

Publication

Asymmetric hydrogenation with iridium C,N and N,P ligand complexes :
characterization of dihydride intermediates with a coordinated alkene**JournalArticle (Originalarbeit in einer wissenschaftlichen Zeitschrift)**

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Previously elusive iridium dihydride alkene complexes have been identified and characterized by NMR spectroscopy in solution. Reactivity studies demonstrated that these complexes are catalytically competent intermediates. Additional H₂ is required to convert the catalyst-bound alkene into the hydrogenation product, supporting an Ir(III) /Ir(V) cycle via an [Ir(III) (H)₂ (alkene)(H₂)(L)](+) intermediate, as originally proposed based on DFT calculations. NMR analyses indicate a reaction pathway proceeding through rapidly equilibrating isomeric dihydride alkene intermediates with a subsequent slow enantioselectivity-determining step. As in the classical example of asymmetric hydrogenation with rhodium diphosphine catalysts, it is a minor, less stable intermediate that is converted into the major product enantiomer.

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