Iron(II) Complexes of Chiral, C₂-Symmetric, P- or C-Stereogenic PNP Pincer Ligands and their Application in the H₂ Hydrogenation of Ketones

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Chiral pincer ligands for iron(II) have been recently developed and applied in the direct H_2 hydrogenation of ketones.^{1,2} We report here the preparation and characterization of iron(II) dibromocarbonyl complexes 1, 2, and 3 of the type [FeBr₂(CO)(L)], where L is one of the tridentate, P-C-stereogenic, C_2 -symmetric PNP pincer or ligands (S_{P}, S_{P}) -2,6-bis((cyclohexyl(methyl)phosphanyl) methyl)pyridine (4), 2,6-bis(((2R,5R)-2,5-dimethylphospholan-1-yl)methyl)pyridine (5), $(S_{\rm P}, S_{\rm P})$ -2,6-bis(or (tert-butyl(methyl)phosphanyl)methyl) pyridine (6).



The corresponding bromocarbonylhydride complexes were prepared by addition of NaBHEt₃ (1 equiv.) and either isolated or directly used in catalysis. They were active in the direct H_2 hydrogenation of a variety of arylalkyl ketones under 50 bar of H_2 pressure and in the presence of KO^tBu as base. The enantioselectivity reached 61% ee with (*S*)-1-(2-naphthyl)ethanol. The origin of enantioselectivity was investigated using DFT calculations.



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