

Poster

Rhodium(I) Carbonyl Complexes as Model Nano-Wired Assemblies and Catalysts**P.P. Mokolokolo,¹ M. Schutte-Smith,¹ A. Brink, and A. Roodt¹**¹*Department of Chemistry, University of the Free State, 205 Nelson Mandela Drive, Bloemfontein, 9300, South Africa*[*ppmokolokolo@gmail.com*](mailto:ppmokolokolo@gmail.com)

Square planar rhodium(I) complexes of the type $[\text{Rh}(\text{L},\text{L}'\text{-Bid})(\text{CO})(\text{PPX}_3)]$, where L,L'-Bid = monoanionic bidentate ligands and PPX₃ are tertiary phosphine ligands, have been extensively investigated as potential catalyst precursors in different conversion reactions [1-5].

The main objective of this current study is to use solution and solid state ³¹P NMR spectroscopy in conjunction with X-ray crystallography to investigate the structure and reactivity relationship of the rhodium(I) complexes for potential application in catalysis. The employment of solid-state NMR spectroscopy techniques in this study provides an opportunity to have a much closer look at the solid vs. solution state behaviour of the compounds which might enable an improved prediction and translation between the solution state with respect to possible structural relationship(s).

A range of complexes of the type $[\text{Rh}(\text{L},\text{L}'\text{-Bid})(\text{CO})(\text{PPX}_3)]$ containing systematic manipulation of the steric and electronic properties were synthesized and characterized using IR, UV/Vis and NMR spectroscopy including MAS solid-state NMR. These rhodium(I) complexes were obtained from the substitution of one carbonyl ligand in the complexes $[\text{Rh}(\text{L},\text{L}'\text{-Bid})(\text{CO})_2]$, by simple stoichiometric reaction with monodentate tertiary phosphines. Correlations of different parameters such as the first-order coupling constant ¹J_{Rh-P}, chemical shift and the Rh-P bond-distances were evaluated in order to understand the coordination environment around the metal centre and variations which could occur in the transition from solid to solution state, in particular its effect on the construction of model nano-wired assemblies.

[1] Roodt A., Visser H.G., Brink A. *Crystallogr. Rev.* 2011. 17. 241.

[2] Warsink S., Fesha F.G., Purcell W., Venter J.A. *J. Organomet. Chem.* 2013. 726. 14.

[3] Conradie M.M., P. H.van Rooyen, P.H., Pretorius C., Roodt A., Conradie J., *J. Mol. Struct.* 2017.1144. 280.

[4] Brink A., Roodt A., Steyl G., Visser H.G. *Dalton Trans.* 2010. 39. 5572.

[5] Warsink S., Kotze P.D.K., Janse Van Rensburg J.M., Venter J.A., Otto S., Botha E., Roodt A. *Eur. J. Inorg. Chem.* 2018. 2018. 3615.

This work was supported by the South African National Research Foundation, SASOL and the University of the Free State.