS 2015,– Columbia, Missouri, 26-31 May 2015.**ufs-022891**
3. **von Eschwege, K. G.** 2015. Synthetic fuel from CO₂ – The Ultimate Answer? (invited lecture). Carbon Capture Workshop, University of Western Cape, South Africa, 2-4 March 2015.**ufs-022923**
4. **Venter, G.J.S., Steyl, G. and Roodt, A.** 2015. Influencing Rh(I) dicarbonyl and phosphine complexes with substituted enaminoketones. (Poster). 29th European Crystallographic Meeting, Rovinj, Croatia, 23-28 August 2015.**ufs-022925**
5. **Schutte-Smith, M., Visser, H.G., Roodt, A.** 2015. A mechanistic study of rhenium (I) complexes: aqua vs methanol substitution (Poster). Indaba 8, Skukuza, Kruger National Park, South Africa, 16 – 21 August 2015.**ufs-022927**
6. **Conradie, J.** 2015. Electronic influence of different β -diketonato ligands on the electrochemical behaviour of tris(β -diketonato)M(III) complexes, M = Cr, Mn and Fe. (Invited Keynote Lecture). The 3rd International Symposium on Electrochemistry, University of the Western Cape, Bellville, South Africa, 26–28 May 2015.**ufs-022928**
7. **Conradie, J.** 2015. A Frontier orbital energy approach to redox potentials. (Lecture). IC-MSQUARE, The 4th International Conference on Mathematical Modeling in Physical Sciences, Mykonos, Greece, 5-8 June 2015.**ufs-022929**
8. **Landman, M., Conradie, J. and van Rooyen, P.H.** 2015. Computational chemistry insights on the REDOX Behaviour of Cr and W Fisher carbenes. (Poster). IC-MSQUARE, The 4th International Conference on Mathematical Modeling in Physical Sciences, Mykonos, Greece, 5-8 June 2015.**ufs-022930**
9. **von Eschwege, K.G.; Conradie, J. and Ferreira, H.** 2015. “Theoretical Design in Dye-Sensitized Solar Cells”. 3rd International Congress on Energy Efficiency and Energy Related Materials (ENEFM 2015), 19-23 Oct. 2015, Oludeniz, Turkey.**ufs-022932**

10. **Malefo, G., Purcell, W., Nete, M. and Nel, J.T.** 2015. The quantification of hafnium in hafnium-containing compounds. (Poster) Nuclear Materials Development Network Conference 2015, Port Elizabeth, 28-30 October 2015. (peer-reviewed)**ufs-022933**
11. **Mokgawa, J.L., Tutu, H., Nel, J.T. and Nete, M.** 2015. Method development for determination of trace element impurities in zirconium sponge by ICP-OES and ICP-MS. (Poster) Nuclear Materials Development Network Conference 2015, Port Elizabeth, 28-30 October 2015. (peer-reviewed)**ufs-022937**
12. **Nete, M., Purcell, W. and Nel, J.T.** 2015. Element distribution between particle size fractions of a tantalite sample. (Poster) Nuclear Materials Development Network Conference 2015, Port Elizabeth, 28-30 October 2015. (peer-reviewed)**ufs-022939**
13. **Venter, J.A.** 2015. The road less travelled? How solvents are involved during methyl migration in rhodium(III) cupferrate complexes. (poster) XXI EuCheMS International Conference on Organometallic Chemistry, Bratislava, Slovakia, 5-9 July 2015.**ufs-022941**
14. **Purcell, W.** 2015. Oxidative addition between [Ir(cod)(sacac)] and CH₃I: A mechanistic study. (poster) XXI EuCheMS International Conference on Organometallic Chemistry, Bratislava, Slovakia, 5-9 July 2015.**ufs-022944**
15. **von Eschwege, K.G.; Conradie, J. and Ferreira, H.** 2015. Redox and Spectral Tuning of Dyes in Solar Cells – a DFT Approach. (Oral) 42nd National Convention of the South African Chemical Institute, 29/11–4 Dec 2015, Durban, South Africa.**ufs-022946**
16. **Wilhelm, A., van der Westhuizen, J.H., Bonnet, S.L., Phungula, K.V., van Rensburg, E., Zietsman, P.C., and Hering, S.** An investigation into consumed South African plant species as potential hERG channel blockers. (Poster) 63rd GA Conference, Budapest, Hungary, 23-27 August 2015.**ufs-022951**
17. **van Rensburg, E., Zietsman, P.C., Wilhelm, A., van der Westhuizen, J.H., Bonnet, S.L.** hERG channel inhibitors in South African medicinal plants with the focus on *Boophane disticha* (Amaryllidaceae) bulbs, IPUF- SEB 2015, Clanwilliam, South Africa, 28 June – 2 July 2015.**ufs-022977**
18. **Govender, M., Swarts, J.C. and Fourie, E.** 2015. Sintese, karakterisering en elektrochemie van osmoseenbevattende alkohole. (poster) *Studentesimposium in die natuurwetenskappe*, Bloemfontein, 29-30 Oktober 2015.**ufs-022978**
19. **Drost, R.M., Milani, B., de Bruin, B. and Elsevier, C.J.** 2015. Catalyst Species Identification: Find the true catalyst (Poster). The 17th SACI Inorganic Chemistry Conference, Grahamstown, South Africa, 28 June – 2 July, 2015.**ufs-022988**
20. **Conradie, J.** 2015. Mono-, di- and tetranuclear bis(β -diketonato)-dichlorotitanium(IV) complexes: Isomer distribution and hydrolysis. (Keynote Lecture). Centre for High Performance Computing (CHPC) National Meeting, CSIR ICC, Pretoria, South Africa, 30 November – 4 December 2015.**ufs-022991**

21. **Ferreira, H., Conradie, J. and Conradie, M.M.** 2015. 'n Sintese, katalitiese, elektrochemiese en berekeningschemie studie van $\text{Rh}(\text{CH}_3\text{CNPhCHCOCH}_3\text{)}\text{-(CO)(PPh}_3\text{)}$. Translated title: A Synthetic, catalytic, electrochemical and computational study of $\text{Rh}(\text{CH}_3\text{CNPhCHCOCH}_3\text{)}\text{-(CO)(PPh}_3\text{)}$. (Oral Presentation in Afrikaans). The Natural Sciences Symposium for Postgraduate Students, University of the Free State, Bloemfontein, South Africa, 29–30 October 2015.[ufs-022993](#)
22. **Malan, F.P., Singleton, E., Landman, M., Van Rooyen, P.H. and Conradie, J.** 2015. Die sintese, karakterisering, elektrochemiese eienskappe en katalitiese toepassing van nuwe $[\text{CpNiBr(NHC)}]$ komplekse. Translated title: The synthesis, characterisation, electrochemical properties and catalytic application of novel $[\text{CpNiBr(NHC)}]$ complexes. (Poster Presentation in Afrikaans). The Natural Sciences Symposium for Postgraduate Students, University of the Free State, Bloemfontein, South Africa, 29–30 October 2015.[ufs-022996](#)
23. **Von Eschwege, K.G., Conradie, J. and Ferreira, H.** 2015. Theoretical Design in Dye – Sensitized Solar Cells. (Lecture). 3rd International Congress on Energy Efficiency and Energy Related Materials (ENEFM 2015), Oludeniz, Mugla, Turkey, 19–23 October 2015.[ufs-022997](#)
24. **Jansen van Rensburg, A., Landman, M., Van Rooyen, P.H., Conradie, J.** 2015. Pnictogen-Substituted Fischer Ethoxycarbene Complexes: Synthesis, Structure, Electrochemistry and Catalysis. (Poster Presentation). Catalysis Society of South Africa (CATSA) Conference 2015, Arabella Hotel & Spa, Kleinmond, Cape Town, South Africa, 15–18 November 2015.[ufs-022998](#)
25. **Esterhuysen, M., Visser, H. G., Brink, A., Zbačnik, M. and Roodt, A.** 2015. Different compounds obtained from the same starting material: serendipity, misfortune or different reaction conditions? (Poster). 29th European Crystallographic Meeting, Rovinj, Croatia, 23-28 August 2015.[ufs-023000](#)
26. **Conradie, M.** 2015. DFT Mechanistic Investigation of a Large Molecular Catalytic System. (Lecture). Centre for High Performance Computing (CHPC) National Meeting and Conference, CSIR ICC, Pretoria, South Africa, 30 November – 4 December 2015.[ufs-023001](#)
27. **Cambridge, A.N., Chambrier, I., Cook, M.J., Langner, E.H.G., Rahman, M., Swarts, J.C.** 2015. Liquid crystallinity of some metalated 1,4,8,11,15,18,22,25-octaalkyl tetrabenzo $[b,g,l,q][5,10,15]$ triazaporphyrin (TBTAP) derivatives. (Talk). Applications in Thermal Analysis conference by ThermSA, Stellenbosch, South Africa, 17 - 18 August 2015.[ufs-023002](#)
28. **Langner, E.H.G., Tsai, C-W, Peens, F.H.** 2015. Post-synthetic modification of selected Metal Organic Frameworks. (Talk). South Africa – UK Workshop: Materials-Based Hydrogen Storage, Pretoria, South Africa 1 - 4 September 2015.[ufs-023003](#)
29. **Peens, F.H., Langner, E.H.G.** 2015. Sintese van Amino-MIL-53(Al) met Adsorpsie van Ferroseen en Ferroseenkarboksiesuur. (Oral). Studentesimposium in die Natuurwetenskappe, Bloemfontein, South Africa, 29 - 30 October 2015.[ufs-023004](#)

30. **Crause, A., Langner, E.H.G.** 2015. Sintese van Metaal Organiese Netwerk, Co-MOF-74. (Poster). Studentesimposium in die Natuurwetenskappe 2015, Bloemfontein, South Africa, 29 – 30 October 2015.**ufs-023006**
31. **Visser, H.G., Brink, A., Alexander, O., Swart, H.C., Duvenhage, M-M. and Ntwaeaborwa, M.** 2015. Structure and Spectroscopic Properties of $M(Qn)_3$ complexes (M = Aluminium, Gallium, Indium, Europium; Qn = 8-hydroxyquinoline and derivatives thereof) Mabula 2015, 6 th Conference on Photonic Materials, Mabula Game Reserve, South Africa, 4 to 8 of May 2015.**ufs-022898 (ingelees Fisika)**
32. **Roodt, A., Brink, A., Schutte-Smith, M. and Visser, H.G.** 2015. Structure and function of coordination compounds for radiopharmaceutical application. (Oral) 29th European Crystallographic Meeting, 23-28 August 2015, Rovinj, Croatia. (Acta Cryst. (2015). A71, s113).**ufs-023017**
33. **Pretorius C., Brink, A. and Roodt, A.** 2015. Novel 1-D rhodium polymeric chain systems via rhodium-rhodium interactions. (Oral). 29th European Crystallographic Meeting, 23-28 August 2015, Rovinj, Croatia (Acta Cryst. (2015). A71, s117).**ufs-023018**
34. **Brink, A.** 2015. Through the looking glass: anomalies and packing. (Poster). 29th European Crystallographic Meeting, 23-28 August 2015, Rovinj, Croatia (Acta Cryst. (2015). A71, s436).**ufs-023019**
35. **Conradie, J.** 2015. A Frontier orbital energy approach to redox potentials. *Journal of Physics: Conference Series* **633** 4th International Conference on Mathematical Modeling in Physical Sciences, 5-8 June 2015, Mykonos, Greece. (peer-reviewed).**ufs-023020**
36. **Landman, M., Conradie, J. and van Rooyen, P.H.** 2015. Computational chemistry insights in the REDOX behaviour of Cr and W Fischer carbene complexes. *Journal of Physics: Conference Series* **633**: [12068-12073](#). 4th International Conference on Mathematical Modeling in Physical Sciences, 5-8 June 2015, Mykonos, Greece. (peer-reviewed).**ufs-023023**
37. **Pretorius, C., Brink, A. and Roodt, A.** 2015. *Assembly of one-dimensional metal chains via metallophilic interactions using Rh(I) metal centres* (poster), Indaba8, Skukuza, 16-21 August 2015.**ufs-023584**
38. **Gerber, S.J. and Erasmus, E.** 2015. Edelmetaal Kataliste op metal oksied ondersteunings material deur 'n gesamentlike presipitasie metode vir lae temperatuur selektiewe hidrogenering (poster) Studentesimposium in die Natuurwetenskappe, Bloemfontein, South Africa, 29 - 30 October 2015.**ufs-023573**
39. **Gerber, S.J. and Erasmus, E.** 2015. Noble metal catalysts on metal oxide support by Co-precipitation for low temperature selective hydrogenation (poster) Catalysis Society of South Africa (CATSA) Conference 2015, Arabella Hotel & Spa, Kleinmond, Cape Town, South Africa, 15–18 November 2015.**ufs-023681**

40. **Lewtak, J.P. and Swarts, J.C.** 2015. Synthesis and electrochemical properties of phthalocyanines bearing $\text{Fc}(\text{CH}_2)_n\text{S-}$ and dodecyl substituents in non-peripheral positions. (Lecture). 227th Electrochemical Society Meeting, Chicago, United States of America, 24-28 May. **ufs-023684**
41. **Swarts, J.C.** 2015. Comparative electrochemical properties of phthalocyanines bearing $\text{Fc}(\text{CH}_2)_n\text{-}$ and/or alkyl substituents in non-peripheral and/or peripheral positions. (Lecture). 227th Electrochemical Society Meeting, Chicago, United States of America, 24-28 May. **ufs-023693**
42. **Swarts, J.C. and Siegert, U.** 2015 Polysiloxanes as carriers for rhodium-ferrocenyl complexes with potential catalytic applications. . (Lecture). 25th International Conference on Coordination and Bioinorganic Chemistry, Smolenice, Slovakia, 31 May-5 June 2015. **ufs-023822**
43. **Swarts, J.C., Magqi, N. and Erasmus, E.** 2015. Silver and Platinum Catalysts for oxidation hydrogenation and aromatisation: From two-dimensional models on silicon wafers to three-dimensional zeolite-supported systems. (Invited Lecture). Advanced Materials World Congress, Stockholm, Sweden, 23-26 August 2015. **ufs-023823**
44. **Swarts, J.C.** 2015. Different functionalisation strategies to tune the physical properties of phthalocyanines. (Keynote Lecture). South African Chemical Institute Inorganic Chemistry Conference (INORG 2015), Grahamstown, South Africa, 28 June – 2 July 2015. **ufs-023825**
45. **Belay, N.A., Venter, J.A. and Drost, R.** 2015. Synthesis and characterization of Nb(V) complexes with *O,O'* bidentate ligands. Indaba8 Serendipity vs Prediction Conference, (poster) Skukuza in the Kruger National Park, South Africa, 16-21 August 2015. **ufs-024494**
46. **Elmakki, M., Venter, J.A. Drost, R.** 2015. Synthesis and characterisation of rhodium cupferrate and substituted cupferrate complexes (Poster). Indaba 8, Kruger National Park, South Africa, 16-21 August 2015. **ufs-024500**
47. **Roodt, A.** 2015. Perspectives on the 2nd European Crystallographic School (Invited Opening Lecture). 2nd European Crystallographic School, Mieres, Asturias, Spain, 30 August-5 September 2015. **ufs-024501**
48. **Roodt, A.** 2015. Outcomes of the South African Summit Meeting in Bloemfontein. (Invited Lecture). Crystallography for the next Generation, Rabat, Morocco, 22-24 April 2015. **ufs-024507**
49. **Roodt, A.** 2015. Applications of Crystallography in Chemistry (Invited Lecture). 2nd European Crystallographic School, Mieres, Asturias, Spain, 30 August - 5 September 2015. **ufs-024511**

50. **Roodt, A., Brink, A., Schutte-Smith, M., Visser, H.G.** 2015. Intimate mechanism of substitution reactions at organometallic octahedral / square planar metal sites via state-of-the art kinetic studies (Invited Lecture). International Conference 'Organometallic and Coordination Chemistry: Achievements and Challenges'. Volga river, Nizhny Novgorod, Russia, 18-23 September 2015.**ufs-024514**
51. **Roodt, A.** Are detailed reaction mechanisms really necessary in (applied) Organometallic and Coordination Chemistry? (Invited special lecture). Special seminar from the Russian Academy of Sciences; State University of Saint Petersburg, St. Petersburg, Russia. 22 September 2015.**ufs-024517**
52. **Roodt, A.** A few perspectives of Cedric Holzapfel from an 'Inorganic' Chemist (Invited Lecture). C.W. Holzapfel Symposium, University of Johannesburg, Johannesburg. 2 October 2015.**ufs-024523**
53. **Roodt, A., Alberto, R.** Multi-functional Cyclopentadienyl and Carbonyl Complexes for Theranostic Applications (Invited Lecture). Mid-term Conference and Workshop of the Swiss South Africa Joint Research Programme, Basel, 22-23 October 2015.**ufs-024526**
54. **Renier Koen, Visser, H.G., Roodt, A.** 2015. Comparing tantalum and niobium: The β -diketone approach. Indaba8 Serendipity vs Prediction Conference, (poster) presented at Skukuza in the Kruger National Park, South Africa, 16-21 August 2015.**ufs-024535**
55. **Renier Koen, Visser, H.G., Roodt, A.** 2015. A redetermination of the structure of Tetraethylammonium *mer*-oxidorichlorido (thenoyltrifluoroacetato- K^2O,O')niobate (V) - $(NEt_4)[NbOCl_3(ttfa)]$. Oral presented at AMI Nuclear Metals 2015, Port Elizabeth, South Africa, 2015, 28-30 October 2015. **ufs-024538**
56. **Alexander, O.T., Duvenhage, M.M., Brink, A., Mueller, P., Swart, H.C., Visser H.G.,** 2015. Effects on the luminescence properties of two Gallium(III)-*tris*-(5,7-dimethyl-8-hydroxyquinolino) complexes. (Poster). Indaba 8, Skukuza, Kruger National Park, South Africa, 16 – 21 August 2015.**ufs-024644**