

Identification of lowest excited states in the organometallic iron-nitrile complexes

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Electronic absorption spectra for the complexes $[\text{CpFe}(\text{dppe})\text{NC-R}]\text{PF}_6$ R = $\text{CH}_2\text{-C}_6\text{H}_4\text{-ON}_3\text{P}_3(\text{OC}$
 $6\text{H}_4\text{t-Bu})_5$ (1), R = $\text{CH}_2\text{-C}_6\text{H}_4\text{-OH}$ (2) and R = CH_3 (3) in different solvents have been measured.

The two absorption bands at the lowest energy value for (1) and (2) are assigned to a metal - ligand charge - transfer transition (MLCT) on the basis of the solvent effect and extended Hückel MO calculations. The possible implications of a low-lying excited states in these complexes are discussed.