

Faculty of Natural and Agricultural Sciences

Department of Chemistry

Publications 2018

1. **Mokolokolo, Pennie P., Frei, A., Tsosane, M.S., Kama, D.V., Schutte-Smith, M., Brink, A., Visser, H.G., Meola, G., Alberto, R. and Roodt, A.** 2018. Nuclearity manipulation in Schiff-base fac-tricarbonyl complexes of Mn(I) and Re(I). *Inorganica Chimica Acta* **471**: 249-256. [ufs-031376](#)
2. **von Eschwege, K.G. and Conradie, J.** 2018. Iron phenanthrolines: A density functional theory study. *Inorganica Chimica Acta* **471**: 391-396. [ufs-031404](#)
3. **Mngomezulu, M.E., Luyt, A.S., Chapple, S.A. and John, M.H.** 2018. Poly(lactic acid)-starch/Expandable Graphite (PLA-starch/EG) Flame Retardant Composites. *Journal of Renew Materials* **6**:1 26-37. [ufs-031407](#)
4. **Mokhena, T.C., Jacobs, N.V. and Luyt, A.S.** 2018. Nanofibrous alginate membrane coated with cellulose nanowhiskers for water purification. *Cellulose* **25**: 417-427. [ufs-031411](#)
5. **Jacobs, F.J.F., Venter, G.J.S. and Brink A.** 2018. Crystal structure of benzoato-κO-bis(1,3,5-triaza-7-phosphaadamantane-κP)silver(I) monohydrate C₁₉H₃₁AgN₆O₃P₂. *Zeitschrift fur Kristallographie: New Crystal Structures* **233(2)**: 311-313. [ufs-031420](#)
6. **Venter, G.J.S.** 2018. A magnetic spin transfer NMR study of tertiary phosphine exchange in rhodium(I) complexes. *Journal of Organometallic Chemistry* **866**: 200-205. [ufs-031423](#)
7. **Alexander, O.T., Donka, R., van Tonder, J.H., Bezuidenhoudt, B.C.B. and Visser, H.G.** 2018. The crystal structure of 6-(4-bromobenzyl)-1,2,5-trimethyl-7-[henyl-1,5-dihydro-2H-pyrrolo[3,2-d]pyrimidine-2,1(3H)-dione, C₂₂H₂₀BrN₃O₂. *Zeitschrift fur Kristallographie: New Crystal Structures* **233(3)**: 395-397. [ufs-031430](#)
8. **Kuhn, A. and Conradie, J.** 2018. Orbital control over the metal vs ligand reduction in a series of neutral and cationic bis(cyclopentadienyl) Ti(IV) complexes. *New Journal of Chemistry* **42**: 662. [ufs-031431](#)
9. **Landman, M., Jansen van Rensburg, A., van Rooyen, P.H., Conradie, M.M. and Conradie, J.** 2018. Triphenylstibine-substituted Fischer carbene complexes of tungsten(0): synthesis, structure, DFT and electrochemistry. *New Journal of Chemistry* **42**: 7301. [ufs-031450](#)
10. **Malloum, A., Fifen, J.J. and Conradie, J.** 2018. Structures and Spectroscopy of the Ammonia Eicosamer, (NH₃)_{n=20}. *Journal of Chemical Physics* **149**: 024304-1 – 024304-8. [ufs-031461](#)
11. **Conradie, J., Conradie, M.M., Tawfiq, K.M., Al-Jeboori, M.J., Coles, S.J., Wilson, C. and Potgieter, J.H.** 2018. Synthesis, characterization, experimental and theoretical structure of novel Dichloro(bis{2-{1-(4-methoxyphenyl)-1H-1,2,3-triazol-4-yl-κN³}pyridine-κN})metal(II) compounds, metal = Mn, Co and Ni. *Journal of Molecular Structure* **1161**: 89-99. [ufs-031463](#)

12. **Stuurman, N.F., Buitendach, B.E., Twigge, L., Swarts, P.J. and Conradie, J.** 2018. Rhodium(triphenylphosphine)carbonyl-2,4-dioxo-3-pentyl-4-decanyloxybenzoate: synthesis, electrochemistry and oxidative addition kinetics. *New Journal of Chemistry* **42**: 4121-4132. [ufs-031464](#)
13. **Conradie, J., Conradie, M.M., Tawfiq, K.M., Al-Jeboori, M.J., Coles, S.J., Wilson, C. and Potgieter, J.H.** 2018. Novel dichloro(bis{1-(4-methylphenyl)-1H-1,2,3-triazol-4-yl- κ N³}pyridine- κ N}metal(II) coordination compounds of seven transition metals (Mn, Fe, Co, Ni, Cu, Zn and Cd). *Polyhedron* **151**: 243-254. [ufs-031465](#)
14. **Malan, F.P., Singleton, E., Conradie, J. and Landman, M.** 2018. Electrochemistry of a series of symmetric and asymmetric CpNiBr(NHC) complexes: Probing the electrochemical environment due to push-pull effects. *Journal of Electroanalytical Chemistry* **814**: 66-76. [ufs-031471](#)
15. **Mair, C.E., Grienke, U., Wilhelm, A., Urban, E., Zehl, M., Schmidtke, M. and Rollinger, J.M.** 2018. Anti-Influenza Triterpene Saponins from the Bark of *Burkea Africana*. *Journal of Natural Products* **81**: 515-523. [ufs-031478](#)
16. **Noreljaleel, A.E.M., Wilhelm, A., Bonnet, S.L. and van der Westhuizen, J.H.** 2018. Synthesis and Bioactivity of Reduced Chalcones Containing Sulfonamide Side Chains. *Journal of Natural Products* **81**: 41-48. [ufs-031487](#)
17. **Swart, M.R., Twigge, L., Marais, C. and Bezuidenhoudt, B.C.B.** 2017. A variable temperature NMR analysis and resonance assignment of the Grubbs second generation catalyst. *Polyhedron* **152**: 31-36. [ufs-031495](#)
18. **Manicum, A-L, Alexander, O., Schutte-Smith, M. and Visser, H.G.** 2018. Crystal structure of *fac*-(acetylacetonato- κ^2 O,O')tricarbonyl(tri-*m*-tolyl phosphane- κ P)rhenium(I), C₂₉H₂₈O₅tPre. *Zeitschrift fur Kristallographie: New Crystal Structures* **233:1** 23-25. [ufs-031514](#)
19. **Manicum, A-L., Schutte-Smith, M., Visser, H.G.** 2018. The synthesis and structural comparison of *fac*-[Re(CO)₃]⁺ containing complexes with altered β -diketone and phosphine ligands. *Polyhedron* **145**: 80-87. [ufs-031580](#)
20. **Buitendach, B.H., Erasmus, E., Niemandtsverdriet, J.W., and Swarts, J.C.,** 2018. Can Electrochemical Measurements Be Used To Predict X-ray Photoelectron Spectroscopic Data? The Case of Ferrocenyl- β -Diketonato Complexes of Manganese(III). *Transition Metal Chemistry* **43**: 409-420. [ufs-031582](#)
21. **Erasmus, E.** 2018. X-ray photoelectron spectroscopy: Charge transfer in Fe 2p peaks and inner-sphere reorganization of ferrocenyl-containing chalcones. *Journal of Electron Spectroscopy and Related Phenomena* **223**: 84-88. [ufs-031597](#)
22. **Parrott, L.K. and Erasmus, E.** 2018. Metal Hexacyanometallate Nanoparticles: Spectroscopic Investigation on the Influence of Oxidation State of Metals on Catalytic Activity. *Catalysis Letters* **148:7** 2008-2018. [ufs-031645](#)
23. **Gerber, S.J. and Erasmus, E.** 2018. Electronic effects of metal hexacyanoferrates: An XPS and FTIR study. *Chemistry and Physics* **203**: 73-81. [ufs-031646](#)
24. **Botha, E., Landman, M., van Rooyen, P.H., and Erasmus, E.** 2018. Electronic properties of ferrocenyl-terpyridine coordination complexes: An electrochemical and X-ray photoelectron spectroscopic approach. *Inorganica Chimica Acta* **482**: 514-521. [ufs-031658](#)
25. **Gerber, S.J. and Erasmus, E.** 2018. Surfactant-stabilized nano-metal hexacyanoferrates with electrocatalytic and heterogeneous catalytic applications. *Transition Metal Chemistry* **43**: 409-420. [ufs-031708](#)

26. **Tsai, C-W., Niemantsverdriet, J.W. and Langner, E.H.G.** 2018. Enhanced CO₂ adsorption in nano-ZIF-8 modified by solvent assisted ligand exchange. *Microporous and Mesoporous Materials* **262**: 98-105. [ufs-031-031717](#)
27. **Dennis, C.R., Swarts, J.C. and Langner, E.H.G.** 2018. Nucleophilic ligand substitution in triply deprotonated tetrapeptide complexes of copper(II) and nickel(II) with 1,10-phenanthroline and 2,2-bipyridine. *Transition Metal Chemistry* **43**: 387-395. [ufs-031842](#)
28. **Adeniyi, A.A. and Conradie, J.** 2018. The stability, kinetic and inter-fragment electron communication of the tautomers of twelve selected β -diketone molecules: A computational study. *Journal of Molecular Graphics and Modelling* **85**: 25-39. [ufs-031909](#)
29. **Hill, T.N. and Roodt, A.** 2018. Solid-state and Computational Study of "Venus fly-trap" Geometric Parameters for 1,5-Cyclooctadiene in Pd^{II} and Pt^{II} β -Enaminonato Complexes. *Zeitschrift für anorganische und allgemeine Chemie* **644:14** 763-774. [ufs-031914](#)
30. **Frei, A., Mokolokolo, P.P., Bolliger, R., Braband, H., Tsosane, M.S., Brink, A., Roodt, A. and Alberto, R.** 2018. Self-Assembled Multinuclear Complexes Incorporating ^{99m}Tc. *Chemistry-A European Journal* **24:41** 10397-10402. [ufs-031916](#)
31. **Burianova, V.K., Mikherdov, A.S., Bolotin, D.S., Novikov, A.S., Mokolokolo, P.P., Roodt, A., Boyarskiy, V.P., Suslonov, V.V., Zhdanov, A.P., Zhizhin, K.Yu and Kuznetsov, N.T.** 2018. Electrophilicity of aliphatic nitrilium *closo*-decaborate clusters: Hyperconjugation provides an unexpected inverse reactivity order. *Journal of Organometallic Chemistry* **870**: 97-103. [ufs-031937](#)
32. **Otto, S., Botha, E. and Roodt, A.** 2018. Structure and Reactivity Relationships in Methyl and Hydrido Complexes of Platinum (II) by Group 15 Donor Atom Ligands. *Croatica Chemica Acta* **91:2** 265–279. [ufs-031943](#)
33. **Burianova, V.K., Bolotin, D.S., Mikherdov, A.S., Novikov, A.S., Mokolokolo, P. P. A. Roodt, A., Boyarskiy, V. P., Dar'in, D., Krasavin, M., Suslonov, V.V., Zhdanov, A.P., Zhizhind, K.Yu. and Kuznetsov, N.T.** 2018. Mechanism of generation of *closo*-decaborato amidrazones. Intramolecular non-covalent B–H \cdots π (Ph) interaction determines stabilization of the configuration around the amidrazone C=N bond. *New Journal of Chemistry* **42:11** 8693-8703. [ufs-031944](#)
34. **Brink, A., Kroon, R.E., Visser, H.G., van Rensburg, C.E.J. and Roodt, A.** 2018. Designing model imino bifunctional chelators for radiopharmaceuticals—in vitro antitumor activity, photoluminescence and structural analysis. *New Journal of Chemistry* **42**: 5193-5203. [ufs-031640](#)
35. **Raleaooa, P.V., Roodt, A, Mhlongo, G.G., Motaung, D.E. and Ntwaeaborwa, O.M.** 2018. Analysis of the structure, particle morphology and photoluminescent properties of ZnS: Mn²⁺ nanoparticulate phosphors. *Optik-International Journal for Light and Electron Optics* **153**: 31-42. [ufs-031955](#)
36. **Ponra, S., Gohain, M., Donka, R., van Tonder, J.H. and Bezuidenhout, B.C.B.** 2018. Al(OTf)₃-catalyzed one-pot synthesis of pyrrolo[3,2-*d*]pyrimidinedione derivatives. *Tetrahedron Letters* **59**: 2909-2912. [ufs-031962](#)
37. **Warsink, S., Kotze, P.D.R., Janse van Rensburg, J.M., Venter, J.A., Otto, S., Botha, E. and Roodt, A.** 2018. Kinetic-Mechanistic and Solid-State Study of the Oxidative Addition and Migratory Insertion of Iodomethane to [Rhodium(S,O-BdiPT or N,O-ox)(CO)(PR¹R²R³)] Complexes. *European Journal of Inorganic Chemistry* **32**: 3615-3625. [ufs-031980](#)
38. **Loke, P.F., Kotze, E., du Preez, C.C. and Twigge, T.** 2018. Long-term effects of wheat production management practices on some carbon fractions of a semiarid Plinthustalfs. *Soil Research* **56**: 601-614. [ufs-031981](#)

39. **Skipina, B., Luyt, A.S., Csóka, L., Djoković, V. and Dudić, D.** 2018. Generation of photo charge in poly(ethyleneimine)-TiO₂-anthocyanin modified papers conditioned at different humidities. *Dyes and Pigments* **149**: 51-58. [ufs-031985](#)
40. **Gumede, P., Luyt, A.S. and Muller, A.J.** 2018. Review on PCL, PBS, and PCL/PBS blends containing carbon nanotubes. *Express Polymer Letters* **12:6** 505-529. [ufs-031987](#)
41. **Gumede, T.P., Luyt, A.S., Pérez-Camargo, R.A., Tercjak, A. and Müller, A.J.** 2018. Morphology, Nucleation, and Isothermal Crystallization Kinetics of Poly(Butylene Succinate) Mixed with Polycarbonate/MWCNT Masterbatch. *Polymers* **10**: **424** 1-22. [ufs-031988](#)
42. **Foroutan-Nejad, C., Larsen, S., Conradie, J. and Ghosh, A.** 2018. Isocorroles as Homoaromatic NIR-Absorbing Chromophores: A First Quantum Chemical Study, *Scientific Reports* **8:11952** 1-10. [ufs-031994](#)
43. **Ferreira, H., Conradie M.M. and Conradie, J.** 2018. Electrochemical properties of a series of Co(II) complexes, containing phenanthroline functionalized ligands. *Data in Brief* **21**: 866-877. [ufs-031995](#)
44. **Conradie, J., Conradie, M.M., Tawfiq, K.M., Coles, S.J., Tizzard G.J., Wilson, C. and Potgieter, J.H.** 2018, Jahn-Teller distortion in 2-pyridyl-(1,2,3)-triazole-containing copper(II) compounds. *New Journal of Chemistry* **42**: 16335 – 16345. [ufs-032058](#)
45. **Ganguly, S., McCormick, L., Conradie, J., Gagnon, K., Sarangi, R. and Ghosh, A.** 2018. Electronic Structure of Manganese Corroles Revisited: X-ray structures, Optical and X-ray Absorption Spectroscopies, and Electrochemistry as Probes of Ligand Noninnocence, *Inorganic Chemistry* **57**: **16** 9656–9669. [ufs-032067](#).
46. **Conradie, J., Conradie, M.M., Mtshali, Z. and Potgieter, J.H.** 2018. DFT and CV data of 4-phenyl-substituted Dichloro(*bis*{2-[1-(phenyl)-1H-1,2,3-triazol-4-yl-κN³]pyridine-κN})iron(II) coordination compounds. *Data in Brief* **21**: 1458-1471. [ufs-032074](#)
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48. **Demissie, T.B., Conradie, J., Vazquez-Lima, H., Ruud, K. and Ghosh, A.** 2018. Rare and Nonexistent Nitrosyls: Periodic Trends and Relativistic Effects in Ruthenium and Osmium Porphyrin-Based {MNO}⁷ Complexes. *ACS Omega* **3**: 10513–10516. [ufs-032115](#)
49. **Conradie, J., Conradie, M.M., Tawfiq, K.M., Al-Jeboori, M.J., Coles, S.J., Wilson, C., D'Silva, C. and Potgieter, J.H.** 2018. Chemical and structural data of (1,2,3-triazol-4-yl)pyridine-containing coordination compounds. *Data in Brief* **20**: 1397-1408. [ufs-032123](#)
50. **Ghosh, A., Larsen, S., Conradie, J. and Foroutan-Nejad, C.** 2018. Local versus Global Aromaticity in Azuliporphyrin and Benziporphyrin Derivatives. *Organic Biomolecular Chemistry*. **16**: 7964-7970 [ufs-032725](#)
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52. **Conradie, J.** 2018. Structural and electronic data of three first-row transition octahedral hexaaquametal(II) ions, metal = Cr, Ni or Cu, *Data in Brief* **21**: 2051–2058. [ufs-032796](#)

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55. **Ntoi, Lumanyano L.A., Alexander, Orbett T. and von Eschwege*, Karel G.** 2018. Synthesis and kinetics of photochromic carboxy-substituted dithizonatophenylmercury(II). *Journal of Photochemistry & Photobiology*, **368**: 219-226 [ufs-032892](#)
56. **Malloum, A., Fifen, J.J. and Conradie, J.** 2018. Structures and infrared spectroscopy of large sized protonated ammonia clusters. *The Journal of Chemical Physics* **149**: 244301-244310 [ufs-032897](#)
57. **Ponra, Sudipta, Gohain, Mukut, Donka, Rajashekar, van Tonder, Johannes H., and Bezuidenhoudt*, Barend C.B.** 2018 Al(OTf)₃-catalyzed one-pot synthesis of pyrrolo[3,2-*d*]pyrimidinedione derivatives. *Tetrahedron Letters*. **59**: 2909-2912 [ufs-032981](#)
58. **Šulce, Anda Backenköhler, Jana, Schrader, Imke, Delle Piane, Massimo, Müller, Christian, Wark, André, Ciacchi, Lucio Colombi, Azov, Vladimir and Kunz, Sebastian.** 2018. Ligand-functionalized Pt nanoparticles as asymmetric heterogeneous catalysts: molecular reaction control by ligand–reactant interactions. *Catalysis Science & Technology*. **8**: 6062-6075 [ufs-032983](#)
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