

CONFERENCES 2018

1. **Nete, M., Purcell, W. and Nel, J.T.** 2017. Analysis of Non-Conducting Tantalite Minerals by Glow Discharge Optical Emission Spectrometry. **Chapter in Book**, pages 11-21. International Conference on Pure and Applied Chemistry (ICPAC 2016).Mauritius, in July 2016.**ufs-029215**.
2. **Lötter, S.J., Purcell, W., Nel, J.T. and van Brecht, B.** 2017. Cation Influence on Zirconium/Hafnium Fluoride Coordination. **Chapter in Book**, pages 239-265. International Conference on Pure and Applied Chemistry (ICPAC 2016). Mauritius, in July 2016.**ufs-029217**
3. **Nete, M. and Purcell, W.** 2017. Beneficiation of Niobium and Tantalum from Tantalite Ore Using Physical and Chemical Processes. **Chapter in book**. Pages 267-283. International Conference on Pure and Applied Chemistry (ICPAC 2016). Mauritius, in July 2016.**ufs-029219**
4. **Conradie, J.** 2018. (lecture) A DFT view of CH₃I Oxidative Addition to Monocarbonylphosphine [Rh(b-diketonato)(CO)(PPh₃)] Complexes: Steric and Electronic Effects. 28th International Conference on Organometallic Chemistry (ICOMC), Congress and Exhibition Centre, Florence, Italy, 15 – 20 July 2018. **ufs-033124**
5. **Conradie, J., and Kuhn, A.**, 2018. (poster) A DFT view of the reduction of bis(cyclopentadienyl) mono(β -diketonato) titanium(IV) cationic complexes. (poster) 28th International Conference on Organometallic Chemistry (ICOMC), Congress and Exhibition Centre, Florence, Italy, 15-20 July 2018. **ufs-033160**
6. **F.P. Malan, E. Singleton, P.H. van Rooyen, J. Conradie, M. Landman**, 2018. (poster) Base-free Glucose Dehydration Catalysed by NHC-stabilised Heterohalo cyclopentadienyl Cr(III) complexes. 28th International Conference on Organometallic Chemistry (ICOMC), Congress and Exhibition Centre, Florence, Italy, July, 15-20, 2018. **ufs-033162**
7. **Venter, J.A., Belay, A.N. & Roodt, A.** 2018. (poster) Crystallographic and kinetic study of Niobium(V) and Tantalum(V) complexes with O,O'-bidentate ligands. (poster) 28th International Conference on Organometallic Chemistry (ICOMC), Florence, Italy, 15-20 July 2018. . **ufs-033165**
8. **Venter, J.A.** 2018. (poster) Structural and reactivity studies on related rhodium phosphine complexes. (Oral) 28th International Conference on Organometallic Chemistry (ICOMC), Florence, Italy, 15-20 July 2018. . **ufs-033167**

9. **Wilhelm, A., Moradi-Afrapoli, F., van der Merwe, H., Swart, K., Stadler, M. and de Meiri, M.** 2018. (oral) HPLC-based activity profiling for GABAA receptor modulators in *Searsia pyroides* using a larval zebrafish locomotor assay. First Conference of Biomedical and Natural Sciences and Therapeutics (CoBNeST). Spier Estate Stellenbosch, 7-10 October 2018. . **ufs-033168**

10. **SL Bonnet, A Wilhelm, K Phungula, M Stadler, S Hering.** 2018. (oral) *In vitro* screening of South African plant extracts for GABAergic activity via an automated two-microelectrode voltage clamp assay on *Xenopus* oocytes. First Conference of Biomedical and Natural Sciences and Therapeutics (CoBNeST). Spier Estate Stellenbosch, 7-10 October 2018. . **ufs-033169**

11. **Conradie, J.** 2018. (lecture) HPC insights into chemistry mysteries, Conference program p9, Centre for High Performance Computing (CHPC) National Conference, Century City Conference Centre, Cape Town, South Africa, 2-6 December 2018. www.chpcconf.co.za. **ufs-033170**

12. **Conradie, J.** (poster) 2018. REDOX behaviour of Metal-b-diketonato Complexes: A Frontier Molecular Orbital Energy approach, Centre for High Performance Computing (CHPC) National Conference, Century City Conference Centre, Cape Town, South Africa, 2-6 December 2018. . **ufs-033171**

13. **Adeniyi, A.A., Conradie, J.** 2018. (lecture), Anticholinesterase activities of peptidomimetic drugs physostigmine ((-)-phy) and its three analogues (-)-her, (-)-phe and (+)-phe in their interaction with Acetylcholinesterase (AChE) and butyrylcholinesterases (BChE). at CECAM conference on Protein-peptide interactions: peptide identification, binding prediction and design, October 16, 2018 to October 19, 2018 at CECAM-FR-MOSER University Paris-Diderot Amphi Turing Bâtiment Sophie Germain 8 place Aurélie Nemours - 75013 Paris. **ufs-033172**

14. **Adeniyi, A.A., Conradie, J.** 2018, (lecture) The theoretical investigation of reduction potentials and spectroscopic properties of nitrobenzene and keto-enol molecules, Conference program p12, Centre for High Performance Computing (CHPC) National Conference, Century City Conference Centre, Cape Town, South Africa, 2-6 December 2018. **ufs-033177**

15. **Swarts, P.J., Conradie, J., Swarts, J.C.** 2018. (poster) International Conference on Porphyrins and Phthalocyanines (ICPP-10), 1 – 6 July 2018, Munich, Germany, Synthesis, electrochemical and spectroscopic studies on new subphthalocyanines. **ufs-033178**

16. **Adeniyi, A.A., Conradie, J.** 2018. (poster) The theoretical investigation of reduction potentials and spectroscopic properties of nitrobenzene and keto-enol molecules, Centre for High Performance Computing (CHPC - Main) National Conference, Century City Conference Centre, Cape Town, South Africa, 2-6 December 2018. **ufs-033179**

17. **van der Westhuizen, D., Conradie, J., von Eschwege, K.** 2018. (poster) DFT Studies of Fe, Ru & Os Light-Sensitive Energy Conversion Dyes/Catalysts, Centre for High Performance Computing (CHPC) National Conference, Century City Conference Centre, Cape Town, South Africa, 2-6 December 2018. **ufs-033214**

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| 18. Xaba, S M, Nete, M and Purcell, W. 2018. Concentration of rare earth elements from monazite by selective precipitation. <i>IOP Conference Series: Materials Science and Engineering</i> . 23-26 October 2018, Vanderbijlpark, South Africa, 430: 36-42. ufs-033433 (Waiting for Peer Review Letter) |
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19. **Alexander, O.T., Khasemene, M., Alberto, R.A., Roodt, A.** 2018. (lecture) Some General Aspects on Cobalt Chemistry and Optimistic Forecast on its Water (In)Soluble Complexes as Potential Water Splitting Catalysts. ReMec1: 1st Symposium on Reaction Mechanisms, Bloemfontein, South Africa. 13-14 November 2018. **ufs-033216**
20. **Alexander, O.T., Khasemene, M., Alberto, R.A., Roodt, A.** 2018. (Flash oral presentation and Poster). Exploring Potential Catalytic Behavior Of Water (In)Soluble N-Based Ligand Cobalt Complexes as Water Splitting Catalyst. Indaba 9, Skukuza, Kruger National Park, South Africa, 2-7 September 2018. **ufs-033218**
21. **Botha, E., Roodt, A., Alberto, R.A., Hernandez, D.** 2018. (lecture) Carbon dioxide fixation in succulent plants, synthesis and characterization of metal carboxylates, Plastic recycling, water purification and heavy metal recovery. ReMec1: 1st Symposium on Reaction Mechanisms, Bloemfontein, South Africa. 13-14 November 2018. **ufs-033219**
22. **Brink, A.** (Keynote Lecture) The Challenges of Interoperability between Chemical and Protein Crystallography. ReMec1: 1st Symposium on Reaction Mechanisms, Bloemfontein, South Africa. 13-14 November 2018. **ufs-033220**
23. **Botha, E., Roodt, A.** 2018. (Lecture) Carbon Dioxide Fixation in Succulent Plants: A Crystal Engineering, Solid State Modeling and Kinetics Approach, 31st European Crystallographic Meeting, Oviedo, Spain, 22-27 Aug 2018. **ufs-033221**
24. **Elmakki, M., Venter, J.A., Venter, G.J.S., Roodt, A.** 2018. (lecture) Influence of Selected Bidentate Ligands on the reactivity of Rh(I) Complexes. ReMec1: 1st Symposium on Reaction Mechanisms, Bloemfontein, South Africa. 13-14 November 2018. **ufs-033222**
25. **Jacobs, F.J.F., Brink, A., Venter, G.J.S.** 2018. (lecture) Rhenium radiopharmaceutical models inspired by biological moieties. ReMec1: 1st Symposium on Reaction Mechanisms, Bloemfontein, South Africa. 13-14 November 2018. **ufs-033223**
26. **Kama, D.V., Brink, A., Alberto, R.A., Roodt, A.** (Flash oral presentation and Poster). Systematic phosphine ligand design: Some structural implications on catalysis and radiopharmaceuticals. Indaba 9, Skukuza, Kruger National Park, South Africa, 2-7 September 2018. **ufs-033225**
27. **Kama, D.V., Brink, A., Schutte-Smith, M., Swart, C., Alberto, R.A., Roodt, A.** 2018. (lecture) Selective Diphosphinoamine Ligand Design: For Platinum-Group Metal Catalysts and Group 7 Theranostic Synthons. ReMec1: 1st Symposium on Reaction Mechanisms, Bloemfontein, South Africa. 13-14 November 2018. **ufs-033227**

28. **Khasemene, M., Roodt, A.** 2018. (lecture) Middle and late transition metal complexes as model water reduction catalysts. ReMec1: 1st Symposium on Reaction Mechanisms, Bloemfontein, South Africa. 13-14 November 2018. **ufs-033228**
29. **Mokolokolo, P.P., Pretorius, C., Schutte-Smith, M., Brink, A., Roodt, A.** 2018. (Flash Oral presentation and Poster). Rhodium(I) Carbonyl Complexes as Model Nano-Wired Assemblies and Catalysts. Indaba 9, Skukuza, Kruger National Park, South Africa, 2-7 September 2018. **ufs-033229**
30. **Mokolokolo, P.P., Tsosane, M.S., Kama, D.V., Schutte-Smith, M., Brink, A., Visser, H.G., Meola, G., Frei, A., Alberto, R.A., Roodt, A.** 2018. (lecture) Electronic and steric manipulation of Schiff-base and Oxine-type ligand systems to selected middle and late transition metal carbonyl cores. ReMec1: 1st Symposium on Reaction Mechanisms, Bloemfontein, South Africa. 13-14 November 2018 **ufs-033230**
31. **Kamiński, R., Jarzemska, K. N., Paliwoda, D., Petříček, V., Pretorius, C., Roodt, A.** 2018. (Poster) High-pressure single-crystal X-ray diffraction study of a model Rh complex exhibiting metallophilic interactions in the solid state. 31st European Crystallographic Meeting, Oviedo, Spain, 22-27 Aug 2018. **ufs-033239**
32. **Morerwa, Z.G., Andreas Roodt, A., Venter, G.J.S.** 2018. (lecture) Environmentally Friendly Rhodium(I) Model Catalysts. ReMec1: 1st Symposium on Reaction Mechanisms, Bloemfontein, South Africa. 13-14 November 2018. **ufs-033252**
33. **Motente, M., Schutte-Smith, M., Roodt, A.** 2018. (lecture) Radiopharmaceuticals: Developing potential radiopharmaceutical agents using natural product ligand systems. ReMec1: 1st Symposium on Reaction Mechanisms, Bloemfontein, South Africa. 13-14 November 2018. **ufs-033253**
34. **Nkoe, P.I., Brink, A., Schutte-Smith, M.** 2018. (lecture) Investigation of the coordination behavior of nitrogen and oxygen containing ligands with rhenium(I) tricarbonyl and the potential use as radiopharmaceuticals. ReMec1: 1st Symposium on Reaction Mechanisms, Bloemfontein, South Africa. 13-14 November 2018. **ufs-033233**
35. **Roodt, A.** 2018. (Keynote Lecture). Successful modeling of the total chemical process: is this viable and possible? Indaba 9, Skukuza, Kruger National Park, South Africa, 2-7 September 2018. **ufs-033234**
36. **Roodt, A.** (Keynote Lecture) Detailed Reaction Mechanisms: Quo Vadis? ReMec1: 1st Symposium on Reaction Mechanisms, Bloemfontein, South Africa. 13-14 November 2018. **ufs-033235**
37. **Roodt, A.** 2018. (Keynote Lecture). Expanding diagnostic nuclear medicine: some perspectives. Official Inauguration and IUCr Open laboratory, Abidjan, Ivory Coast, 22-31 March 2018. **ufs-033236**
38. **Taoana, T.N., Twigge, L., Venter, J.A.** 2018. (Lecture) Structural and mechanistic study on a rhodium acetylacetonato derivative. ReMec1: 1st Symposium on Reaction Mechanisms, Bloemfontein, South Africa. 13-14 November 2018. **ufs-033237**
39. **Roodt, A.** 2018. (Invited Lecture). Advanced studies of reaction mechanisms. New Frontiers in Chemical Science (NFCS), Indian Institute for Technology Bombay, Mumbai, India. 13-14 December 2018. **ufs-033238**

40. **Schutte-Smith, M., Twigge, L., Alexander, O.T., Visser, H.G., Roodt, A., Manicum, A.-L.** 2018. (Keynote Lecture) Carbonyl Activation in Rhenium(I) Complexes – a solid and solution state study. ReMec1: 1st Symposium on Reaction Mechanisms, Bloemfontein, South Africa. 13-14 November 2018. **ufs-033240**
41. **Roodt, A.** 2018. (Plenary lecture) Properties and applications of crystals/crystallography. 5th European Crystallographic School, University of Stellenbosch, South Africa. 8-14 July 2018. **ufs-033241**
42. **Venter, G.J.S.** (Keynote Lecture) β -diketones and their derivatives in Rh(I) dicarbonyl and phosphine complexes. ReMec1: 1st Symposium on Reaction Mechanisms, Bloemfontein, South Africa. 13-14 November 2018. **ufs-033242**
43. **Redgard, S., Roodt, A.** 2018. (lecture) Nucleophile assisted CO₂ fixation for a cleaner environment. ReMec1: 1st Symposium on Reaction Mechanisms, Bloemfontein, South Africa. 13-14 November 2018. **ufs-033243**
44. **Venter, J.A., Drost, R.M., Warsink, S.** 2018. (Keynote Lecture) Steric and electronic relationships in selected rhodium phosphine complexes. ReMec1: 1st Symposium on Reaction Mechanisms, Bloemfontein, South Africa. 13-14 November 2018. **ufs-033244**
45. **Viljoen, J.A., Roodt, A., Visser, H.G.** 2018. (lecture) Some Aspects of the Coordination Environment of Hafnium. ReMec1: 1st Symposium on Reaction Mechanisms, Bloemfontein, South Africa. 13-14 November 2018. **ufs-033245**
46. **Schutte-Smith, M., Manicum, A.L., Visser, H.G.** ‘A Solid State and Mechanistic Study of Carbonyl Activation in Rhenium (I) Complexes’. 7th EuCheMS Chemistry Congress, 26-30 August 2018, Liverpool, England, UK. (Oral Presentation) **ufs-033246**
47. **Invited Lecture: Brink, A.** 2018. *Small Molecule to Macromolecular – A Wonderland Journey for Radiopharmaceuticals* (Oral). SciDataCon 2018 – International Data Week, Gaborone, Botswana, 5-8 Nov 2018. <https://www.scidatacon.org/IDW2018/sessions/223/> **ufs-033247**
48. **Brink, A.** 2018. *Modifying the RheManTec Triad – A small molecule meanders into the macromolecular world.* (Poster). 31st European Crystallographic Meeting, Oviedo, Spain, 22-27 Aug 2018, Acta Cryst., 2018, A74, e381. **ufs-033248**
49. **Azov, V. A.** 2018. (Lecture) Dynamic Molecular Architectures Based on Tetrathiafulvalenes. 43rd National Convention of the South African Chemical Institute SACI-2018, Pretoria, South Africa. 2-7 December 2018. **ufs-033249**
50. **Xantini, Z., Erasmus, E.** 2018. *Preparation, characterisation and comparing 3 different catalytic supports for hydrogenation of unsaturated carbonyl compounds.* (Poster) CATSA 2018, Legend Golf & Safari Resort, Limpopo, South Africa, 11-14 November 2018. **ufs-033254**
51. **Masene, M., Erasmus, E.** 2018. *Bimetal cyanometallates used as a heterogeneous catalyst.* (Oral) CATSA 2018, Legend Golf & Safari Resort, Limpopo, South Africa, 11-14 November 2018. **ufs-033256**

53. **Meyer, N., Swarts, J.C.** 2018. (poster) Electrochemical and spectroscopic studies on sterically hindered corroles and their gold(III) complexes, 10th International Conference on Porphyrins and Phthalocyanines (ICPP-10), Munich, Germany. **ufs-033257**
54. **Crause, A., Swarts, J.C.** 2018. (poster) Synthesis, spectroscopic and electrochemical properties of contracted and expanded porphyrins. 10th International Conference on Porphyrins and Phthalocyanines (ICPP-10), Munich, Germany **ufs-033259**
55. **Swarts, J.C., Lewtak, J., Langner E.H.G.** 2018. (oral) Synthetic, electrochemical and spectroscopic studies on new subphthalocyanines. 10th International Conference on Porphyrins and Phthalocyanines (ICPP-10), Munich, Germany **ufs-033260**
56. **C.-W. Tsai, E.H.G. Langner, J.J. Terblans, H.C. Swart, R.A. Harris.** 2018. (poster) Computational study of ZIF with functional groups for CO₂ adsorption, 63rd Annual Conference of the South African Institute of Physics, Bloemfontein, 25-29 June 2018. **ufs-033261**
57. **Mogale, R., EHG, Langner, E.H.G.,** 2018. (oral) ZIF-8(Zn) and NH₂-MIL-53(Al) As Supports For Pd and Ag Crystallites with Application in Heterogeneous Catalysis. CATSA 2018, Legend Golf & Safari Resort, Limpopo, South Africa, 11-14 November 2018. **ufs-033262**
58. **Mphuthi L., Langner E.H.G.,** 2018. (poster) Metal exchange in nZIF-8 and nZIF-67 with Fe(II) for heterogeneous catalytic applications, NanoSmat-Africa 2018, NH The Lord Charles Hotel, Western Cape, South Africa, 19-23 November 2018 **ufs-033336**
59. **Mogale, R., Langner E.H.G.,** 2018. (oral) ZIF-8(Zn) and NH₂-MIL-53(Al) As Supports For Pd and Ag Crystallites with Application in Heterogeneous Catalysis, NanoSmat-Africa 2018, NH The Lord Charles Hotel, Western Cape, South Africa, 19-23 November 2018 **ufs-033337**
60. **C.-W. Tsai, E.H.G. Langner, J.J. Terblans, H.C. Swart, R.A. Harris.** 2018. (poster) Zeolitic Imidazolate Framework nanomaterial with functional groups for CO₂ adsorption, NanoSmat-Africa 2018, NH The Lord Charles Hotel, Western Cape, South Africa, 19-23 November 2018 **ufs-033339**
61. **Mensah, P., Katerere, D., Hachigonta, S., Roodt, A.** 2018. **Book** – 1st Edition (Springer, p. 1-329). Systems Analysis Approach for Complex Global Challenges. ISBN 978-3-319-71486-8. Cham, Switzerland > **ufs-033368**
62. **Roodt, A., Alberto, R.A., Frei, A., Mokolokolo, P.P., Bollinger, R., Brink, A., Kama, D.V. Patent.** PCT INTERNATIONAL PATENT > **ufs-033376**