

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

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

#### **Publications 2020**

1. **Conradie J**, (2020). Computational DFT data related to the redox behaviour of tris( $\beta$ -diketonato)ruthenium(III) compounds. Data in Brief, 2020 30 105617. [ufs-037413](#)
2. **Swarts PJ, Conradie J** (2020). Redox data of ferrocenylcarboxylic acids in dichloromethane and acetonitrile, Data in Brief, 2020 30 105650. [ufs-037415](#)
3. **Gostynski, R., van Rooyen, P.H. and Conradie, J** (2020). X-ray diffraction and QTAIM calculations of the non-covalent intermolecular fluorine-fluorine interactions in  $[\text{Mn}^{\text{III}}(\text{trifluoroacetylacetonato})_3]$ . Journal of Molecular Structure (1201)127119. [ufs-037463](#)
4. **Swarts, P.J. and Conradie, J.** (2020), Electrochemical behaviour of chloro- and hydroxy-subphthalocyanines, Electrochimica Acta 329 135165. [ufs-037465](#)
5. **Malloum, A., Fifen, J.J., and Conradie, J.** (2020), Large Sized Ammonia Clusters and Solvation Energies of the Proton in Ammonia, Journal of Computational Chemistry, 41, 21–30. ...[ufs-037469](#)
6. **Conradie, J.** (2020), Tris( $\beta$ -ketoiminato)ruthenium(III) – Structural and electronic data of the neutral, oxidized and reduced forms. Data in brief 28 104833. [ufs-037470](#)
7. **Muller, F.A.M., Conradie, J. and von Eschwege, K.G.** (2020), Conformational preference of nitroformazans: a computational study, Journal of Molecular Structure 1203, 127463. [ufs-037471](#)
8. **Truscott, J.C., Kama, D.V., Visser, H.G., Conradie, J** (2020)., Synthesis, Structure and DFT study of novel Ga(III) complexes containing a tetradentate ligand. Journal of Molecular Structure 1203 (2020) 127334. [ufs-037472](#)
9. **Swarts, P.J. and Conradie, J.** (2020), Oxidation and reduction data of subphthalocyanines. Data in Brief 28 (2020) 105039. [ufs-037473](#)
10. **Thomas, K.E., Desbois, N., Conradie, J., Teat, S. J., Gros, C.P., Ghosh, A.** (2020), Gold Dipyrin-Bisphenolates: A Combined Experimental and DFT Study of Metal-Ligand Interactions, RSC Advances, 2020,10, 533-540 Royal Society of Chemistry Publishing. [ufs-037489](#)

11. **Muller, F.M.A., Conradie, J, von Eschwege, K.G.** (2020) Synthesis, DFT and kinetic studies of chromic S-Methyldithizone, Polyhedron 179 (2020) 114386. [ufs-037497](#)
12. **Conradie, J.** (2020), Redox Behaviour of [Ru( $\beta$ -diketonato)<sub>3</sub>] Complexes. Electrochimica Acta 337 (2020) 135801. [ufs-037499](#)
13. **Adeniyi, A.A. and Conradie, J.** (2020) A Theoretical investigation of the fragments interaction, non-linear optical and electronic properties of tris( $\beta$ -diketonato)iron(III) complexes. Structural Chemistry 2020 31 215–232. [ufs-037502](#)
14. **Chiyindiko, E., Stuurman, N.F., Langner E.H.G. and Conradie, J.** (2020), Electrochemical behaviour of bis( $\beta$ -diketonato)copper(II) complexes containing  $\gamma$ -substituted  $\beta$ -diketones, Journal of Electroanalytical Chemistry, 860, 113929. [ufs-037503](#)
15. **Da-yang, E., Fifen, J.J., Malloum, A., Lahmar, S., Nsangou, M., Conradie, J.** (2020), Structures of the Solvated copper (II) Ion in Ammonia at various temperatures. New Journal of Chemistry 2020 44 3637-3653. [ufs-037504](#)
16. **Pieter J. Swarts, Jeanet Conradie** (2020), Solvent and Substituent Effect on Electrochemistry of Ferrocenylcarboxylic Acid, Journal of Electroanalytical Chemistry, 866 114164. [ufs-037509](#)
17. **Kolle E. Thomas, Jeanet Conradie, Christine M. Beavers and Abhik Ghosh** (2020), Free-Base Porphyrins with Localized NH Protons. Can Substituents Alone Stabilize the Elusive Cis Tautomer? Org. Biomol. Chem.18, 2861-2865. [ufs-037511](#)
18. **Adebayo A. Adeniyi, Cecilia O. Akintayo, Emmanuel T. Akintayo, Jeanet Conradie** (2020), The conformational search, the stability, fragment interaction and resistance to acidic attack of epoxy-polyurethanes in different solvent media, Structural Chemistry 31, 861–875. [ufs-037512](#)
19. **Jeanet Conradie, Karel G. von Eschwege** (2020), Cyclic voltammograms and electrochemical data of Fe<sup>II</sup> polypyridine complexes, Data in brief 31 105754. [ufs-037514](#)
20. **Du Plessis, M, Marais, C., Bezuidenhout, B.C.B.** (2020). Palladium catalyzed hydroesterification of substituted alkenes under microwave conditions. *Arkivoc* 2020 (iii), 40-48. [ufs-037825](#)
21. **Swart, M.R., Bezuidenhout, B.C.B., Marais, C., Erasmus, E.** (2021). Spectroscopic characterization of Grubbs 2<sup>nd</sup> generation catalyst and its *p*-cresol derivatives. *Inorganica Chimica Acta* 2021, 514, 120001. [ufs-037827](#)
22. **Loke, P. F., Kotze, E., Du Preez, C.C., Twigge, L.** (2020). Cross-rangeland comparisons on soil carbon dynamics in the *pedoderm* of semi-arid and arid South African commercial farms. *Geoderma* 2021. [ufs-037828](#)
23. **Parrot, L. K., Erasmus, E.** (2020). Palladium/graphene oxide nanocomposites with carbon nanotubes and or magnetite for the reduction of nitrophenolic compounds. *RSC Advances* 10:32885-32896. [ufs-037822](#)

24. **Xantini, Z, Erasmus, E. (2020).** Platinum supported on nanosilica and fibrous nanosilica for hydrogenation reactions. *Polyhedron* 114769. **ufs-037829**
25. **Parrott, L. K., Erasmus, E. (2020)** Modified palladium/chitosan/graphene nanocomposites for the reduction of nitrophenolic compounds. *Fullerenes, Nanotubes and Carbon Nanostructures*. **ufs-037836**
26. **Moji, R.G., Kroon, R.E., Motlounge, S.V., Motaung, T.E., Ahemen, I. & Koao, L.F. 2020.** Color tuning and white light emission from sol-gel SiO<sub>2</sub> nanoparticles doped with Sr<sup>2+</sup>. *Materials Chemistry and Physics* 242: 122409. **ufs-037760**
27. **Moji, R.G., Kroon, R.E., Motlounge, S.V., Motaung, T.E. & Koao, L.F. 2020.** Morphology, structural and luminescent properties of sol-gel synthesized SiO<sub>2</sub> powders co-doped with Sr<sup>2+</sup> and Tb<sup>3+</sup>. *Physica B: Physics of Condensed Matter* 580: 411817. **ufs-037758**
28. **Erasmus, E (2020).** Morphology-Dependent Ullmann C-O Arylation Using Cu<sub>2</sub>O Nanocrystals. *Journal of Nanomaterial*. **ufs-037837**
29. **Adeniyi, A. A., von Stein, P.F. X, Bosman, G. W., Steenkamp, C. M, Chiweshe, T., von Eschwege, K. G., Conradie, J. (2020).** Probing ultrafast reaction mechanisms of photo-excited dithizone through transient absorption spectroscopy and computational CASCF studies. *Journal of the Optical Society of America B: Optical Physics*: 37 pp. A356-A366. **ufs-037838**
30. **Chukwuma, C. I, Mashele, S. S., Eze, K. C., Matowane, G. R., Islam, S. Md., Bonnet, S. L., Noreljaleel, A. E. M., Ramorobi, L. M. (2020).** A comprehensive review on zinc (II) complexes as anti-diabetic agents: The advances, scientific gaps and prospects. *Pharmacological Research* 155 104744. Pp 1-20. **ufs-037841**
31. **Motlounge, D. M., Mashele, S. S., Matowane, G. R., Swain, S. S., Bonnet, S. L, Noreljaleel, A. E. M., Oyedemi, S. O, Chika I. Chukwuma, C. I. (2020).** Synthesis, characterization, antidiabetic and antioxidative evaluation of a novel Zn (II)-gallic acid complex with multifacet activity. *Journal of Pharmacy and Pharmacology*. Pp 1-15. **ufs-037842**
32. **Kinyok, Mc. J, Wilhelm, A, Kamto, D. E., Mbing, J. N., Bonnet, S. L., Pegnyemb, D. E. (2020).** Chemical constituents of the leaves of *Anthonotha macrophylla* (Leguminosae). *Natural Product Research*. 1478-6427. Pp1-9. **ufs-037843**
33. **Divya, J., Shivaramu, N.J., Purcell, W., Roos, W.D. & Swart, H.C. (2020).** Effects of annealing temperature on the crystal structure, optical and photocatalytic properties of Bi<sub>2</sub>O<sub>3</sub> needles. *Applied Surface Science* 520: 146294. **ufs-037830**
34. **Divya, J., Shivaramu, N.J., Coetsee, E., Kroon, R.E., Purcell, W. & Swart, H.C. 2020.** Enhanced luminescence and photocatalytic activity of Bi<sub>2</sub>O<sub>3</sub>:Ho<sup>3+</sup> needles. *Journal of Alloys and Compounds* 842: 155641. **ufs-037831**

35. **J. Warneke, M. Mayer, M. Rohdenburg, X. Ma, J. K. Y. Liu, M. Grellmann, S. Debnath, V. A. Azov, E. Apra, R. P. Young, C. Jenne, G. E. Johnson, H. I. Kenttämä, K. R. Asmis, J. Laskin.** (2020) "Direct functionalization of C–H bonds by electrophilic anions" *Proc. Natl. Acad. Sci. U.S.A.* 2020, 117, 23374-23379. [ufs-037848](#)
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38. **Conradie, M.M.** (2020). Rhodium(triphenylphosphine)carbonyl-2,4-dioxo-3-pentyl-4-decanyloxybenzoate: a DFT study of oxidative addition and methyl migration. *Inorganica Chimica Acta* 2020, 513, 119954. [ufs-037854](#)
39. **Conradie, M.M.** (2020). Data of the rhodium(triphenylphosphine)carbonyl-2,4-dioxo-3-pentyl-4-hydroxybenzoate plus iodomethane oxidative addition and follow-up reactions. *Data in Brief* 2020, 32, 106253. [ufs-037856](#)
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41. **Li, Y., Li, S., Bäumer, M., Ivanova-Shor, E.A., and Moskaleva, L.V.** (2020). What Changes on the Inverse Catalyst? Insights from CO Oxidation on Au-Supported Ceria Nanoparticles Using Ab Initio Molecular Dynamics, *ACS Catal.* 10, 3164–3174. [ufs-037883](#)
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44. **Gantsho, L.V., Dotou, M., Jakubaszek, M., Goud, B., Gasser, G., Visser, H.G., Schutte-Smith, M.** (2020). Synthesis, characterization, kinetic investigation and biological evaluation of Re(I) di- and tricarbonyl complexes with tertiary phosphine ligands† *Dalton Trans.* 49, 35-46. [ufs-037888](#)
45. **Marogoa, N.R., Kama, D.V., Visser, H.G., Schutte-Smith, M.** (2020). Crystal structures of chlorido-[dihydroxybis-(1-imino-ethoxy)]arsanido-κ<sup>3</sup>N,As,N']platinum(II) and of a polymorph of chlorido-[dihydroxybis-(1-imino-propoxy)]arsanido-κ<sup>3</sup>N,As,N']platinum(II) *Acta Cryst.* E76, 180-185. [ufs-037891](#).

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51. **Malloum, A., Fifen, J.J., Conradie, J.** (2020) Theoretical infrared spectrum of the ethanol hexamer, *International Journal of Quantum Chemistry* 2020 120 e26234. [ufs-038431](#)
52. **Akpomie, K., Conradie. J.** (2020) Advances in application of cotton based adsorbents for heavy metals trapping, surface modifications and future perspectives: A review. *Ecotoxicology and Environmental Safety* 201 (2020) 110825. [ufs-038432](#)
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65. **van der Westhuizen, D., Kannan, A., Conradie, J., von Eschwege, K.G.** (2020) Polypyridine Os<sup>II</sup> complexes electrochemical data. *Data in Brief* 33 (2020) 106454. [ufs-038446](#)
66. **Malimabe, M.A., Dejene, B.F., Swart, H.C., Motloug, S.V., Motaung, T.E. & Koa, L.F.** 2020. Characterization of the incorporated ZnO doped and co-doped with Ce<sup>3+</sup> and Eu<sup>3+</sup> nanophosphor powders into PVC polymer matrix. *Journal of Molecular Structure* 1202: 127339. [ufs-037426](#)
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68. **Rohdenburg, M., Azov, V. A., Warneke, J.** 2020 New Perspectives in the Noble Gas Chemistry Opened by Electrophilic Anions. *Frontiers in Chemistry* 8:580295 [ufs-038453](#)
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70. **Kama, D.V., Brink, A., Roodt, A.** 2020 Crystal structure of dichlorido(N-o-tolyl-1,1-di-p-tolylphosphanamine- $\kappa$ 1P)-(methoxydi-p-tolylphosphane- $\kappa$ 1P)palladium(II), C<sub>36</sub>H<sub>39</sub>Cl<sub>2</sub>NOP<sub>2</sub>Pd. Zeitschrift fur Kristallographie NCS 2020: 235(2): 349-352. [ufs-038459](#)
71. **Kama, D.V., Brink, A., Alberto, R., Roodt, A.** 2020 Crystal structure of hexacarbonyl-( $\mu$ 2-methanoato- $\kappa$ 2O:O')-( $\mu$ 2-bis(di-p-tolylphosphino)cyclohexylamine- $\kappa$ 2P:P')dirhenium(I), C<sub>42</sub>H<sub>45</sub>NO<sub>8</sub>P<sub>2</sub>Re<sub>2</sub>. Zeitschrift fur Kristallographie NCS 2020: 235(2): 303-305. [ufs-038460](#)
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73. **Elmakki, M.A., Alexander, O.T., Roodt, A.** 2020 The crystal structure of trans-carbonyl-(diphenylcyclohexyl-phosphine- $\kappa$ P)iodidomethyl-(2-oxopyridin-1(2H)-olato- $\kappa$ 2O,O')rhodium(III), C<sub>25</sub>H<sub>28</sub>INO<sub>3</sub>PRh. Zeitschrift fur Kristallographie NCS 2020: 235(2): 279-281. [ufs-038462](#)
74. **Hamdi, I., Bkhairia, I., Roodt, A., Roisnel, T., Nasri, M., Naili, H.,** 2020 Synthesis, intermolecular interactions and biological activities of two new organic-inorganic hybrids C<sub>6</sub>H<sub>10</sub>N<sub>2</sub>,<sub>2</sub>Br and C<sub>6</sub>H<sub>10</sub>N<sub>2</sub>,<sub>2</sub>Cl·H<sub>2</sub>O<sup>+</sup>. RSC Adv., 10 2020: 5864-5873. [ufs-038463](#)
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76. **Mokolokolo, P.P., Brink, A., Schutte-Smith, M., Roodt, A.** 2020 *Subtle variation of stereo-electronic effects in rhodium(I) carbonyl Schiff base complexes and their iodomethane oxidative addition kinetics.* J. Coord. Chem., 2020, 2740-2762. [ufs-038468](#)
77. **Jacobs, F.J.F., Brink, A.** 2020 Crystal structure of fac-tricarbonyl-(nitrate- $\kappa$ 1O)- bis(pyridine- $\kappa$ N)-rhenium, C<sub>13</sub>H<sub>10</sub>O<sub>6</sub>N<sub>3</sub>Re. Z. Kristallogr. NCS, 2020, MS-ID: NCRS-2020-0475. [ufs-038470](#)
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88. **Hough, M. A., Conradie, J., Strange, R. W., Antonyuk, S.V., Eady, R.R, Ghosh, A., Hasnain, S.S.,** (2020) Nature of the copper-nitrosyl intermediates of copper nitrite reductases during catalysis, *Chemical Science*, 2020, 11, 12485. **ufs-038568**
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