

Faculty of Natural and Agricultural Sciences

Department of Chemistry

Publications 2022

1. **von Eschwege, K.G, Conradie, J.** (2022). Review of DFT-simulated and experimental electrochemistry properties of the polypyridyl Row-1 Mn, Fe & Co, and Group-8 Fe, Ru and Os MLCT complexes. *Electrochemistry Communications* Vol, 136, 107225, 10.1016/j.elecom.2022.107225. Pg1-7 **Ufs-044129**
2. **Gomez-Arias, A., Yesares, L., Diaz, J., Caraballo, M. A., Maleke, M., Saez, R., van Heerden, E., Vermeulen, D., Nieto, J., Hernandez, C.J.** (2022). Mine waste from carbonatite deposits as potential rare earth resource: Insight into the Phalaborwa (Palabora) Complex. *Journal of Geochemical Exploration*, 232, 106884. 10.1016/j.jgexplo.2021.106884. Pg1-13 **Ufs-044130**
3. **Sinha, M.K., Jordaan, R., Purcell, W.** (2022). Hydrometallurgical Recovery of Manganese from Ferruginous Manganese Ore by Reductive-Acid Leaching with Sodium Dithionite. *Journal of Sustainable Metallurgy* 8:783–794, 10.1007/s40831-022-00529-5. **Ufs- 044131**
4. **Otunola, B.O, Aghoghowia, M.P, Thwala, M., Gómez-Arias, A., Jordaan, R., Hernandez, C.J, Ololade, O.O.** (2022). Influence of Clay Mineral Amendments Characteristics on Heavy Metals Uptake in Vetiver Grass (*Chrysopogon zizanioides* L.Roberty) and Indian Mustard (*Brassica juncea* L. Czern). *Sustainability*, 14(10), 5856; 10.3390/su14105856. **Ufs- 044133**
5. **Wilhelm, A., Bonnet, S.L., Twigge, L., Rarova, L., Stenclova, T., Visser, H.G., Schutte-Smith, M.** (2022). Synthesis, characterization and cytotoxic evaluation of chalcone derivatives. *Journal of Molecular Structure*, Vol 1251, 132001. 10.1016/j.molstruc.2021.132001. **Ufs-044134**
6. **Kapp, L.E., Schutte-Smith, M., Twigge, L., Visser, H.G.** (2022) Synthesis, characterization and DNA binding of four imidazo[4,5- f]1,10-phenanthroline derivatives. *Journal of Molecular Structure*, Vol 1247, 131235. 10.1016/j.molstruc.2021.131235. **Ufs-044136**
7. **Manicum, A.E., Schutte-Smith, M., Malan, F.P., Visser, H.G.** (2022) Steric and electronic influence of Re(I) tricarbonyl complexes with various coordinated β -diketones. *Journal of Molecular Structure*, Vol 1264, 133278. 10.1016/j.molstruc.2022.133278. **Ufs-044137**
8. **Schutte-Smith, M., Visser, H.G.** (2022) Crystal and molecular structures of *fac*-[Re(Bid)(PPh₃)(CO)₃] [Bid is tropolone (TropH) and tribromotropolone (TropBr₃H)]. *Acta Cryst.* C78, 351-359. 10.1107/S205322962200465X. **Ufs-044138**

9. **Swart, G., Fourie, E., Swarts, J.C.** (2022) Octakis(dodecyl)phthalocyanines: Influence of Peripheral versus Non-Peripheral Substitution on Synthetic Routes, Spectroscopy and Electrochemical Behaviour. *Molecules*, 27(5), 1529; <https://doi.org/10.3390/molecules27051529>. **Ufs-044140**
10. **Mogale, R., Akpomie, K.G., Conradie, J., Langner, E.H.G.** (2022) Dye adsorption of aluminium- and zirconium-based Metal Organic Frameworks with azobenzene dicarboxylate linkers. *Journal of Environmental Management*, 304, 114166, 10.1016/j.jenvman.2021.114166. **Ufs-044141**
11. **Foadin, C.S.T., Nya, F.T., Malloum, A., Conradie, J.** (2022) Enhancement of absorption capacity, optical and non-linear optical properties of graphene oxide nanosheet. *Journal of Molecular Graphics and Modelling* 111, 108075, 10.1016/j.jmgm.2021.108075. **Ufs-044142**
12. **Malloum, A., Conradie, J.** (2022) Structures, Binding Energies and Non-Covalent Interactions of Furan Clusters. *Journal of Molecular Graphics and Modelling* 111, 108102, 10.1016/j.jmgm.2021.108102. **Ufs-044143**
13. **Malloum, A., Conradie, J.** (2022) Structures, QTAIM Analysis Dataset for Non-Covalent Interactions in Furan Clusters. *Data in Brief* 40, 107766, 10.1016/j.dib.2021.107766. **Ufs-044151**
14. **Conradie, J.** (2022) Polypyridyl copper complexes as dye sensitizer and redox mediator for Dye-Sensitized Solar Cells (mini Review on invitation for Special Issue on: 'Electrocatalysis in energy conversion and storage systems'). *Electrochemistry Communications* 134, 107182 10.1016/j.elecom.2021.107182. **Ufs-044152**
15. **Malloum, A., Conradie, J.** (2022) Non-Covalent Interactions in Small Thiophene Clusters. *Journal of Molecular Liquids* 347, 118301, 10.1016/j.molliq.2021.118301. **Ufs-044153**
16. **Malloum, A., Conradie, J.** (2022) Potential Energy Surface of the Thiophene Pentamer and Non-Covalent Interactions. *International Journal of Quantum Chemistry*, 122 e26840. 10.1002/qua.26840. **Ufs-044154**
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18. **Malloum, A., Conradie, J.** (2022) Non-Covalent Interactions in Dimethylsulfoxide (DMSO) Clusters and DFT Benchmarking. *Journal of Molecular Liquids* 350, 118522. 10.1016/j.molliq.2022.118522. **Ufs-044156**
19. **Foadin, C.S.T., Nya, F.T., Malloum, A., Conradie, J.** (2022) Data of electronic, reactivity, optoelectronic, linear and non-linear optical parameters of doping graphene oxide nanosheet with aluminum atom. *Data in brief* 41, 107840. 10.1016/j.dib.2022.107840. **Ufs-044157**
20. **Adeniyi, J.N., Adebayo A. Adeniyi, A.A., Moodley, R., Nlooto, M., Ngcobo, M., Gomo, E., Conradie, J.** (2022) Unravelling the drugability of MSI2 RNA recognition motif (RRM) protein and the prediction of their effective antileukemia inhibitors from traditional herb concoctions. *Journal of Biomolecular Structure & Dynamics* 40 2516-2529. 10.1080/07391102.2020.1840442. **Ufs-044163**

21. **Amaku, J.F., Ogundare, S.A., Akpomie, K.G., Conradie, J.** (2022) *Pentaclethra macrophylla* stem bark extract anchored on functionalized MWCNT-spent molecular sieve nanocomposite for the biosorption of hexavalent chromium. *International Journal of Phytoremediation*, 24:3, 301-310, 10.1080/15226514.2021.1937930. **Ufs-044164**
22. **Mogale, R., Conradie, J., Langner, E.H.G.** (2022) *Trans–cis* Kinetic Study of Azobenzene-4,4'-dicarboxylic Acid and Aluminium and Zirconium Based Azobenzene-4,4'-dicarboxylate MOFs. *Molecules*, 27 1370. 10.3390/molecules27041370. **Ufs-044165**
23. **Ferreira, H., Conradie, M.M., Conradie, J.** (2022) Kinetic study of the oxidative addition reaction between methyl iodide and [Rh(imino- β -diketonato)(CO)(PPh)₃] complexes, utilizing UV/vis and IR Spectrophotometry, NMR spectroscopy and DFT calculations. *Molecules*, 27 1931. 10.3390/molecules27061931. **Ufs-044166**
24. **Malloum, A., Conradie, J.** (2022) Dimethylsulfoxide (DMSO) Clusters Dataset: DFT Relative Energies, Non-Covalent Interactions, and Cartesian Coordinates. *Data in brief* 42, 108024. 10.1016/j.dib.2022.108024. **Ufs-044167**
25. **Conradie, J., Vazquez-Lima, H., Alemayehu, A.B., Ghosh, A.** (2022) Comparing Isoelectronic, Quadruple-Bonded Metalloporphyrin and Metalloporphyrin Dimers: Scalar-Relativistic DFT Calculations Predict a > 1-eV Range for Ionization Potential and Electron Affinity. *ACS Phys. Chem Au* 2 2 70-78. 10.1021/acspchemau.1c00030. **Ufs-044168**
26. **Conradie, J., Alemayehu, A.B., Ghosh, A.** (2022) Iridium(VII)-Corrole Terminal Carbides Should Exist as Stable Compounds. *ACS Organic & Inorganic Au*, 2, 159. 10.1021/acscorginorgau.1c00029. **Ufs-044169**
27. **Chiyindiko, E., Langner, E.H.G., Conradie, J.** (2022) Electrochemical behaviour of 2-hydroxybenzophenones and related molecules. *Results in Chemistry* 4, 100332, Part of special issue: SI: *Advances in Electrochemistry*. 10.1016/j.rechem.2022.100332. **Ufs-044171**
28. **Conradie, J.** (2022) Redox chemistry of bis(terpyridine)manganese(II) complexes – a molecular view. *Journal of Electroanalytical Chemistry* 913, 116272. 10.1016/j.jelechem.2022.116272. **Ufs-044170**
29. **Conradie, J.** (2022) DFT Study of bis(1,10-phenanthroline)copper complexes: molecular and electronic structure, redox and spectroscopic properties and application to Solar Cells. *Electrochimica Acta* 418, 140276. 10.1016/j.electacta.2022.140276. **Ufs-044172**
30. **Conradie, J.** (2022) Redox chemistry of tris(β -diketonate)cobalt(III) complexes – a molecular View. *Journal of The Electrochemical Society*, 169 046522. 10.1149/1945-7111/ac6705. **Ufs-044173**
31. **Conradie, J.** (2022) Electronic and structural data of 4'-substituted bis(2,2';6'2''-terpyridine)manganese in *mono-, bis-, tris-* and *tetra-*cationic states from DFT calculations. *Data in Brief* 42, 108221. 10.1016/j.dib.2022.108221. **Ufs-044178**
32. **Amaku, J.F., Ogundare, S.A., Akpomie, K.G., Ngwu, C.M., Conradie, J.** (2022) Enhanced chromium (VI) removal by *Anacardium occidentale* stem bark extract-coated multiwalled carbon nanotubes. *International Journal of Environmental Science and Technology*, 19 4421– 4434. 10.1007/s13762-021-03364-5. **Ufs-044179**

33. **Chiyindiko, E., Langner, E.H.G., Conradie, J.** (2022), Electrochemical behaviour of copper(II) complexes containing 2-hydroxyphenones. *Electrochimica Acta* 424, 140629. 10.1016/j.electacta.2022.140629. **Ufs-044181**
34. **Da-yang, T.E., Fifen, J.J., Conradie, J. Conradie, M.M.** (2022) Structures, Temperature effect, Binding and Clustering Energies of $\text{Cu}^{2+}(\text{MeOH})_{n=1-8}$ clusters and extrapolations. *Journal of Molecular Liquids* 360, 119439. 10.1016/j.molliq.2022.119439. **Ufs-044183**
35. **Conradie, M.M.** (2022) UV-Vis Spectroscopy, Electrochemical and DFT Study of Tris(β -diketonato)iron(III) Complexes with Application in DSSC: Role of Aromatic Thienyl Groups. *Molecules*, 27(12), 3743; 10.3390/molecules27123743 **Ufs-044184.**
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37. **Mtshali, Z., von Eschwege, K.G., Conradie, J.** (2022) Redox Data of Tris(polypyridine)manganese(II) Complexes. *Data* 2022, 7(9), 130; 10.3390/data7090130. **Ufs-044363.**
38. **Messi, A.N., Bonnet, S.L., Owona, B.A., Wilhelm, A., Kamto, D.E., Ndongo, J.T., Siwe-Noundou, X., Poka, M., Demana, P.H., Krause, R. W. M., Mbing, J.N., Pegnyemb, D.E., Bochet, C.G.** (2022) In Vitro and In Silico Potential Inhibitory Effects of New Biflavonoids from *Ochna rhizomatosa* on HIV-1 Integrase and *Plasmodium falciparum*. *Pharmaceutics* 14, 1701, 1-17. 10.3390/pharmaceutics14081701. **Ufs-044388.**
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41. **Mphuthi, L.E., Maseme, M.R., Langner, E.H.G.** (2022) Ti(IV)-Exchanged Nano-ZIF-8 and Nano-ZIF-67 for Enhanced Photocatalytic Oxidation of Hydroquinone. *Journal of Inorganic and Organometallic Polymers and Materials*, 32 (7), pp. 2664-2678. 10.1007/s10904-022-02327-8. **Ufs-044396**
42. **Abraha, Y.W., Tsai, C.-W., Langner, E.H.G.** (2022) Scalable synthesis of mixed-linker (Zn) ZIFs and their application in CO_2 adsorption and fixation. *Journal of Porous Materials*. 10.1007/s10934-022-01326-x. **Ufs-044398**
43. **Pieterse, T., Marais, C., Bezuidenhout, B.C.B.** (2022) Ring-closing metathesis in flavonoid synthesis, part 1: flavenes. *Arkivoc, part v*, 98 – 113. 10.24820/ark.5550190. p011.733. **Ufs-044427**
44. **Pieterse, T., Marais, C., Bezuidenhout, B.C.B.** (2022) Ring-closing metathesis in flavonoid synthesis, part 2: neoflav-3-enes. *Arkivoc, part v*, 217 – 231. 10.24820/ark.5550190. p011.759. **Ufs-044428**

45. **Alebachew, N, Murthy, H.C., Bedassa Abdissa, Demissie, T.B., von Eschwege, K.G, Langner, E.H.G., Coetsee-Hugo, L.** (2022) Synthesis and characterization of CuO@S-doped g-C₃N₄ based nanocomposites for binder-free sensor applications†. *RSC Adv.*, 12, 29959–29974.1039/d2ra04752g. **Ufs-044550.**
46. **Khambule, S.P., Motlounge, S.V., Motaung, T.E., Koao, L.F., Kroon, R.E., Malimabe, M.A.** (2022) Tuneable blue to orange phosphor from Sm³⁺ doped ZnAl₂O₄ nanomaterials. *Results in Optics, Vol 9*, 100280, doi.org/10.1016/j.rio.2022.100280. **Ufs-044586**
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50. **Brink, A., Jacobs, F.J.F., Helliwell, J.R.** (2022) Trends in coordination of rhenium organometallic complexes in the Protein Data Bank. *IUCrJ.*, 9, 180-193, doi.org/10.1107/S2052252522000665. **Ufs-044705**
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53. **Ramorobi, L.M., Matowane, G.R., Mashele, S.S., Bonnet, S.L., Noreljaleel, A.E.M., Swain, S.S., Makhafola, T.J., & Chukwuma, C.I.** (2022). Bioactive synergism between zinc mineral and p-coumaric acid: A multi-mode glyceic control and antioxidative study. *Journal of Food Biochemistry*, 46(10), e14360. doi.org/10.1111/jfbc.14360 . **Ufs-044725**
54. **Matowane, G.R., Ramorobi, L.M., Mashele, S.S., Bonnet, S.L., Noreljaleel, A.E.M., Swain, S.S., Makhafola, T.J., Chukwuma, C.I.** (2022). Complexation potentiated promising anti-diabetic and anti-oxidative synergism between ZN(II) and ferulic acid: A multimode study. *Diabet Med.* 39(9): e14905. 10.1111/dme.14905. **Ufs-044726**
55. **X. Ma, M. Rohdenburg, H. Knorke, S. Kawa, J. K.-Y. Liu, E. Aprà, K. R. Asmis, V. A. Azov, J. Laskin, C. Jenne, H. I. Kenttämä, J. Warneke.** (2022) "Binding of saturated and unsaturated C₆-hydrocarbons to the electrophilic anion [B₁₂Br₁₁]⁻: a systematic mechanistic study" *Phys. Chem. Chem. Phys.* 24, 21759-21772. DOI: 10.1039/d2cp01042a. **Ufs-044727**

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57. **Moherane, L., Alexander, O.T., Schutte-Smith, M., Kroon, R.E., Mokolokolo, P.P., Biswas, S., Prince, S., Visser, H.G., Manicum, A.E.** (2022) Polypyridyl coordinated rhenium (I) tricarbonyl complexes as model devices for cancer diagnosis and treatment. *Polyhedron*, Vol 228, 116178. doi.org/10.1016/j.poly.2022.116178 **Ufs-044731**
58. **Moji, R.G., Motloug, S.V., Motaung, T.E., Koao, L.F.** (2022) Characterization of the incorporated SiO₂ co-doped with Sr²⁺ and Tb³⁺ phosphors into PLA polymer matrix. *Journal of Molecular Structure*, Vol 1263, 133176. doi.org/10.1016/j.molstruc.2022.133176. **Ufs-044737**
59. **Ferreira, H., Conradie, M.M., Conradie, J.** (2022) Redox behaviour of imino-β-diketonato ligands and their rhodium (I) complexes. *Results in Chemistry*, Volume 4, 100517. doi.org/10.1016/j.rechem. **Ufs-044744**
60. **Dennis, C.R., van Zyl, G.J., Fourie, E., Basson, S.S., Swarts, J.C.** (2022) The oxidation of the uranium(IV)tetrachloride by the octacyanotungstate(V)and the octacyanomolybdate(V) ions in perchloric acid medium: A kinetic study. *Reaction Kinetics, Mechanisms and Catalysis*. doi.org/10.1007/s11144-022-02297-5. **Ufs-044745**
61. **Boukar, O., Fifen, J.J., Malloum, A., Nsangou, M., Ghalila, H., Conradie, J.** (2022) Solvation energies of ferrous ion in methanol at various temperatures *Journal of Molecular Liquids* 360 (2022) 119460 .10.1016/j.molliq.2022.119460 **Ufs-044945**
62. **Chiyindikio, E., Langner, E.H.G., Conradie, J.** (2022) Cyclic voltammetry data of 2-hydroxybenzophenones and related molecules *Chemical Data Collections*, 100897 https://doi.org/10.1016/j.cdc.2022.100897 . **Ufs-044946**
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64. **Adegoke, K.A., Oyedotun, K.O., Ighalo, J.O., Amaku, J.F., Olisah, C., Adeola, A.O., Iwuozor, K.O., Akpomie, K.G., Conradie, J.** (2022) Cellulose derivatives and cellulose-metal-organic frameworks for CO₂ adsorption and separation, *Journal of CO₂ Utilization* 64 (2022) 102163 10.1016/j.jcou.2022.102163 **Ufs-044949**
65. **Iwuozor, K.O Akpomie, K.G., Conradie, J., Adegoke, K.A., Oyedotun, K.O., Ighalo, J.O. Amaku, J.F., Olisah, C., Adeola, A.O.** (2022) Aqueous phase adsorption of aromatic organoarsenic compounds: A review, *Journal of Water Process Engineering* *Journal of Water Process Engineering* 49 (2022) 103059 10.1016/j.jwpe.2022.103059 . **Ufs-044951**
66. **Malloum, A., Conradie, J.** (2022) Molecular Simulations of the Adsorption of Aniline From Waste-Water, *Journal of Molecular Graphics and Modelling* 117 (2022) 108287 10.1016/j.jm gm.2022.108287 . **Ufs-044953**
67. **Ighalo, J.O., Amaku, J.F., Olisah, C., Adeola, A.O., Iwuozor, K.O., Akpomie, K.G., Conradie, J., Adegoke, K.A., Oyedotun, K.O.** (2022) Utilisation of Adsorption as a Resource Recovery Technique for Lithium in Geothermal Water. *Journal of Molecular Liquids* 365 (2022) 120107 .10.1016/j.molliq.2022.120107 . **Ufs-045002**

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74. **Ishwarlall, T. Z.; Okpeku, M.; Adeniyi, A. A.; Adeleke, M. A.** (2022) The Search for a Buruli Ulcer Vaccine and the Effectiveness of the Bacillus Calmette–Guérin Vaccine. *Acta Trop.*, 228 (October 2021), 106323. 10.1016/j.actatropica.2022.106323. **Ufs-046298**
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