Electronic Supplementary Material (ESI) for New Journal of Chemistry

Supporting Information for

Amphiphilic iron(II) complexes with short alkyl chains – Crystal Packing and Spin Transition properties

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Figure S1. ^{1}H NMR of the ligand **H_2L** (left). S denotes the residual solvent.

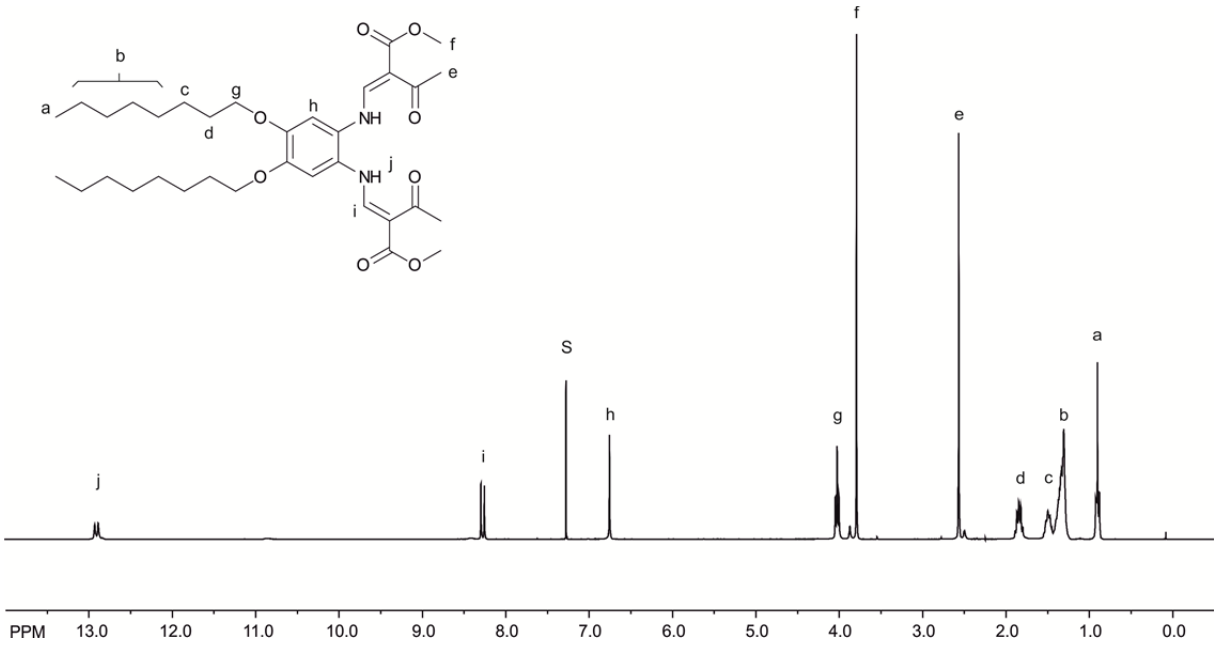

Table S1. Parameters for crystal structure determination of **1a**(HS), **1a**(LS), **1b**, **2a** and **2b**.

Compound reference	**1a**(HS)	**1a**(LS)	**1b**	**2a**	**2b**
Chemical formula	$C_{48}H_{70}FeN_6O_8$·MeOH	$C_{48}H_{70}FeN_6O_8$·MeOH	$C_{48}H_{70}FeN_6O_8$·1.5MeOH	$C_{41}H_{60}FeN_4O_8$	$C_{41}H_{60}FeN_4O_8$
M_r/g mol^{-1}	946.99	946.99	963.01	792.78	792.78
crystal dimensions /mm	0.20×0.27×0.40	0.37×0.40×0.42	0.14×0.19×0.39	0.20×0.26×0.34	0.11×0.12×0.29
radiation /nm	0.71073	0.71073	0.71073	0.71073	0.71073
crystal system	triclinic	triclinic	monoclinic	monoclinic	triclinic
a /Å	12.0361(8)	11.9287(5)	10.599(5)	19.8161(9)	11.9872(7)
b /Å	13.4241(10)	13.1406(5)	31.295(5)	8.2415(4)	12.5380(8)
c /Å	17.3275(13)	17.0569(7)	15.997(5)	25.5905(11)	14.6613(10)
α /°	103.289(6)	103.154(3)	90	90	95.394(5)
β /°	101.608(6)	100.508(3)	101.404(5)	98.224(3)	102.327(5)
γ /°	99.935(6)	100.246(3)	90	90	106.231(5)
Unit cell volume /Å^3	2597.7(3)	2491.76(18)	5201(3)	4136.3(3)	2039.0(2)
Temperature /K	273	133	133	133	133
space group	$P\bar{1}$	$P\bar{1}$	$P2_1/c$	$P2_1/c$	$P\bar{1}$
Z	2	2	4	4	2
μ /mm^{-1}	0.347	0.362	0.349	0.419	0.425
No. of reflections measured	31745	30301	56290	38465/5508	24231
No. of independent reflections	8697	8344	8715	5508	6827
R_{int}	0.154	0.073	0.185	0.00 (0.142)*	0.142
Final R_1 values ($I > 2\sigma(I)$)	0.0660	0.0384	0.0852	0.1008	0.0632
Final R_1 values (all data)	0.1055	0.0531	0.1626	0.1147	0.1335
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.1737	0.0975	0.2514	0.2606	0.1380
Goodness of fit on F^2	0.87	0.93	0.93	1.13	0.88
CCDC number	CCDC 944437	CCDC 944436	CCDC 944434	CCDC 944438	CCDC 944435

* new hkl file generated by PLATON. Original R_{int} in brackets.

Figure S2. Spin crossover behaviour of the reaction products of **[Fe(L)(MeOH)$_2$]** with 20 (triangles), 30 (open squares), 70 (cycles), 90 (squares) and 110 (open cycles) equivalents of dmap.

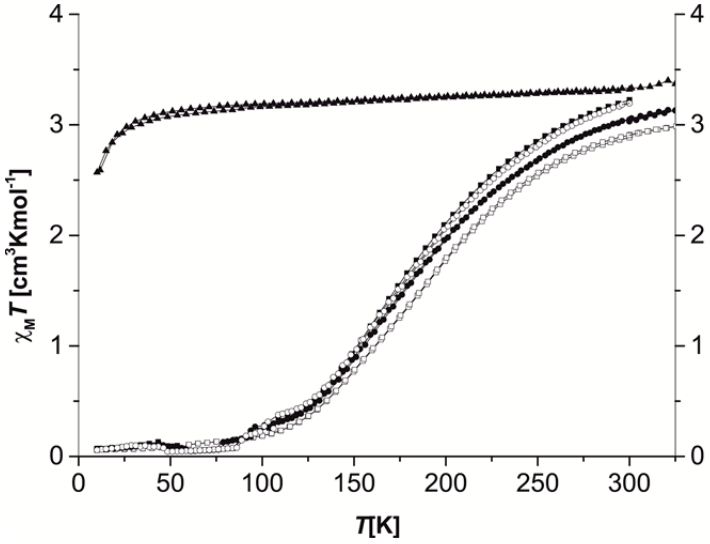

Figure S3. Left: Spin crossover behaviour of fresh crystals of **[Fe(L)(dmap)$_2$] (1c)**. Right: Spin transition curve of **1a** (cycles) and combined curve of the 50:50 weighted contributions of the spin transition curves of **1b** and **1c** (open triangles).

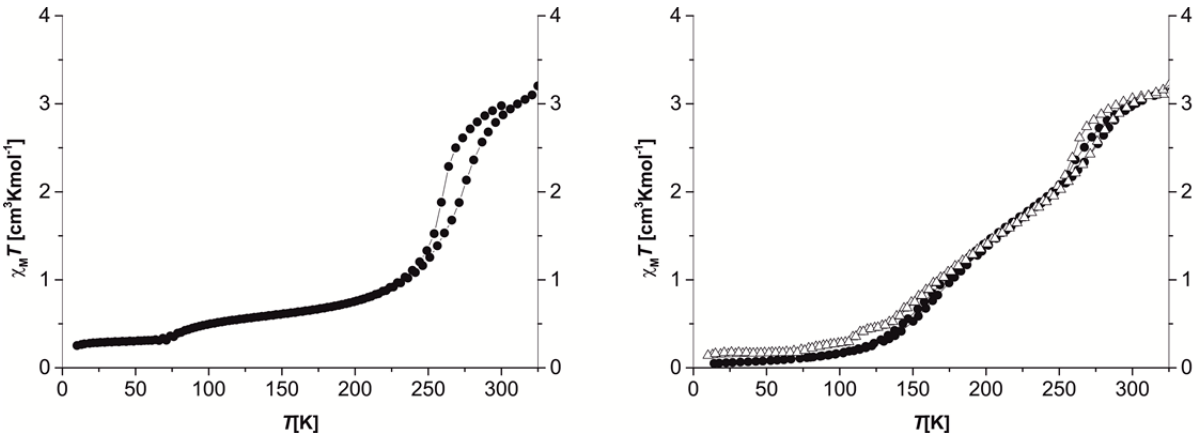

Figure S4. Left: appearance of the high spin state of the solution of **[Fe(L)(MeOH)$_2$]** with 50 equivalents of dmap. Right: low spin state of the solution after cooling with liquid nitrogen.