Electronic Supplementary Information

Room Temperature Spin Crossover Ionic Liquids

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Magnetic Measurements

Variable temperature magnetic susceptibility data for liquid samples of (**2**) and **3** were recorded on a Quantum Design MPMS® XL-7 SQUID magnetometer in a field of 0.1 T between 10 – 380K in heating and cooling modes for (**2**), and between 300 K and 10 K for (**3**), both at 5 K/min warming/cooling rate. A gelatin capsule was used to house the liquid and Teflon tape was wrapped around the seal of the capsule to prevent leaks. Diamagnetic contributions were accounted for using Pascal's constants for the sample, and by measurement for the sample holder. The effect of the loss of solvent on the magnetic profile of complex (**2**) is obvious in Fig. S1. The corrected molecular formula *i.e.* less three water molecules yields a value in line with S = ½ Fe(III) ion for cycles 1-4, Table S1.

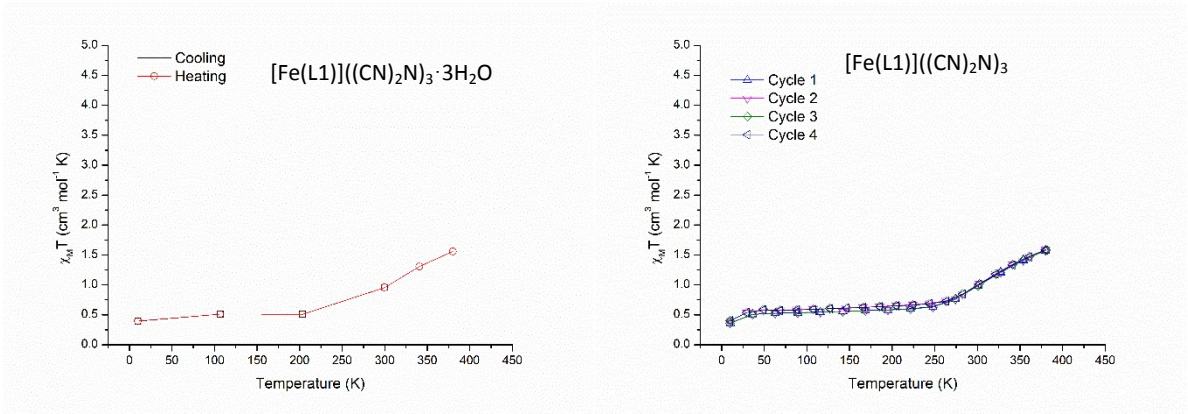

Fig. S1: $\chi_M T$ v T plot for complex (**2**) and (**2'**), exhibiting change in the magnetic moment as a result of water loss.

Table S1: $\chi_M T$ v T for all cycles. Molecular weight used – (**2**) for initial and (**2'**) for Cycles 1-4.

Initial		Cycle 1		Cycle 2		Cycle 3		Cycle 4	
$C_{42}H_{50}FeN_{17}O_2 \cdot 3H_2O$		$C_{42}H_{50}FeN_{17}O_2$		$C_{42}H_{50}FeN_{17}O_2$		$C_{42}H_{50}FeN_{17}O_2$		$C_{42}H_{50}FeN_{17}O_2$	
Temp (K)	$\chi_M T$ ($cm^3mol^{-1}K$)	Temp (K)	$\chi_M T$ ($cm^3mol^{-1}K$)	Temp (K)	$\chi_M T$ ($cm^3mol^{-1}K$)	Temp (K)	$\chi_M T$ ($cm^3mol^{-1}K$)	Temp (K)	$\chi_M T$ ($cm^3mol^{-1}K$)
300.0026	0.9567	9.99711	0.36238	380.0117	1.5893	10.00387	0.40196	10.00387	0.40116
203.4097	0.5087	36.43435	0.5105	360.6685	1.47892	29.47726	0.53944	29.47726	0.53836
106.7014	0.5108	62.85593	0.52907	340.9656	1.34291	48.94713	0.58611	48.94713	0.58494
9.999542	0.395	89.28457	0.5386	321.6123	1.1873	68.45747	0.57358	68.45747	0.57243
9.997768	0.3962	115.7055	0.5493	302.1476	1.01864	87.88965	0.58397	87.88965	0.5828
106.6695	0.511	142.1948	0.55948	282.6995	0.85207	107.3653	0.59337	107.3653	0.59218
203.3307	0.5087	168.6087	0.57175	263.2049	0.73778	126.9215	0.60533	126.9215	0.60412
300.0161	0.9575	194.9884	0.58592	243.7172	0.6917	146.4033	0.61349	146.4033	0.61226
340.6779	1.3067	221.4631	0.60361	224.2446	0.66977	165.8787	0.62488	165.8787	0.62363
380.0285	1.5583	247.8537	0.63624	204.7675	0.65363	185.3352	0.63719	185.3352	0.63591
		274.3194	0.76897	185.286	0.6395	204.8069	0.6506	204.8069	0.6493
		300.74	0.99268	165.8019	0.62688	224.2825	0.66468	224.2825	0.66335
		327.1668	1.21807	146.3278	0.61576	243.742	0.68698	243.742	0.68561
		353.5813	1.42214	126.8573	0.60601	263.2216	0.72895	263.2216	0.72749
		380.0194	1.58648	107.3957	0.59669	282.6969	0.84806	282.6969	0.84637
		380.0194	1.57061	87.92707	0.59025	302.1581	1.0146	302.1581	1.01257
		353.5813	1.40791	68.45466	0.57597	321.6191	1.18269	321.6191	1.18032
		327.1668	1.20589	48.94769	0.57556	341.1095	1.33844	341.1095	1.33576
		300.74	0.98275	29.47227	0.53905	360.5619	1.47267	360.5619	1.46973
		274.3194	0.76128	9.99831	0.40044	380.0448	1.58762	380.0448	1.58444
		247.8537	0.62988	9.99711	0.35876	380.0194	1.57061	380.0448	1.58127
		221.4631	0.59758	36.43435	0.50539	353.5813	1.40791	360.5619	1.46679
		194.9884	0.58006	62.85593	0.52378	327.1668	1.20589	341.1095	1.33309
		168.6087	0.56603	89.28457	0.53321	300.74	0.98275	321.6191	1.17796
		142.1948	0.55389	115.7055	0.5438	274.3194	0.76128	302.1581	1.01054
		115.7055	0.5438	142.1948	0.55389	247.8537	0.62988	282.6969	0.84468
		89.28457	0.53321	168.6087	0.56603	221.4631	0.59758	263.2216	0.72604
		62.85593	0.52378	194.9884	0.58006	194.9884	0.58006	243.742	0.68424
		36.43435	0.50539	221.4631	0.59758	168.6087	0.56603	224.2825	0.66202
		9.99711	0.35876	247.8537	0.62988	142.1948	0.55389	204.8069	0.648
				274.3194	0.76128	115.7055	0.5438	185.3352	0.63464
				300.74	0.98275	89.28457	0.53321	165.8787	0.62238
				327.1668	1.20589	62.85593	0.52378	146.4033	0.61104
				353.5813	1.40791	36.43435	0.50539	126.9215	0.60291
				380.0194	1.57061	9.99711	0.35876	107.3653	0.591
								87.88965	0.58163
								68.45747	0.57129
								48.94713	0.58377
								29.47726	0.53728
								10.00387	0.40036

Thermogravimetric Measurements

Thermogravimetric analysis of (**2**) was recorded on a TA Q500 TGA instrument and fixed mass spectra were recorded by a Hiden Analytical HPR20 and a Thermo OnixTM Prolab spectrometer, Fig. S2.

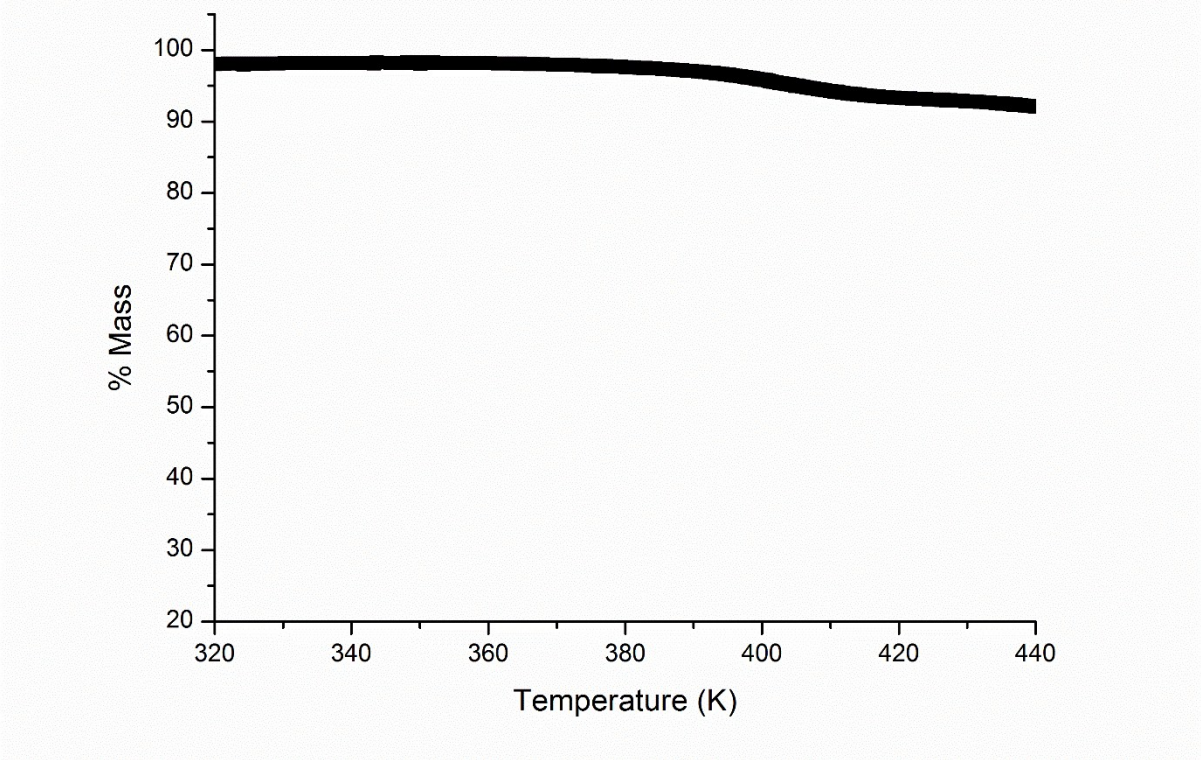

Fig. S2: Thermogravimetric Analysis of complex (**2**) showing water loss at 400 K.

Variable Temperature Electronic Spectroscopy

Variable temperature UV-Vis measurements were conducted on (**2**) to investigate if it shows thermochromism, Fig. S3. By eye there is no change in the colour of the neat liquid when heated above room temperature. This is reflected in the lack of a batho- or hypsochromic shift in the UV data collected in a methanolic solution of (**2**). The hypochromic shift at 260 and 330 nm on warming indicates a change in the MLCT bands due to partial spin transition from S = ½ to S = $^{5}/_{2}$ over this temperature range.

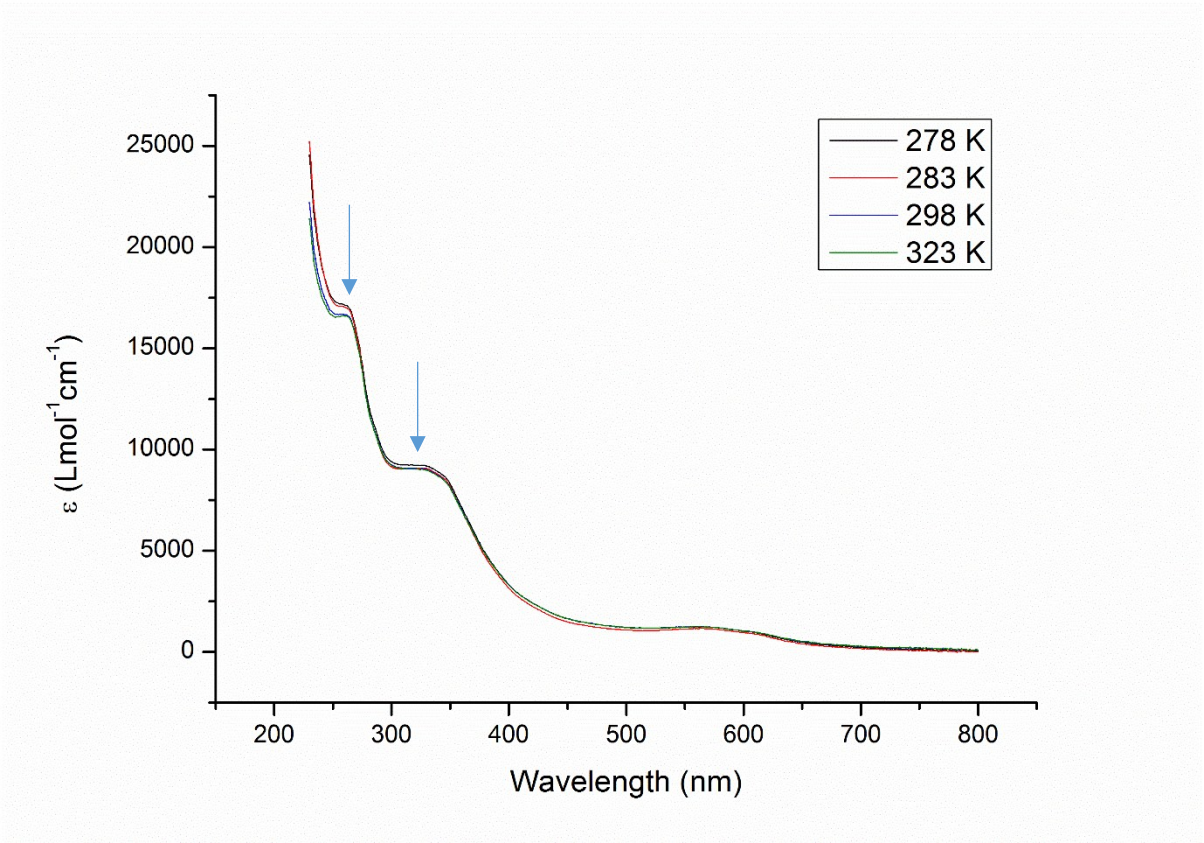

Fig. S3: UV-Vis spectra of complex (**2**) in MeOH at a concentration of 1.9×10^{-5} M.