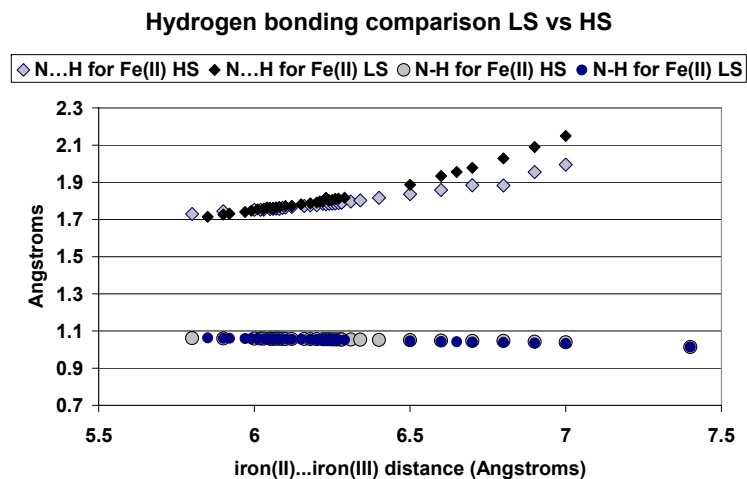


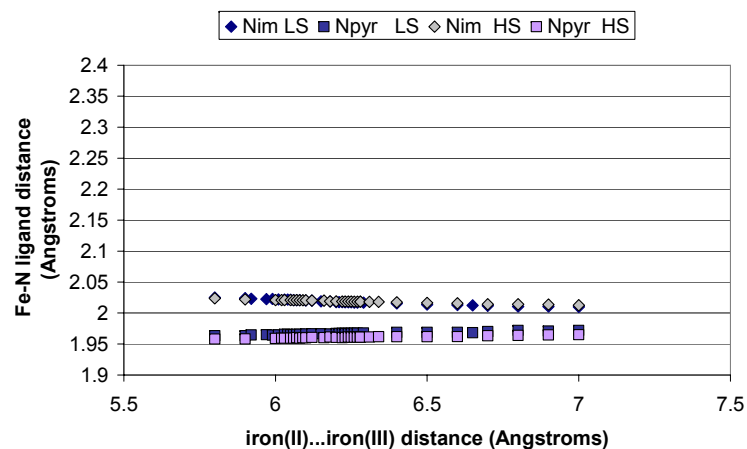
Electronic Supplemental Information for:

**“Synthesis and characterization of homo- and heterodinuclear M(II)-M(III)’
(M(II)= Mn or Fe, M(III)’ = Fe or Co) mixed-valence supramolecular pseudo-dimers.
The effect of hydrogen bonding on spin state selection of M(II)”**

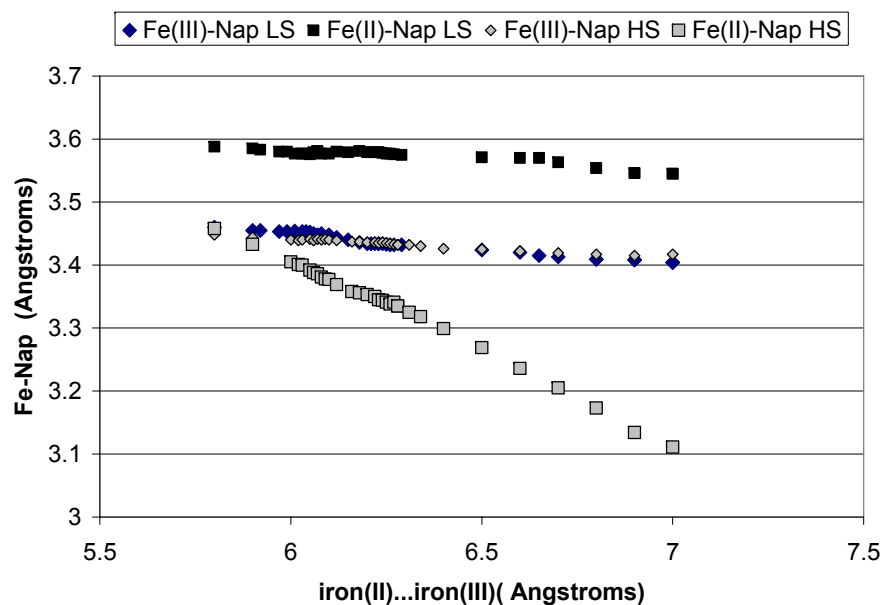


ESI Figure 1. The variation of $N_{\text{pyrazole-H}}$ and $N_{\text{pyrazolate-H}}$ as a function of iron(II)-iron(III) distance in $\{[\text{Fe}(\text{LS})\text{H}_3\text{L}^1][\text{FeL}^1]\}^{2+}$ and $\{[\text{Fe}(\text{HS})\text{H}_3\text{L}^1][\text{FeL}^1]\}^{2+}$.

First coordination sphere geometry around iron(III)



ESI Figure 2. The variation LS Fe(III)-N_{imine} and LS Fe(III)-N_{pyrazolate} bond distances as a function of iron(II)-iron(III) distance in $\{[\text{Fe}(\text{LS})\text{H}_3\text{L}^1][\text{FeL}^1]\}^{2+}$ and $\{[\text{Fe}(\text{HS})\text{H}_3\text{L}^1][\text{FeL}^1]\}^{2+}$. Note that these bonds are essentially invariant with iron(II)-iron(III) distance and the spin state of iron(II) and that the Fe(III)-N_{pyrazolate} distance is less than the Fe(III)-N_{imine} distance as experimentally observed.



ESI Figure 3. The variation of Fe-N_{ap} bond distances as a function of iron(II)-iron(III) distance in $\{[\text{Fe}(\text{LS})\text{H}_3\text{L}^1][\text{FeL}^1]\}^{2+}$ and $\{[\text{Fe}(\text{HS})\text{H}_3\text{L}^1][\text{FeL}^1]\}^{2+}$. Note that only iron(II) HS shows any significant variation and that as the HS iron(II) approaches the LS iron(III) it will undergo a SC requiring a drastically increased Fe(II)-N_{ap} distance as is experimentally observed.