

SYNTHESIS, CHARACTERIZATION, DFT AND TD-DFT STUDY OF THE $[\text{Fe}(\text{mnt})(\text{L})(t\text{-BuNC})_2]$ OCTAHEDRAL COMPLEX (L = phen, bipy)

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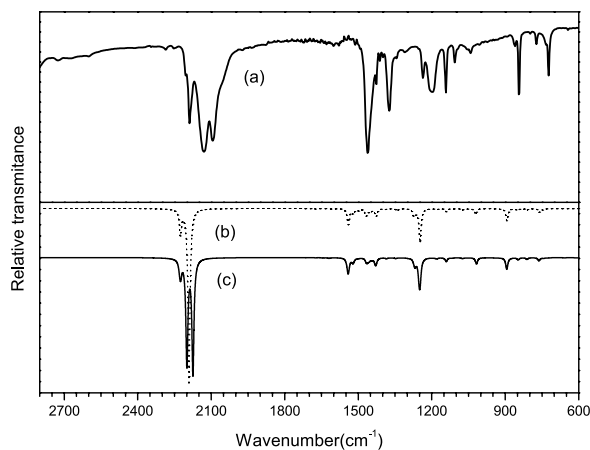


Figure 1S. Infrared Spectrum of $[\text{Fe}(\text{mnt})(\text{phen})(t\text{-BuNC})_2]$ (1) obtained experimentally in nujol mull (a) and calculated for the *trans*-1 (b) and *cis*-1 (c) isomers

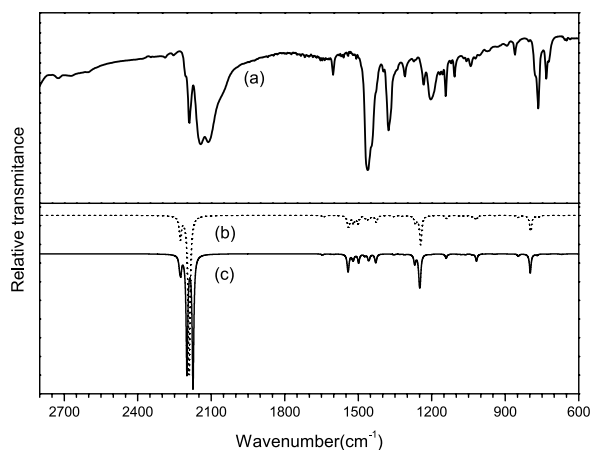


Figure 2S. Infrared Spectrum of $[\text{Fe}(\text{mnt})(\text{bipy})(t\text{-BuNC})_2]$ (2) obtained experimentally in nujol mull (a) and calculated for the *trans*-2 (b) and *cis*-1 (c) isomers

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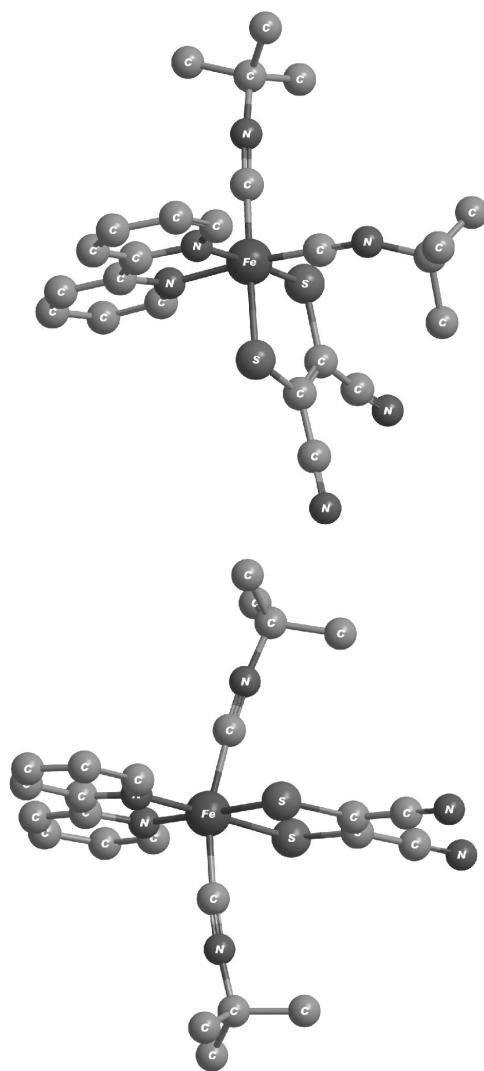


Figure 3S. Optimized Structure of *cis* and *trans* $[Fe(mnt)(bipy)(t-BuNC)_2]$ (hydrogen atom was omitted)

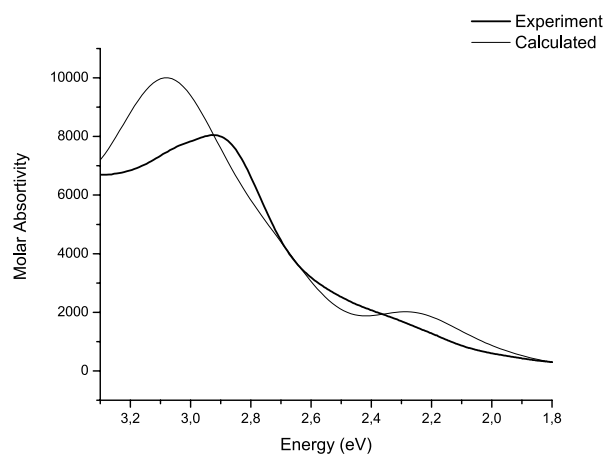


Figure 4S. Absorption Spectrum of **2** and computed TD-DFT of the *cis*-**2** isomer