

Self-Assembly of a Diferrous Triple Stranded Helicate with Bis(2,2'-Bipyridine) Ligands : Thermodynamic and Kinetic Intermediates

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Supporting Information

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Table S1. ^1H NMR Data for $\text{L}_3\text{Fe}_2^{4+}$ Complex in CD_3CN at 25°C .

H_3'	H_5'	H_4'	H_6'	H_3	H_4	H_6	NH	$\text{H}_{i,k}$	H_j
8.59 (dd)	8.06 (m)	7.30 (m)	7.20 (m)	8.46 (d)	8.22 (dd)	8.15 (d)	9.43 (s)	3.55 (m)	1.29
								2.15 (m)	

Table S2 ES-MS Data for Ferrous Complexes of Ligand L^a

Observed Ion	Measured m/z					Calculated m/z
	$\text{p}[\text{H}] = 2.50^b$	$\text{p}[\text{H}] = 10.20^b$	$1/20^c$	$1/1^c$	$3/1^c$	
$[\text{L} + \text{H}]^+$	439.4	439.3				439.5
$[\text{L} + 2\text{H} + \text{ClO}_4]^+$	539.2	539.2				539.9
$[\text{L} + 2\text{H} + \text{Na} + 2\text{ClO}_4]^+$	662.7					662.4
$[\text{L} + \text{Na}]^+$			461.2	461.2	461.2	461.5
$[2\text{L} + \text{Na}]^+$			899.7			900.0
$[\text{L} + \text{Fe}]^{2+}$	246.9	246.9				246.9
$[\text{L} + \text{Fe} + \text{ClO}_4]^+$		593.3				593.2
$[2\text{L} + \text{Fe}]^{2+}$		466.5				466.4
$[2\text{L} + 2\text{Fe} + \text{SO}_4]^{2+}$			542.5	542.3	542.3	542.3
$[3\text{L} + 2\text{Fe}]^{4+}$		356.8				356.8
$[3\text{L} + 2\text{Fe} + \text{ClO}_4]^{3+}$		508.8				508.9
$[3\text{L} + 2\text{Fe} + 2\text{ClO}_4]^{2+}$	813.0	813.0				813.0
$[3\text{L} + 2\text{Fe} + \text{H} + 3\text{ClO}_4]^{2+}$		863.3				863.2
$[3\text{L} + 2\text{Fe} + \text{SO}_4]^{2+}$			761.7	761.7	761.7	761.6

^aSolvent: methanol; $[\text{L}]_{\text{tot}} = 5.10 \times 10^{-5} \text{ M}$; ^b $[\text{Fe(II)}]_{\text{tot}} = 2.55 \times 10^{-5} \text{ M}$; ^c $[\text{Fe(II)}]_{\text{tot}}/[\text{L}]_{\text{tot}}$

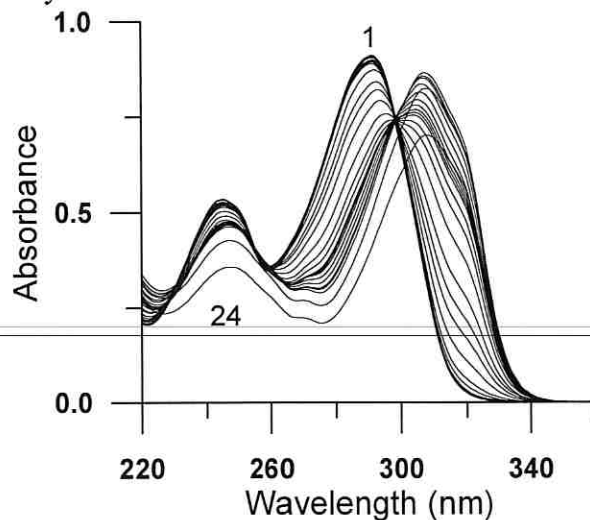
Figure S1. Absorption spectra of ligand L versus $\text{p}[\text{H}]$. Solvent methanol; $I = 0.1 \text{ M}$; $T = 25.0 (2)^\circ\text{C}$; $l = 2 \text{ cm}$; $[\text{L}]_{\text{tot}} = 1.0 \times 10^{-5} \text{ M}$; Spectra 1-24: $\text{p}[\text{H}] = 10.35$; 6.39; 6.21; 5.99; 5.75; 5.32; 5.04; 4.85; 4.67; 4.40; 4.20; 4.09; 4.00; 3.96; 3.93; 9.90; 3.85; 3.74; 3.61; 3.48; 3.42; 3.28; 2.96; 2.67 respectively.

Figure S2. Dissociation kinetics of the ferrous helicate L_3Fe_2 . Solvent: methanol; $I = 0.1$ M; $T = 25.0$ (2) $^{\circ}C$; $[L_3Fe_2]_{tot} = 3.1 \times 10^{-5}$ M; $[OH^-]_{tot} = 9.8 \times 10^{-3}$ M; $l = 0.5$ cm; $\lambda = 540$ nm.

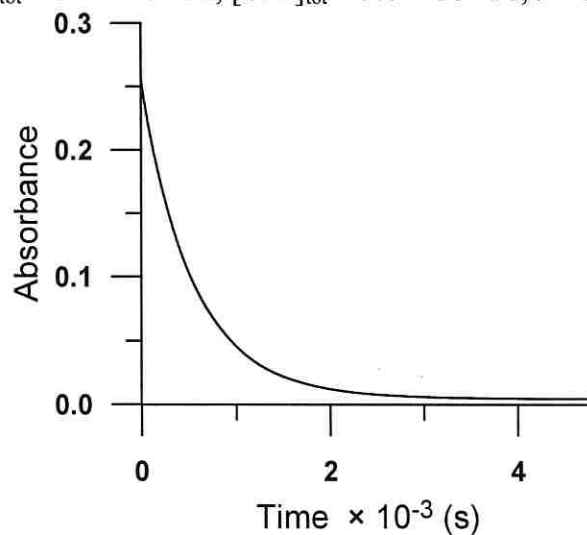


Figure S3. Time-resolved absorption spectra: dissociation kinetics of L_3Fe_2 . Solvent: methanol; $I = 0.1$ M; $T = 25.0$ (2) $^{\circ}C$; $[L_3Fe_2]_{tot} = 3.7 \times 10^{-5}$ M; $[OH^-]_{tot} = 9.8 \times 10^{-4}$ M; $l = 1$ cm. Spectra 1-10 every 12 min and spectra 11-15 every 34 min

