

Faculty of Natural and Agricultural Sciences

Department of Chemistry

Conference Contributions 2021

1. **Wilhelm, A.** (2021). International Organic Chemistry Symposium, Virtual meeting, Invited lecture - Larval zebrafish locomotor assay for the discovery of GABAA-receptor modulators, 15 June 2021. **ufs-040181**
2. **Swart, M.R., Twigge, L., Erasmus, E., Marais, C., Bezuidenhout B.C.B.,** (2021). The riddle of *p*-cresol and Grubbs second generation catalyst (Oral). International Organic Chemistry Symposium, University of the Free State, Virtual Symposium 15 June 2021. **ufs-041084**
3. **Maier, D.I.H., Bezuidenhout, B.C.B., Marais, C.** (2021). New catalytic methodologies towards the synthesis of oxygenated dibenzo[b,f]azepines (Oral). International Organic Chemistry Symposium, University of the Free State, Virtual Symposium, 15 June 2021. **ufs-041085**
4. **Visser, M., Pieterse, T., Twigge, L., Marais, C.; Bezuidenhout, B.C.B.** (2021). Synthesis of flavonoids and benzo[b]furans (Oral). International Organic Chemistry Symposium, University of the Free State, Virtual Symposium, 15 June 2021. **ufs-041086**
5. **De Jager, K.M., Kuo, C.-M., Bezuidenhout, B.C.B., Marais, C.** (2021). Total synthesis of isomeric hydroxylated mono-methoxy homoisoflavanones (Oral). International Organic Chemistry Symposium, University of the Free State, Virtual Symposium, 15 June 2021. **ufs-041089**
6. **Makhathini, B.T., Bezuidenhout, B.C.B., Marais, C.** (2021) Strategies towards the synthesis of a stilbene-related substituted γ -butenolide natural product (Oral). International Organic Chemistry Symposium, University of the Free State, Virtual Symposium, 15 June 2021. **ufs-041090**
7. **Faber, J., Marais, C., Wilhelm, A.** (2021) Investigation of the C-glucosylated xanthone, mangiferin, under oxidative conditions (Oral). International Organic Chemistry Symposium, University of the Free State, Virtual Symposium, 15 June 2021. **ufs-041091**
8. **Makhathini, B.T., Bezuidenhout, B.C.B., Marais, C.** (2021) Strategies towards the synthesis of a stilbene-related substituted γ -butenolide natural product (Poster). Young Chemist's Symposium 2021 (SACI National), Virtual, 8 – 9 July 2021. **ufs-041092**

9. **Visser, M., Pieterse, T., Twigge, L., Marais, C.; Bezuidenhout, B.C.B.** (2021) Synthesis of flavonoids and benzo[b]furans (Oral). Young Chemist's Symposium 2021 (SACI National), Virtual, 8 – 9 July 2021. **ufs-041093**
10. **Makhathini, B.T., Bezuidenhout, B.C.B., Marais, C.** (2021) Strategies towards the synthesis of a stilbene-related substituted γ -butenolide natural product. Natural and Agricultural Sciences: Flash Fact Competition, Virtual, 26 - 27 July 2021 (MSc winner). **ufs-041094**
11. **Azov, V.A., Hennecke, U., Ballet, S., Martin, C. (Invited lecture).** (2021) P-STAC: Stabilizing peptide nanoStructures with tetraThiafulvalenebased donors and Acceptors. International Organic Chemistry Symposium, University of the Free State, Virtual Symposium, 15 June 2021. **ufs-041100**
12. **Bonnet, S.L., Wilhelm, A., (Invited lecture).** (2021) In vitro screening of South African plant extracts for GABAergic activity. International Organic Chemistry Symposium, University of the Free State, Virtual Symposium, 15 June 2021. **ufs-041102**
13. **De Beer, F.J., Twigge, L., Azov, V.A.** (2021). Synthesis of amino acids with donor and acceptor substituents (Oral presentation). International Organic Chemistry Symposium, University of the Free State, Virtual Symposium, 15 June 2021. **ufs-041103**
14. **Twigge, L., Roodt, A., Alberto, R., Visser, H.G., Kirsten, L., Koen, R., Schutte-Smith, M.** (2021). Structure of a rhenium(II) complex with 3-hydroxyflavone as O,O'-bidentate ligand and confirmation of π -stacking by solid-state NMR spectroscopy (Oral presentation). International Organic Chemistry Symposium, University of the Free State, Virtual Symposium, 15 June 2021. **ufs-041104**
15. **Mncwangi, S.N., Azov, V.A.** (2021) Synthesis of bis-tetrathiafulvalene derivatives with variable degree of π -conjugation (Oral presentation). International Organic Chemistry Symposium, University of the Free State, Virtual Symposium, 15 June 2021. **ufs-041105**
16. **Noreljaleel, A.E.M, Wilhelm, A., van der Westhuizen, J.H., Bonnet, S.L.** (2021) Synthesis and bioactivity of reduced chalcones containing sulphonamide side chains (Oral presentation). International Organic Chemistry Symposium, University of the Free State, Virtual Symposium, 15 June 2021. **ufs-041106**
17. **Molahloe, T.S, Zietsman, P.C., Wilhelm, A., Bonnet, S.L.** (2021) Structure elucidation of iridoid glycosides from *Aptosimum elongatum* extracts (Oral presentation). International Organic Chemistry Symposium, University of the Free State, Virtual Symposium, 15 June 2021. **ufs-041107**
18. **Brink, A. Invited Lecture:** (2021) *The harvesting of small molecule structure and dynamic data for macromolecular and catalytic usage.* (Oral). IUCr 2021: XXV General Assembly and Congress of the International Union of Crystallography. 14-22 August 2021, Prague, Czech Republic. **ufs-041783**

19. **Jacobs, FJF., Brink, A.** (2021) Bridging the gap between nature and industry: Fundamentals of capturing entering entities for industrial and medical applications. RheManTec^{III}: “Solar Light-driven Homogeneous Catalysis for Greener Industrial Processes with H₂ as Energy Source and CO₂ as C1 Building Block”. Joint virtual seminar between UFS and UZH, SSAJRP IZLZS2_170856., South Africa & Switzerland. 28 May 2021. [ufs-041784](#)
20. **Moreerwa, Z.G., Roodt, A., Brink, A.** (2021) Towards water soluble catalysts for CO/CO₂ fixation and conversion. RheManTec^{III}: “Solar Light-driven Homogeneous Catalysis for Greener Industrial Processes with H₂ as Energy Source and CO₂ as C1 Building Block”. Joint virtual seminar between UFS and UZH, SSAJRP IZLZS2_170856., South Africa & Switzerland. 28 May 2021. [ufs-041785](#)
21. **Jacobs, FJF., Brink, A.** (2021) Functionalised nitrogen based ligands in dinuclear rhenium model radiopharmaceuticals with applications to protein coordination (Poster and presentation) CCP4 Crystallographic School: Data Collection to Structure Refinement and Beyond (Digital Conference), University of Cape Town, South Africa, 22 February - 5 March 2021. [ufs-041786](#)
22. **Van Dyk, H., Brink, A.** (2021) Functionalised Schiff Base Ligands With Applications In Protein Crystallization Coordination, Catalysis And Luminescence. (Poster) CCP4 Crystallographic School: Data Collection to Structure Refinement and Beyond (Digital Conference), University of Cape Town, South Africa, 22 February - 5 March 2021 [ufs-041787](#)
23. **Moreerwa, Z.G., Brink, A., Roodt, A.** (2021) Environmentally Friendly Rhodium(I) Model Catalysts tailored by various bidentate and monodentate (water-soluble) ligand. (Poster). IUCr 2021: XXV General Assembly and Congress of the International Union of Crystallography. 14-22 August 2021, Prague, Czech Republic. [ufs-041788](#)
24. **Jacobs, FJF., Brink, A.** (2021) Understanding small rhenium molecules kinetically and structurally in a macromolecular setting. (Poster). IUCr 2021: XXV General Assembly and Congress of the International Union of Crystallography. 14-22 August 2021, Prague, Czech Republic. [ufs-041790](#)
25. **Bosman, L., Kama, D., Brink, A.** (2021) Halogenated rhodium(I) complexes as model catalysts for methanol carbonylation. (Poster). IUCr 2021: XXV General Assembly and Congress of the International Union of Crystallography. 14-22 August 2021, Prague, Czech Republic. [ufs-041791](#)
26. **Van Dyk, H., Jacobs, F.J.F., Brink, A.** (2021) Catalytic development and medical application of transition metal complexes (Re, Co, Cu) containing novel Salicylidene Schiff bases. (Poster). IUCr 2021: XXV General Assembly and Congress of the International Union of Crystallography. 14-22 August 2021, Prague, Czech Republic. [ufs-041794](#)
27. **Motente, M., Venter, J.A., Brink, A.** (2021) Rhodium(I) (O,O'; N,O) Hydroxamic Acid Complexes As Model Catalysts. (Poster). IUCr 2021: XXV General Assembly and Congress of the International Union of Crystallography. 14-22 August 2021, Prague, Czech Republic. [ufs-041795](#)

28. **Kama, D., Brink, A., Roodt, A.** (2021) Exploring Structural Implications of diphosphinamine ligands in Medicine and Catalysis. (Poster). IUCr 2021: XXV General Assembly and Congress of the International Union of Crystallography. 14-22 August 2021, Prague, Czech Republic. [ufs-041796](#)
29. **Mokolokolo, P.P., Brink, A., Pretorius, C., Roodt, A.** (2021) Structure and Reactivity of Rhodium(I) Carbonyl complexes as Model Nano-Wired Assemblies and Catalyst. (Poster). IUCr 2021: XXV General Assembly and Congress of the International Union of Crystallography. 14-22 August 2021, Prague, Czech Republic. [ufs-041797](#)
30. **Jacobs, F.J.F., Brink, A.** (2021) Structural and kinetic variations of rhenium tricarbonyl complexes for biological and catalytic evaluation. (Poster). Joint virtual meeting of the AfLS3-2021: African Light Source and the ePCCr: Pan-African Conference on Crystallography Online. 15-19 November 2021. Hosted by X-TechLab, Cotonou, Benin. [ufs-041798](#)
31. **Bosman, L., Kama, D.V., Brink, A.** (2021) Schiff-ting into a greener future utilizing Rh(I) N,O model catalysts. (Poster). Joint virtual meeting of the AfLS3-2021: African Light Source and the ePCCr: Pan-African Conference on Crystallography Online. 15-19 November 2021. Hosted by X-TechLab, Cotonou, Benin. [ufs-041800](#)
32. **van Dyk, H., Jacobs, F. J. F., Mokolokolo, P.P., Brink, A.** (2021) Application of functionalized salicylidene Schiff base ligands in catalysis, luminescence, and radiopharmacy. (Poster). ePCCr: Pan African Conference on Crystallography Online held jointly with the African Physical Society (AfPS) and the African Light Source (AfLS) conferences. 15-19 November 2021, Hosted by X-TechLab, Cotonou, Benin. [ufs-041801](#)
33. **van Staden, C, Visser, H.G., Schutte-Smith, M.** (2021) 25th Congress of the International Union of Crystallography, IUCr 2021, 14-22 August 2021, Hybrid congress – Prague, Czech Republic and Virtual. Poster presentation – ‘The manipulation of metal-metal bonding distances by variation of the size of N-substituents on PNP ligand systems. [ufs-042473](#)
34. **Kapp, L., Visser, H.G., Schutte-Smith, M.** (2021) 25th Congress of the International Union of Crystallography, IUCr 2021, 14-22 August 2021, Hybrid congress – Prague, Czech Republic and Virtual. Poster presentation – ‘Structure activity relationship of imidazo[4,5-f] ligands and their Rhenium(I) complexes- photoluminescence and DNA intercalation.’ [ufs-042480](#)
35. **Mokolokolo, P.P., Schutte-Smith, M., Brink, A., Roodt, A.** (2021) 25th Congress of the International Union of Crystallography, IUCr 2021, 14-22 August 2021, Hybrid congress – Prague, Czech Republic and Virtual. Poster presentation – ‘Structure and Reactivity of Rhodium(I) Carbonyl complexes as Model Nano-Wired Assemblies and Catalyst’. [ufs-042481](#)
36. **Liebenberg, L., Visser, H.G., Schutte-Smith, M.** (2021) Student Symposium in Natural Sciences 2021, 28-29 Oktober 2021, Potchefstroom / Virtual. Oral Presentation – ‘Rhenium(I) trikarbonielkomplekse van 1’-(alkielamino)aurone en amino-auronimiene as potensiele chemoterapeutiese middels’. [ufs-042482](#)

37. **Oosthuizen, U., Schutte-Smith, M., Visser, H.G.,** (2021) Student Symposium in Natural Sciences, 28-29 Oktober 2021, Potchefstroom / Virtual. Oral Presentation – ‘Studie van Renuim en Goud metaalverbindinge as anti-kanker en anti-mikrobiale middels’. [ufs-042483](#)
38. **Blignaut, J., Visser, H.G., Schutte-Smith, M.** (2021) Pan African Conference on Crystallography (ePCCr), 15-19 November 2021, Virtual. Poster Presentation – ‘Crystallographic characterization of Ru(II)-PC(n)P-Au(I) bimetallic complexes with varying PC(n)P-ligands’. [ufs-042486](#)
39. **van Staden, C., Visser, H.G., Schutte-Smith, M., Kama, D.V.** (2021) Pan African Conference on Crystallography (ePCCr), 15-19 November 2021, Virtual. Poster presentation - ‘The structural comparison of dimeric Ag(I) and Au(I) complexes with bridging bidentate phosphine ligand systems.’ [ufs-042493](#)
40. **van Staden, C., Moskaleva, L.V., Kroon, R.E., Kama, D.V., Schutte-Smith, M., Visser, H.G.** (2021) Material Science and Beyond, 2 - 3 Desember 2021, Virtual. Oral presentation - ‘Journey to the structural optimisation of gold(I) complexes to investigate the experimental manipulation potential of aurophilic interactions by ligand design.’ [ufs-042506](#)
41. **Swart, M.R., Twigge, L., Erasmus, E., Marais, C., Bezuidenhoudt, B.C.B.** (2021) Alkene metathesis, p-Cresol and the Second -Generation Grubbs Catalyst: Fitting the Pieces. Catalysis Science & Technology 10th Anniversary Symposium, Virtual event, 16-17 November 2021. [ufs-042507](#)
42. **Visser, M., Pieterse, T., Twigge, L., Marais, C., Bezuidenhoudt, B.C.B.,** (2021) Universele metodiek vir die sintese van flavonoïede en benzo[b]furane. Studentesimposium in die Natuurwetenskappe, Virtueel, 28 – 29 Oktober 2021. (2de prys). [ufs-042508](#)
43. **Conradie, J., Penelope Brothers, Ghosh, A.** (2021) Invited oral, Energetics of Exotic Porphyrinoid Systems, 11th International Conference on Porphyrins and Phthalocyanines, ICPP-11 virtual meeting, 26 June – 2 July 2021. [ufs-042510](#)
44. **Conradie, J., Swarts, P.J.** (2021) - Poster Synthesis, Electrochemical and DFT Study of an Electron Rich Subphthalocyanine, 11th International Conference on Porphyrins and Phthalocyanines, ICPP-11 virtual meeting, 26 June – 2 July 2021, Symposia 01. SubPcs, SubPzs, SubPors and Related Contracted Porphyrinoids, poster S01-P-001 July, 2021. (Accredited), Book of Abstracts p 9: talk BST-04. [ufs-042511](#)
45. **Conradie, J., von Eschwege, K.G.** (2021) Poster, DFT Studies of Redox Tendencies observed in a Phenyl-substituted Tetraphenylporphyrin Series, 11th International Conference on Porphyrins and Phthalocyanines, ICPP-11 virtual meeting, 26 June – 2 July 2021, Symposia 17. Optical, Electrical and Optoelectronic Phenomena in Porphyrins and Phthalocyanines poster S17-P-007 . [ufs-042512](#)

46. **Chiyindiko, E., Conradie, J.** (2021) Poster, Practical Chemistry during a Pandemic: from lab to laptop, International Symposium of Microscale Chemistry (ISMC2021) and the RSC Secondary and Further Education Group Conference, Practical Chemistry during a Pandemic including a microscale approach, 6th conference, 13-14 July 2021, online, United Kingdom. [ufs-042513](#)
47. **Akpmie K.G, Ezeofor C.C, Conradie J.** (2021) ZnO nanoparticle impregnated biomass sorbent for the adsorption of celestine blue: thermodynamics, isotherm, kinetics and reusability. The 4th African conference/workshop on applications of nanotechnology to energy, environment, agriculture and health. Nanotechnology: A Springboard for National Development, University of Nigeria, Nsukka, 19th – 23rd July, 2021. (Accredited). Book of Abstracts p 10: talk BGD 02. [ufs-042514](#)
48. **Malloum, A., Conradie J.** (2021) Oral presentation, Non-covalent interactions in thiophene clusters and furan clusters, International FreeStatePhyChem-2021 Symposium, University of the Free State, Bloemfontein, South Africa, 28 Oct 2021; abstract: P1. [ufs-042522](#)
49. **Akpmie K.G, Conradie J.** (2021) Oral presentation, 1st place for best student speaker, Experimental and DFT investigations on the ultrasonic-aided adsorption of anionic and cationic dyes onto low-temperature derived biochar, International FreeStatePhyChem-2021 Symposium, University of the Free State, Bloemfontein, South Africa, 28 Oct 2021; abstract: P2. [ufs-042523](#)
50. **Mogale, R., Akpmie K.G, Conradie J., Langner, E.** (2021) Oral presentation, 2nd place for best student speaker, Dye adsorption of aluminium- and zirconium-based metal organic frameworks with azobenzene dicarboxylate linkers, International FreeStatePhyChem-2021 Symposium, University of the Free State, Bloemfontein, South Africa, 28 Oct 2021; abstract: P5 [ufs-042524](#)
51. **Chiyindiko, E.** (2021) Breaking the walls of darkness, Falling Walls Science Summit 7–9 Nov 2021, Berlin, 2nd place for “Breakthrough of the year in the emerging talents category”. [ufs-042525](#)
52. **Mateyise, N.G.S., Conradie, M.M., Conradie, J.** (2021) Poster, DFT and kinetic study of the oligothiophene-containing rhodium model catalysts, RSC/SACI Young Chemists’ Symposium 2021 (YCS), online, 8-9 July 2021. South Africa. Abstract book p 59. [ufs-042526](#)
53. **Mtshali, Z., von Eschwege, K. G., Conradie, J.** (2021) Poster, functionalised polyridine manganese (II) complexes probed with DFT and cyclic voltammetry, RSC/SACI Young Chemists’ Symposium 2021 (YCS), online, 8-9 July 2021. South Africa. Abstract book p 72. [ufs-042527](#)
54. **Da-yang, T.E., Fifen, J.J., Dhaouadi, Z. Nsangou, M, Conradie J.** (2021) Oral presentation, Structures of the solvated copper (II) in methanol at various temperature, Prochaines Journées Scientifiques de la Faculté des Sciences (Scientific Days of the Faculty of Sciences), Faculté des Sciences - Université de Maroua, Cameroon, 15 - 17 April 2021. [ufs-042528](#)

55. **Amaku, J.F., Ogundare, S., Akpomie, K.G., Ibeji, C.U., Conradie, J.** (2021) MWCNTs-quartzite nanocomposite coated with Dacryodes edulis stem bark extract for the attenuation of hexavalent chromium. Nanotechnology: A Springboard for National Development, University of Nigeria, Nsukka, 19th – 23rd July, 2021. (Accredited), Book of Abstracts p 9: talk BST-04. [ufs-042529](#)
56. **Malloum, A., Conradie, J.** (2021) CHPC Micro Talks – Professional, DMSO Clusters: Non-Covalent Interactions and DFT Benchmarking, CHPC National Conference 2021. 1-3 December 2021, online, South Africa. [ufs-042533](#)
57. **Khokho, E.C.Y., Nya, F.T., Malloum, A., Conradie, J.** (2021) CHPC Micro Talks MSc/Hons. Students, Computational study of the electronic and nonlinear optical properties of the molecules diphenanthro [3,4,5,6-efghi:3',4',5',6'-uvabc] ovalene and tribenzo [jk. mn.pq] dibenzo [5.6:7,8] pentapheno [2,1,14,13,12-stuvabcd]: influence of potassium functionalization, CHPC National Conference 2021. 1-3 December 2021, online, South Africa. [ufs-042536](#)
58. **Bouba, M.O., Nya, F.T., Malloum, A., Conradie, J.** (2021) CHPC Micro Talks – PhD Students, DFT, TDDFT and CCSD(T) predictions of electronic structure and optical properties of large molecular structures: a huge challenge for the CHPC, CHPC National Conference 2021. 1-3 December 2021, online, South Africa. [ufs-042537](#)
59. **Foadina, C.S.T, Nya, F.T., Malloum, A., Conradie, J.** (2021) CHPC Micro Talks – PhD Students, Computational study of increasing absorption capacity, optical and non-linear optical properties of graphene oxide molecule, CHPC National Conference 2021. 1-3 December 2021, online, South Africa. [ufs-042538](#)
60. **Teimouri, S., Potgieter, J.H., Conradie, J.** (2021) CHPC Micro Talks – PhD Students, DFT Modelled Deep Eutectic Solvent (DES) – Pyrite interactions, CHPC National Conference 2021. 1-3 December 2021, online, South Africa. [ufs-042539](#)
61. **Moskaleva, L., Li, Y., Li, S., Ivanova-Shor, E., Bäumer, M.** (2021) Ceria nanoparticle supported on Au(111) as a model for inverse catalysis. An ab initio molecular dynamics study of the role of oxide-metal interface in catalytic reactions. (Oral Presentation) 31st Catalysis Society of South Africa (CATSA) Conference - Virtual, 7-10 November 2021. [ufs-042540](#)
62. **Carroll, L., Moskaleva, L.** (2021) Studying the wet and dry CO oxidation of nanoporous Au using static DFT Computations. (Poster). International Conference on Theoretical Aspects of Catalysis (ICTAC) Online Meeting 2021, 15, 22, 30 June 2021. [ufs-042541](#)
63. **Carroll, L., Moskaleva, L.** (2021) Studying the wet and dry CO oxidation of nanoporous Au using static DFT Computations. (Pre-Recorded Video Poster). SACI YCS2021 National Conference Online, 8-9 July 2021. [ufs-042543](#)
64. **Carroll, L., Moskaleva, L.** (2021) Studying the wet and dry CO oxidation of nanoporous Au using static DFT Computations. (Oral Presentation). FreeStatePhyChem Symposium, 28 October 2021, Bloemfontein, South Africa. [ufs-042544](#)

65. **Olaniyan, O., Moskaleva, L.** (2021) The reactivity of –O-Au-O- chain structures on the Au (321) surface with Ag impurities: a computational study. (Oral Presentation). FreeStatePhyChem Symposium, 28 October 2021, Bloemfontein, South Africa. [ufs-042545](#)
66. **Carroll, L., Moskaleva, L.** (2021) Studying the wet and dry CO oxidation of nanoporous Au using static DFT Computations and AIMD simulations. (Micro Talk). CHPC National Conference Online, 1-3 December 2021. [ufs-042546](#)
67. **Abraha, Y.W., Tsai, C-W., Langner, E.H.G.** (2021) Oral presentation, Rapid gram-scale synthesis of mixed-linker (Zn) ZIFs and their application in CO₂ adsorption and fixation, International FreeStatePhyChem-2021 Symposium, University of the Free State, Bloemfontein, South Africa, 28 Oct 2021; abstract: P6. [ufs-042796](#)
68. **Gawe, S., Langner, E.H.G.** (2021) Oral presentation, Post-synthetic ligand exchange of ZIF-8 and ZIF-67 nanoparticles to act as drug carriers, International FreeStatePhyChem-2021 Symposium, University of the Free State, Bloemfontein, South Africa, 28 Oct 2021; abstract: P7. [ufs-042797](#)
69. **Roodt, A.** (2021) Invited lecture. “And then there was AfCA (African Crystallographic Association)....” Joint virtual meeting of the AfLS3-2021: African Light Source and the ePCCr: Pan-African Conference on Crystallography (ePCCr). Hosted by X-TechLab, Cotonou, Benin. 15-19 November 2021. [ufs-043023](#)
70. **Redgard, S., Roodt, A., Venter, J.A.** (2021) Oral presentation. “CO₂ fixation using 5-coordinate Pt and Pd complexes and its anomalies”. RheManTec^{III}: “Solar Light-driven Homogeneous Catalysis for Greener Industrial Processes with H₂ as Energy Source and CO₂ as C1 Building Block”. Joint virtual seminar between UFS and UZH, SSAJRP IZLZS2_170856., South Africa & Switzerland. 28 May 2021. [ufs-043024](#)