

## Publications: Research Articles 2009

1. **Bem, D.B., Luyt, A.S., Dejene, F.B., Botha, J.R. & Swart, H.C.** 2009. Structural, luminescent and thermal properties of blue  $\text{SrAl}_2\text{O}_4:\text{Eu}^{2+}, \text{Dy}^{3+}$  phosphor filled low-density polyethylene composites. *Physica B* 404: 4504-4508.
2. **Brink, A., Roodt., A. & Visser, H.G.** 2009. 2-(*m*-Tolyliminomethyl)phenol. *Acta Crystallographica Section E* E65: o3175-o3176.
3. **Bungu, P.N. & Otto, S.** 2009. 2-Isobutyl-2-phosphabicyclo[3.3.1]nonane 2-selenide. *Acta Crystallographica Section E* E65: o560-o561.
4. **Bungu, P.N. & Otto, S.** 2009. *cis*-Dichloridobis{dimethyl[3-(9-phosphabicyclo[3.3.1]non-9-yl)propyl]amine- $\kappa P$ }platinum(II). *Acta Crystallographica Section C* C65: m152-m155.
5. **Chambrier, I., Swarts, J.C., Hughes, D.L. & Cook, M.J.** 2009. Triple-decker cadmium phthalocyanine sandwich complexes: Self-assembled EPR active complexes. *Journal of Porphyrins and Phthalocyanines* 13: 175-187.
6. **Cloete, N., Visser, H.G., Roodt, A. & Gabrielli, W.F.** 2009. *N,N*-Bis(diphenylphosphine)ethylamine. *Acta Crystallographica Section E* E65: o3081.
7. **Conradie, J.** 2009. A computational study and fragment analysis of the back-bonding in Titanocenyl Complexes containing a five-member L,L'-cyclic ligand, L,L' = O,O'; S,S' or Se,Se'. *Journal of Molecular Structure. THEOCHEM* 915: 51-57.
8. **Conradie, J. & Swarts, J.C.** 2009. Oxidative addition of  $\text{CH}_3\text{I}$  and CO migratory insertion in a series of Ferrocene-containing Carbonyl Phosphine  $\beta$ -Diketonato Rhodium(I) Complexes. *Organometallics* 28: 1018-1026.
9. **Conradie, M. & Conradie, J.** 2009. Stereochemistry of the reaction products of the oxidative addition reaction of methyl iodide to  $[\text{Rh}((\text{C}_4\text{H}_3\text{S})\text{COCHCOR})(\text{CO})(\text{PPh}_3)]$ : A NMR and computational study. R =  $\text{CF}_3$ ,  $\text{C}_6\text{H}_5$ ,  $\text{C}_4\text{H}_3\text{S}$ . *Inorganica Chimica Acta* 362: 519-530.
10. **Conradie, M.M. & Conradie, J.** 2009. 'n Eksperimentele en kwantumberekeningschemie-studie van die reaksie tussen die karbonileringskatalisator  $[\text{Rh}((\text{C}_5\text{H}_4\text{S})\text{COCHCOR})(\text{CO})(\text{PPh}_3)]$  en metieljodied (R =  $\text{CF}_3$ ,  $\text{C}_6\text{H}_5$ ,  $\text{C}_4\text{H}_3\text{S}$ ). *Suid-Afrikaanse Tydskrif vir Natuurwetenskap en Tegnologie* 28: 241-242.
11. **Cook, M.J., Chambrier, I., White, G.F., Fourie, E. & Swarts, J.C.** 2009. Electrochemical and EPR studies of two substituted bis-cadmium tris-phthalocyanine complexes: Elucidation of unexpectedly different free-radical character. *Dalton Transactions*: 1136-1144.

12. **Dikobe, D.G. & Luyt, A.S.** 2009. Morphology and properties of polypropylene/ethylene vinyl acetate copolymer/wood powder blend composites. *eXPRESS Polymer Letters* 3: 190-199.
13. **Fourie, E., Swarts, J.C., Chambrier, I. & Cook, M.J.** 2009. Electrochemical and spectroscopic detection of self-association of octa-alkyl phthalocyaninato cadmium compounds into dimeric species. *Dalton Transactions*: 1145-1154.
14. **Goetz, B.I., Wang, P., Shields, H.W., Basu, S., Grubina, R., Haung, J., Conradie, J., Huang, Z., Jeffers, A., Jiang, A., He, X., Azarov, I., Seibert, R., Mehta, A., Patel, R., King, S.B., Ghosh, A., Hogg, N., Gladwin, M.T. & Kim-Shapiro, D.B.** 2009. Nitrite-methemoglobin inadequate for hypoxic vasodilation (Correspondence). *Nature Chemical Biology* 5: 366-367.
15. **Grobbelaar, E., Lötter, S., Visser, D., Conradie, J. & Purcell, W.** 2009. Investigation of the electron density of Iridium(I) Vaska-type complexes using DFT calculations and structural results: Structure of trans-carbonyl-chloro-bis(tricyclohexylphosphine)-iridium(I). *Inorganica Chimica Acta* 362: 3949-3954.
16. **Hopmann, K.H. & Conradie, J.** 2009. A density functional theory study of substitution at the Square-Planar Acetylacetonato-dicarbonyl-rhodium(I) complex. *Organometallics* 28: 3710-3715.
17. **Hopmann, K.H., Conradie, J. & Ghosh, A.** 2009. Broken-symmetry DFT spin densities of Iron Nitrosyls, including Roussin's red and black salts: Striking differences between pure and hybrid functionals. *Journal of Physical Chemistry B* 113: 10540-10547.
18. **Kirsten, L. & Steyl, G.** 2009. Dibromidobis(triphenylarsine)-palladium(II). *Acta Crystallographica Section E* E65: m218.
19. **Kirsten, L. & Steyl, G.** 2009. *Trans*-Dibromidobis[tris(4-chlorophenyl)phosphine]palladium(II). *Acta Crystallographica Section E* E65: m1565.
20. **Kirsten, L., Steyl, G. & Roodt, A.** 2009. *Trans*-Dibromidobis(tri-*p*-tolylarsine)-palladium(II). *Acta Crystallographica Section E* E65: m1449.
21. **Kirsten, L., Steyl, G. & Roodt, A.** 2009. *Trans*-Dibromidobis[diphenyl(*p*-tolyl)-phosphine]palladium(II). *Acta Crystallographica Section E* E65: m1564.
22. **Kuhn, A., Muller, A. & Conradie, J.** 2009. Syntheses, crystal structure and theoretical modeling of tetrahedral mono- $\beta$ -diketonato titanocenyl complexes. *Polyhedron* 28: 966-974.
23. **Kuhn, A., Tsotetsi, T.A., Muller, A. & Conradie, J.** 2009. Isomer distribution and structure of (2,2'-biphenyldiolato)bis( $\beta$ -diketonato)titanium(IV) complexes: A single crystal X-ray, solution NMR and computational study. *Inorganica Chimica Acta* 362: 3088-3096.

24. **Lötter, S., Purcell, W. & Nel, J.T.** 2009. Die vertering en kwantifisering van onsuiwerhede in sirkoon en plasmagedissoosieerde sirkoon (pdz). *Suid-Afrikaanse Tydskrif vir Natuurwetenskap en Tegnologie* 28: 252-253.
25. **Luyt, A.S. & Krupa, I.** 2009. Phase change materials formed by uv curable epoxy matrix and Fischer-Tropsch paraffin wax. *Energy Conversion and Management* 50: 57-61
26. **Luyt, A.S., Dramičanin, M.D., Antić, Ž. & Djoković, V.** 2009. Morphology, mechanical and thermal properties of composites of polypropylene and nanostructured wollastonite filler. *Polymer Testing* 28: 348-356.
27. **Marston, A., Van der Westhuizen, J.H. & Zietsman, P.** 2009. Investigation of South African Amaryllidaceae for inhibitors of acetylcholinesterase. *Planta Medica* 75: 877-1094.
28. **Matabola, K.P., De Vries, A.R., Moolman, F.S. & Luyt, A.S.** 2009. Single polymer composites: a review. *Journal of Material Science* 44: 6213-6222.
29. **Meera, A.P., Said, S., Grohens, Y., Luyt, A.S. & Thomas, S.** 2009. Tensile stress relaxation studies of TiO<sub>2</sub> and natural rubber composites. *Industrial & Engineering Chemistry Research* 48: 3410-3416.
30. **Meijboom, R., Bowen, R.J. & Berner-Price, S.J.** 2009. Coordination complexes of silver(I) with tertiary phosphine and related ligands. *Coordination Chemistry Reviews* 253: 325-342.
31. **Meijboom, R., Dhirori, P. & Mavunkal, I.J.** 2009. Synthesis and characterization of an unusual equatorially substituted di-manganese compound. The first structural determination of a phosphate compound of type [Mn<sub>2</sub>(CO)<sub>9</sub>P]. *Inorganica Chimica Acta* 362: 617-620.
32. **Mishra, S.B. & Luyt, A.S.** 2009. Effect of organic peroxides on the morphology and properties of EVA/Cloisite 15A Nanocomposites. *Journal of Applied Polymer Science* 112: 218-225.
33. **Molefi, J.A., Luyt, A.S. & Krupa, I.** 2009. Comparison of the influence of Cu micro- and nano-particles on the thermal properties of polyethylene/Cu composites. *eXPRESS Polymer Letters* 3: 639-649.
34. **Ochigbo, S.S., Luyt, A.S. & Focke, W.W.** 2009. Latex derived blends of poly(vinyl acetate) and natural rubber: Thermal and mechanical properties. *Journal of Material Science* 44: 3248-3254.
35. **Omondi, B., Venter, G.J.S., Roodt, A. & Meijboom, R.** 2009. Isomorphism in monomeric 1:3 complexes of silver(I) salts with tri-*p*-tolylphosphine. *Acta Crystallographica Section B* B65: 699-706.

36. **Otto, S., Roodt, A. & Elding, K.I.** 2009. Bridge-splitting of *trans*-[PtCl<sub>2</sub>( $\eta^2$ -CH<sub>2</sub>=CH<sub>2</sub>)<sub>2</sub>] by weak nucleophiles: Crystal and molecular structure of *trans*-[PtCl<sub>2</sub>( $\eta^2$ -CH<sub>2</sub>=CH<sub>2</sub>)(MeCN)]. *Inorganic Chemistry Communications* 12: 766-768.
37. **Ramontja, J., Ray, S.S., Pillai, S.K. & Luyt, A.S.** 2009. High-performance carbon nanotube-reinforced bioplastic. *Macromolecular Materials and Engineering* 294: 839-846.
38. **Schutte, M., Visser, H.G. & Brink, A.** 2009. [N,N-Bis(diphenylphosphino)propylamine- $\kappa^2P,P$ ]bromidotricarbonylrhenium(I). *Acta Crystallographica Section E* E65: m1575-m1576.
39. **Steyl, G.** 2009. Bis[tris(4-fluorophenyl)phosphine- $\kappa P$ ](tropolonato- $\kappa^2O,O'$ )copper(I). *Acta Crystallographica Section E* E65: m448.
40. **Steyl, G.** 2009. Nitratotris(triphenylphosphine)copper(I) methanol solvate. *Acta Crystallographica Section E* E65: m272.
41. **Steyl, G. & Hill, T.N.** 2009. (3,5,7-Tribromotropolonato- $\kappa^2O,O'$ )tris-(triphenylphosphine- $\kappa P$ )silver(I). *Acta Crystallographica Section E* E65: m191.
42. **Steyl, G. & Hill, T.N.** 2009. Bis(triphenylphosphine- $\kappa P$ )(tropolonato- $\kappa^2O,O'$ )silver(I) dichloromethane solvate. *Acta Crystallographica Section E* E65: m233.
43. **Stuurman, N.F. & Conradie, J.** 2009. Iodomethane oxidative addition and CO migratory insertion in monocarbonylphosphine complexes of the type [Rh((C<sub>6</sub>H<sub>5</sub>)COCHCO(CH<sub>2</sub>)<sub>n</sub>CH<sub>3</sub>)(CO)(PPh<sub>3</sub>)]: Steric and electronic effects. *Journal of Organometallic Chemistry* 694: 259-268.
44. **Suthiram, J., Mhlaba, K., Zeevaart, J.R., Visser, H.G. & Roodt, A.** 2009. Tetraethylammonium tricarbonylchlorido(pyrazine-2-carboxylato-*N*<sup>1</sup>,*O*)rhenate(I). *Acta Crystallographica Section E* E65: m1395.
45. **Swarts, J.C., Nafady, A., Roudebush, J.H., Trupia, S. & Geiger, W.E.** 2009. One-Electron oxidation of Ruthenocene: Reactions of the Ruthenocenium Ion in gentle electrolyte media. *Inorganic Chemistry* 48: 2156-2165.
46. **Tsotetsi, T.A., Kuhn, A., Muller, A. & Conradie, J.** 2009. Substitution kinetics of biphenol at dichlorobis(acetylacetonato-*O,O'*)titanium(IV): Isolation, characterization, crystal structure and enhanced hydrolytic stability of the product bis(acetylacetonato-*O,O'*)titanium(IV). *Polyhedron* 28: 209-214.
47. **Van der Merwe, K.A., Visser, H.G. & Venter, J.A.** 2009. Diammonium diaquabis(methylenediphosphonato- $\kappa^2O,O'$ )cobaltate(II). *Acta Crystallographica Section E* E65: m1394.
48. **Van Tonder, J.H., Bezuidenhoudt, B.C.B. & Janse van Rensburg, J.M.** 2009. Tricarbonyl( $\eta^6$ -flavone)chromium(O). *Acta Crystallographica Section E* E65: m1346.

49. **Van Tonder, J.H., Bezuidenhoudt, B.C.B. & Janse van Rensburg, J.M.** 2009. Tricarbonyl( $\eta^6$ -4',7-dimethoxyisoflavone)chromium(O). *Acta Crystallographica Section E* E65: m1343.
50. **Venter, G.J.S., Roodt, A. & Meijboom, R.** 2009. Polymorphism in iodotris(*tri-p-tolylphosphine*)silver(I). *Acta Crystallographica Section B* B65: 182-188.
51. **Venter, G.J.S., Roodt, A. & Meijboom, R.** 2009. Self-assembly in tetrameric 1:1 silver(I) halide-*tri-p-tolylphosphine* complexes: An in-depth structural investigation. *Inorganica Chimica Acta* 362: 2475-2479.
52. **Venter, G.J.S., Steyl, G. & Roodt, A.** 2009. Carbonyl[4-(2,3-dimethylphenylamino)-pent-3-en-2-onato- $\kappa^2 N,O$ ](triphenyl-phosphine- $\kappa P$ )rhodium(I). *Acta Crystallographica Section E* E65: m1321-1322.
53. **Venter, G.J.S., Steyl, G. & Roodt, A.** 2009. Carbonyl[4-(2,6-dimethylphenylamino)pent-3-en-2-onato- $\kappa^2 N,O$ ]triphenylphosphine- $\kappa P$ )rhodium(I) acetone hemisolvate. *Acta Crystallographica Section E* E65: m1606-m1607.
54. **Venter, J.A., Purcell, W. & Visser, H.G.** 2009. Di- $\mu$ -iodido-bis[acetyl(4-methyl-2,6,7-trioxa-1-phosphabicyclo[2.2.2]octane)(*N*-nitroso-*N*-oxidoaniline- $\kappa^2 O,O'$ )rhodium(III)]. *Acta Crystallographica Section E* E65: m1528-m1529.
55. **Venter, J.A., Purcell, W., Visser, H.G. & Muller, T.J.** 2009. Carbonyl(*N*-nitroso-*N*-oxido-1-naphtylamine- $\kappa^2 O,O'$ )(triphenylphosphine- $\kappa P$ )rhodium(I) acetone solvate. *Acta Crystallographica Section E* E65: m1578.
56. **Viljoen, J.A., Visser, H.G., Roodt, A. & Steyn, M.** 2009. Di- $\mu$ -hydroxido-bis[tris(1,1,1,5,5,5-hexafluoroacetylacetonato- $\kappa^2 O,O'$ )hafnium(IV) acetone solvate]. *Acta Crystallographica Section E* E65: m1367-m1368.
57. **Viljoen, J.A., Visser, H.G., Roodt, A. & Steyn, M.** 2009. Tetrakis(quinolin-8-olato- $\kappa^2 N,O$ )hafnium(IV) toluene disolvate. *Acta Crystallographica Section E* E65: m1514-m1515.
58. **Von Eschwege, K.G. & Muller, A.** 2009. 2,3-Bis(2-methoxyphenyl)tetrazolium-5-thiolate-acetone-dichloromethane (1/0.4/0.1). *Acta Crystallographica Section E* E65: o2.
59. **Von Eschwege, K.G. & Muller, A.** 2009. 2,3-Bis(3-fluorophenyl)tetrazolium-5-thiolate. *Acta Crystallographica Section E* E65: o1864.
60. **Zobi, F., Blacque, O., Steyl, G., Spingler, B. & Alberto, R.** 2009. Formation and reactivity of [(tacn)-*N*-CO-Re<sup>II</sup>Br(CO)<sub>2</sub>]<sup>+</sup> in Water: A theoretical and experimental study. *Inorganic Chemistry* 48: 4963-4970.

## **Books 2009**

1. **Ghosh, A., Conradie, J. & Hopmann, K.H.** 2009. Electronic structure of transition Metal-NO Complexes. In *Computational Inorganic and Bioinorganic Chemistry*, part 3 of the *Encyclopedia of Inorganic Chemistry*; edited by Edward I. Solomon, Robert A. Scott and R. Bruce King. Chichester, UK: John Wiley & Sons. pp. 389-410.

## **Patents 2009**

1. **Achilonu, M.C., Bonnet, S.L. & Van der Westhuizen.** 2009. *Method for the preparation of C-4 coupled flavonoids, proanthocyanidins and analogues thereof.* PCT Application number PCT/IB2009/052396.
2. **Van der Westhuizen, J.H., Ferreira, D. & Joubert, E.** 2009. *Method for the synthesis of asphalatin and analogues thereof.* Method A: 2009/08304 (with the South African Medical Research Council).
3. **Van der Westhuizen, J.H., Ferreira, D. & Joubert, E.** 2009. *Method for the synthesis of asphalatin and analogues thereof.* Method B: 2009/08308 (with the South African Medical Research Council).
4. **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).
5. **Achilonu, M.C., Bonnet, S.L. & Van der Westhuizen, J.H.** 2009. *The synthesis of 3-Aryl flavenes and C-3 Coupled Biflavonoids.* Patent number 2009/05765.