

Ionization of the FeX bond in polar solvents: A spectroscopic study of CpFe(dppe)X complexes

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Electronic absorption spectra for complexes CpFe(dppe)X [with X = Cl, I and CN; dppe = (Ph)₂PCH₂CH₂P(Ph)₂; Cp = η^5 -C₅H₅] and the cationic derivative [CpFe(dppe)NCCH₃]PF₆ in different solvents have been measured. The lower energy bands were assigned to iron d-d orbital transitions on the basis of intensities, solvent effects and extended Hückel MO calculations. The complexes CpFe(dppe)X (with X = Cl and I) undergo ionization in polar solvents to give the cationic solvated species [CpFe(dppe) (solvent)]⁺. This behaviour can be explained on the basis of the theoretical calculations. © 1993.