

Electronic Structure of Iron Complexes Containing Bipyridine-based PNN Pincer Ligands

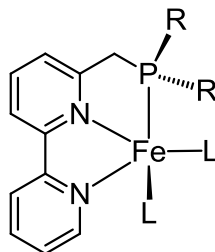
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Pincer ligands are used in many transition metal complexes, and these complexes serve as effective catalysts for various reactions. In particular, a complex of Ru and a bipyridine-based pincer ligand was shown to catalyze various environmentally benign reactions, such as the hydrogenation of amides to the corresponding alcohols and amines[1] and the hydrogenation of urea derivatives to amines and methanol[2]. This broad application of the Ru pincer complex encourages investigation of bipyridine-based pincer ligands coordinated to an iron center. Herein, we present a study in which we examine the electronic structure of iron pincer complexes containing the bpy moiety. Our attention is especially concentrated on answering the question of whether the bpy moiety is a spectator ligand or a redox-active ligand. This question arises from study by Scarborough *et al.*[3] who showed several examples of complexes containing bipyridine (bpy) that behave as non-innocent ligand and the complexes have a biradical character.



[1] Balaraman, E., Gnanaprakasam, B., Shimon, L. J.W., Milstein, D. *J. Am. Chem. Soc.*, 132:16756–16758, 2010.

[2] Balaraman, E., Ben-David, Y., Milstein, D. *Angew. Chem., Int. Ed.*, 50:11702–11705, 2011.

[3] Scarborough, C. C., Wieghardt, K. *Inorg. Chem.*, 50:9773–9793, 2011.