



NATURAL AND
AGRICULTURAL SCIENCES
NATUUR- EN
LANDBOUWETENSKAPPE

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PUBLIKASIES/PUBLICATIONS - 2015

1. **Kumar, V., Swart, H.C., Gohain, M., Bezuidenhout, B.C.B., van Vuuren, A.J., Lee, M. and Ntwaeaborwa, O.M.** 2015. The role of neutral and ionized oxygen defects in the emission of tin oxide nanocrystals for near white light application. *Nanotechnology* **26**: 295703 (1-11). **ufs-021741(ingelees Fisika)**
2. **Sefadi, S.J., Luyt, A.S. and Pionteck, J.** 2015. Effect of Surfactant on EG Dispersion in EVA and Thermal and Mechanical Properties of the System. *Journal of Applied Polymer Science* **132**:4 41352 (1 – 11). **ufs-021700**
3. **Abay, E.T., van der Westhuizen, J.H., Swart, K.J., Gibhard, L., Lawrence, N., Dambuza, N., Wilhelm, A., Pravin, K. and Wiesner, L.** 2015. Efficacy and pharmacokinetic evaluation of a novel anti-malarial compound (NP046) in a mouse model. *Malaria Journal* **14**:8 1-7. **ufs-021701**
4. **Motsoeneng, T.S., van Reenen, A.J. and Luyt, A.** 2015. Structure and properties of a β -nucleated polypropylene impact copolymer. *Polymer International* **64**: 222-228. **ufs-021702**
5. **Gohain, M., Kumar, V., van Tonder, J.H., Swart, H.C., Ntwaeaborwa, O.M. and Bezuidenhout, B.C.B.** 2015. Nano CuFe_2O_4 : an efficient, magnetically separable catalyst for transesterification of β -ketoesters. *RSC Advances* **5**: 18972-18976. **ufs-021703**
6. **Pionteck, J., Valdez, E.M.M., Piana, F., O, M., Luyt, A.S. and Voit, B.** 2015. Reduced percolation concentration in polypropylene/expanded graphite composites: Effect of viscosity and polypyrrole. *Journal of Applied Polymer* **132**:20 41994 (1-12). **ufs-021704**
7. **Mochane, M.J. and Luyt, A.S.** 2015. Synergistic effect of expanded graphite, diammonium phosphate and Cloisite 15A on flame retardant properties of EVA and EVA/wax phase-change blends. *Journal of Material Science* **50**: 3485-3494. **ufs-021706**
8. **Mofokeng, J.P. and Luyt, A.S.** 2015. Morphology and thermal degradation studies of melt-mixed poly(hydroxybutyrate-co-valerate)(PHBV)/poly(ϵ -caprolactone)(PCL) biodegradable polymer blend nanocomposites with TiO_2 as filler. *Journal of Material Science* **50**: 3812-3824. **ufs-021707**
9. **Mofekeng, J.P. and Luyt, A.S.** 2015. Morphology and thermal degradation studies of melt-mixed PLA/PHBV biodegradable polymer blend nanocomposites with TiO_2 as filler. *Journal of Applied Polymer Science* **132**:25 (1-11). **ufs-021709**
10. **Manicum, A., Schutte-Smith, M., Kemp, G. and Visser, H.G.** 2015. Illustration of the electronic influence of coordinated β -diketone type ligands: A kinetic and structural study. *Polyhedron* **85**: 190-195. **ufs-021710**

11. **Ponra, S., Gohain, M., van Tonder, J.H. and Bezuidenhoudt, B.C.B.** 2015. Al(OTf)₃-Catalyzed Preparation of 4-Hydroxy-3-propargylic Coumarins and Subsequent Regioselective Cyclization towards Furo- or Pyrano[3,2-c]coumarins. *Synlett* **26**: 745-750.[ufs-021710](#)
12. **Mokhothu, T.H., Luyt, A.S., Morselli, D., Bondioli, F. and Messori, M.** 2015. Influence of *In Situ*-Generated Silica Nanoparticles on EPDM Morphology, Thermal, Thermomechanical, and Mechanical Properties. *Polymer Composites* **36**:5 825-833.[ufs-021711](#)
13. **Kuhn, A and Conradie, J.** 2015. Observed hydrolysis of fluorine substituted bis(β -diketonato)-dichlorotitanium(IV) complexes. *Dalton Transactions* **44**: 5106-5113.[ufs-021712](#)
14. **Conradie, M.M. and Conradie, J.** 2015. Electrochemical behavior of Tris(β -diketonato)iron(III) complexes: A DFT and experimental study. *Electrochimica Acta* **152**: 512-519.[ufs-021713](#)
15. **Manicum, A-L, Visser, H.G., Engelbrecht, I. and Roodt, A.** 2015. Crystal structure of *fac*-(acetylacetonato- κ^2 O,O')tricarbonyl(carclohexyl-diphenylphosphine- κ P)rhenium(I), C₂₆H₂₈O₅Pre. *Zeitschrift fur Kristallographie: New Crystal Structures* **230**: 150-152.[ufs-021726](#)
16. **Mofokeng, J.P. and Luyt, A.S.** 2015. Morphology and thermal degradation studies of melt-mixed poly(lactic acid) (PLA/poly(ϵ -caprolactone) (PCL) diodegradable polymer blend nanocomposites with TiO₂ as filler. *Polymer Testing* **45**: 93-100.[ufs-021751](#)
17. **Mofokeng, J.P. and Luyt, A.S.** 2015. Dynamic mechanical properties of PLA/PHBV, PLA/PCL, PHBV/PCL blends and their nanocomposites with TiO₂ as nanofiller. *Therochimica Acta* **613**: 41-53.[ufs-021752](#)
18. **Mochane, M.J. and Luyt, A.S.** 2015. The Effect of Expanded Graphite on the Thermal Stability, Latent Heat, and Flammability Properties of EVA/Wax Phase Change Blends. *Polymer Engineering and Science* **55**:6 1255-1262.[ufs-021753](#)
19. **Mokhothu, T.H., Luyt, A.S., Morselli, D., Bondioli, F. and Messori, M.** 2015. Influence of *In Situ*-Generated Silica Nanoparticles on EPDM Morphology, Thermal, Thermomechanical, and Mechanical Properties. *Polymer Composites* **36**: 825-833.[ufs-021754](#)
20. **Sefadi, J.S., Luyt, A.S., Pionteck, J. and Gohs, U.** 2015. Effect of surfactant and radiation treatment on the morphology and properties of PP/EG composites. *Journal of Material Science* **50**: 6021-6031.[ufs-021755](#)
21. **Landman, M., Fraser, R., Twigge, L. and Conradie, J.** 2015. Fischer aminocarbene conformers containing a 2-thienyl or 2-furyl ring: a crystallographic, NMR, and DFT study. *Journal of Coordination Chemistry* **68**:14, 2388-2408.[ufs-021759](#)

22. **Kuo, C.-M., Hill T.N. and Bezuidenhoudt. B.C.B.** 2015. Crystal structure of 7-benzyloxy-5,6-dihydroxyflavone $C_{22}H_{16}O_5$. *Zeitschrift für Kristallographie, NCS*, **230**:193-194.[ufs-021762](#)
23. **Hill T.N., Kuo, C.-M., and Bezuidenhoudt. B.C.B.** 2015. Crystal structure of 3-bromo-4,6-dibenzyloxy-2-hydroxy acetophenone. *Zeitschrift für Kristallographie, NCS*, **230**: 251-252.[ufs-021768](#)
24. **Du, K., de Mieri, M., Saxena, P., Phungul, K.V., Wilhelm, A., Hrubaru, M.M., van Rensburg, E., Zietsman, P.C., Hering, S., van der Westhuizen, J.H. and Hamburger, M.** 2015. HPLC-Based Activity Profiling for hERG Channel Inhibitors in the South African Medicinal Plant *Galenia Africana*. *Planta Medica* **81**: (12-13): 1154-1162.[ufs-021779](#)
25. **Schutte-Smith, M. and Visser, H.G.** 2015. The versatility of pyridine-2,5-dicarboxylic acid in the synthesis of *fac*-M(CO)₃ complexes (M = Re, ^{99m}Tc): Reactivity toward substitution reactions and derivatization after coordination to a metal. *Polyhedron* **89**: 122-128.[ufs-021786](#)
26. **Twala, T.N., Schutte-Smith, M., Roodt, A. and Visser, H.G.** 2015. Activation of the manganese(I) tricarbonyl core by selective variation of bidentate ligands (L,L'-Bid = N,N' and N,O donor atom sets) in *fac*-[Mn(CO)₃(L,L'-Bid)(CH₃OH)]ⁿ complexes. *Dalton Transactions* **44**: 3278 – 3288.[ufs-021788](#)
27. **Mochane, M.J. and Luyt, A.S.** 2015. The effect of expanded graphite on the flammability and thermal conductivity properties of phase change material based on PP/wax blends. *Polymer Bulletin* **72**: 2263-2283.[ufs-021789](#)
28. **Molaba, M.P., Dudic, D. and Luyt, A.S.** 2015. Influence of the presence of medium-soft paraffin wax on the morphology and properties of iPP/silver nanocomposites. *eXPRESS Polymer Letters* **9**:10 901-915.[ufs-021790](#)
29. **Mokhena, T.C., Jacobs, V. and Luyt, A.S.** 2015. A review on electrospun bio-based polymers for water treatment. *eXPRESS Polymer Letter* **9**:10 839-880.[ufs-021791](#)
30. **Landman, M., Levell, T.J., Buitendach, B.E., Conradie, M.M and Conradie, J.** 2015. Effect of CO substitution on the redox properties of Fischer Mo(0) carbene complexes Mo(CO)₅=C(Y)(2-Furyl), Y = OEt, NHCy or NH₂. *Electrochimica Acta* **174**: 252-289.[ufs-021809](#)
31. **Landman, M., Levell, T.J., Conradie, M.M., van Rooyen, P.H. and Conradie J.** 2015. Structural and conformational study of pentacarbonyl and phosphine substituted Fischer alkoxy- and aminocarbene complexes of molybdenum. *Journal of Molecular Structure* **1086**: 190-200.[ufs-021810](#)
32. **Landman, M., Buitendach, B.E., Conradie, M.M., Fraser, R., van Rooyen, P.H. and Conradie, J.** 2015. Fischer mono and biscarbene complexes of tungsten with mono and dimeric heteroaromatic substituents. *Journal of Electroanalytical Chemistry* **739**: 202-210.[ufs-021818](#)

33. **Kuhn, A. and Conradie, J.** 2015. Structural investigation of trifluoromethyl substituted bis(β -diketonato)-dichlorotitanium(IV) complexes displaying a mono-dinuclear equilibrium hydrolysis reaction. *Journal of Molecular Structure* **1098**: 267-276.[ufs-021819](#)

34. **van As, A., Joubert, C.C., Buitendach, B.E., Erasmus, E., Conradie, J., Cammidge, A.N., Chambrier, I., Cook, M.J. and Swarts, J.C.** 2015. Tetrabenzoporphyrin and -mono-, -cis-di- and Tetrabenzotriazaporphyrin Derivatives: Electrochemical and Spectroscopic Implications of meso CH Group Replacement with Nitrogen. *Inorganic Chemistry*, **54**: 5329-5341.[ufs-021832](#)

35. **Duvenhage, M-M, Ntwaeaborwa, M., Visser, H.G., Swarts, P.J., Swarts, J.C. and Swart, H.C.** 2015. Determination of the optical band *gap* of Alq₃ and its derivatives for the use in two-layer OLEDs. *Optical Materials* **42**: 193-198.[ufs-021698](#) ([ingelees Fisika](#)).

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38. **Freitag, R. and Conradie, J.** 2015. Electrochemical and Computational Chemistry Study of Mn(β -diketonato)₃ complexes. *Electrochimica Acta* **158**: 418-426.[ufs-021949](#)

39. **Landman, M., Levell, T.J., Buitendach, B.E., Conradie, M.M. and Conradie, J.** 2015. Effect of CO substitution on the redox properties of Fischer Mo(0) carbene complexes Mo(CO)₅ = C(Y)(2-Furyl), Y = OEt, NHCy or NH₂. *Electrochimica Acta* **174**: 282-289.[ufs-021954](#)

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41. **Conradie, J., Patra, A.K., Harrop, T.C. and Ghosh, A.** 2015. Square-Antiprismatic Eight-Coordinate Complexes of Divalent First-Row Transition Metal Cations: A Density Functional Theory Exploration of the Electronic-Structural Landscape. *Inorganic Chemistry* **54**: 1375-1383.[ufs-022151](#)

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45. **Conradie, J., Berg, S. and Ghosh, A.** 2015. Mechanisms of Oxygen Atom Transfer between Main-Group Elements. *European Journal of Inorganic Chemistry* 4138-4144.[ufs-022197](#)
46. **Capar, J., Conradie, J., Beavers, C.M. and Ghosh, A.** 2015. Molecular Structures of Free-Base Corroles: Nonplanarity, Chirality, and Enantiomerization. *The Journal of Physical Chemistry A* **119**: 3452-3457.[ufs-022249](#)
47. **Chiweshe, T.T., Purcell, W. and Venter, J.A.** 2015. ICP-OES Monitoring of the Instability of $[\text{OsCl}_6]^{2-}$ and Evaluation of $[\text{OsO}_2(\text{CN})_4]^{2-}$ as Alternative Standard for Osmium Quantification. *Bulletin of the Chemical Society of Japan* **88**:8 1054-1063.[ufs-022255](#)
48. **Gohain, M., van Tonder, J.H. and Bezuidenhoudt, B.C.B.** 2015. $\text{NaHSO}_4\text{-SiO}_2$: An Efficient Reusable Green Catalyst for Selective C-3 Propargylation of Indoles with Tertiary Propargylic Alcohols. *Iranian Journal of Chemistry & Chemical Engineering – International English Edition* **34**: 3 11-17.[ufs-022289](#)
49. **Marake, D.T., Mokolokolo, P.P., Visser, H.G., Brink, A.** 2015. Structural comparison of group 7 tricarbonyl complexes of 2-[[2-(1H-imidazol-4-yl)ethyl]iminomethyl]-5-methylphenolate *Acta Crystallographica Section C: Structural Chemistry* **71**, 1, 423-429.[ufs-022296](#)
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53. **Mphure, L.T., Visser, H.G., Roodt, A. and Brink, A.** 2015. Crystal structure of dichloro-*N,N*-bis(pyridine-2-ylmethyl)cyclohexamino copper(II), $\text{C}_{18}\text{H}_{23}\text{Cl}_2\text{CuN}_3$. *Zeitschrift für Kristallographie: New Crystal Structures* **230**: 156-158.[ufs-022589](#)
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57. **Purcell, W. and Visser, H.G.** 2015. Rhenium(V)-nitrido complexes with different nitrogen donor bidentate ligands. *Transition Metal Chemistry* **40**: 899-906.**ufs-022733**
58. **Kumar, V., Gohain, M., van Tonder, J.H., Ponra, S., Bezuidenhoudt, B.C.B., Ntwaeaborwa, O.M. and Swart, H.C.** 2015. Synthesis of quinolone based heterocyclic compounds for blue lighting application. *Optical Materials* **50**: 275-281 **ufs-022439 (ingelees deur Fisika)**
59. **Jansen van Rensburg, A., Landman, M., Van der Westhuizen, D., Conradie, M.M. and Conradie, J.** 2015. Electrochemistry of Triphenylarsine-substituted Tungsten(0) Fischer carbene complexes. *Electrochimica Acta* **186**: 321–327.**ufs-022756**
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62. **Bonnet, S.L., Wilhelm A., Willcox, M. and Phungula.** 2015. Retrospective treatment outcome analysis on the use of medicinal plants to alleviate diarrhoea in the Thaba Nchu area of the Free State Province, South Africa. *Planta Medica* **81**: 99.**ufs-022919**
63. **Noto, L.L., Roos, W.D., Ntwaeaborwa, O.M., Gohain, M., Yagoub, M.Y.S., Coetsee, E. and Swart, H.C.** 2015. The role of Flux Material on the Enhancing of the Luminescent Intensity and Persistent Emission of $\text{ZnTa}_2\text{O}_6\text{:Pr}^{3+}$ Phosphor. *Science of Advanced Materials* **7**: 1-10.**ufs-022799 (ingelees deur Fisika)**
64. **Herbst, L., Visser, H.G., Roodt, A., Steyn, M and Loganathan, N.** 2015. Crystal structure of (2-(benzoyl)phenolato- k^2O, O')-trans-dichlorido-cis(methoxido)niobium(V), $\text{C}_{15}\text{H}_{15}\text{Cl}_2\text{NbO}_4$. *Zeitschrift für Kristallographie: New Crystal Structures* **230:4** 345-347.**ufs-022841**
65. **Muller, K.A., Venter, J.A. and Visser, H.G.** 2015. Crystal structure of potassium dizqua dihydroxy(methylenediphosphonato- k^2O, O')cobaltate(III), $\text{Ch}_{10}\text{CoKO}_{10}\text{P}_2$. *Zeitschrift für Kristallographie: New Crystal Structures* **230:4** 349-351.**ufs-022863**
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