

Asymmetric Hydrogenation: Novel Rh(I) Catalysts & Predictive DFT Calculations

Graeme J Gainsford, Andrew Falshaw, Cees Lensink, Stephen White, *Industrial Research Limited, P O Box 31-310, Lower Hutt, New Zealand 6009*. E-mail: g.gainsford@irl.cri.nz

Recent advances in the calculation of molecular energetics based on Density Functional Theory (DFT) have raised the hope that both properties and transition state energy profiles could be predicted.¹ We have been investigating homogeneous Rhodium(I) catalysts coordinated to novel carbohydrate-phosphinite ligands and now report our attempts to predict by calculation the enantiomeric excess (ee) values for hydrogenation using variants of these ligands. We have characterized by X-ray diffraction analyses two components: "CandyPhos"(1D-3,4-(bis(O-diphenylphosphino)-1,2,5,6-tetra-O-methyl-chiro-inositol) and the active complex (CandyPhos)(η^4 -(Z,Z)-cyclo-octa-1,5-diene)-rhodium(I) tetrafluoroborate CHCl_3 solvate.

DFT calculations have been carried out using the Amsterdam Density Function programme suite² utilizing these diffraction coordinates and the previous in-depth analysis by Feldgus & Landis³. We will report the crystallographic details and the interim calculation results for model enamides in comparison with our in-house determined ee values. We acknowledge with gratitude the support of Professor Tom Ziegler & Dr Michael Seth of the University of Calgary, Calgary, Canada.

[1] Ziegler T., *Can. J. Chem.*, 1995, **73**, 743-761. [2] *SCIENTIFIC COMPUTING & MODELLING NV*, ADF Program Suite, Vrije Universiteit, Theoretical Chemistry, Amsterdam, The Netherlands. [3] Feldgus S, Landis C.R., *J. Am. Chem. Soc.*, 2000, **122**, 12714-12727.

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