Supplementary material

Pentacoordinated chloro-Iron(III) Complexes with Unsymmetrically-substituted N_2O_2 quadridentate Schiff-Base Ligands: Syntheses, structures, magnetic and redox properties

Jonathan Cisterna, Vania Artigas, Mauricio Fuentealba, Paul Hamon, Carolina Manzur, Jean-René Hamon, and David Carrillo

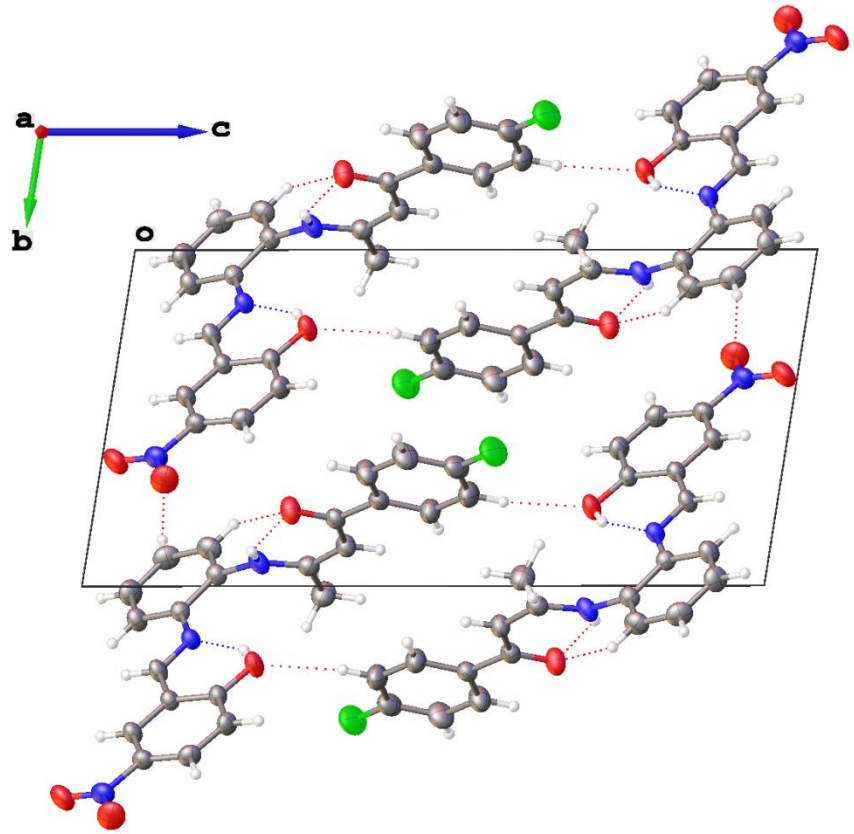

Figure S1. Packing diagram of **2** showing the hydrogen bonding interactions.

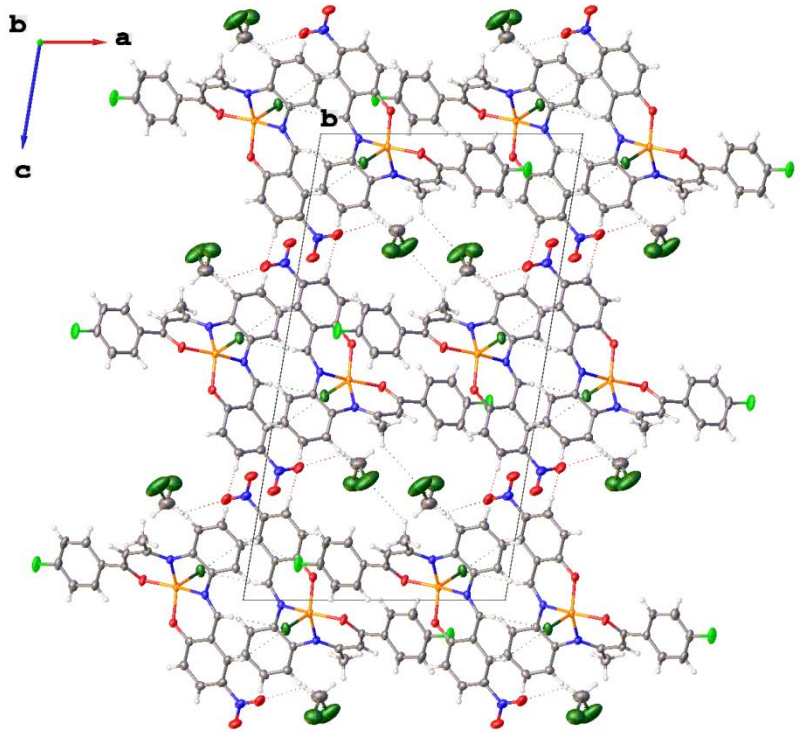

Figure S2. Packing diagram of **3**·CH_2Cl_2 showing the hydrogen bonding interactions implying the dichloromethane crystallization molecules.

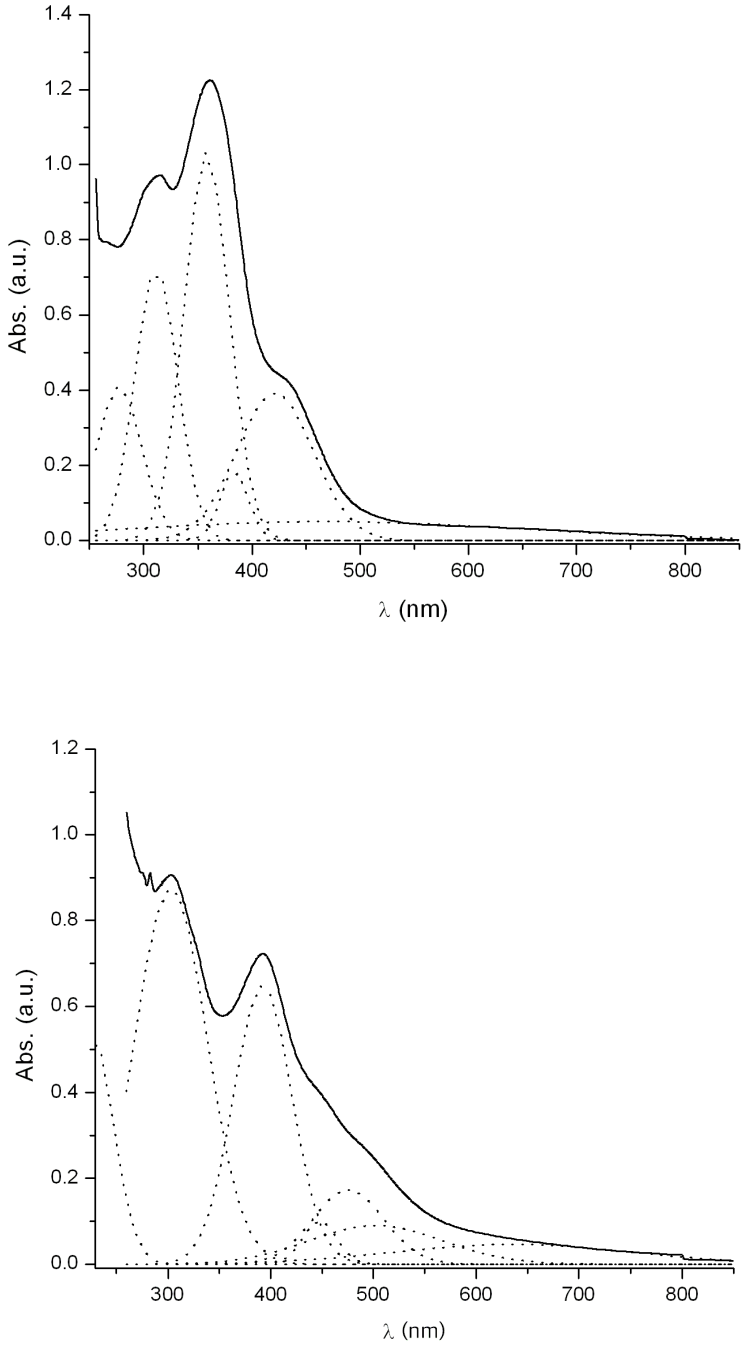

Figure S3. Experimental UV-vis spectra of complexes 3 (top, full line) and 5 (bottom, full line) recorded in DMSO at 20 °C, and their respective deconvoluted spectra (dotted lines).

Table S1. Selected bond distances (Å)and angles (°) for compounds **3**·CH_2Cl_2.

Bond distances	
O(1)-C(7)	1.292(5)
O(2)-C(19)	1.303(5)
N(1)-C(9)	1.323(5)
N(1)-C(11)	1.419(5)
N(2)-C(16)	1.408(5)
N(2)-C(17)	1.301(5)
C(7)-C(8)	1.376(6)
C(8)-C(9)	1.398(6)
C(11)-C(16)	1.404(5)
C(17)-C(18)	1.422(6)
C(18)-C(19)	1.434(5)
F(1)-C(1)	1.356(5)
N(3)-C(22)	1.461(6)
N(3)-O(3)	1.222(6)
N(3)-O(4)	1.221(6)
Bond angles	
Fe(1)-O(1)-C(7)	131.4(3)
Fe(1)-O(2)-C(19)	132.2(3)
Fe(1)-N(1)-C(9)	124.4(3)
Fe(1)-N(1)-C(11)	111.4(2)
Fe(1)-N(2)-C(16)	111.2(2)
Fe(1)-N(2)-C(17)	125.6(3)
O(1)-C(7)-C(8)	123.3(4)
C(7)-C(8)-C(9)	126.1(4)
C(8)-C(9)-N(1)	122.8(4)
O(2)-C(19)-C(18)	122.2(4)
N(2)-C(17)-C(18)	124.4(3)
C(17)-C(18)-C(19)	123.7(3)

Table S2. Selected bond distances (Å) and angles (°) for compound **5**·0.5MeCN.

Bond distances			
O(1)-C(11)	1.311(11)	O(2)-C(23)	1.353(11)
N(1)-C(13)	1.321(12)	N(1)-C(15)	1.417(12)
N(2)-C(20)	1.414(11)	N(2)-C(21)	1.305(11)
O(3)-C(27)	1.388(13)	O(3)-C(28)	1.427(18)
C(10)-C(11)	1.482(12)	C(11)-C(12)	1.361(14)
C(12)-C(13)	1.361(14)	C(15)-C(20)	1.403(13)
C(21)-C(22)	1.428(12)	C(22)-C(23)	1.395(13)
Fe(2)-C(Cp) avg	2.05(2)	Fe(2)-C(Cp′) avg	2.026(13)
Bond angles			
Fe(1)-O(1)-C(11)	128.0(6)	Fe(1)-O(2)-C(23)	129.2(6)
Fe(1)-N(1)-C(13)	125.0(6)	Fe(1)-N(1)-C(15)	111.2(6)
Fe(1)-N(2)-C(20)	112.1(6)	Fe(1)-N(2)-C(21)	126.9(6)
O(1)-C(11)-C(12)	122.6(9)	O(2)-C(23)-C(22)	124.2(8)
N(1)-C(13)-C(12)	120.5(8)	N(2)-C(21)-C(22)	122.8(8)
C(11)-C(12)-C(13)	128.2(9)	C(21)-C(22)-C(23)	123.2(8)

Abbreviations: Cp = C_5H_5, Cp′ = C_5H_4

Table S3. Atomic occupancy for complex **5**.

Atom	Occupancy	Atom	Occupancy	Atom	Occupancy
C(2)	0.67(2)	H(2)	0.67(2)	C(1)	0.67(2)
H(1)	0.67(2)	C(5)	0.67(2)	H(5)	0.67(2)
C(4)	0.67(2)	H(4)	0.67(2)	C(3)	0.67(2)
H(3)	0.67(2)	N(1S)	0.5	C(1S)	0.5
C(2S)	0.5	H(4A)	0.5	H(4B)	0.5
H(4C)	0.5	C(1A)	0.33(2)	H(4AB)	0.33(2)
C(2A)	0.33(2)	H(0AB)	0.33(2)	C(3A)	0.33(2)
H(1AB)	0.33(2)	C(4A)	0.33(2)	H(2AB)	0.33(2)
C(5A)	0.33(2)	H(3AB)	0.33(2)		

Table S4. Hydrogen bond interaction parameters for proligand **2**.

D-H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
O(2)-H(2)···N(2)	0.82	1.85	2.586(2)	148.4
N(1)-H(1)…O(1)	0.86	1.98	2.638(2)	132.6