

Faculty of Natural and Agricultural Sciences

Department of Chemistry

Conference Contributions 2022

1. **Azov, V.A., Hennecke, U., Martin, C., Ballet, S., De Beer, F.J., Mashweu, A.R. (Invited lecture).** (2022) Stabilizing peptide nano-structures using non-canonical amino acids with donors and acceptors. International Organic Chemistry Symposium, University of the Free State, Bloemfontein, 20 June 2022. **Ufs-044732**
2. **Mashweu, A.R., Azov, V.A.** (Oral presentation). (2022) Synthesis of unnatural amino acids with acceptor and donor moieties starting from asparagine and glutamine. International Organic Chemistry Symposium, University of the Free State, Bloemfontein, 20 June 2022. **Ufs-044733**
3. **De Beer, F.J., Bertouille, J., Mashweu, A.R., Martin, C., Ballet, S., Hennecke, U., Azov, V.A.**(Oral presentation). (2022) Incorporation of acceptor amino acids into an amphiphilic peptide sequence. International Organic Chemistry Symposium, University of the Free State, Bloemfontein, 20 June 2022. **Ufs-044734**
4. **Jacobs, F.J.F., De Beer, F.J, Kama, D.V., Azov, V.A.** (Poster). (2022) Chlorinated and iodinated alanine derivatives in the crystal phase: polar interactions vs. halogen bonds. International Organic Chemistry Symposium, University of the Free State, Bloemfontein, 20 June 2022. **Ufs-044736**
5. **De Beer, F.J, Azov, V.A.** (Poster). (2022) Synthesis of amino acids with donor and acceptor substituents by means of Pd-catalyzed coupling reactions. International Organic Chemistry Symposium, University of the Free State, Bloemfontein, 20 June 2022. **Ufs-044739**
6. **Tshehla, P.K., Azov, V.A.** (Poster) (2022) Synthesis of redox-responsive tetrathiafulvalene derivatives with amphiphilic properties to be used in soft materials. NanoAfrica2022, Cape Town, 26-28 October 2022. **Ufs-044740**
7. **Wilhelm, A., Ehlers, K., Bonnet, S.L.** (Oral Presentation) (2022) GABAergic and larval zebrafish locomotor activity of *Bolusanthus speciosus* and *Asparagus laricinus*. International Organic Chemistry Symposium, University of the Free State, Bloemfontein, 20 June 2021. **Ufs-044742**
8. **Makhathini, B., Bezuidenhoudt, B.C.B, Marais, C.** (Poster) (2022) Strategies towards the synthesis of a stilbene-related substituted γ -butenolide natural product. International Organic Chemistry Symposium, University of the Free State, Bloemfontein, 20 June 2021. **Ufs-044743**

9. **Purkait, K., Kapp, L.E., Schutte-Smith, M., Visser, H.G., Gasser, G.** (2022) *16th European Biological Inorganic Chemistry Conference (EuroBIC), 17-21 July 2022, Grenoble, France.* Poster presentation – ‘Exploring the structure-activity relationship of Rhenium(I)-tricarbonyl complexes of 1H-imidazo[4,5-f][1,10]phenanthroline derivatized ligands.’ **Ufs-046444**
10. **Oosthuizen, U., Visser, H.G., Schutte-Smith, M.** (2022) *SACI Central section Young Chemists Symposium, 19 August 2022, Virtual.* Oral presentation – ‘Study of Rhenium and Gold complexes as anticancer and anti-microbial agents.’ **Ufs-046445**
11. **Nzhadzhaba, N.N., Schutte-Smith, M., Visser, H.G.** (2022) *SACI Central section Young Chemists Symposium, 19 August 2022, Virtual.* Oral presentation – ‘Synthesis, characterising, luminescence and cytotoxicity of Rhenium(I) tricarbonyl complexes bearing N,N'- bidentate ligands.’ **Ufs-046446**
12. **Liebenberg, L., Visser, H.G., Schutte-Smith, M.** (2022) *SACI Central section Young Chemists Symposium, 19 August 2022, Virtual.* Poster presentation – ‘Alkylamino aurones and its rhenium(I) tricarbonyl complexes as potential anticancer agents.’ **Ufs-046447**
13. **van Staden, C., Schutte-Smith, Kama, D.V., Visser, H.G.** (2022) *SACI Central section Young Chemists Symposium, 19 August 2022, Virtual.* Poster presentation – ‘Argentophilic vs. Auophilic Interactions in Identical Dimeric Diphosphine Complexes.’ **Ufs-046449**
14. **Liebenberg, L., Visser, H.G., Schutte-Smith, M.** (2022) *SACI National Young Chemist Symposium, 3-4 October 2022.* Poster presentation – ‘The synthesis and evaluation of a series of aminoaurone derivatives and its rhenium(I) tricarbonyl complexes as possible pharmaceutical agents.’ **Ufs-046450**
15. **Oosthuizen, U., Schutte-Smith, M, Visser, H.G.** (2022) *SACI National Young Chemist Symposium, 3-4 October 2022.* Poster presentation – ‘Photoluminescence of Rhenium(I)tricarbonyl complexes and its preliminary anti-microbial activity.’ **Ufs-046451**
16. **Nzhadzhaba, N.N., Schutte-Smith, M., Visser, H.G.** (2022) *SACI National Young Chemist Symposium, 3-4 October 2022.* Oral presentation – ‘Synthesis, characterisation, luminescence and cytotoxicity of Rhenium and it's N,N'- bidentate ligands.’ **Ufs-046452**
17. **van Staden, C., Schutte-Smith, M., Moskaleva, L., Kama, D.V., Visser, H.G.** (2022) *SACI National Young Chemist Symposium, 3-4 October 2022.* Oral presentation – ‘Development of the T-angle as a solid state cone angle for the quantification of the steric bulk in bis(diphenylphosphino)amine gold(I) complexes.’ **Ufs-046453**
18. **Makhathini, B.T., Bezuidenhoudt, B.C.B., Marais, C.** (2022) Poster Strategies towards the synthesis of a stilbene-related substituted γ -butenolide natural product; International Organic Chemistry Symposium, University of the Free State, Bloemfontein, 20 June 2022. **Ufs-046455**
19. **van Dyk, H., Brink, A., Mokolokolo, P.P., Jacobs, F.J.F., Kroon, R.E., Makhafola, T.J.** (2022). Synthesis, Characterization & Biological Activity of Functionalized Salicylidene Compounds. (Poster). UFS-VUB Joint International Organic Chemistry Symposium 2022. 20 June 2022, Bloemfontein, South Africa. **Ufs-046457**

20. **van Dyk, H., Brink, A., Mokolokolo, P.P., Jacobs, F.J.F., Kroon, R.E., Makhafola, T.J.** (2022). Nitro Salicylidene Compounds: Cytotoxicity, luminescence, and structural manipulation of model *N,O* bifunctional chelators. (Poster). SACI National Young Chemists' Symposium (Virtual). 3-4 October 2022, Johannesburg, South Africa. **Awarded: First Place in the MSc Poster Presentation category. Ufs-046458**
21. **Bosman, L., Kama, D.V., Brink, A.** (2022) Rhodium(I) complexes as model catalysts for methanol carbonylation. (Poster). SACI National Young Chemists' Symposium (Virtual). 3-4 October 2022, Johannesburg, South Africa. **Ufs-046464**
22. **Jacobs, F.J.F., Brink, A.,** (2022). Rhenium organometallic complexes in proteins for targeted cancer treatment. (Oral presentation) The Legacy of START: Synchrotron Techniques for African Research and Technology. 6-8 October 2022, Cape Town, South Africa. **Ufs-046465**
23. **Jacobs, F.J.F., Brink, A.,** (2022). Small organic to protein - molecular trends applicable to radiopharmaceutical development. (Oral presentation) International Organic Chemistry Symposium. 20 June 2022, Bloemfontein, South Africa. **Ufs-046466**
24. **Jacobs, F.J.F., Brink, A.,** (2022). Klein organometaalverbindinge na proteïne - die geheim van molekules in fundamentele kristalruimtes. (Oral presentation) Studentesimposium in die Natuurwetenskappe. 3-4 November 2022, Pretoria, South Africa. **Ufs-046467**
25. **Bosman, L., Kama, D.V., Brink, A.** (2022) Schiff base Rhodium(I) complexes as model catalysts for homogeneous catalysis. (Poster). International FreeStatePhyChem-2022 Symposium. 18 November 2022, Bloemfontein, South Africa. **Ufs-046468**
26. **Kama, D.V., Brink, A., Alberto, R., Roodt, A.** (2022) The hidden versatility of diphosphinoamine chelating ligands. (Oral presentation). International Organic Chemistry Symposium, University of the Free State, Bloemfontein, 20 June 2022. **Ufs-046469**
27. **Jacobs, F.J.F., De Beer, F.J., Kama, D.V., Azov, V.A.** (2022) Chlorinated and iodinated alanine derivatives in the crystal phase: polar interactions vs. halogen bonds. (Poster). International Organic Chemistry Symposium, University of the Free State, Bloemfontein, 20 June 2022. **Ufs-04671**
28. **Brink, A.** (2022) Invited Seminar Lecture: A Complex Journey for a Multi-nuclear Theranostic Agent. (2022). Joint live/virtual seminar lecture: Cambridge Crystallographic Data Centre (CCDC), Cambridge University, United Kingdom, 23 June 2022. **Ufs-046470**
29. **Brink, A.,** (2022). Exploring Rabbit-holes for the Wonderland of Radiopharmaceuticals. (Oral). Conference of the Department of Higher Education and Training: National Collaboration Project: Future Professors Programme Phase One. Stellenbosch University, 3-6 November 2022. **Ufs-046472**
30. **Moskaleva, L.V., Carroll, L.L., Olaniyan, O., Li, S.** (2022) Formation and catalytic activity of 1D chains of gold oxide from density functional theory. (Keynote lecture). 32th Annual Conference of the Catalysis Society of South Africa (CATSA). 13 – 16 November 2022, Champagne Sports Resort, Central Drakensberg, South Africa. **Ufs-046480**

31. **Moskaleva, L.V.** (2022) Ab initio molecular dynamics study of the role of oxide-metal interface in catalytic reactions. (Invited lecture). COSYES Summer Meeting, June 2-3, 2022, Madrid, Spain. [Ufs-046484](#)
32. **Moskaleva, L.V.** (2022) Computational Studies of Oxidation Catalysis on nanoporous Gold. (Invited lecture). Symposium of the Research Unit NAGOCAT, May 30-June 1, 2022, Soderstorf, Germany. [Ufs-046486](#)
33. **Cele, S.A., Matthews, C., Moskaleva, L.V.** (2022) Computational modelling of the prototypical photocatalyst: a zeolite encapsulated TiO₂-supported Cu₅ cluster. (Poster). 32th Annual Conference of the Catalysis Society of South Africa (CATSA). 13 – 16 November 2022, Champagne Sports Resort, Central Drakensberg, South Africa. [Ufs-046487](#)
34. **Cele, S.A., Matthews, C., Moskaleva, L.V.** (2022) Computational modelling of the prototypical photocatalyst: a zeolite encapsulated TiO₂-supported Cu₅ cluster. (Poster). FreeState PhyChem-2022 Symposium. 18 November 2022. Bloemfontein, South Africa. [Ufs-046489](#)
35. **Cele, S.A., Matthews, C., Moskaleva, L.V.** (2022) Computational modelling of the prototypical photocatalyst: a zeolite encapsulated TiO₂-supported Cu₅ cluster. (Microtalk). CHPC 2022: Centre for High Performance Computing 2022 National Conference. 30 November – 02 December 2022, Pretoria, South Africa. [Ufs-046491](#)
36. **Otukile, K., Kandpal, S., Matthews, C., Chakraborty, S., Moskaleva, L., Ramakrishnan, R.** (2022) DFT vs. Composite Methods: Search for an Accurate and Inexpensive Approach to Generate a Database of Energies and Rate Constants of Combustion Reactions. (Poster). Psi-k 2022. 22-25 August 2022, Lausanne, Switzerland. [Ufs-046492](#)
37. **Otukile, K., Kandpal, S., Matthews, C., Chakraborty, S., Moskaleva, L., Ramakrishnan, R.** (2022) Performance of DFT and Composite Methods on the Hydrocarbon and Molecular Oxygen Reactions Thermodynamics and Kinetics. (Poster). 32th Annual Conference of the Catalysis Society of South Africa (CATSA). 13-16 November 2022, Champagne Sports Resort, Central Drakensberg, South Africa. [Ufs-046493](#)
38. **Otukile, K., Kandpal, S., Matthews, C., Chakraborty, S., Moskaleva, L., Ramakrishnan, R.** (2022) Accurate Thermochemistry of Selected Hydrocarbon Combustion Reactions by DFT and Composite Quantum Chemistry Methods. (Oral). FreeStatePhyChem2022 Physical and Theoretical Chemistry, 18 November 2022, University of the Free State, South Africa. [Ufs-046494](#)
39. **Carroll, L., Moskaleva, L.** (2022) Computational modelling of catalysis on nanoporous gold: Self-organisation and reactivity of surface oxygen using AIMD simulations. (Oral Presentation). Psi-k 2022 Conference, 22-25 August 2022, Lausanne, Switzerland. [Ufs-046496](#)
40. **Carroll, L., Moskaleva, L.** (2022) Self-organization of oxygen atoms and restructuring of Au(221), with and without Carbon Monoxide. (Oral Presentation). CAMOM 2022 Conference (Online & In-Person Hybrid Conference), 19-21 September 2022, Online. [Ufs-046497](#)
41. **Carroll, L., Moskaleva, L.** (2022) Nanoporous gold catalysis modelling: Self-organisation and reactivity of surface oxygen using AIMD simulations. (Oral Presentation). Nano Africa Conference 2022, 26-28 October 2022, Cape Town, South Africa. [Ufs-046498](#)

42. **Carroll, L., Moskaleva, L.** (2022) Studying the self-organization of oxygen atoms on stepped model nanoporous gold surfaces with and without additional adsorbates. (Oral Presentation). FreeStatePhyChem Symposium, 18 November 2022, Bloemfontein, South Africa. **Ufs-046500**
43. **Olaniyan, O., Moskaleva, L.V.** (2022) Electrocapillary coupling coefficient of Au(221) with adsorbed oxygen atoms: a first-principles study. (Oral Presentation). FreeStatePhyChem Symposium, 18 November 2022, Bloemfontein, South Africa. **Ufs-046502**
44. **Olaniyan, O., Carrol, L., Li, S., Loginova, A., Moskaleva, L.V.** (2022) Static and dynamic DFT study of CO oxidation by O chains on gold and determination of electrocapillary Coupling Coefficient for Au(111) with adsorbed O atoms. (Poster). Symposium of the Research Unit NAGOCAT, May 30-June 1, 2022, Soderstorf, Germany. **Ufs-046502**
45. **Matthews, C., Van Staden, C., Kroon, R.E., Moskaleva, L.V., Otukile, K.P., Kama, D.V., Schutte-Smith, M., Visser, H.G.** (2022) A Python script for evaluating 3D 'Tolman cone angle'-based steric descriptors of N-substituents and their modulation of the Au..Au distance of dinuclear gold complexes with PNP-ligands. (Oral Presentation). FreeStatePhyChem Symposium, 18 November 2022, Bloemfontein, South Africa. **Ufs-046504**
46. **Matthews, C.** (2022) Energy and charge density analysis of non-covalent interactions within conformers of bis(2-pyridylmethyl)amine, using ab initio coupled-cluster and MP2 theory: a molecular tailoring approach. (Microtalk). CHPC 2022: Centre for High Performance Computing 2022 National Conference. 30 November – 02 December 2022, Pretoria, South Africa. **Ufs-046505**
47. **Von Eschwege, K. G., Conradie, J.** (2022) DFT and Electrochemistry. (Oral Presentation). FreeStatePhyChem Symposium, 18 November 2022, Bloemfontein, South Africa. **Ufs-046506**
48. **Mashweu, A.R, de Beer, F.J., Bertouille, J., Martin, C., Ballet, S., Hennecke, U., V. Azov, V.A.** (2022) "P-STAC: Stabilizing Peptide NanoStructures with Tetrathiafulvalene-based Donors and Acceptors" Poster, *24th Merck Organic Chemistry Symposium (MOCS)*, Blankenberge, Belgium, 1–2.12.2022; abstract: P45. **Ufs-046507**
49. **Mzinjani, V., Azov, V.A., Langner, E.H.G.** (2022) "Amphiphile-coated magnetic iron oxide nanoparticles for the extraction of contaminants from the aqueous media" Poster, *FreeStatePhyChem-2022*, Bloemfontein, South Africa, 18.11.2022; abstract: PR7. **Ufs-046508**
50. **de Beer, F.J., Azov, V.A.,** (2022) "Synthesis of Amino Acids with Donor and Acceptor Substituents utilising Pd-catalyzed coupling reactions" Oral presentation, *CATSA 2022*, Drakensberg, South Africa, 13–16.11.2022; abstract: OP 14. **Ufs-046509**
51. **Roodt, A. Venter, J.A. and Redgard, S.** (2022). *NMR, Kinetic-mechanistic and SC-XRD study of carbon dioxide capturing model molecular materials.* (Poster), 33rd European Crystallographic Meeting (ECM33), 23-27 August 2022, Versailles, France. **Ufs-046527**
52. **Conradie, J.** (2022) Invited keynote. Redox Chemistry of Benzophenones, International Society of Electrochemistry (ISE). Regional Meeting in Prague, August 15th to 19th, 2022, Clarion Congress Hotel, Freyova 33, Prague, Czech. **Ufs-046529**

53. **Conradie, J., Mateyise, N.G.S., Conradie, M.M.** (2022) Redox Chemistry of Polypyridines (Poster). International Society of Electrochemistry (ISE), Regional Meeting in Prague, August 15th to 19th, 2022, Clarion Congress Hotel, Freyova 33, Prague, Czech. **Ufs-046530**
54. **Akporie, K.G., Ofomatah, A.C., Chukwuemeka-Okorie, H.O., Ani, J.U., Agbo, S.C., Odewole, O.A., Ojo, F.K., Alum, O.L., Conradie, J.** (2022) Equilibrium isotherm investigation on the sequestration of ciprofloxacin from solution via adsorption onto yam peel powder (Paper). 5th International Conference and Training Workshop on Energy for Sustainable Development in Africa (ICTWSEDA), 17 -19th May 2022, National Centre for Energy Research and Development, University of Nigeria Nsukka. **Ufs-046531**
55. **Malloum, A., Conradie, J.** (2022) Simulations of Aniline Adsorption: Solvent and Temperature effects, 1st International congress on Advanced Computational Modelling of Materials (CAMOM), 18 – 22 September 2022, University of Pretoria, South Africa (and online). **Ufs-046532**
56. **Teimouri, S., Potgieter, J.H., Billing, C., Conradie, J.** (2022) CHPC Micro Talks – PhD Students, Indium and Gallium Extraction Using Ionic liquids: Theoretical Investigation with DFT, Abstract ID: 9, CHPC National Conference. 30 November-2 December 2022, CSIR ICC in Pretoria (plus online), South Africa. **Ufs-046533**
57. **Khokho, E. C.Y., Nya, F.T., Malloum, A., Conradie, J.** (2022) CHPC Micro Talks – PhD Students, DFT calculation of the electronic, linear and non-linear optical properties of the 2,5,8,11,14,17-hexa-tert-butyl-hexa-peri-hexabenzocoronene molecule and its derivatives molecules functionalized with one and two potassium atoms: influence of doping, Abstract ID: 51, CHPC National Conference 2022. 30 November-2 December 2022, CSIR ICC in Pretoria (plus online), South Africa. **Ufs-046534**
58. **Mtshali, Z., Conradie, J.** (2022) CHPC Micro Talks – MSc Students, Computational calculations of tris(bipyridine)nickel molecules, using Density Functional Theory, Abstract ID: 20, CHPC National Conference 2022. 30 November-2 December 2022, CSIR ICC in Pretoria (plus online), South Africa. **Ufs-046535**
59. **Kenfack, G.M.D., Nya, F.T., Bouba, M.A., Malloum, A., Conradie, J.** (2022) CHPC Micro Talks – PhD Students, Optoelectrical, electronic and thermodynamic DFT study of a carbon nanoring and its derivative – HPC application as a computational chemistry resource, Abstract ID: 75, CHPC National Conference 2022. 30 November-2 December 2022, CSIR ICC in Pretoria (plus online), South Africa. **Ufs-046536**
60. **Conradie, J., Mateyise, N.G.S., Conradie, M.M.** (2022) CV and DFT of terpyridine ligands (Poster) 3rd Commonwealth Chemistry Posters, Royal Society of Chemistry online, 28-29 Sept 2022. **Ufs-046537**
61. **Mtshali, Z., von Eschwege, K.G., Conradie, J.** (2022) Redox behavior of first row group 7, 8 and 9 transition metal complexes containing substituted bipyridines and phenanthrolines. (Poster) 3rd Commonwealth Chemistry Posters, Royal Society of Chemistry online, 28-29 Sept 2022. **Ufs-046538**
62. **Conradie, J., von Eschwege, K.G.** (2022) Oral, DFT-simulated and experimental electrochemistry properties of the polypyridyl Row-1 Mn, Fe & Co, and Group-8 Fe, Ru and Os MLCT complexes, International FreeStatePhyChem-2022 Symposium, University of the Free State, Bloemfontein, South Africa, 18 Nov 2022. **Ufs-046540**

63. **Liebenberg, L., Visser, H.G., Schutte-Smith, M.** (2022). Oral presentation - 'Die sintese en evaluasie van 'n reeks amino-ouroonderivate en hul renium(I) trikarbonielkomplekse as moontlike antikankermiddels'. *Studentesimposium in die Natuurwetenskappe, 3-4 November 2022, Potchefstroom Virtueel*. **Ufs-046541**
64. **du Plessis, U., Visser, H.G., Schutte-Smith, M.** (2022). Oral presentation - 'Fotoluminesensie en die voorlopige toetsing van anti-mikrobiale aktiwiteit van Renium(I) trikarboniel komplekse en bimetaal verbindings'. *Studentesimposium in die Natuurwetenskappe 2022, 3-4 November 2022, Potchefstroom Virtueel*. **Ufs-046542**
65. **van Staden, C., Schutte-Smith, M., Moskaleva, L., Kama, D.V., Visser, H.G.** (2022) Oral presentation. 'Die ontwikkeling van die T-hoek as 'n metode vir die kwantifisering van die steriese massa in bis(difenielfosfien)amien goud(I) komplekse'. *Studentesimposium in die Natuurwetenskappe 2022, 3-4 November 2022, Potchefstroom Virtueel*. **Ufs-046543**
66. **Conradie, M.M.** (2022) Oral, Photophysical Properties of Tris(beta-diketonato)iron(III) Complexes - Influence of Aromatic Thienyl Groups., International FreeStatePhyChem-2022 Symposium, University of the Free State, Bloemfontein, South Africa, 18 Nov 2022. **Ufs-046549**
67. **Abraha Y.W., Tsai, C-W., Langner, E.H.G.** (2022) Scaleable synthesis of mixed-linker (Zn) ZIFs and their application in CO₂ adsorption and fixation. (Poster). 32th Annual Conference of the Catalysis Society of South Africa (CATSA). 13 – 16 November 2022, Champagne Sports Resort, Central Drakensberg, South Africa. **Ufs-046573**
68. **Abraha Y.W., Tsai, C-W., Langner, E.H.G.** (2022) " Scaleable synthesis of mixed-linker (Zn) ZIFs and their application in CO₂ adsorption and fixation" Poster, *FreeStatePhyChem-2022*, Bloemfontein, South Africa, 18.11.2022; abstract: PR8 **Ufs-046575**