

Faculty of Natural and Agricultural Sciences

Department of Chemistry

Conference Contributions 2020

1. **Wilhelm, A., Bonnet, S.L., Hering, S.** (2020) Establishing a locomotive zebrafish larvae bioassay using GABAA receptor modulators... Virtual 11th European Zebrafish Meeting 2020, Virtual, 26-27 October 2020. **ufs-038074**
2. **J. van der Merwe, C. Smith, M Vlok, Y. Powrie, H. Reuter, A Wilhelm, K. Swart.** (2020) Use of a larval zebrafish locomotor assay to identify and isolate GABA_A receptor modulators in *Ammocharis coranica*. Virtual Annual Academic Day, Faculty of Medicine & Health Sciences, Stellenbosch University, Tygerberg Campus, South Africa. 26-27 August 2020. **ufs-038447**
3. **Brink, A.** *The nuclearity manipulation of radiopharmaceuticals - how to bridge the CSD & PDB.* (Oral) Cambridge Crystallographic Data Center (CCDC) Global User Group Meeting, Cambridge University, UK, Virtual Zoom Meeting. 14 October 2020. **ufs-038475**
4. **Brink, A.** *Inorganic Chemistry to Protein - The advantages of tuneable radiation.* (Oral) BrightnESS2: Mini Symposium for Neutron Techniques, Stellenbosch University, South Africa, Virtual Zoom Meeting, 25 August 2020. **ufs-038477**
5. **Jacobs, FJF., Brink, A.** *From Radiopharmaceuticals to Potential H₂ /CO₂ Catalysts.* (Oral). Virtual Seminar between University of the Free State and University of Zurich, Conference grant code: SSAJRP IZLSZ2_170856, South Africa & Switzerland, August 19, 2020. **ufs-038478**
6. **Jacobs, FJF., Venter, G.J.S., Roodt, A., Brink, A.** *Understanding weak interactions of radiopharmaceuticals for use in macromolecular structures.* (Poster & Oral). ISXB-4 Virtual 2020: 4th International Symposium on Halogen Bonding, Stellenbosch University, South Africa, Virtual Meeting, 2-5 November 2020. **ufs-038480**
7. **Conradie, J., Swarts, P.** 2020 Poster. Influence of the Axial, Peripheral and Non-peripheral Substituents on the Redox Properties of Subphthalocyanines: an Electrochemical and DFT Study. The 71th Annual Meeting of the International Society of Electrochemistry. Belgrade Online, 31-Aug 2020 - 04-Sep 2020. <https://annual71.ise-online.org/index.php> contribution s15-011. **ufs-038581**

8. **Sibongile Mateyise, N.G.S, Conradie, M.M., Conradie, J.** 5 min student microtalk. HPC calculations to identify the correct DFT approach of the iodomethane oxidative addition to rhodium reaction. 14th CHPC National Conference. 30 Nov to 2 Dec 2020, Birchwood, South Africa. www.chpcconf.co.za. **ufs-038582**
9. **Mtshali, Z., von Eschwege, K.G., Conradie, J.** 5 min student microtalk. Density Functional Theory Calculations of Manganese-polypyridine Complexes. 14th CHPC National Conference. 30 Nov to 2 Dec 2020, Birchwood, South Africa. www.chpcconf.co.za. **ufs-038583**
10. **Chiyindiko, E., Conradie, J.** 5 min student microtalk. Exploring the reduction of benzophenones and electron distribution with High Performance Computing. 14th CHPC National Conference. 30 Nov to 2 Dec 2020, Birchwood, South Africa. www.chpcconf.co.za. **ufs-038584**
11. **Malloum, A., Conradie, J.** 10 min micro-talk Solvation Free Energy of the Proton in Acetonitrile. 14th CHPC National Conference. 30 Nov to 2 Dec 2020, Birchwood, South Africa. www.chpcconf.co.za. **ufs-038585**
12. **Akpomie, K.G., Odewole, O.A, Conradie, J.** One-Pot Synthesis and Characterization of an Inorganic-Organic Composite 27 (Zno@BM) For Oil Water Separation, International Virtual Conference of Organic Synthesis/Medicinal Chemistry Research Group Department of Pure and Industrial Chemistry, Faculty of Physical Sciences, University of Nigeria, Nsukka, 10-12 August 2020, Book of Abstracts p 27: talk SMC-18. **ufs-038586**
13. **Akpomie, K.G., Odewole, O.A, Conradie, J.** Synthesis and Characterization of a Magnetic-Organic Composite for Dye Adsorption 28, International Virtual Conference of Organic Synthesis/Medicinal Chemistry Research Group Department of Pure and Industrial Chemistry, Faculty of Physical Sciences, University of Nigeria, Nsukka, 10-12 August 2020, Book of Abstracts p 28: talk SMC-19. **ufs-038587**
14. **Malloum, A., Conradie, J.** 5 min Poster-talk, Water-Ammonia Proton Transfer Free Energy and Enthalpy, International FreeStatePhyChem-2020 Symposium, University of the Free State, Bloemfontein, South Africa, 30 October 2020; abstract: P3. Second prize in MSc category. fb.me/FreeStatePhyChem. **ufs-038588**
15. **Mtshali, Z., von Eschwege, K.G., Conradie, J.** 5 min Poster-talk, Electrochemical study of Tris(1,10-phenanthroline)manganese(II): effect of concentration and scan rate, International FreeStatePhyChem-2020 Symposium, University of the Free State, Bloemfontein, South Africa, 30 October 2020; abstract: P8. fb.me/FreeStatePhyChem. **ufs-038589**
16. **Chiyindiko, E., Conradie, J.** 5 min Poster-talk, Electrochemical study of benzophenones: effect of substituents and solvent, International FreeStatePhyChem-2020 Symposium, University of the Free State, Bloemfontein, South Africa, 30 October 2020; abstract: P9. Second prize in PhD category. fb.me/FreeStatePhyChem. **ufs-038590**
17. **Akpomie, K.G., Conradie J.,** 5 min Poster-talk, Ultrasonic assisted sorption of oil from oil-in-water emulsion onto *Ananas comosus* peel-silver nanocomposite, International FreeStatePhyChem-2020 Symposium, University of the Free State, Bloemfontein, South Africa, 30 October 2020; abstract: P10. Second prize in Post Doctoral category. fb.me/FreeStatePhyChem. **ufs-038591**

18. **Sibongile Mateyise, N.G.S, Conradie, M.M., Conradie, J.** 5 min Poster-talk, Kinetic study of a model catalyst: $[\text{Rh}((\text{C}_4\text{H}_3\text{S}-\text{C}_4\text{H}_2\text{S})\text{COCHCOF}_3)(\text{CO})(\text{PPh}_3)] + \text{CH}_3\text{I}$, International FreeStatePhyChem-2020 Symposium, University of the Free State, Bloemfontein, South Africa, 30 October 2020; abstract: P11. Second prize in MSc category. fb.me/FreeStatePhyChem. **ufs-038592**
19. **Alhadji Malloum and Jeanet Conradie**, Water-Ammonia Proton Transfer Free Energy and Enthalpy, Poster, African Physical Society (AfPS) International Conference, 18-20 November 2020, Trieste, Italy. Poster 04. <http://indico.ictp.it/event/9121/overview> . **ufs-038593**
20. **Dhlamini, K.S., Moskaleva L.** Computational study of carbon monoxide reactivity when adsorbed on a stepped Au(221) surface and interacting with water and oxygen species. (Oral) FreeStatePhyChem-2020 Symposium Online, University of the Free State, SA, Virtual Meeting. 30 October 2020. **ufs-038603**
21. **Dhlamini, K.S., Moskaleva L.** Computational study of carbon monoxide reactivity when adsorbed on a stepped Au(221) surface and interacting with water and oxygen species. (Oral) The South African Chemical Institute Young Chemists Symposium 2020, University of Johannesburg, SA, Virtual Meeting. 18 November 2020. (1st place among MSc student talks). **ufs-038604**
22. **Dhlamini, K.S., Moskaleva L.** Computational study of carbon monoxide reactivity when adsorbed on a stepped Au(221) surface and interacting with water and oxygen species. (Oral) 2020 CHPC National Conference, CHPC, SA, Virtual conference. 1-3 December 2020. **ufs-038606**
23. **Olaniyan, O., Moskaleva L.** Characterization of thermal properties of graphene and hexagonal boron nitride composite with alternating boron nitride and carbon chains: a first principles study. (Oral) FreeStatePhyChem-2020 Symposium Online, University of the Free State, SA, Virtual Meeting. 30 October 2020. **ufs-038615**
24. **Olaniyan, O., Moskaleva L.** Thermal properties of an intermediate two-dimensional material between graphene and hexagonal boron nitride: a first-principles study. (Oral) 2020 CHPC National Conference, CHPC, SA, Virtual conference. 1-3 December 2020. **ufs-038616**
25. **Van Staden, C., Kama, D.V., Moskaleva, L., Kroon, R.E., Schutte-Smith, M., Visser, H.G.** The Manipulation of Auophilic Interactions by Altering Phosphorous Based Ligand Systems. (Poster & Oral). ISXB-4 Virtual 2020: 4th International Symposium on Halogen Bonding, Stellenbosch University, South Africa, Virtual Meeting, 2-5 November 2020. **ufs-038617**
26. **Van Staden, C., Moskaleva, L., Kroon, R.E., Kama, D.V., Schutte-Smith, M., Visser, H.G.** Luminescent Au(I) Complexes with potential application for chemosensing and pollution treatment. (Oral) The South African Chemical Institute Young Chemists Symposium 2020, University of Johannesburg, SA, Virtual Meeting. 18 November 2020. (2nd place among PhD student talks). **ufs-038618**
27. **Mogale, R., Langner, E.H.G.,** The synthesis and characterisation of azobenzene dicarboxylate MOFs with different metal centers ($\text{M} = \text{Al}^{3+}, \text{Fe}^{3+}, \text{Zr}^{4+}, \text{Ti}^{4+}$) and their Application in Catalytic CO_2 Conversion, (Oral). 2020 CHPC National Conference, CHPC, SA, Virtual conference. 1-3 December 2020. **ufs-039324**

28. **Abraha, Y.W., Tsai, C-W., Niemantsverdriet, J.W., Langner, E.H.G.**, Ligand Exchanged ZIF-8 Derivatives with Greatly Improved CO₂ Adsorption Capacity, International FreeStatePhyChem-2020 Symposium, University of the Free State, Bloemfontein, South Africa, 30 October 2020; abstract: P 4. fb.me/FreeStatePhyChem. **ufs-039326**
29. **Masiu, M.P., Langner, E.H.G.**, Cytotoxicity studies of Ferrocenecarboxylic acid and cisplatin prodrug anchored on the surface of ZIF-8 nanoparticles, International FreeStatePhyChem-2020 Symposium, University of the Free State, Bloemfontein, South Africa, 30 October 2020; abstract: P 6. fb.me/FreeStatePhyChem. **ufs-039327**
30. **Mogale, R., Langner, E.H.G.**, The synthesis and characterisation of azobenzene dicarboxylate MOFs with different metal centers (M = Al³⁺, Fe³⁺, Zr⁴⁺, Ti⁴⁺) and their Application in Catalytic CO₂ Conversion, International FreeStatePhyChem-2020 Symposium, University of the Free State, Bloemfontein, South Africa, 30 October 2020; abstract: fb.me/FreeStatePhyChem. **ufs-039328**
31. **Belay, A.N., Venter, J.A. and Alexander, O.T.** 2020. *Crystal structure of 4-(dimethylamino)pyridin-1-ium-2,5-dichloro-3,6-dioxocyclohexa-1,4-diene-1,4-bis(olate) 4-dimethylaminopyridine(2:1) water undeca-solvate*. Poster presented at the 4th International Symposium on Halogen Bonding (ISXB4), Virtual Event, Hosted by Stellenbosch University, South Africa, 2-5 November 2020. **ufs-039853**