Enhanced Catalytic Activity of Iridium(III) Complexes by Facile Modification of C,Nbidentate Chelating Pyridylideneamide Ligands

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Non-innocent ligands that can significantly modulate their donor properties have become increasingly popular as a powerful class of ligands for a variety of homogenous catalytic applications, since they can stabilize different metal configurations.¹ Pyridylideneamines (PYEs) and pyridylideneamides (PYAs) are electronically highly flexible N-donor sites that can coordinate to the metal center as a π -acidic imine or as a π -basic pyridinium amide. Their flexibility is represented by the two limiting resonance forms comprised of a diene heterocycle and a neutral imine donor site with minimal charge separation and a zwitterionic form, which features an anionic amide donor site and aromatic stabilization of the pyridinium residue.²

Here, we applied this concept for facile catalyst tailoring by incorporating donor substituents in different positions of the phenyl ring of the C,N-bidentate chelating PYA ligand (Fig. 1). These modifications greatly enhance the catalytic activity of the coordinated iridium center.



[1] Hartwig, J. Organotransition Metal Chemistry, *University Science Books*, Mill Hill Valley California, **2010.**

[2] a) Donnelly, K. F.; Segarra, C.; Shao, L.; Suen, R.; Müller-Bunz, H.; Albrecht, M.; Organometallics **2015**, *34*, 4076–4084. b) Navarro, M.; Li, M.; Müller-Bunz, H.; Bernhard, S.; Albrecht, M.; Chem. Eur. J. **2016**, *22*, 6740–6745.