NATURAL AND AGRICULTURAL SCIENCES
NATUUR- EN LANDBOUWETENSKAPPE
UFS·UV

PUBLIKASIES/PUBLICATIONS – 2016

1. **Purcell, W., Conradie, J., Kumar, S. and Venter, J.A.** 2016. Characterisation and mechanistic study of the oxidative addition reactions of [Ir(cod)(sacac)]. *Journal of Organometallic Chemistry* **801**: 80-86.**ufs-025224**

2. **Nete, M., Purcell, W. and Nel, J.T**. 2016. Hydrometallurgical Separation of Niobium and Tantalum: A Fundamental Approach. *The Journal of The Minerals, Metals & Materials Society* **68(2):** 556-566.**ufs-025226**

3.. **Purcell, W. and Visser, H.G**. 2016. Evidence of Unusually Long Metal-Aqua Interaction: The Crystal Structure of Tetraphenylphosponium Rhenium(V)aquatetracyanonitrido Monohydrate Tri-terpyridine. *Journal of Chemical Crystallography* **46:** 15-20.**ufs-025230**

4. **du Plessis, M., Marais, C. and Bezuidenhoudt, B.C.B.** 2016. Parameters Influencing Reactivity and Regioselectivity in the Methoxycarbonylation of Arylalkenes, *Synthesis* **48:** 557-565.**ufs-025258**

5. **Tsosane, M.S., Visser, H.G. and Brink, A.** 2016. Crystal structure of (E)-2-(((1,10-phenanthrolin-5-yl)imino)methyl)-5-methylphenol monohydrate, $C_{20}H_{15}N_3O \cdot H_2O$. *Zeitschrift fur Kristallographie: New Crystal Structures* **231(1):** 237-239.**ufs-025279**

6. **Marake, D.T., Roodt, A. and Brink, A.** 2016. Crystal structure of *fac*-tricarbonyl(2-(isopropylimino)methyl-5-methylphenolatido-k^2N,O)(pyridine-kN)rhenium(I), $C_{10}H_{19}N_2O_4Re$. *Zeitschrift fur Kristallographie: New Crystal Structures* **231(1):** 251-254.**ufs-025287**

7. **Pieterse, T., Visser, M., Marais, C. and Bezuidenhoudt, B.C.B.** 2016. $Al(OTf)_3$: An Efficient Lewis Acid Additive for Domino Addition-Elimination of Grignard Reagents to Activated Ketones. *Synlett* **27:** 1541-1546.**ufs-025290**

8. **Gibhard, L., Pravin, K., Abay, E., Wilhelm, A., Swart, K., Lawrence, N., Khoury, R., van der Westhuizen, J., Smith, P. and Wiesner, L.** 2016. *In Vitro* and *In Vivo* Pharmacokinetics of Aminoalkylated Diarylpropanes NP085 and NP102. *American Society for Microbiology Antimicrobial Agents and Chemotherapy* **60(5):** 3065-3069.**ufs-025292**

9. **Rajasekhar, D., Srinivasulu, D., Sridhar, C., Kumar, G.V.N. and Ramesh, P.** Synthesis, Spectral Characterization and Antioxidant Activity of Novel Zafirlukast Sulfonyl Derivatives. *Journal of the Chinese Chemical Society* **63:** 267-274.**ufs-025295**

10. **Marais, C., Meintjes, R., Dennis, C.R. and Swarts, J.C.** 2016. Performance in Chemistry of students who started in the University Preparation Programme: The ripple effect. *South African Journal of Science* **112(7/8):** 1-3.**ufs-025303**

11. **Chiweshe, T.T., Purcell, W. and Venter, J.A.** 2016. Evaluation of PGE Liberation and Chromium Isolation in a Solid UG2 Chromitite Concentrates at Moderate Temperatures Using ICP-OES. *The Journal of the Minerals, Metals & Materials Society* **68(6):** 1691-1700.**ufs-025309**

12. **Chiweshe, T.T., Purcell, W. and Venter, J.A.** 2016. Evaluation of Different Internal Standards for previous metals quantification. *Bulletin Chemical Society Ethiopia* **30(1)** 55-70.**ufs-025322**

13. **Chiweshe, T.T., Landman, M., Conradie, J. and von Eschwege, K.G.** 2016. Synthesis and structure of dithizonato complexes of copper(II), antimony(III) and tin(IV). *Journal of Coordination Chemistry* **69(5):** 788-800.**ufs-025331**

14. **Manicum, A.-L., Schutte-Smith, M., Visser, H.G., Pretorius, C., Roodt, A.** 2016. Crystal structure of tetraethylammonium *fac*-tricarbonyl(hexafluoroacetylacetonato-κ^2O,O)-(nitrato-O)rhenium(I), $C_{16}H_{21}O_8N_2F_6Re$. *Zeitschrift fur Kristallographie: New Crystal Structures* **231(1)**: 263-266. **ufs-025353**

15. **Schutte-Smith, M., Visser, H.G., Roodt, A.** 2016. Crystal structure of tetraethylammonium 3,5-dinitrosalicylate, $C_{15}H_{23}N_3O_7$. *Zeitschrift fur Kristallographie: New Crystal Structures* **231(1)**: 77-79.**ufs-025354**

16. **Schutte-Smith, M., Visser, H.G., Roodt, A.** 2016. Crystal structure of *fac*-hexacarbonylbisμ_2-(3-carboxy-3'-carboxylato-2,2'-bipyridine)-κ^3*N,N':O*-dirhenium(I) tetrahydrate, $C_{30}H_{22}N_4O_{18}Re_2$. *Zeitschrift fur Kristallographie: New Crystal Structures* **231(2)**: 335-338.**ufs-025358**

17. **Nkoe, P.I., Koen, R., Brink, A., Schutte-Smith, M.** 2016. Crystal structure of hexacarbonyl bis(μ_2-2-methoxybenzenethiolato-κ^2*S*)pyridine(triphenylphosphane)= dirhenium(I),$C_{43}H_{34}NO_8PS_2Re_2$. *Zeitschrift fur Kristallographie: New Crystal Structures* **231(2)**: 461-464.**ufs-025359**

18. **Schutte-Smith, M., Bungu, P.S.E., Steyl, G., Roodt, A.** 2016. Crystal structure of 3,5,7-tris(morpholinomethyl)tropolone 0.67 hydrate, $C_{22}H_{33}N_3O_5{\cdot}0.67H_2O$. *Zeitschrift fur Kristallographie: New Crystal Structures* **231(3):** 999-1002.**ufs-025360**

19. **Jansen van Rensburg, A., Landman, M., van Rooyen, P.H., Conradie, M.M. and Conradie, J.** 2016. Synthesis and Structure of novel Triphenylarsine-substituted Tungsten(0) Fischer carbene complexes. *Journal of Molecular Structure* **1105:** 205-213.**ufs-025364**

20. **Conradie, M.M., van Rooyen, P.H. and Conradie, J.** 2016. X-ray and electronic structure of tris(benzoylacetonato-k2O,O')iron(III). *Journal of Molecular Structure* **1123:** 199-205.**ufs-025365**

21. **Elmakki, M.A., Koen, R., Venter, J.A. and Drost, R.** 2016. Crystal structure of dicarbonyl(pyridine-2-olate-1-oxido-κ^2O,O')rhodium(I), $C_7H_4NO_4Rh$. *Zeitschrift fur Kristallographie: New Crystal Structures* **231(3):** 703-705.**ufs-025372**

22. **Elmakki, M.A., Koen, R., Drost, R.M., Alexander, O.T., Venter, G.J.S. and Venter, J.A.** 2016. Crystal structure of carbonyl(2-oxopyridin-1(2H-olato-κ^2O,O')(triphenylphosphine-κP)rhodium(I), $C_{24}H_{19}NO_3PRh$. *Zeitschrift fur Kristallographie: New Crystal Structures* **231(3):** 781-783.**ufs-025373**

23. **Dutta, S., Sharma, S.K., Kumar, V., Som, S., Swart, H.C. and Vissert, H.G.** 2016. Ion-induced modification of structural, optical and luminescence behavior of Gd_2MoO_6 nanmaterials: A Comparative approach. *Vacuum* **128:** 146-157.**ufs-025336 (ingelees Fisika)**

24. **Erasmus, E.** 2016. Synthesis and electrochemistry of *p*-substituted phenyl diphenylphosphinite rhodium(I) complexes. *Polyhedron* 106: 18-26.**ufs-025374**

25. **Buitendach, B.E. , Erasmus, E., Landman, M., Niemantsverdriet, J.W.H. and Swarts, J.C.** 2016. Consequences of Electron-Density Manipulations on the X-Ray Photoelectron Spectroscopic Properties of Ferrocenyl-β-diketonato Complexes of Manganese(III). Structure of $[Mn(FcCOCHCOCH_3)_3]$. *Inorganic Chemistry* 55: 1992-2000.**ufs-025388**

26. **Dutta, S., Som, S., Kunti, A.K., Sharma, S.K., Kumar, V., H.C. Swart and Visser, H.G.** 2016. Ag^{7+} ion induced modification of morphohologu, optical and luminescence behavirour of charge compensated $CaMoO_4$ nanophosphor. *Nuclear Instruments and Methods in Physics Research B.* **384:** 76-85.**ufs-025344 (ingelees deur Fisika)**

27. **Erasmus, E.** 2016. Spectroscopic monitoring of carbonylation reactions on zeolite supported rhodium(I) carbonyls. *Inorganica Chimica Acta* 451: 197-201.**ufs-025389**

28 **Liu, R., Conradie, J., and Erasmus E**. 2015. Comparison of X-ray photoelectron spectroscopy multiplet splitting of Cr 2p peaks from chromium tris(β-diketonates) with chemical effects. *Journal of Electron Spectroscopy and Related Phenomena* 206: 46-51.**ufs-025390**

29. **Drost, R.M., Koen, R., Roodt, A. and Venter, J.A**. 2016. Crystal structure of monocarbonyl(N-nitroso-N-oxido-phenylamine-κ^2,O')(triphenylarsine-κAs) rhodium(I), $C_{25}H_{20}AsN_2O_3Rh$. *Zeitschrift fur Kristallographie: New Crystal Structures* **231(2):** 493-495.**ufs-025391**

30. **Belay, A.N., Koen, R., Venter, J.A. and Drost, R.M.** 2016. Crystal structure of tris (N-nitroso-N-oxyanilino-κ^2O,O')oxidoniobium(V), $C_{18}H_{15}H_6O_7Nb$. *Zeitschrift fur Kristallographie: New Crystal Structures* **231(2):** 513-515.**ufs-025392**

31. **Som, S., Kumar, V., Kumar, V., Gohain, M., Pandey A., Duvenhage, M., Terblans, J.J., Bezuidenhoudt, B.C.B. and Swart, H.C.** 2016. Dopant distribution and influence of sonication temperature on the pure red light emission of mixed oxide phosphor for solid state lighting. *Ultrasonics* **28:** 79-89. **ufs-021920 (ingelees deur A-M Pienaar)**

32. **Al Mahdi, A.A.G.A., Hussein, M., Fourie, E., Swarts, J.C. and Dennis, C.R.** 2016. Influence of the decomposition of Tris(2.2-bipyridine)iron(II) and (III) on the reduction of Tris(2,2-bipyridine)iron(III) by hydrazine in aqueous acidic medium: a kinetic study. *Transition Metal Chemistry* **41:** 25-34. **ufs-022732 (ingelees deur A-M Pienaar)**

33. **Erasmus, E., Claassen, J.O. and van der Westhuizen, W.A.** 2015. Catalytic wet oxidation of formic acid in wastewater with natural occuring iron ore. *Water SA* 42: 442-448.**ufs-025396**

34. **Kumar, V., Gohain, M., Som, S., Kumar, V., Bezuidenhoudt, B.C.B. and Swart, H.C.** 2016. Microwave assistedsynthesis of ZnO nanoparticles for lighting and dye removal application. *Physica B* **480:** 36-41. **ufs-025160 (ingelees Fisika)**

35. **Gostynski, R., van Rooyen, P.H. and Conradie, J.** 2016. Jahn-Teller Distortion in Tris[4,4,4-Trifluoro-1-(2-thienyl)-1,3-butanedionato]manganese(III) Isomers: an X-ray and Computational Study. *Journal of Molecular Structure.* **1119**: 48-53.**ufs-025398**

36. **Conradie, J. and Ghosh, A.** 2016. Metalloporphyrin-Nitroxyl Interactions: A DFT Study of the Low-Energy States of Reduced Manganese, Iron, and Cobalt Porphyrin Nitrosyls. *Journal of Physical Chemistry B* **120:22** 4972-4979.**ufs-025399**

37. **Mokolokolo, P.P., Brink, A. and Visser, H.G.** 2016. Crystal structure of bis(μ_2-2-((3-methylphenyl)imino)methylphenolato-κ^2N,O:O)hexacarbonyldimanganese(I), $C_{34}H_{24}Mn_2N_2O_8$. *Zeitschrift fur Kristallographie: New Crystal Structures* **231(2):** 613-615.**ufs-025725**

38. **van Rooyen, P.H. and Conradie, J.** 2016: Orientation of Trimethylolethane Cyclic Phosphite in Rhodium Complexes: Structure of [Rh($CH_3COCHCOCH_3$)(CO)(P(OCH_2)$_3$$CCH_3$)]. *Polyhedron* **111**: 161-166.**ufs-25406**

39. **Malan, F.P., Singleton, E., Landman, M., van Rooyen, P.H. and Conradie, J.** 2016. The Synthesis, Characterisation, Electrochemistry, and the Catalytic Application of new [CpNiBr(NHC)] Complexes. *Suid-Afrikaanse Tydskrif vir Natuurwetenskap en Tegnologie* **35: 1**, 2 bladsye.**ufs-025407**

40. **Conradie, J.** 2016. Bond Stretch Isomers of d^4 Tris(benzoylacetonato-κ^2O,O')Mn(III). *Computational and Theoretical Chemistry* **1087**: 1-5.**ufs-025408**

41. **Conradie, J. and Ghosh, A.** 2016. The Valence States of Copernicium and Flerovium. *European Journal of Inorganic Chemistry* **2016:18** 2989–2992.**ufs-025574**

42. **Kuhn, A., Tischlik, S., Hopmann, K.H., Landman, M., van Rooyen, P.H. and Conradie, J.** 2016. Structure, Substitution and Hydrolysis of Bis(trifluorobenzoylacetonato-O,O') Dichloro Titanium(IV): An Experimental and Computational Study. *Inorganic Chimica Acta* **453**: 345-356.**ufs-025578**

43. **Kuhn, A. and Conradie, J.** 2016. Synthesis, electrochemical and DFT study of octahedral bis(β-diketonato)-titanium(IV) complexes. *Inorganic Chimica Acta* **453**: 247-256.**ufs-025586**

44. **Liu, R., van Rooyen, P.H. and Conradie, J.** 2016. Geometrical isomers of Tris(beta-diketonato)metal(III) complexes for M = Cr or Co: synthesis, X-ray structures and DFT study. *Inorganica Chimica Acta*, **447**: 59-65.**ufs-025592**

45. **Mochane, M.J. and Luyt, A.S.** 2016. The Effect of Expanded Graphite on the Physical Properties of Conductive EVA/Wax Phase Change Blends for Thermal Energy Storage. *Polymer Composites* **37:10** 3025-3032.**ufs-025621**

46. **Sibeko, M.A., Saladino, M.L., Luyt, A.S. and Caponetti, E.** 2016. Morphology and properties of poly(methyl methacrylate) (PMMA) filled with mesoporous silica (MCM-41) prepared by melt compounding. *Journal of Material Science* **51** 3957-3970.**ufs-025623**

47. **Gumede, T.P., Luyt, A.S., Perez-Camargo, R.A., Iturrospe, A., Arbe, A., Zubitur, M., Mugica, A. and Muller, A.J.** 2016. Plasticization and Cocrystallization in LLDPE/Wax Blends. *Journal of Polymer Science Part B-Polymer Physics* **54:** 1469-1482.**ufs-025633**

48. **Mofokeng, J.P., Kelnar, I. and Luyt, A.S.** 2016. Effect of layered silicates on the thermal stability of PCL/PLA microfibrillar composites. *Polymer Testing* **50: 9-14.ufs-025673**

49. **Saladino, M.L., Armetta, F. Sibeko, M.A., Luyt, A.S., Martino, D.F.C. and Caponetti, E.** 2016. Preparation and characterization of Ce:YAG –polycarbonate composites for white LED. *Journal of Alloys and Compounds* **664:** 726-731.**ufs-025678**

50. **Armetta, F. Sibeko, M.A., Luyt, A.S., Martino, D.F.C., Spinella, A. and Saladino, M.L.** 2016. Influence of the Ce:YAG Amount on Structure and Optical Properties of Ce:YAG-PMMA Composites for White LED. *Zeitschrift fur Physikalische Chemie-International Journal ofd Research in Physical Chemistry & Chemical Physics* **230:9** 1219-1231.**ufs-025688**

51. **Tsai, C-W, Langner, E.H.G.** 2016. The effect of synthesis temperature on the particle size of nano-ZIF-8. *Microporous and Mesoporous Materials* **221:** 8-13.**ufs-025726**

52. **Jansen van Rensburg, A., Landman, M., Erasmus, E., van der Westhuizen, D., Ferreira, H., Conradie, M.M. and Conradie, J.** 2016. Electrochemical and X-ray photoelectron spectroscopic insights into Molybdenum(0) Fischer ethoxycarbene complexes *Electrochimica Acta* **219:** 204-213.**ufs-025727**

53. **Conradie, J. and Erasmus, E.,** 2016. XPS Fe 2p peaks from iron tris(β-diketonates): Electronic effect of the β-diketonato ligand. *Polyhedron* **119:** 142-150.**ufs-025749**

54. **Nete, M., Purcell, W. and Nel, J.T.** 2016. Separation of Niobium and Tantalum Pentafluoride by Selective Precipitation Using ρ-Phenylenediamine. *The Journal of the Minerals, Metals & Materials Society* **68: 11** 2817-2823.**ufs-025803**

55. **Ferreira, H., Von Eschwege, K.G., Conradie, J.** 2016. Electronic Properties of Iron Charge Transfer Complexes – A Combined Experimental and Theoretical Approach. *Electrochimica Acta* **216: 339-346**.**ufs-025804**

56. **Kama, D.V., Brink, A. and Visser, H.G.** 2016. Crystal structure of bis(μ2-chloro)-bis(di-p-tolylhydroxyphosphine-P)-bis(di-p-tolylphosphite-P)-di-palladium. *Zeitschrift fur Kristallographie: New Crystal Structures* **231(4):** 1081–1083.**ufs-025806**

57. **Frei, A., Sidler, D., Mokolokolo, P., Braband, H., Fox, T., Spingler, B., Roodt, A., Alberto, R.** 2016. Kinetics and Mechanism of CO Exchange in $[MBr_2(solvent)(CO)_3]^-$ (M = Re, ^{99}Tc). *Inorg. Chem*. **55**, 9352−9360.**ufs-025810**

58. **Vazquez-Lima, H., Conradie, J. and Ghosh, A.** 2016. Metallocorrole-Mediated Sensing of Carbon Monoxide, Nitric Oxide, and the Nitroxyl Anion. A DFT Survey of Low-Energy Bound States. *Inorganic Chemistry* **55**: 8248-8250.**ufs-025817**

59. **Walter, M.R., Dzul, S.P., Rodrigues, A.V., Stemmler, T.L., Telser, J., Conradie, J., Ghosh, A. and Harrop, T.C.** 2016. Synthesis of Co^{II}-NO^- Complexes and Their Reactivity as a Source of Nitroxyl. *Journal of the American Chemical Society* **138**: 12459–12471.**ufs-025869**

60. **Bolotin, D.S., Il'in, M.V., Kolesnikov, I.E., Suslonov, V.B., Novozhilov, Y., Ronzhina, O., Krasavin, M., Boyarskiy, V.P., Koen, R. and Roodt, A.** 2016. Fluorescent (pyrazolyl acetoxime)Zn^{II} complexes: Synthetic, structural, and photophysical studies. *Inorganica Chimica Acata* **455:** 9-14.**ufs-025876**

61. **Landman, M., Gostynski, R. and Conradie, J.** 2016: Electrochemical Behaviour of Cr and W Fischer Ethoxy Carbene Complexes: a comparative study. *Journal of Nano Research* **44**: 1-9.**ufs-026256**

62. **Koen, R., Roodt, A. and Visser, H.G.** 2016. Exploring differences in various Nb(V)- and Ta(V) tropolonato complexes by a solid-state structural comparison study. *The Journal of the Southern African Institute of Mining and Metallurgy* **116:** 895-899.ufs-**026010**

63. **Erasmus, E., Muller, A.J., Siegert, U. and Swarts, J.C**. 2016. Synthesis by ligand exchange and electrochemistry of ruthenocenylcontaining β-diketonato complexes of titanocene. Structure of $[TiCp_2(RcCOCHCOCH_3)][ClO_4]$. *Journal of Organometallic Chemistry* **861:** 62-70.**ufs-026015**

64. **Novak-Krol, A., Fourie, E., Joubert, C. C., Gryko, D., Gryko, D. T., Swarts, J. C.** 2016. Stable, Low-Melting *trans*-A_2B-Corroles. *Journal of Porphyrins and phthalocyanines*, **20:** 1-12.**ufs-026022**

65. **Korb, M., Swarts, P. J., Miesel, D., Hildebrandt, A., Swarts, J. C., Lang, H.** 2016. Nucleophilic Aromatic Substitution Reactions for the Synthesis of Ferrocenyl Aryl Ether. *Organometallics*, **35:** 1287-1300.**ufs-026054**

66. **Lewtak, J. P., Landman, M., Fernández I., Swarts, J. C.** 2016. A DFT-Elucidated Comparison of the Solution-Phase and SAM Electrochemical Properties of Short-Chain Mercaptoalkylferrocenes: Synthetic and Spectroscopic Aspects, and the Structure of $FcCH_2CH_2$-S-S-CH_2CH_2Fc. *Inorganic Chemistry*, **55:** 2584-2596.**ufs-026070**

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68. **Conradie, M.M.**, **Gostynski, R., Liu, R. and Conradie, J.** 2016: Electronic influence of different β-diketonato ligands on the electrochemical behaviour of tris(β-diketonato)M(III) complexes, M = Cr, Mn and Fe. *Journal of Nano Research* **44**: 252-264.**ufs-026257**

69. v**an Tonder, J. A., Visser, H. G. and Koen, R.** 2016. The crystal structure of 6-chloro-2,4-diphenylquinoline. *Zeitschrift fur Kristallographie: New Crystal Structures* **231(2):** 233-235**.ufs-026475**

70. **Koen, R., Visser, H. G. and Roodt A. 2016.** Crystal structure of tetraethylammonium hexachloridotantalate (V). *Zeitschrift fur Kristallographie: New Crystal Structures* **231:** 227-229.**ufs-026477**

71. **Erasmus, E.** 2016. The influence of thermal treatment on properties of kaolin. *Hemijska Industrija* **70(5):** 595-601.**ufs-026875**

wag **M. Esterhuysen, A. Brink, H. G. Visser, A. Roodt, M. Zbačnik, J. P. Slabbert, P. R. Beukes**. 2016. Synthesis, Structure and Biological Study of Gallium(III) Complexes as Model Radiopharmaceuticals.; *European Journal of Medical Physics*, **32(9):** Supplement 2, 167…….

wag75.**Ayyavoo Kannan, Ramasamy Anandhan and Perumal Rajakumar**. 2016. Synthesis and optical, electrochemical properties of glucose cored ferrocenyl dendrimers, *Synth. Commun.*, **2016**, DOI: 10.1080/00397911.2016.1245752. (Article in press)…**wag**…..