

MS31-P16 | STRUCTURE / REACTIVITY RELATIONSHIPS FROM DETAILED REACTION MECHANISMS

Roodt, Andreas (Univ of the Free State, Bloemfontein, ZAF); Mokolokolo, Pennie P (Univ of the Free State, Bloemfontein, ZAF); Alexander, Orbett T (Univ of the Free State, Bloemfontein, ZAF); Kama, Dumisani V (Univ of the Free State, Bloemfontein, ZAF); Brink, Alice (Univ of the Free State, Bloemfontein, AUT); Schutte Smith, Marietjie (Univ of the Free State, Bloemfontein, ZAF)

This presentation addresses some fundamental issues of importance in selected process reactions currently employed or with potential scope to be implemented (in industry). Different processes were chosen and include examples from homogeneous catalysis, radiopharmaceutical models, with some comment aimed at environmental issues.

Extracts of key points to be discussed include the following:

The first reaction involves the basic oxidative addition of substrates to catalyst models, a *fundamental* process in many a homogeneous catalytic cycle [such as hydroformylation, hydrogenation, carbonylation and others] [1,2]. It will highlight complex (modified) characteristics, substrate behavior and knowledge thereof in predicting outcomes within the process.

A next reaction to be discussed involves *theranostic* models in radiopharmacy and how intimate mechanistic understanding is critical for basic design of agents, whether it is only for diagnostics, or only for therapy, or for both [3]. Some expanded aspects of detailed mechanisms, also of importance in metal beneficiation and green chemistry will be further presented [4].

[1] S. Warsink, P.D.R. Kotze, J.M. Janse van Rensburg, J.A. Venter, S. Otto, E. Botha, A. Roodt. *European Journal of Inorganic Chemistry* **2018**, 32, 3615.

[2] M.V. Dobrynin, C. Pretorius, D.V. Kama, A. Roodt, V.P. Boyarskiy, R.M. Islamova. Rhodium(I)-catalysed cross-linking of polysiloxanes conducted at room temperature. *Journal of Catalysis* **2019**, 372, 193.

[3] A. Frei, P.P. Mokolokolo, R. Bolliger, H. Braband, M.S Tsosane, A. Brink, A. Roodt, R. Alberto. *Chemistry-A European Journal* **2018**, 24, 10397.

[4] M. Schutte-Smith, A. Roodt, H.G. Visser. *Dalton Transactions* **2019**, 48, 9984.