



Faculty of Natural and Agricultural Sciences
Department of Chemistry

Publications 2021

1. **Swart, M.R., Bezuidenhoudt, B.C.B, Marais, C., Erasmus, E.** (2021). NMR data of a Grubbs 2nd generation catalyst p-cresolate derivative. Data in Brief, 34 (2021) 106634. **Ufs-040057**
2. **Swart, M.R., Bezuidenhoudt, B.C.B, Marais, C., Erasmus, E.** (2021). Spectroscopic characterisation of Grubbs 2nd generation catalyst and its p-cresol derivatives. Inorganica Chimica Acta, 514 (2021) 120001. **Ufs-040058**
3. **Swart, M.R., Bezuidenhoudt, B.C.B, Marais, C., Erasmus, E.** (2021). Olefin Metathesis, p-Cresol, and the Second Generation Grubbs Catalyst: Fitting the Pieces. Eur. J. Inorg. Chem. 2021, 1752-1762. **Ufs-040062**
4. **Elmakki, M. A., Alexander, O.T., Venter, J. A., Roodt, A.** (2021). Crystal structure of carbonyl(2-methylquinolin-8-olato κ^2N,O)(triphenylarsine- κ As)rhodium(I), $C_{29}H_{23}AsNO_2Rh$. Z. Kristallogr. NCS 2021; 236(1):215-217. **Ufs-040099**
5. **Elmakki, M. A., Alexander, O.T., Venter, J. A., Roodt, A.** (2021). Crystal structure of carbonyl(2-oxopyridin-1(2H)-olato- κ^2O,O')(triphenylarsine- κ As)rhodium(I), $C_{24}H_{19}AsNO_3Rh$. Z. Kristallogr. NCS 2021; 236(1):223-225. **Ufs-040100**.
6. **Elmakki, M. A., Alexander, O.T., Venter, G. J. S., Venter, J. A., Roodt, A.** (2021). Synthesis and structural determination of $[Rh(opo)(CO)(PR_3)]$ complexes (opo^- = 2-oxopyridin-1-olate) and *in situ* isomeric behavior from preliminary kinetic study of iodomethane oxidative addition. Journal of Coordination Chemistry 2021, Vol. 74, NOS.1-3, 444-446. **Ufs-040103**
7. **Mikherdov, A. S., Popov, R. A., Kinzhalov, M. A., Haukka, M., Polukeev, V. A., Boyarskiy, V. P., Roodt, A.** (2021) Reaction mechanism of regiosomerization in binuclear (diaminocarbene) PdII complexes. Inorganica Chimica Acta 514 (2021), 120012, Pg 1-8. **Ufs-040106**
8. **Hamdi, I., Mhadhbi, N., Issaoui, N., Roodt, A., Turnbull, M. M., Naïli, H.** (2021) Design, synthesis and physico-chemical studies of a Co(II)/Co(III)mixed-valence complex: An experimental and DFT approach. Journal of Molecular Structure 1237 (2021), 130385, Pg 1-12. **Ufs-040136**

9. **Mentoor, K., Twigge, L., Niemantsverdriet, J. W. H., Swarts, J. C., Erasmus, E.** (2021) Silica Nanopowder Supported Frustrated Lewis Pairs for CO₂ Capture and Conversion to Formic Acid. Inorg. Chem. 2021, 60, Pg. 55-69. **Ufs-040169**
10. **Swarts, P. J., Erasmus, E., Fourie, E.** (2021) Comparison of synthetic, spectroscopic, computational and electrochemical aspects of ferrocenyl-containing β-diketones, β-ketoesters and β-ketoamides. Polyhedron (2021), Vol 205. 115279. Pg. 1-11. **Ufs-040173**
11. **Maseme, M.R., Buitendach, B.E., Erasmus, E., Swarts, J.C.** (2021) The chemistry of spin-coated rhodium-ferrocenyl complexes supported on silanol-capped silicon wafers. Polyhedron (2021), Vol 204. 115277. Pg. 1-12. **Ufs-040174**
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13. **Malloum, A, Fifen, J. J, Conradie, J.** (2021), Determination of the absolute solvation free energy and enthalpy of the proton in solutions (Review), Journal of Molecular Liquids 322 114919. **Ufs-042619**
14. **Malloum, A, Conradie, J.** (2021), Structures of Water Clusters in the Solvent Phase and Relative Stability Compared to Gas Phase, Polyhedron, 2021, 193, 114856. **Ufs-040390**
15. **Akpomie, K., Conradie, J.** (2021) Ultrasonic aided sorption of oil from oil-in-water emulsion onto oleophilic natural organic-silver nanocomposite. Chemical Engineering Research and Design (Official journal of the European Federation of Chemical Engineering: Part A 165 12-24. **Ufs-040394**
16. **Adeniyi, A., Conradie, J., R. Fukae, R., Yoshimura, M., Nishinari, K., Lawal, O. S.** (2021) Enhancing the loading and swelling capacity of cellulose crystal through difunctional and multifunctional epoxy cross-linkers and the effects on the elasticity and plasticity: A computational study, Journal of Molecular Structure 2021, 1228 129436. **Ufs-040397**
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19. **Mateyise, N.G.S, Conradie, J., Conradie, M.M.** (2021). Density functional theory calculated data of the iodomethane oxidative addition to oligothiophene-containing rhodium complexes – importance of dispersion correction, Data in Brief 35 (2021) 106929. **Ufs-040450**

20. **Mateyise, N.G.S, Conradie, J., Conradie, M.M. (2021)** Synthesis, Characterization, Electrochemistry, DFT and Kinetic Study of the Oligothiophene-containing Complex [Rh((C₄H₃SC₄H₂S)COCHCOCF₃)(CO)(PPh₃)], Polyhedron 199 (2021) 115095 . **Ufs-040449**
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22. **Malloum, A., Conradie, J., (2021)** Computational and Theoretical Chemistry 1199 (2021) 113189. **Ufs-042622**
23. **Malloum, A., Conradie, J., (2021)** Accurate Binding Energies of Ammonia Clusters and Benchmarking of Hybrid DFT Functionals, Computational and Theoretical Chemistry, 1200 (2021) 113236. **Ufs-040452**
24. **Malloum, A., Conradie, J., (2021)** Solvation Free Energy of the Proton in Acetonitrile, Journal of Molecular Liquids 335 (2021) 116032. **Ufs-040453**
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68. **Jacobs, FJF, Brink, A., (2021)** Crystal structure of *fac*-tricarbonyl-(nitrato- $\kappa^1 O$)- bis(pyridine- κN)-rhenium, C₁₃H₁₀O₆N₃Re. *Z. Kristallogr. NCS.* 2021, **236**, 253-255. **Ufs-038470**
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