Overlooked and Misbehaving: Unsymmetric Tetrazine Ligands Coordinated to Iron(II)

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Abstract: Metal complexes of redox-active ligands have potential for use as catalysts in water splitting and as functional components of molecular-scale machines. Using compounds such as terpyridine as inspiration, we designed, synthesized, and studied a terdentate ligand containing previously untapped unsymmetric tetrazines bridged by a pyridine, 2,6-bis(3-methyl-1,2,4,5-tetrazin-6-yl)pyridine (BisTzP). An analysis of the crystal structure for the BisTzP ligand and the bisligated Fe(II) complex revealed an equivocal valence state. Physical studies are presented that help to characterize the nature of this electronic ambiguity.