

Regulating Redox and Spin State Behavior of bis-Terpy Fe(II) via Steric and Inductive Influence of Ligand Substituents

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A series of complexes with the general formula $[\text{Fe}(\text{R-terpy})_2]^{2+}$ where R = Me, OCH₃, OCH₂CH₃, OCH(CH₃)₂, CH₃, C₂H₅, C₂Si(CH₃)₃, Cl, Br, and I... were synthetically prepared to investigate the steric and inductive influence these substituent groups on the 6' position of 2,2':6',2'-terpyridine (R-terpy) have on the electronic properties of Fe(II). All of the R-terpy ligands were characterized by way of ¹H and ¹³C NMR followed by coordination onto the metal center in a bis-manner. The Fe(III/II) redox couple of each complex was characterized by way of cyclic voltammetry in which their redox behavior was observed to correlate well with the substituents inductive influence. NMR methodology was used for measuring room temperature magnetic susceptibilities of each Fe(II) complex under solution conditions. Several of the Fe(II) complexes exhibited spin equilibrium (low and high spin states) that strongly correlated with the 6'- substituents steric influence.