

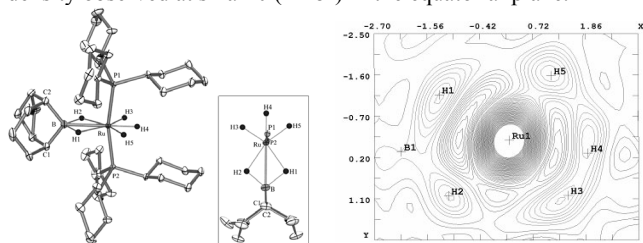
X-ray Structural Study of σ -borane and Dihydridoborate Ruthenium Complexes

L. Vendier, S. Lachaize, S. Sabo-Etienne, *Laboratoire de Chimie de coordination, Toulouse* E-mail: vendier@lcc-toulouse.fr

In this work, we present 3 X-ray structures of a new family of σ -borane and dihydridoborate complexes. Two σ -borane and one dihydridoborate complexes have been produced: respectively $\text{RuH}_2(\eta^2\text{-HBpin})(\eta^2\text{-H}_2)(\text{PCy}_3)_2$ (2Bpin) and $\text{RuH}_2(\eta^2\text{-HBcat})(\eta^2\text{-H}_2)(\text{PCy}_3)_2$ (2Bcat), and $\text{RuH}[(\mu\text{-H})_2\text{BBN}](\eta^2\text{-H}_2)(\text{PCy}_3)_2$ (2BBN).

The formulation of each complex has been ascertained by an X-ray structural study. Each experiment was carried out at 100 °K, in order to prevent as much as possible dihydrogen rotation, and to help the localisation of all the hydrogen atoms around the ruthenium. These complexes have been studied as well by NMR spectroscopy and by DFT/B3LYP calculations.

In the case of 2-BBN, the highly delocalized electronic density precluded any good location in the region of the equatorial plane *trans* to the dihydridoborate, and the hydride positions should be considered as artefacts. To solve this problem, our X-ray structural study has been completed by calculating Fourier differences map of the electronic density observed at small θ ($< 18^\circ$) in the equatorial plane.



Keywords: low temperature, hydride structures, Fourier maps