

## Publications: Research Articles 2010

1. **Bem, D.B., Swart, H.C., Luyt, A.S., Coetzee, E. & Dejene, F.B.** 2010. Properties of Green  $\text{SrAl}_2\text{O}_4$  Phosphor in LDPE and PMMA Polymers. *Journal of Applied Polymer Science* 117: 2635-2640.
2. **Božanić, D.K., Trandafilović, L.V., Luyt, A.S. & Djoković, V.** 2010. 'Green' synthesis and optical properties of silver-chitosan complexes and nanocomposites. *Reactive & Functional Polymers* 70: 869-873.
3. **Brink, A., Roodt, A., Steyl, G. & Visser, H.G.** 2010. Steric vs. electronic anomaly observed from iodomethane oxidative addition to tertiary phosphine modified rhodium(I) acetylacetonato complexes following progressive phenyl replacement by cyclohexyl [ $\text{PR}_3 = \text{PPh}_3, \text{PPh}_2\text{Cy}, \text{PPhCy}_2$  and  $\text{PCy}_3$ ]. *Dalton Transactions* 39: 5572-5578.
4. **Capar, C., Hansen, L-K., Conradie, J. & Ghosh, A.** 2010.  $\beta$ -octabromo-meso-tris(pentafluorophenyl)corrole: reductive demetalation-based synthesis of a heretofore inaccessible, perhalogenated free-base corrole. *Journal of Porphyrins and Phthalocyanines* 14: 509-512.
5. **Cloete, N., Visser, H.G. & Roodt, A.** 2010. [*N,N*-Bis(diphenylphosphino)propylamine- $\kappa^2\text{P},\text{P}$ ]dichloridoplatinum(II). *Acta Crystallographica Section E* E66: m51-m52.
6. **Conradie, J. & Ghosh, A.** 2010. Electronic Structure of an Iron-Porphyrin-Nitrene Complex. *Inorganic Chemistry* 49: 243-248.
7. **Conradie, J.** 2010. A DFT and NBO Analysis of the Bonding in Titanocenyl Complexes containing a Five-membered  $\text{L},\text{L}'$ -cyclic Ligand:  $\text{L},\text{L}' = \text{O},\text{O}'; \text{S},\text{S}'$  or  $\text{Se}, \text{Se}'$ . *South African Journal of Chemistry* 63: 65-71.
8. **Conradie, J.** 2010. Bonding in Titanocenyl Complexes Containing  $\text{O},\text{O}'$ -Cyclic Ligands. *International Journal of Quantum Chemistry* 110: 1100-1107.
9. **Conradie, J., Hopmann, K.H. & Ghosh, A.** 2010. Understanding the Unusually Straight: A Search For MO Insights into Linear  $\{\text{FeNO}\}^7$ . *Journal of Physical Chemistry B* 114: 8517-8524.
10. **Conradie, M.M. & Conradie, J.** 2010. A density functional theory study of the oxidative addition of methyl iodide to square planar  $[\text{Rh}(\text{acac})(\text{P}(\text{OPh})_3)_2]$  complex and simplified model systems. *Journal of Organometallic Chemistry* 695: 2126-2133.
11. **Conradie, M.M., & Conradie, J.** 2010. Vereenvoudigde chemiese modellering van rodiumkatalisator - wen of verloor? *Suid-Afrikaanse Tydskrif vir Natuurwetenskap en Tegnologie* 29(3): 147-148.
12. **Conradie, M.M., Conradie, J. & Ghosh, A.** 2010. Capturing the spin state diversity of iron(III)-aryl porphyrins: OLYP is better than TPSSh. *Journal of Inorganic Biochemistry* 105: 84-91.
13. **Dennis, C.R., Potgieter, I.M. & Basson, S.S.** 2010. A kinetic study of the reduction of the octacyanomolybdate(V) ion by the hydroxide ion. *Reaction Kinetics Mechanisms and Catalysis* 99:63-68.

14. **Dennis, I., Pretorius J. & G Steyl.** 2010. Effect of fracture zone on DNAPL transport and dispersion: a numerical approach. *Environmental Earth Science* 61: 1531-1540.
15. **Dikobe, D.G. & Luyt, A.S.** 2010. Comparative study of the morphology and properties of PP/LLDPE/wood powder and MAPP/LLDPE/wood powder polymer blend composites. *Express Polymer Letters* 4: 729-741.
16. **Dikobe, D.G. & Luyt, A.S.** 2010. Morphology and Thermal properties of Maleic Anhydride Grafted Polypropylene/Ethylene-Vinyl Acetate Copolymer/Wood Powder Blend Composites. *Journal of Applied Polymer Science* 116: 3193-3201.
17. **Engelbrecht, I., Visser, H.G. & Roodt, A.** 2010. Bis[*N,N*-bis(diphenylphosphanyl)pentylamine- $\kappa^2P,P'$ ]platinum(II) bis(hexafluoridophosphate) dichloromethane disolvate. *Acta Crystallographica Section E* E66: m922-m923.
18. **Engelbrecht, I., Visser, H.G. & Roodt, A.** 2010. Bis[*N,N*-bis(diphenylphosphanyl)cyclohexylamine- $\kappa^2P,P'$ ]platinum(II) bis(hexafluoridophosphate) dichloromethane disolvate. *Acta Crystallographica Section E* E66: m994-m995.
19. **Engelbrecht, I., Visser, H.G. & Roodt, A.** 2010. *N,N*-Bis(diphenylphosphanyl)cyclopentanamine. *Acta Crystallographica Section E* E66: o3322-o3323.
20. **Engelbrecht, I., Visser, H.G. & Roodt, A.** 2010. *N,N*-Bis(diphenylphosphanyl)cyclopropylamine. *Acta Crystallographica Section E* E66: o2881.
21. **Fourie, E., Swarts, J.C., Lorcy, D. & Bellec, N.** 2010. Synthesis, Substitution Kinetics, and Electrochemistry of the First Tetrathiafulvalene-Containing  $\square$ -Diketonato Complexes of Rhodium(I). *Inorganic Chemistry* 49: 952-959.
22. **Gericke, H.J., Barnard, N.I., Erasmus, E., Swarts, J.C., Cook, M.J. & Aquino, M.A.S.** 2010. Solvent and electrolyte effects in enhancing the identification of intramolecular electronic communication in a multi redox-active diruthenium tetraferrocenoate complex, a triple-sandwiched dicadmium phthalocyanine and a ruthenocene-containing  $\square$ -diketone. *Inorganic Chimica Acta* 363: 2222-2232.
23. **Grove, J.J.C., Van Heerden, P.S., Ferreira, D. & Bezuidenhoudt, B.C.B.** 2010. Conversion of pravastatin into an advanced intermediate for the synthesis of the HMG-CoA reductase inhibitor BB-476. *Tetrahedron Letters* 51: 57-59.
24. **Hato, M.J., Ray, S.S. & Luyt, A.S.** 2010. The Thermal and Rheological Properties of POSS-Containing Poly(methyl methacrylate) Nanocomposites. *Advanced Science Letters* 3: 1-7.
25. **Herbst, L., Koen, R., Roodt, A. & Visser, H.G.** 2010. (Acetylacetonato- $\kappa^2O,O'$ )chloride-trimethanolatoniobium(V). *Acta Crystallographica Section E* E66: m801-m802.
26. **Hildebrandt, A., Rüffer, Erasmus, E., Swarts, J.C. & Lang, H.** 2010. A Star-Shaped Supercrowded 2,3,4,5-Tetraferrocenylthiophene: Synthesis, Solid-State Structure, and Electrochemistry. *Organometallics* 29: 4900-4905.
27. **Hill, T.N. & Steyl, G.** 2010. [*N,N'*-Bis(4-chlorophenyl)pentane-2,4-diiminato]-dicarbonylrhodium(I). *Acta Crystallographica Section E* E66: m205.

28. **Hopmann, K.H., Stuurman, N.F., Muller, A. & Conradie, J.** 2010. Substitution and Isomerization of Asymmetric  $\beta$ -Diketonato Rhodium(I) Complexes: A Crystallographic and Computational Study. *Organometallics* 29:2446-2458.
29. **Johnson, M.T., Johansson, R., Kondrashov, M.V., Steyl, G., Ahlquist, M.S.G., Roodt, A. & Wendt, O.F.** 2010. Mechanisms of the CO<sub>2</sub> Insertion into (PCP) Palladium Allyl and Methyl  $\sigma$ -Bonds. A Kinetic and Computational Study. *Organometallics* 29: 3521-3529.
30. **Kotze, P.D.R., Roodt, A., Venter, J.A. & Otto, S.** 2010. (N-Benzoyl-N'-phenylthiourea- $\kappa$ S)-chlorido( $\eta^4$ -1,5-cyclooctadiene)-rhodium(I). *Acta Crystallographica Section E* E66: m1028-1029.
31. **Kuhn, A. & Conradie, J.** 2010. Electrochemical and density functional theory study of bis(cyclo-pentadienyl)mono( $\square$ -diketonato) titanium(VI) cationic complexes. *Electrochimica Acta* 56: 257-264.
32. **Luyt, A.S., Krupa, I., Assumption, H.J., Admad, E.E.M. & Mofokeng, J.P.** 2010. Blends of polyamide 12 and maleic anhydride grafted paraffin wax as potential phase change materials. *Polymer Testing* 29: 100-106.
33. **Marston, A., Cawood, M., Van der Westhuizen, J. & Zietsman P.** 2010. High-performance countercurrent chromatography for the efficient isolation of alkaloid acetylcholinesterase inhibitors from *Nerine* species (Amaryllidaceae). *Planta Medica* 76: 1208.
34. **Marston, A., Van der Westhuizen, J.H. & Zietsman, P.** 2010. Investigation of South African Amaryllidaceae for inhibitors of acetylcholinesterase. *Planta Medica* 75: 944.
35. **Mishra, S.B., Mishra, A.K., Luyt, A.S., Revaprasadu, N., Hillie, K.T., Van der Merwe Steyn, W.J., Coetsee, E. & Swart, H.C.** 2010. Ethyl Vinyl Acetate Copolymer-SrAl<sub>2</sub>O<sub>4</sub>:Eu,Dy and Sr<sub>4</sub>Al<sub>14</sub>O<sub>25</sub>:Eu,Dy Phosphor-Based Composites: Preparation and Material Properties. *Journal of Applied Polymer Science* 115: 579-587.
36. **Mngomezulu, M.E., Luyt, A.S. & Krupa, I.** 2010. Structure and Properties of Phase Change Materials Based on HDPE, Soft Fischer-Tropsch Paraffin Wax, and Wood Flour. *Journal of Applied Polymer Science* 118: 1541-1551.
37. **Molefi, J.A., Luyt, A.S. & Krupa, I.** 2010. Comparison of LDPE, LLDPE and HDPE as matrices for phase change materials based on a soft Fischer-Tropsch paraffin wax. *Thermochimica Acta* 500: 88-92.
38. **Molefi, J.A., Luyt, A.S. & Krupa, I.** 2010. Comparison of the influence of copper micro- and nano-particles on the mechanical properties of polyethylene/copper composites. *Journal of Material Science* 45: 82-88.
39. **Molefi, J.A., Luyt, A.S. & Krupa, I.** 2010. Investigation of Thermally Conducting Phase-Change Materials Based on Polyethylene/Wax Blends Filled with Copper Particles. *Journal of Applied Polymer Science* 116: 1766-1774.
40. **Mosoabisane, T & Van der Westhuizen, J.** 2010. A novel approach towards the syntheses of proanthocyanidins and biflavonoids. *Planta Medica* 76: 1164.

41. **Motaung, T.E. & Luyt, A.S.** 2010. Effect of maleic anhydride grafting and the presence of oxidized wax on the thermal and mechanical behaviour of LDPE/silica nanocomposites. *Materials Science and Engineering A* 527: 761-768.
42. **Muller, A.J., Conradie, J., Purcell, W., Basson, S.S. & Venter, J.A.** 2010. Characterization and Oxidative Addition Reactions of Different Rhodium and Iridium Triazolato Complexes. *South African Journal of Chemistry* 63: 11-19.
43. **Nete, M., Purcell, W., Snyders, E. & Nel, J.T.** 2010. Alternative dissolution methods for analysis of niobium containing samples. *South African Journal of Chemistry* 63: 130-134.
44. **Osthoff, G., Hugo, A., Bouwman, H., Buss, P., Govender, D., Joubert, C.C. & Swarts, J.C.** 2010. Comparison of the lipid properties of captive, healthy wild, and pansteatitis-affected wild Nile crocodiles (*Crocodylus niloticus*). *Comparative Biochemistry and Physiology, Part A* 155: 64-49.
45. **Otto, S.** 2010. Structure and solution behaviour of cyclooctadiene complexes of platinum(II). *Inorganica Chimica Acta* 363: 3316-3320.
46. **Patra, A.K., Dube, K.S., Papaefthymiou, G.C., Conradie, J., Ghosh, A. & Harrop, T.C.** 2010. *Inorganic Chemistry* 49: 2032-2034.
47. **Schutte, M., Visser, H.G. & Roodt, A.** 2010. Tetraethylammonium bromidotricarbonyl-(tropolonato)rhenate(I). *Acta Crystallographica Section E* E66: m859-m860.
48. **Sisa, M., Bonnet, S.L., Ferreira, D. & Van der Westhuizen, J.H.** 2010. Photochemistry of Flavonoids. *Molecules* 15: 5196-5245.
49. **Steyl, G., Muller, T.J. & Roodt, A.** 2010. Bis(2-(*N*-methylamino)troponato)copper(II). *Acta Crystallographica Section E* E66: m1508-m1508.
50. **Suthiram, J., Zeevaart, J.R., Visser, H.G. & Roodt, A.** 2010. Tetraethylammonium tricarbonyl-chlorido(quinoxaline-2-carboxylato- $\kappa^2 N^1, O$ )rhenate(I). *Acta Crystallographica Section E* E66: m1042-m1043.
51. **Tábi, T., Sajó, I.E., Szabó, F., Luyt, A.S. & Kovács, J.G.** 2010. Crystalline structure of annealed polylactic acid and its relation to processing. *eXPRESS Polymer Letters* 4: 659-668.
52. **Tangen, E., Conradie, J., Franz, K., Friedle, S., Telser, J., Lippard, S.J. & Ghosh, A.** 2010. Electronic Structure of a Paramagnetic  $\{MnO\}^6$  Complex: MnNO 5,5-Tropocoronand. *Inorganic Chemistry* 49: 2701-2705.
53. **Van der Merwe, K.A., Visser, H.G. & Venter, J.A.** 2010. Pyridinium diaquabis(methylene-diphosphonato- $\kappa^2 O, O'$ )chromate(III) tetrahydrate. *Acta Crystallographica Section E* E66: m1011-m1012.
54. **Van der Westhuizen, H.J., Meijboom, R., Schutte, M. & Roodt, A.** 2010. Mechanism for the Formation of Substituted Manganese(V) Cyanidonitrido Complexes: Crystallographic and Kinetic Study of the Substitution Reactions of *trans*- $[MnH(H_2O)(CN)_4]^{2-}$  with Monodentate Pyridine and Bidentate Pyridine-Carboxylate Ligands. *Inorganic Chemistry* 49: 9599-9608.

55. **Van der Westhuizen, H.J., Roodt, A. & Meijboom, R.** 2010. Equilibrium and kinetic studies of reactions of  $[\text{MnN}(\text{H}_2\text{O})(\text{CN})_4]^{2-}$  with monodentate ligands and the molecular structure of  $[\text{MnN}(\text{NCS})(\text{CN})_4]^{3-}$ . *Polyhedron* 29: 470-476.
56. **Van der Westhuizen, H.J., Roodt, A. & Meijboom, R.** 2010. Kinetics of thermal decomposition and of the reaction with oxygen, ethane and 1-octene of first generation Grubbs' catalyst precursor. *Polyhedron* 29: 2776-2779.
57. **Van Tonder, J.H., Bezuidenhoudt, B.C.B. & Janse van Rensburg, J.M.** 2010. Racemic tricarbonyl( $\eta^6$ -flavan)-chromium(O). *Acta Crystallographica Section E* E66: m1086.
58. **Van Tonder, J.H., Bezuidenhoudt, B.C.B. & Janse van Rensburg, J.M.** 2010. Racemic tricarbonyl( $\eta^6$ -7-methoxy-flavan)chromium(O). *Acta Crystallographica Section E* E66: m907-m908.
59. **Van Tonder, J.H., Marais, C., Cole-Hamilton, D.J. & Bezuidenhoudt, B.C.B.** 2010. Regioselective Hydrogenation of  $\alpha,\beta$ -Unsaturated Ketones over Wilkinson's Catalyst. *Synthesis*: 0421-0424.
60. **Van Tonder, J.H., Muller, T.J. & Bezuidenhoudt, B.C.B.** 2010. 2',3,4,4'-Tetramethoxy-chalcone. *Acta Crystallographica Section E* E66: o1798-o1799.
61. **Van Tonder, J.H., Muller, T.J. & Bezuidenhoudt, B.C.B.** 2010. 2',3,4,4',5-Pentamethoxychalcone. *Acta Crystallographica Section E* E66: o2889-o2890.
62. **Venter, G.J.S., Steyl, G. & Roodt, A.** 2010. 4-(2-Methylanilino)pent-3-en-2-one. *Acta Crystallographica Section E* E66: o1593-o1594.
63. **Venter, G.J.S., Steyl, G. & Roodt, A.** 2010. 4-[(4-Methylphenyl)amino]pent-3-en-2-one. *Acta Crystallographica Section E* E66: o3011-o3012.
64. **Viljoen, J.A., Visser, H.G. & Roodt, A.** 2010. Tetrakis(1,3-diphenylpropane-1,3-dionato)hafnium(IV). *Acta Crystallographica Section E* E66: m1053-m1054.
65. **Viljoen, J.A., Visser, H.G. & Roodt, A.** 2010. Tetrakis(8-quinolinolato- $\kappa^2\text{N},\text{O}$ )hafnium(IV) dimethylformamide solvate monohydrate. *Acta Crystallographica Section E* E66: m603-m604.
66. **Visser, H.G. & Clegg, J.K.** 2010. Bis(tetraphenylarsonium) di- $\mu$ -hydroxido-bis[(nitrilotriacetato)cobalt(III)] octahydrate. *Acta Crystallographica Section E* E66: m1401-m1402.
67. **Visser, H.G., Venter, J.A. & Van der Merwe, K.A.** 2010. Dipotassium diaquabis(methylene-diphosphonato- $\kappa^2\text{O},\text{O}'$ )cobaltate(II). *Acta Crystallographica Section E* E66: m159.
68. **Von Eschwege, K.G. & Kuhn, A.** 2010. Low-temperature redetermination of 1,3-bis(pentafluorophenyl)triazene. *Acta Crystallographica Section E* E66: o3177.
69. **Von Eschwege, K.G. & Swarts, J.C.** 2010. Chemical and electrochemical oxidation and reduction of dithizone. *Polyhedron* 29: 1727-1733.

## Patents 2010

1. **Van der Westhuizen, J.H., Ferreira, D. & Joubert, E.** 2009. *Method for the synthesis of asphalatin and analogues thereof*. Method C: 2009/08309 (with the South African Medical Research Council).