



## Publikasies 2013 - RIMS

1. **von Eschwege, K.G.** 2013. Synthesis and kinetics of electronically altered photochromic dithizonatopenylmercury(II) complexes. *Journal of Photochemistry and Photobiology A: Chemistry* **252**: 159-166.
2. **Zanotto A. Luyt, A.S., Spinella, A. and Caponetti, E.** 2013. Improvement of interaction in and properties of PMMA-MWNT nanocomposites through microwave assisted acid treatment of MWNT. *European Polymer Journal* **49**: 61-69.
3. **He, W., Zhuang, M., Yanxin, Li., Luyt, A.S. and Ge, T-J.** 2013. In-Situ Polymerization Organic-Inorganic Hybrid Materials Monomer Casting Polyamide 6/ Nanorods Yttrium Hydroxide. *Advanced Materials Research* **662**: 24-27.
4. **Venter, G.J.S., Steyl, G. and Roodt, A.** 2013. 2,6-Dichloroaniline-4-(2,6-dichloro-anilino)pent-3-en-2-one (1/2). *Acta Crystallographica Section E* **E69**: o34-o35.
5. **Ahmad, E.E., Luyt, A.S. and Djokovic, V.** 2013. Thermal and dynamic mechanical properties of bio-based poly(furfuryl alcohol)/sisal whiskers nanocomposites. *Polymer Bull.* **70**: 1265-1276.
6. **Klepac, D., Scetar, M., Kurek, M., Mallon, P.E., Luyt, A.S., Galic, K. and Valic, S.** 2013. Oxygen permeability, electron spin resonance, differential scanning calorimetry and positron annihilation lifetime spectroscopy studies of uniaxially deformed linear low-density polyethylene film. *Polymer Int* **62**: 474-481.
7. **Motaung, T.E., Luyt, A.S., Saladino, M.L. and Caponetti, E.** 2013. Study of Morphology, Mechanical Properties, and Thermal Degradation of Polycarbonate-Titania Nanocomposites as Function of Titania Crystalline Phase and Content. *Polymer Composites* **34**: 164-172.
8. **Morselli, D., Nondioli, F., Luyt, A.S., Mokhothu, T.H. and Messori, M.** 2013. Preparation and Characterization of EPDM Rubber Modified with *in Situ* Generated Silica. *Journal of Applied Polymer* **128**: 2525-2532.
9. **Purcell, W., Conradie, J., Chiweshe, T.T., Venter, J.A., Visser, H.G. and Coetzee, M.P.** 2013. Characterization of acetylacetonato carbonyl diphenyl-2-pyridylphosphine rhodium(I): Comparison with other carbonyl complexes. *Journal of Molecular Structure* **1038**: 220-229.
10. **Warsink, S., Fessha, F.G., Purcell, W.P. and Venter, J.A.** 2013. Synthesis and characterization of rhodium(I) 2-methylcupferrate complexes and their kinetic behavior in iodomethane oxidative addition. *Journal of Organometallic Chemistry* **726**: 14-20.

11. **Steyn, M., Visser, H.G. and Roodt, A.** 2013. Evaluation of oxine-type ligand coordination to zirconium(IV). *The Journal of The Southern African Institute of Mining and Metallurgy* **113**: 105-108.
12. **Ndlovu, S.S., van Reenen, A.J. and Luyt, A.S.** 2013. LDPE-wood composites utilizing degraded LDPE as compatibilizer. *Composites: Part A* **51**: 80-88.
13. **Sluijter, D.N., Warsink, S., Lutz, M. and Elsevier, C.J.** 2013. Synthesis of palladium(O) and -(II) complexes with chelating *bis*(*N*-heterocyclic carbene) ligands and their application in semihydrogenation. *Dalton Transactions* **42**: 7365-7372.
14. **Bozanic, D.K., Luyt, A.S., Trandafilovic, L.V. and Djokovic, V.** 2013. Glycogen and gold nanoparticle bioconjugates: controlled plasmon resonance *via* glycogen-induced nanoparticle aggregation. *RSC Advances* **3**: 8705-8713.
15. **Hill, T.N.** 2013. Crystal structure of phosphide-*tris*-(triphenylphosphine)copper(I) acetone solvate, C<sub>57</sub>H<sub>51</sub>CuOP<sub>4</sub>. *Zeitschrift für Crystallographie: New Crystal Structures* **228**: 120-122.
16. **Hill, T., Roodt, A. and Steyl, G.** 2013. Probing the 'Venus fly-trap' parameters of cyclo-octadiene in selected  $\beta$ -diketonato complexes of platinum(II) and the nickel-triad from a spectroscopic, X-ray crystallographic and DFT study. *Polyhedron* **50**: 82-89.
17. **Hill, T.N., Roodt, A. and Steyl, G.** 2013. Electronic influence of  $\beta$ -diketonato-type ligands on the coordination of 1,5-cyclooctadiene to palladium(II) as defined by 'Venus fly trap' geometric parameters. *Acta Crystallographica Section B Structural Science, Crystal Engineering and Materials* **B69**: 36-42.
18. **Cloete, N., Visser, H.G., Engelbrecht, I., Overett, M.J., Gabrielli, W.F. and Roodt, A.** 2013. Ethylene Tr- and Tetramerization: a Steric Parameter Selectivity Switch from X-ray Crystallography and Computational Analysis. *Inorganic Chemistry* **52**: 2268-2270.
19. **Brink, A., Visser, H.G. and Roodt, A.** 2013. Novel imino rhenium(I) tricarbonyl complexes of salicylidene-derived ligands: Synthesis, X-ray crystallographic studies, spectroscopic characterization and DFT calculations. *Polyhedron* **52**: 416-423.
20. **Motaung, T.E., Daldino, M.L., Luyt, A.S. and Martino, D.C.** 2013. Influence of the modification, induced by zirconia nanoparticles, on the structure and preoperties of polycarbonate. *European Polymer Journal* **49**: 2011-2030.
21. **Kuo, C-M., Bezuidenhoudt, B.C.B. and Conradie, J.** 2013. Determination of the relationship between theoretical vibrational frequencies and experimental IR absorbance bands in organic molecules: computational study of oxane, chromane and flavan. *Journal of Physical Organic Chemistry* **26**: 327-334.
22. **Conradie, J.** 2013. A DFT study of the reactivity of  $\beta$ -diketonato-1,5-cyclo-octadieneiridium(I) complexes. *Polyhedron* **51**: 164-167.

23. **Conradie, J.** 2013. Carbonyl Substitution in  $\beta$ -Diketonatodicarbonyl-rhodium(I) by Cyclo-octadiene: Relationships with Experimental, Electronic and Calculated Parameters. *South Africa Journal of Chemistry* **66**: 54-59.
24. **Stuurman, N.F., Muller, A. and Conradie, J.** 2013. Structural trends in  $[\text{Rh}(\text{PhCOCHCO}(\text{CH}_2)_n\text{CH}_3)(\text{CO})(\text{PPh}_3)]$  ( $n = 0-3$ ) and related complexes: crystal structure of  $[\text{Rh}(\text{PhCOCHCO}(\text{CH}_2)_2(\text{CO})(\text{PPh}_3)]$ . *Transition Metal Chemistry* **38**: 4290440.
25. **Erasmus, J.J.C. and Conradie, J.** 2013. Chemical and electrochemical oxidation of  $[\text{Rh}(\beta\text{-diketonato})(\text{CO})(\text{P}(\text{OCH}_2)_3\text{CCH}_3)]$ : an experimental and DFT study. *Dalton Transactions* **42**: 8655-8666.
26. **Stuurman, N.F., Muller, Muller, A. and Conradie, J.** 2013. Conformational analysis of triphenylphosphine in square planar  $[\text{Rh}(\beta\text{-diketonato})(\text{CO})(\text{PPh}_3)]$  complexes. Crystal structure of  $[\text{Rh}(\text{PhCOCHCO}(\text{CH}_2)_3\text{CH}_3(\text{CO})(\text{PPh}_3)]$ . *Inorganica Chimica ACTA* **395**: 237-244.
27. **Gohain, M., Van Tonder, J.H., and Bezuidenhoudt, B.C.B.** 2013.  $\text{Bi}(\text{OTf})_3$ -catalyzed solvent-free synthesis of pyrano[3,2-c]-coumarins through a tandem addition/annulation reaction between chalcones and 4-hydroxycoumarins. *Tetrahedron Lett.*, **54**: 3773-3776.
28. **Sunil, A.C., Langner, E.H.G., Marais, C., Bezuidenhoudt, B.C.B.** 2013. Thermo-analytical determination of intermediates in the copper catalysed rearrangement of o-toluic acid to meta-cresol. *Catal. Sci. Technol.*, **3**: 2227-2233.
29. **Duvenhage, M-M., Swart, H.C., Ntwaeaborwa, O.M. and Visser, H.G.** 2013. Synthesis, crystal structure, luminescent properties and photo degradation of *mer-tris*(8-Hydroxy-quinolinato-N,O)-indium(iii) hydrate 0.5 methanol solvate. *Optical Materials*, **35**: 2355-2371.
30. **Brink, A., Visser, H.G. and Roodt, A.** 2013. Activation of Rhenium(I) Toward Substitution in *fac*- $[\text{Re}(\text{N},\text{O}'\text{-Bid})(\text{CO})_3(\text{HOCH}_3)]$  by Schiff-Base Bidentate Ligands (N,O'-Bid). *Inorganic Chemistry* **52**: 8950-8961.
31. **Gomo, M., van Tonder, G.J. en Steyl, G.** 2013. Investigation of the hydrogeochemical processes in an alluvial channel aquifer located in a typical Karoo Basin of Southern Africa. *Environ Earth Sci* **70**: 227-238.
32. **Purcell, W., Conradie, J., Chiweshe, T.T., Venter, J.A., Twigge, L. and Coetzee, M.P.** 2013. Characterization and oxidative addition reactions of rhodium(I) carbonyl cupferrate diphenyl-2-pyridylphosphine complexes. *Journal of Organometallic Chemistry* **745-746**: 439-453.
33. **Hennion, C., Jonasson, K.J., Wendt, O.F. and Roodt, A.** 2013. Kinetic and mechanistic investigation of the substitution reactions of four and five co-ordinated rhodium stibine complexes with a bulky phosphite. *Dalton Transactions* **42**: 14134-14139.

34. **Sibeko, M.A. and Luyt, A.S.** 2013. Preparation and Characterization of Vinylsilane Crosslinked High-Density Polyethylene Composites Filled with Nanoclays. *Polymer Composites* **34**: 1720-1727.
35. **Pieterse, T.** 2013. *N*-Methylmorpholine *N*-Oxide. *Synlett* **24**: 2175-2176.
36. **von Eschwege, K.G., van As, L., Joubert, C.C., Swarts, J.C., Aquino, M.A.S. and Cameron, T.S.** 2013. Intramolecular interactions in a new *tris*-dithizonatocobalt(III) complex. *Electrochimica Acta* **112**: 747-755.
37. **du Plessis, M.** 2013. Aluminum Trifluoromethanesulfonate. *Synlett* **24**: 2329-2330.
38. **Warsink, S., Roodt, A., Venter, J.A., Kotze, P.D.R. and Otto, S.** 2013. Crystal structure of (*N*-benzoyl-*N'*-(2,4,6-trimethylphenyl)thiourea- $\kappa$ S)chloride( $\eta$ 4-cycloocta-1,5-diene) rhodium(I), C<sub>25</sub>H<sub>30</sub>ClN<sub>2</sub>ORhS). *Zeitschrift fur Kristallographie: New Crystal Structures* **228**: 335-336.
39. **Warsink, S., Roodt, A., Venter, J.A., Kotze, P.D.R. and Otto, S.** 2013. Crystal structure of is(triphenylphosphine)(carbonyl)(*N*-benzoyl-*N'*-(2-methyl-4-hydroxyphenyl)thiourea- $\kappa$ S, $\kappa$ N)rhodium(I), C<sub>52</sub>H<sub>43</sub>N<sub>2</sub>O<sub>3</sub>P<sub>2</sub>RhS. *Zeitschrift fur Kristallographie: New Crystal Structures* **228**: 428-430.
40. **Venter, G.J.S., Steyl, G. and Roodt, A.** 2013. Crystal structure of carbonyl-(4-2,6-dichlorophenylamino)pent-3-en-2-onato- $\kappa$ 2N,O)-(triphenylphosphine- $\kappa$ P)-rhodium(I) acetone solvate, C<sub>31.5</sub>H<sub>28</sub>Cl<sub>2</sub>NO<sub>2.5</sub>PRh. 2013. *Zeitschrift fur Kristallographie: New Crystal Structures* **228**: 410-412.
41. **Steyn, M., Visser, H.G. and Roodt, A.** 2013. Crystal structure of tetrakis(5,7-dichloroquinolin-8-olato- $\kappa^2$ N,O)zirconium(IV) dimethylformamide disolvate, C<sub>42</sub>H<sub>30</sub>Cl<sub>8</sub>N<sub>6</sub>O<sub>6</sub>Zr. *Zeitschrift fur Kystallographie: New Crystal Structures* **228**: 413-415.
42. **Herbst, L., Visser, H.G. and Roodt, A.** 2013. Crystal structure of (benzoylacetato- $\kappa^2$ O,O')dichloridodimerthoxidotantalum(V), C<sub>12</sub>H<sub>15</sub>Cl<sub>2</sub>O<sub>4</sub>Ta. *Zeitschrift fur Kristallographie: New Crystal Structures* 397-398.
43. **Joubert, C.C., van As, L., Jakob, A., Speck, J.M., Lang, H. and Swarts, J.C.** 2013. Intramolecular electronic communication in ferrocene-based  $\beta$ -diketonato copper(II) complexes as observed by an electrochemical study. *Polyhedron* **55**: 80-86.
44. **Siegert, U., Muller, T.J. and Swarts, J.C.** 2013. Synthesis and electrochemical properties of ferrocene-containing *N*-allylcarbamates: Structure of CH<sub>2</sub>=CHCH<sub>2</sub>-NHCOO-CH<sub>2</sub>Fc. *Polyhedron* **51**: 41-45.
45. **Claus, R., Lewtak, J.P., Muller, T.J. and Swarts, J.C.** 2013. Structural influences on the electrochemistry of 1,1'-di(hydroxylalkyl) ferrocenes. Structure of [Fe{ $\eta^5$ -C<sub>5</sub>H<sub>4</sub>-CH(OH)-(CH<sub>2</sub>)<sub>3</sub>OH}]}<sub>2</sub>]. *Journal of Organometallic Chemistry* **740**: 61-69.

46. **van der Westhuizen, B., Swarts, P.J., Strydom, I., Liles, D.C., Fernandez, I., Swarts, J.C. and Bezuidenhout, D.I.** 2013. Electrochemical illumination of thienyl and ferrocenyl chromium(0) Fischer carbene complexes. *Dalton Transactions* **42**: 5367–5378.
47. **Rüffer, T., Jakob, A., Swarts, J.C. and Lang, H.** 2013. Ferrocenyl  $\beta$ -diketonato - based Cu(II)-oxo clusters with Cu<sub>7</sub> and Cu<sub>10</sub> cores. *Journal of Coordination Chemistry* **66**: 2: 329-333.
48. **van der Westhuizen, B., Swarts, P.J., van Jaarsveld, L.M., Liles, D.C., Siegert, U., Swarts, J.C., Fernandez, I. and Bezuidenhout, D.I.** 2013. Substituent Effects on the Electrochemical, Spectroscopic, and Structural Properties of Fischer Mono- and Biscarbene Complexes of Chromium(0). *Inorganic Chemistry* **52**: 6674-6684.
49. **Erasmus, E. and Swarts, J.C.** 2013. Intramolecular communication and electrochemical observation of the 17-electron ruthenocenium cation in fluorinated ruthenocene-containing  $\beta$ -diketones; polymorphism of C<sub>10</sub>H<sub>21</sub> and C<sub>10</sub>F<sub>21</sub> derivatives. *New J Chemistry* **37**: 2862-2873.
50. **Trzebiatowska-Gusowska, M., Gabor, A., Coetsee, E., Erasmus, E., Swart, H.C. and Swarts, J.C.** 2013. Nano islet formation of formyl- and carboxyferrocene, - ruthenocene, -osmocene and cobaltocenium on amine-functionalized silicon wafers highlighted by crystallographic, AFM and XPS studies. *Journal of Organometallic Chemistry* **745-746**: 393-403.
51. **Buitendach, B.E., Gagor, A. and Swarts, J.C.** 2013. Electrochemical Evidence of Intramolecular Electronic Communication in Zr and Hf Phthalocyanines Bearing Ferrocene-Containing  $\beta$ -Diketonato Axial Ligands: Structure of [PcHf(FcCOCHCOC<sub>6</sub>H<sub>5</sub>)<sub>2</sub>]. *Inorganic Chemistry* **52**: 10245-10257.
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54. **Conradie, M.M. and Conradie, J.** 2013. Solid state packing of [Rh( $\beta$ -diketonato)(CO)<sub>2</sub>] complexes. Crystal structure of [Rh(PhCOCHCOC<sub>4</sub>H<sub>3</sub>S)(CO)<sub>2</sub>]. *Journal of Molecular Structure* **1051**: 137-143.
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58. **Novak, I., Popelka, A., Luyt, A.S., Chehimi, M.M., Spirkova, M., Janigova, I., Kleinova, A., Stopka, P., Slouf, M., Vanko, V., Chodak, I. and Valentin, M.** 2013. Adhesive properties of polyester treated by cold plasma in oxygen and nitrogen atmospheres. *Surface & Coatings Technology* **235**: 407-416.
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65. **Loganathan, N. and Roodt, A.** 2013. Crystal structure of  $\mu$ -oxo-di- $\mu$ -sulfato- $\kappa^2$ O:O'-bis[(2,2'-bipyridine- $\kappa^{2Acta Cryst}$  N,N')-bis(dimethylsulfoxide- $\kappa$ O)-diiron(III)monohydrate, C<sub>24</sub>H<sub>30</sub>Fe<sub>2</sub>N<sub>4</sub>O<sub>12</sub>S<sub>4</sub>. *Zeitschrift fur Kristallographie: New Crystal Structures* **228**: 1-3.
66. **Viljoen, J.A., Visser, H.G., Roodt, A. And Engelbrecht, I.** 2013. Crystal structure of tetrakis(5,7-dibromoquinolin-8-olato- $\kappa^2$ N,O)hafnium(IV) dimethylformamide trisolvate, C<sub>45</sub>H<sub>37</sub>Br<sub>8</sub>HfN<sub>7</sub>O<sub>7</sub>. *Zeitschrift fur Kristallographie: New Crystal Structures* **228**: 485-487.

67. **Herbst, L., Visser, H.G. and Roodt.** 2013. Crystal structure of (benzoylacetonato- $\kappa^2$ O,O)dichloridodimetoxido niobium(V),  $C_{12}H_{15}Cl_2NbO$ . *Zeitschrift für Kristallographie: New Crystal Structures* **228**: 451-452.
68. **Gohain, M., Jacobs, Jc., Marais, C. and Bezuidenhoudt, BCB.** 2013.  $Al(OTf)_3$  Catalysed Friedel Crafts Michael Type Addition of Indoles to  $\alpha,\beta$ -Unsaturated Ketones with PEG-200 as Recyclable Solvent. *Aust. J. Chem* **66**: 1594-1599.
69. **Bezuidenhoudt, D.I., Fernandez, I., van der Westhuizen, B., Swarts, P.J. and Swarts, J.C.** 2013. Electrochemical and Computational Study of Tungsten(O) Ferrocene Complexes: Observation of the Mono-Oxidized Tungsten(O) Ferrocenium Species and Intramolecular Electronic Interactions. *Organometallics* **32**: 7334-7344.