

## ***Faculty of Natural and Agricultural Sciences***

### ***Department of Chemistry***

#### **Publications 2019**

1. **Ntoi LLA, Alexander OT, Von Eschwege KG** (2019). Synthesis and kinetics of photochromic carboxy-substituted dithizonatophenyl mercury (II). *Journal of Photochemistry and Photobiology A-Chemistry*, 368 pp. 219 - 226... **ufs-032892**
2. **Tay A, Frogley B, Ware D, Conradie J, Ghosh A, Brothers P**(2019). Tetrahedral Pegs in Square Holes: Stereochemistry of Diboron Porphyrazines and Phthalocyanines *Angewandte Chemie-International Edition*, 58 (10), pp. 3057 - 3061... **ufs-034199**
3. **Ferreira H, Conradie-Bekker MM, Conradie J** (2019). Cyclic voltammetry data of polypyridine ligands and Co (II)-polypyridine complexes. *Data in Brief*, 22 pp. 436 - 445... **ufs-034227**
4. **Ngake, T.L., Potgieter, J.H. and Conradie, J.** (2019). Electrochemical behaviour of amino substituted  $\beta$ -amino  $\alpha,\beta$  unsaturated ketones: A computational chemistry and experimental study. *Electrochimica Acta*. 2019, 296, 1070-1082 DOI: 10.1016/j.electacta.2018.11.144 Elsevier <http://www.journals.elsevier.com/electrochimica-acta/> **ufs-034228**
5. **Adeniyi AA, Conradie J** (2019). Influence of substituents on the reduction potential and pKa values of  $\beta$ -diketones tautomers: A theoretical study. *Electrochimica Acta*, 297 pp. 947 - 960... **ufs-034234**
6. **Ferreira H, Conradie-Bekker MM, Conradie J** (2019). Electrochemical and electronic properties of a series of substituted polypyridine ligands and their Co (II) complexes. *Inorganica Chimica Acta*, 486 pp. 26 - 35. **ufs-034236**
7. **Conradie J, Conradie-Bekker MM, Mtshali Z, Van Der Westhuizen D, Tawfiq K, Al-Jeboori M, Coles S, Wilson C, Potgieter J** (2019). Synthesis, characterisation and electrochemistry of eight Fe coordination compounds containing substituted 2-(1-(4-R-phenyl-1H-1, 2, 3-triazol-4-yl) pyridine ligands, R=CH<sub>3</sub>, OCH<sub>3</sub>, COOH, F, Cl, CN, H and CF<sub>3</sub>. *Inorganica Chimica Acta*, 484 pp. 375 - 385... **ufs-034241**
8. **Conradie J** (2019). Jahn-Teller effect in high spin d<sub>4</sub> and d<sub>9</sub> octahedral metal complexes. *Inorganica Chimica Acta*, 486 pp. 193 - 199... **ufs-034264**
9. **Ghosh A, Conradie J** (2019). Stereochemistry of Transition-Metal Dinitrosyl Complexes. A Molecular Orbital Rationale for the Attracto and Repulso Conformations. *Inorganic Chemistry*, 58 pp. 5943 - 5948... **ufs-034269**

10. **Conradie J, Brothers P, Ghosh A** (2019). Main-Group-Element Isophlorin Complexes Revisited: The Question of a Subvalent Central Atom Inorganic Chemistry, 58 pp. 4634 - 4640.. [ufs-034274](#)
11. **Chiyindiko E, Conradie J** (2019). Redox behaviour of bis ( $\beta$ -diketonato) copper (II) complexes. Journal of Electroanalytical Chemistry, 837 pp. 76 - 85... [ufs-034282](#)
12. **Adeniyi AA, Conradie J** (2019). Computational insight into the contribution of para-substituents on the reduction potential, proton affinity, and electronic properties of nitrobenzene compounds. Journal of Molecular Modeling, 25 (3), pp. 78-1 - 78-20... [ufs-034287](#)
13. **Twigge L, Swarts JC, Conradie J** (2019).  $^{103}\text{Rh}$  NMR shifts of RHI- $\beta$ -diketonato and RHI- $\beta$ -aminoketonato complexes influenced by different substituents. Polyhedron, 169 pp. 14 - 23... [ufs-034296](#)
14. **Zhuang Z, Li Y, Huang J, Li Z, Zhao K, Zhao J, Xu L, Zhou L, Moskaleva L, Mai L**(2019). Sisyphus effects in hydrogen electrochemistry on metal silicides enabled by silicene subunit edge. Science Bulletin, 64 pp. 617 - 624... [ufs-034342](#)
15. **Šulce A, Nico M, Azov V, Kunz S** (2019). Molecular Insights into the Ligand-Reactant Interactions of Pt Nanoparticles Functionalized with  $\alpha$ -Amino Acids as Asymmetric Catalysts for  $\beta$ -Keto Esters. Chemcatchem, 11 pp. 2732 -2742... [ufs-034432](#)
16. **Malloum A, Fifen J, Conradie J** (2019). Exploration of the potential energy surface of the ethanol hexamer. Journal of Chemical Physics, 150 pp. 124308-1 - 124308-8... [ufs-034437](#)
17. **Syafni N, Moradi-Afrapoli F, Danton O, Wilhelm A, Stadler M, Hering S, Potterat O, Hamburger M** (2019). HPLC-Based Activity Profiling for GABAA Receptor Modulators In *Murraya exotica*. Natural Product Communications, 14 (1), pp. 41 - 45... [ufs-034467](#)
18. **Schutte-Smith M, Roodt A, Visser HG** (2019). Ambient and high-pressure kinetic investigation of methanol substitution in fac [Re (Trop) (CO)  $_3$ (MeOH)] by different monodentate nucleophiles. Dalton Transactions, 48 pp. 9984 - 9997... [ufs-034468](#)
19. **Jansen Van Vuuren L, Visser HG, Schutte-Smith M** (2019). Crystal structure of 2-(methylamino) tropone. Acta Crystallographica Section E: Crystallographic Communications, E75 pp. 1128 - 1132... [ufs-034474](#)
20. **Smit JBM, Marais C, Malan F, Bezuidenhoudt BCB** (2019). Crystal structure of (2,4-dimethoxybenzyl) triphenylphosphonium trifluoroacetate— trifluoroacetic acid (1/1), C $_{31}\text{H}_{27}\text{F}_6\text{O}_6\text{P}$ . Zeitschrift Fur Kristallographie-New Crystal Structures, 234 (4), pp. 621 - 623...[ufs-034479](#)
21. **Du J, Yong L, Liu H, Shi W, Moskaleva L, Cheng P** (2019). Formation of One-Dimensional Coordination Chains for High Performance Anode Materials of Lithium-Ion Batteries via a Bottom-Up Approach. ACS Applied Materials & Interfaces, 11 pp. 25863 - 25869... [ufs-034490](#)
22. **Smit JBM, Marais C, Malan F, Bezuidenhoudt BCB** (2019). Crystal structure of 3-(4-methoxyphenyl)-1-phenylprop-2-yn-1-one, C $_{16}\text{H}_{12}\text{O}_2$ . Zeitschrift für Kristallographie, 234 (2), pp. 359 - 360... [ufs-032877](#)
23. **Conradie J, Foroutan-Nejad C, Ghosh A** (2019). Norcorrole as a Delocalized, Antiaromatic System. Scientific Reports, 9 (4852), pp. 1 - 6... [ufs-034301](#)

24. **Kimberly A, Coleman C, Mei W, Bharathi A, Bonnet SL, Lindsey L, Bridget D, Boon P, Ferreira D** (2019). Structural Characterization of Cranberry Arabinoxylglucan Oligosaccharides. *Journal of Natural Products*, 82 pp. 606 - 620... [ufs-034343](#)
25. **Mayer M, van Lessen v, Rohdenburg M, Hou G, Yang Z, Exner R, Apra E, Azov V, Grabowsky S, Xantheas S, Asmis K, Wang X, Jenne C, Warneke J** (2019). Rational design of an argon-binding superelectrophilic anion. *Proceedings of the National Academy of Sciences of the United States of America*, 116 pp. 8167 - 8172... [ufs-034360](#)
26. **Noreljaleel AEM, Wilhelm A, Van Der Westhuizen JH, Bonnet SL** (2019). Analysis of commercial proanthocyanidins. Part5: A high-resolution mass spectrometry investigation of the chemical composition of sulfited wattle (*Acacia mearnsii* De Wild.) bark extract. *Phytochemistry*, 162 pp. 109 - 120... [ufs-034370](#)
27. **Dennis CR, Potgieter IJM, Langner EHG, Fourie E, Swarts JC** (2019). The oxidation of acetaldehyde by the octacyanomolybdate (V) ion in an aqueous alkaline medium. *Transition Metal Chemistry*, 44 pp. 161 - 165... [ufs-034374](#)
28. **Manicum AE, Schutte-Smith M, Alexander OT, Twigge L, Roodt A, Visser HG** (2019). First kinetic data of the CO substitution in fac-[Re(L,L'-Bid)(CO)<sub>3</sub>(X)] complexes (L,L'- Bid=acetylacetonate or tropolonate) by tertiary phosphines PTA and PPh<sub>3</sub>: Synthesis and crystal structures of water-soluble rhenium(I) tri- and dicarbonyl complexes with 1,3,5-triaza-7-phosphaadamantane (PTA). *Inorganic Chemistry Communications*, 101 pp. 93 - 98... [ufs-034386](#)
29. **Dononelli W, Tomaschun g, Kluner T, Moskaleva L** (2019). Understanding Oxygen Activation on Nanoporous Gold. *ACS Catalysis*, 9 pp. 5204 - 5216... [ufs-034393](#)
30. **Purcell W, Sinha MK** (2019). Reducing agents in the leaching of manganese ores: A Comprehensive review. *Hydrometallurgy*, 187 pp. 168 - 186... [ufs-034452](#)
31. **Schutte-Smith M, Roodt A, Alberto R, Twigge L, Visser HG, Kirsten L, Koen R** (2019). Structures of rhenium (I) complexes with 3-hydroxyflavone and benzhydroxamic acid as O, O'-bidentate ligands and confirmation of  $\pi$ -stacking by solid-state NMR spectroscopy. *Acta Crystallographica Section C-Structural Chemistry*, C75 pp. 378 - 387... [ufs-034481](#)
32. **Van Der Westhuizen D, Von Eschwege KG, Conradie J** (2019). Electrochemistry and spectroscopy of substituted [Ru(phen)<sub>3</sub>]<sup>2+</sup> and [Ru(bpy)<sub>3</sub>]<sup>2+</sup> complexes. *Electrochimica Acta*, 320 pp. 134540-1 - 134540-9... [ufs-034500](#)
33. **Boukar O, Fifen J, Malloum A, Dhaoaidi Z, Ghalila H, Conradie J** (2019). Structures of solvated ferrous ion clusters in ammonia and spin-crossover at various temperatures. *New Journal of Chemistry*, 43 pp. 9902 - 9915... [ufs-034504](#)
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35. **Shan W, Desbois N, Pacquelet S, Brandes S, Rousselin Y, Conradie J, Ghosh A, Gros C, Kadish K** (2019). Ligand Noninnocence in Cobalt Dipyrrin-Bisphenols: Spectroscopic, Electrochemical and Theoretical Insights Indicating an Emerging Analogy with Corroles. *Inorganic Chemistry*, 58 pp. 7677 - 7689... [ufs-034518](#)

36. **Loke PF, Kotze E, Du Preez CC, Twigge L** (2019). Dynamics of Soil Carbon Concentrations and Quality Induced by Agricultural Land Use in Central South Africa. *Soil Science Society Of America Journal*, 83 pp. 366 - 379.. **ufs-034724**
37. **Oosthuizen U, Schutte-Smith M, Visser HG** (2019). 6-Nitro-1, 10-phenanthroline-5-amine. *lucrj*, 4 pp. x191016-1 - x191016-3... **ufs-034786**
38. **Truscott, J.C., Visser, H.G., Conradie, J., Swart H.C. and Duvenhage, M** (2019). Synthesis, Crystal Structures, Photoluminescence, Electrochemistry and DFT study of Ga(III) and Al(III) complexes containing a novel tetradentate Schiff-base ligand, *Acta Crystallographica Section C: Structural Chemistry* 2019, C75, 1045-1052 <https://doi.org/10.1107/S2053229619008805> International Union of Crystallography (IUCr). **Ufs-034969**
39. **Alexander OT, Kroon RE, Brink A, Visser HG** (2019). Symmetry correlations between crystallographic and photoluminescence study of ternary  $\beta$ -diketone europium (III) based complexes using 1, 10-phenanthroline as the ancillary ligand. *Dalton Transactions*, (40), pp. 1 - 9... **ufs-034979**
40. **Janardhana D, Nagarasanakote Jayaramu S, Purcell W, Roos WD, Swart HC** (2019). Multifunction applications of Bi<sub>2</sub>O<sub>3</sub>:Eu<sup>3+</sup> nanophosphor for red light emission and photocatalytic activity. *Applied Surface Science*, 497 pp. 143748-1 - 143748-12... **ufs-035101**
41. **Tsai C, Langner EHG, Harris RA** (2019). Computational study of ZIF-8 analogues with electron donating and withdrawing groups for CO<sub>2</sub> adsorption. *Microporous and Mesoporous Materials*, 288 pp. 109613-1 - 109613-6... **ufs-035102**
42. **Mabaleha MB, Zietsman PC, Wilhelm A, Bonnet SL** (2019). Ethnobotanical Survey of Medicinal Plants used to treat Mental Illnesses in the Berea, Leribe and Maseru Districts of Lesotho. *Sage Journal*. pp. 1-13... **ufs-035109**
43. **Buitendach BE, Conradie J, Malan FP, Niemantsverdriet JW, Swarts JC** (2019) Synthesis, Spectroscopy and Electrochemistry in Relation to DFT Computed Energies of Ferrocene- and Ruthenocene-Containing  $\beta$ -Diketonato Iridium (III) Heteroleptic Complexes. Structure of [(2-Pyridylphenyl)<sub>2</sub>Ir(RcCOCHCOCH<sub>3</sub>)<sub>2</sub>] Molecules. pp1-20... **ufs-035139**
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46. **Van der Westhuizen D, Von Eschwege KG, Conradie J** (2019). Electrochemical data of polypyridine complexes of Ru (II). *Data in Brief*, 27 (104759), pp. 1 – 11. **ufs-035353**

47. **Brink A, Helliwell J (2019).** Why is interoperability between the two fields of chemical crystallography and protein crystallography so difficult? *IUCrJ*, 6 (5), pp. 788 - 793. **Publication has been recommended in F1000Prime as being of special significance in its field.** Vicens Q: *F1000Prime Recommendation of [Brink A and Helliwell JR, IUCrJ 2019 6(5):788-793]. In F1000Prime, 07 Oct 2019; 10.3410/f.736544810.793565710. ufs-035402*
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50. **R.-Z. Li, Q. Yuan, Z. Yang, E. Aprà, Z. Li, V. A. Azov, K. Kirakci, J. Warneke,\* X.-B. Wang,\*** "Photoelectron spectroscopy of  $[\text{Mo}_6\text{X}_{14}]^{2-}$  dianions (X = Cl-I)" *J. Chem. Phys.* **2019**, 151, 194310. **ufs-035407**
51. **Brink A, Kama DV, Alberto R, Roodt A (2019).** Crystal structure of hexacarbonyl-( $\mu_2$ -methanoato- $\kappa_2\text{O}:\text{O}'$ )-( $\mu_2$ -bis(di-ptolylphosphino)cyclohexylamine- $\kappa_2\text{P}:\text{P}'$ ) dirhenium (I),  $\text{C}_{42}\text{H}_{45}\text{NO}_8\text{P}_2\text{Re}_2$ . *Zeitschrift Fur Kristallographie-New Crystal Structures*, 235 (2), pp. 1 - 3. **ufs-035688**
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57. **Malloum, A., Fifen, J.J., Dhaouadi, Z., Engo S.G.N. and Conradie, J (2019).** Structures of Neutral Water Clusters, (H<sub>2</sub>O)<sub>2-30</sub>: Results from NewDFT Functionals. *New Journal of Chemistry*, 2019 (43), pp. 13020 - 13037. **ufs-036018**
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64. **Conradie, J. (2019)**. Density functional theory calculated data of different electronic states and bond stretch isomers of tris (trifluoroacetylacetonato)-manganese (III). *Data in brief* 27 pp.1-6 **ufs – 036081**
65. **Kenneth P. Caulfield, Jeanet Conradie, Hadi D. Arman, Abhik Ghosh, and Zachary J. Tonzetich, (2019)** Iron(II) Corrole Anions, *Inorganic Chemistry*. 2019, 58, 22, 15225-15235. American Chemical Society Publications. **ufs-036213**
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