Supporting Information

Structures and Chromogenic Ion-Pair Recognition of Catechol Functionalization of 1, 8-Anthraquinone Macrocycle in DMSO

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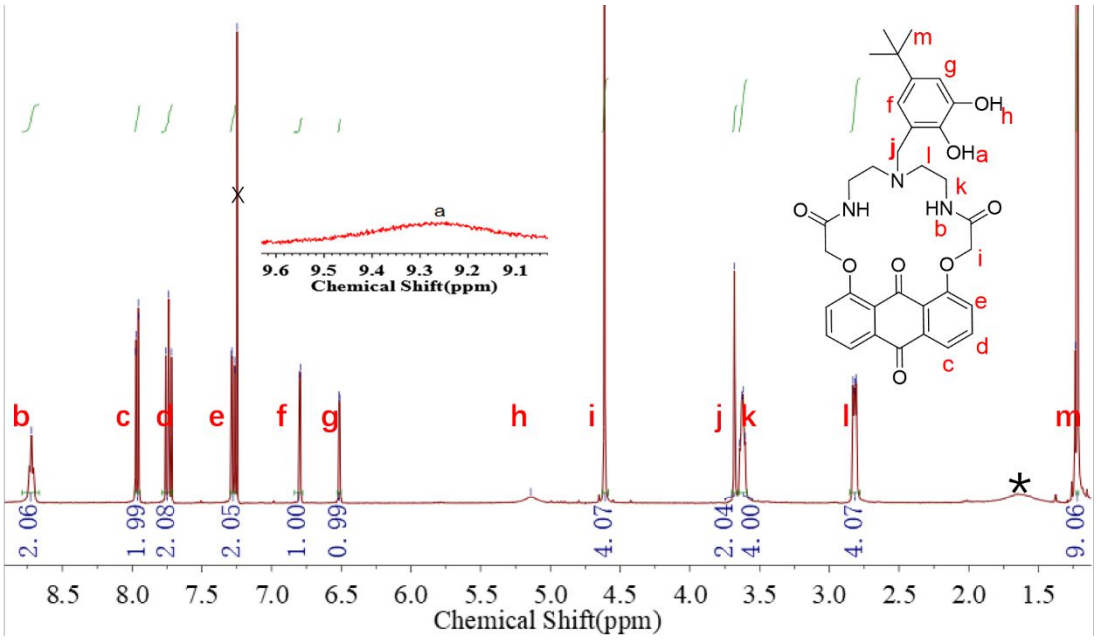

Figure S1. ^{1}H NMR of H_2L in $CDCl_3$

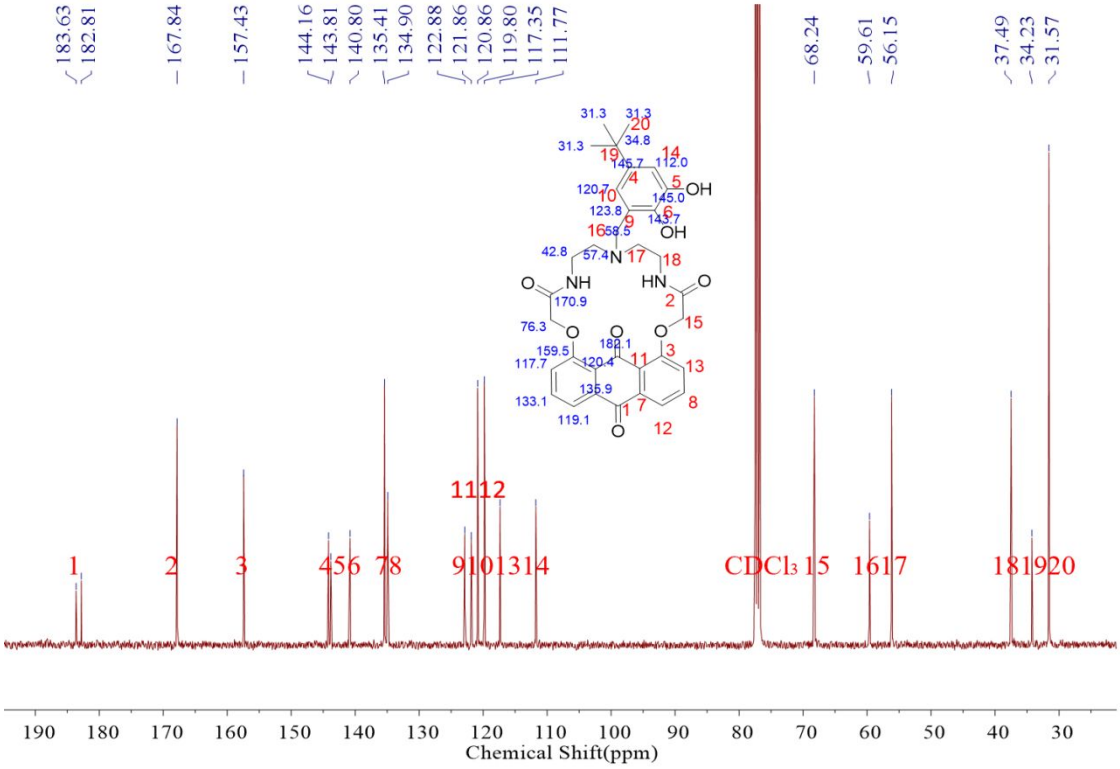

Figure S2. ^{13}C NMR of H_2L in $CDCl_3$

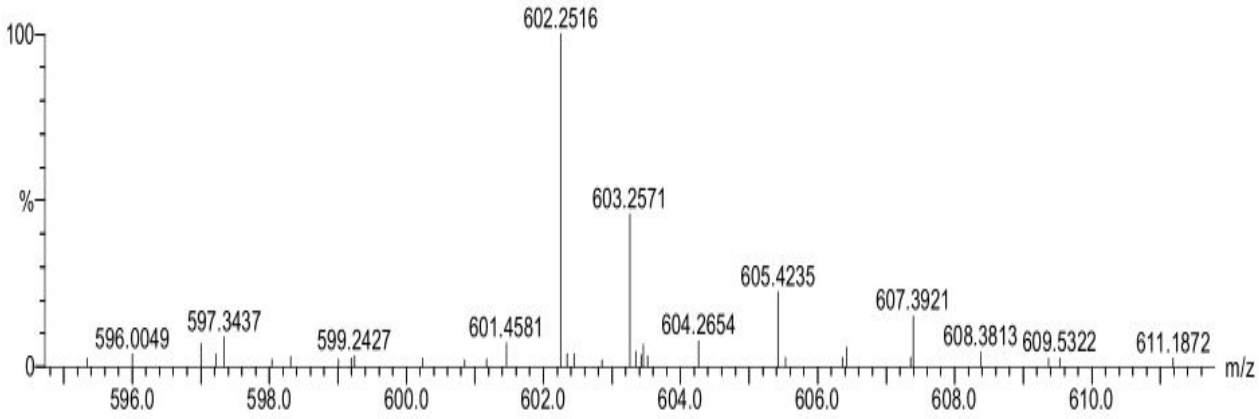

Figure S3. MS of H_2L in CH_3OH

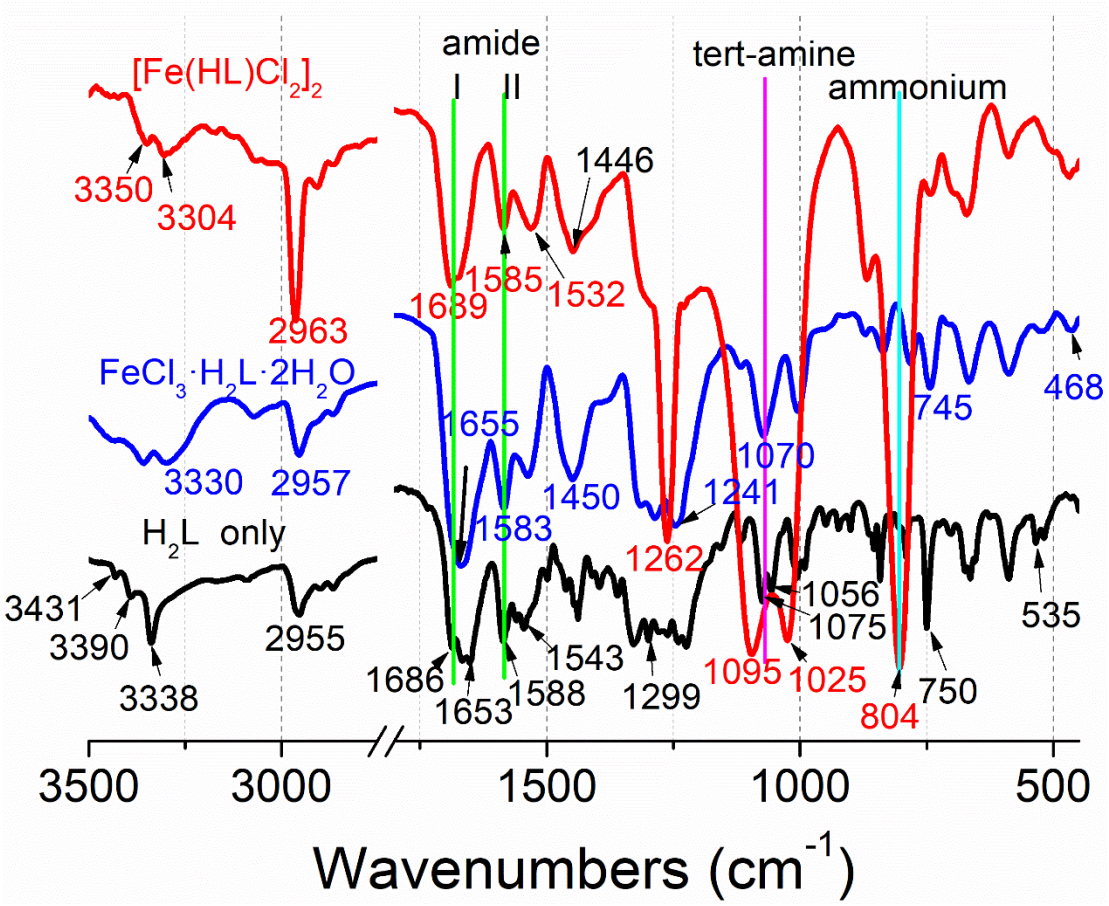

Figure S4. IR of H_2L, $FeCl_3 \cdot H_2L \cdot 2H_2O$ powder and $Fe_2(HL)_2Cl_4$ crystal (KBr disc)

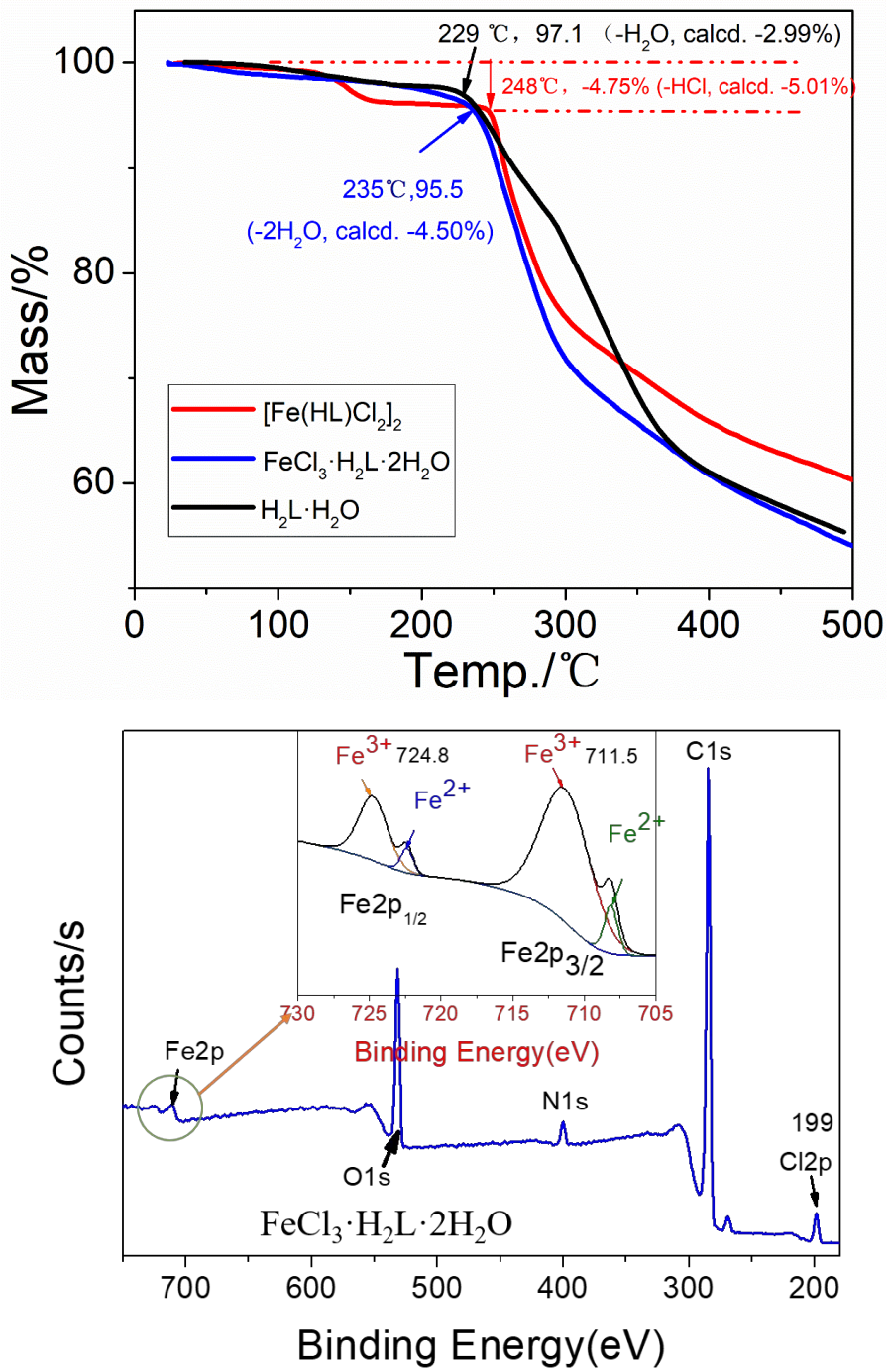

Figure S5. TG of $H_2L·H_2O$, $Fe_2(HL)_2Cl_4$ and $FeCl_3·H_2L·2H_2O$ (top) and XPS of $FeCl_3·H_2L·2H_2O$ (bottom)

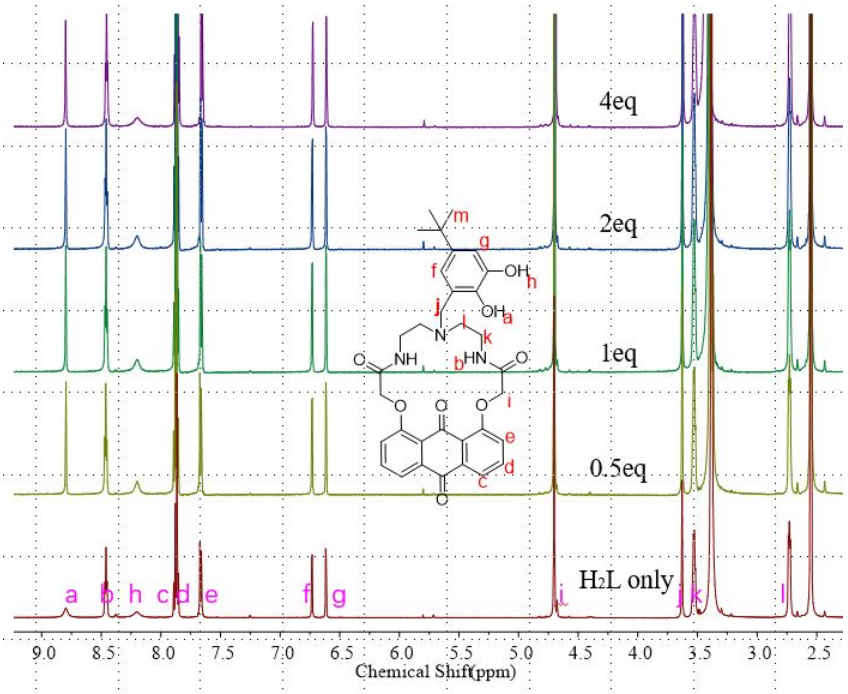

Figure S6. ^{1}H NMR spectra of H_2L in presence of different equivalents of $Zn(ClO_4)_2$ in d_6-DMSO.

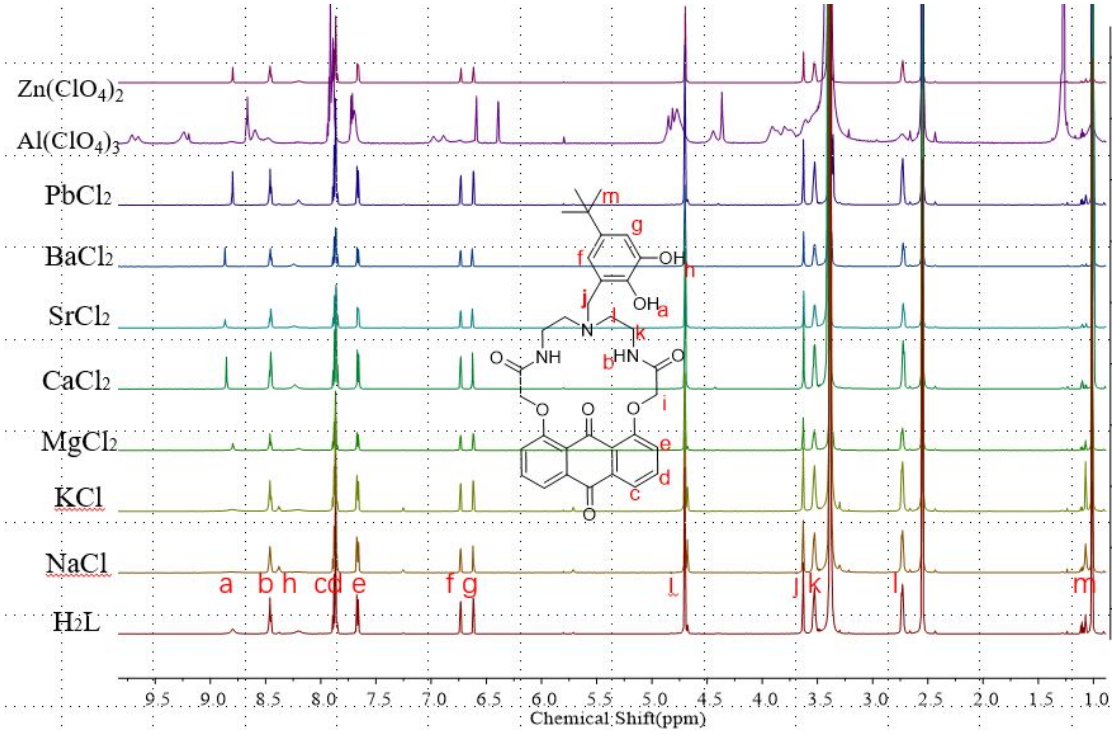

Figure S7. ^{1}H NMR spectra of H_2L in the absence and presence of 2 eq metal salts in d_6-DMSO.

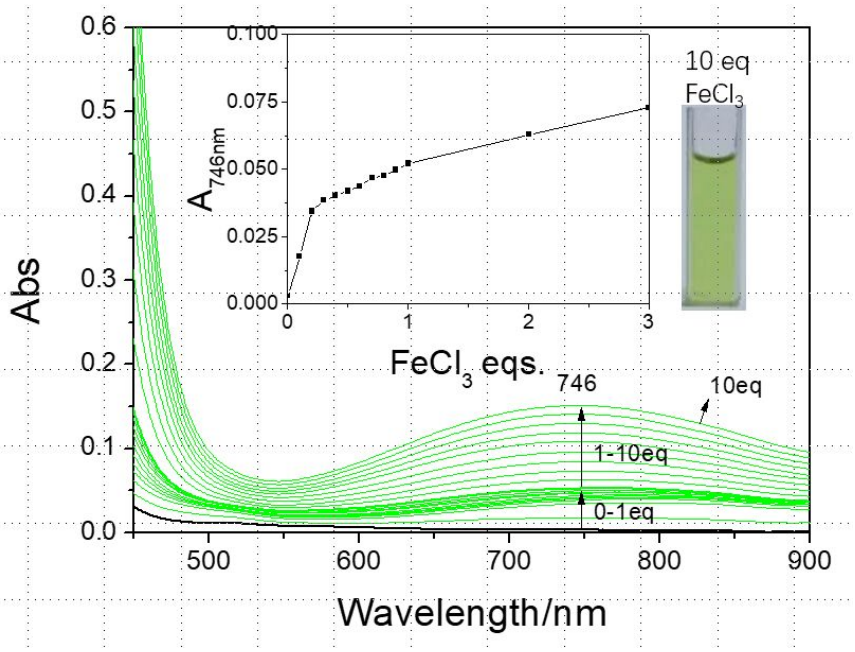

Figure S8. UV-vis spectra of 5.0×10^{-4} M TBC in the presence of different eq. of $FeCl_3$ in DMSO.

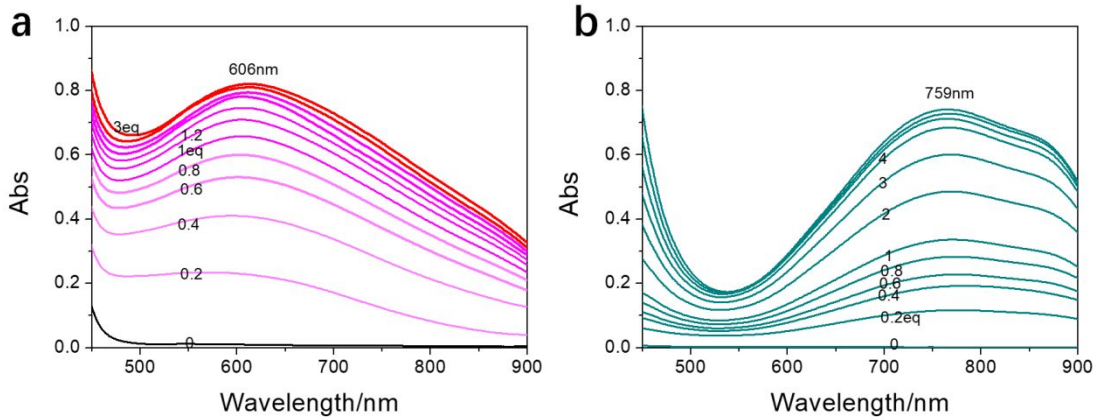

Figure S9. UV-vis spectra of 5×10^{-4} M H_2L(a) and 5×10^{-4} M TBC(b) in the presence of different eq. of $FeCl_3$ in EtOH.

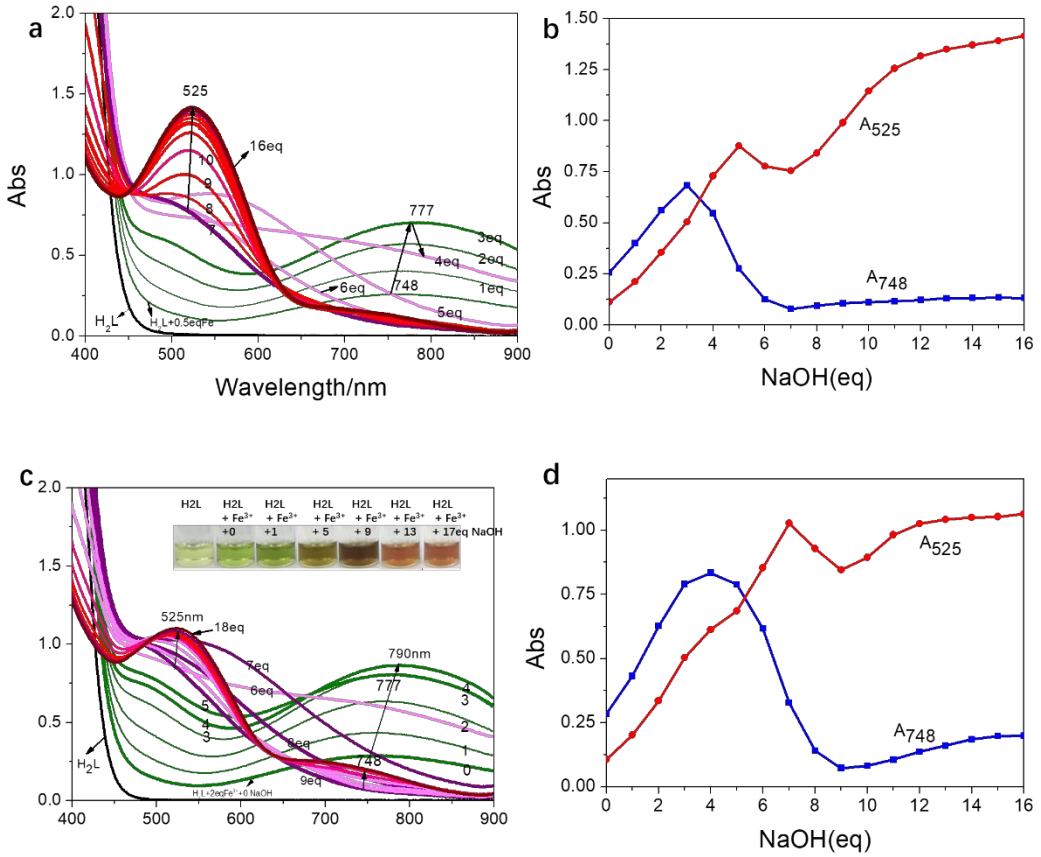

Figure S10. UV-vis spectra of 5.0×10^{-4} M H_2L and 1eq $FeCl_3$(a), 2eq $FeCl_3$(c) upon gradual addition of different equiv. of NaOH and Maximum absorbances of 1eq $FeCl_3$(b), 2eq $FeCl_3$(d) vs. NaOH eq. in DMSO.

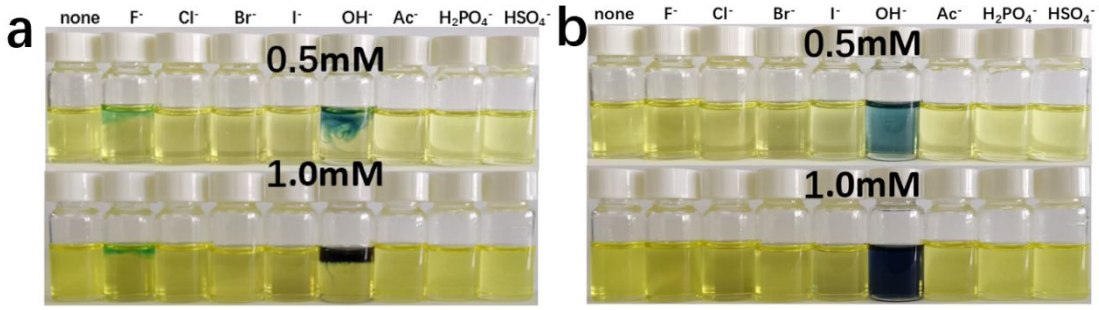

Figure S11. Visual color changes of 0.5 mM and1.0 mM H_2L in the absence and presence of different anions (2eq) in DMSO (a: Without shake, b: Shaking evenly). All anions are tetrabutyl ammonium salts.

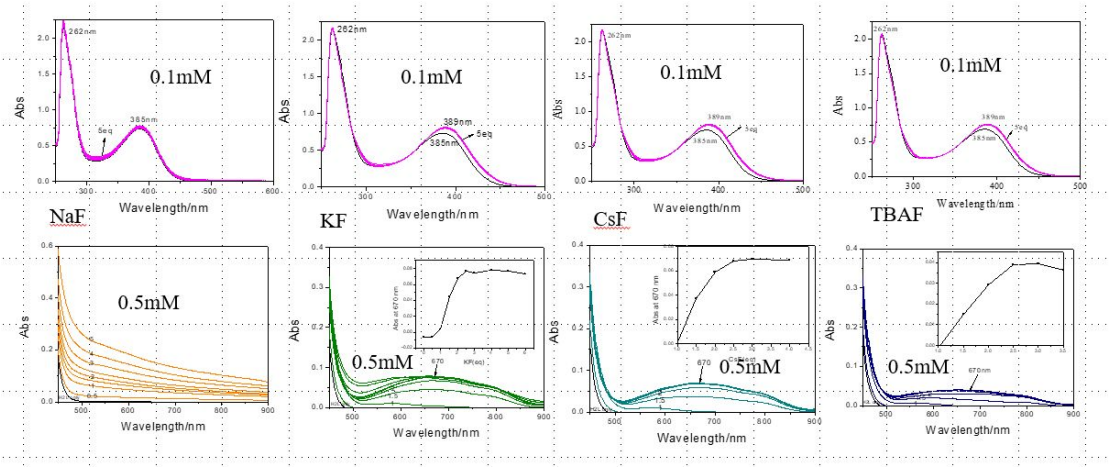

Figure S12. UV-vis spectra of 1.0×10^{-4} M (top) and 5.0×10^{-4}M (bottom) H_2L in the presence of different eq. of NaF, KF, CsF and TBAF in DMSO.

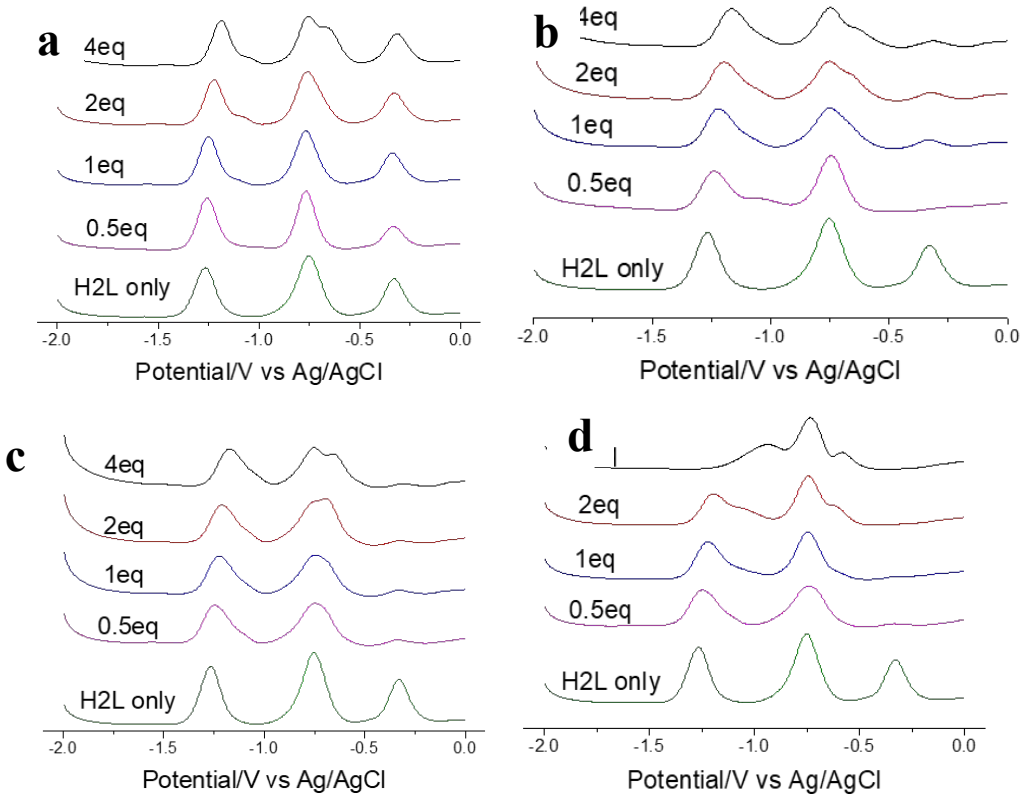

Figure S13. Differential pulse voltammograms of 1.00 mM H_2L in the absence and presence of different eq. of NaF(a), KF(b),CsF(c),TBAF(d) in 50 mM $TBAPF_6$/DMSO solution.

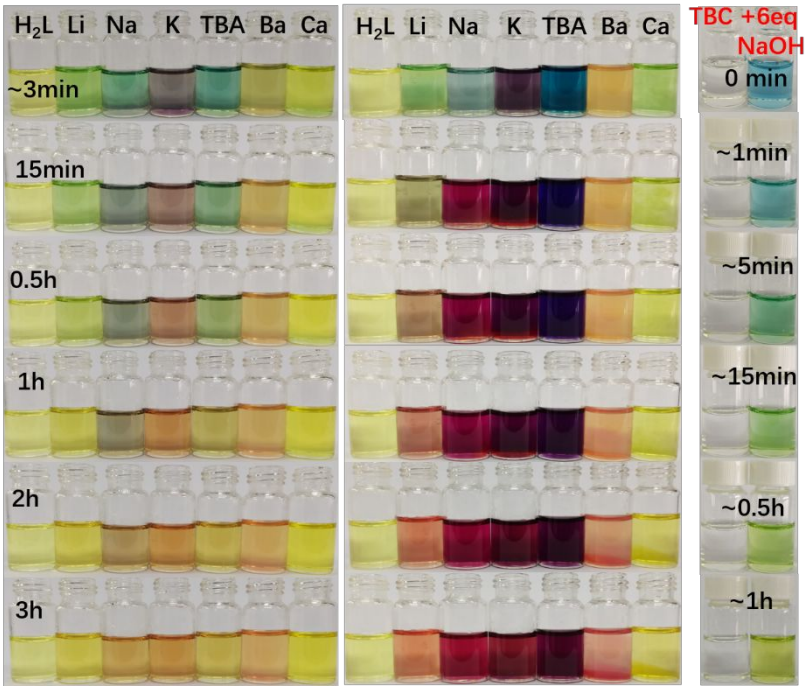

Figure S14. Photograph of 0.50 mM H_2L in the presence of 2 (left) and 6 (middle) eq different hydroxides in DMSO. 0.50 mM TBC in the presence of 6 eq NaOH are pictured in right for comparison

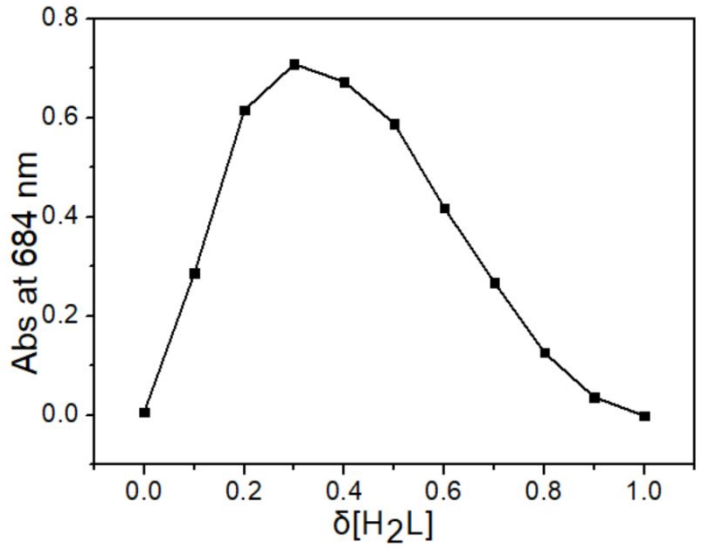

Figure S15. Job plot of 5.0×10^{-3} M [H_2L + NaOH] in DMSO at 684 nm

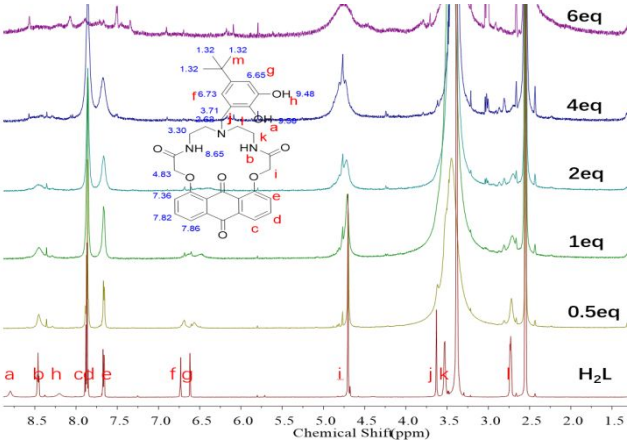

Figure S16. ^{1}H NMR spectra of H_2L in the absence and presence of different eqs. of NaOD in d_6-DMSO.

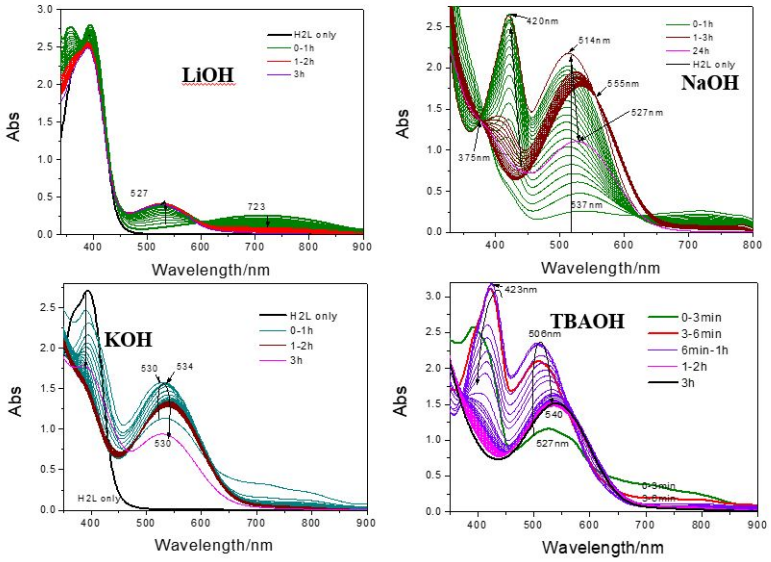

Figure S17. UV-vis spectra of 5.0×10^{-4} M H_2L in the presence of 6 eq. of LiOH, NaOH, KOH, TBAOH in DMSO within 3h.

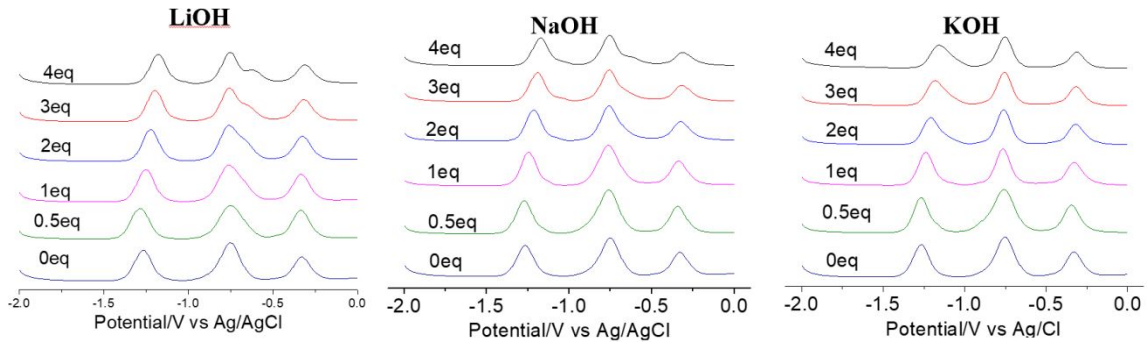

Figure S18. Differential pulse voltammograms of 1.00 mM H_2L in the presence of different equivalents of LiOH、NaOH 、KOH in 0.05 M $TBAPF_6$/DMSO solution.

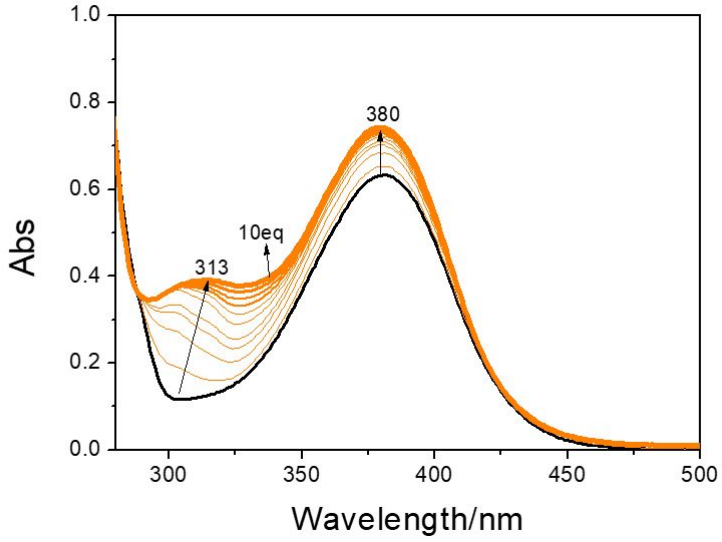

Figure S19. UV-vis spectra of 1.0×10^{-4} M H_2L in the presence of different eq. of NaOH in EtOH.

Table S1. Crystallographic data

Complex	L1·3H_2O	HL1·NO_3·2H_2O	$H_2L·H_2O$	[Fe (HL) Cl_2]$_2$
Empirical formula	C_{22} H_{13} N_3 O_9	C_{22} H_{26} N_4 O_{11}	C_{33} H_{35} N_3 O_8*	C_{66} H_{68} Cl_4 Fe_2 N_6 O_{16}
Formula weight	463.35	522.47	601.64	1454.76
Temperature(K)	173(2)	173(2)	173(2)	303(2)
Wavelength(Å)	1.54178	1.54178	1.54178	1.54178
Crystal system	Orthorhombic	Monoclinic	Monoclinic	Monoclinic
Space group	Cmc2(1)	P2(1)/c	P 21/c	P 21/c
a(Å)	14.2454(4)	12.8883(19)	20.30(2)	16.9262(10)
b(Å)	22.1444(4)	6.8979(13)	6.850(5)	12.4129(7)
c(Å)	6.9237(2)	25.701(3)	26.12(2)	17.4441(10)
a (deg)	90	90	90	90
β (deg)	90	98.195(12)	97.56(6)	102.320(3)
γ (deg)	90	90	90	90
V, Å^3	2184.12(10)	2261.5(6)	3600(5)	3580.7(4)
Z	4	4	4	2
D_c (Mg/m^3)	1.409	1.535	1.110	1.347
μ(mm^{-1})	0.960	1.067	0.660	5.186
F(000)	952	1096	1272	1504
R_{int}	0.0363	0.0409	0.0734	0.0413
Reflections collected	8735	15079	27851	26013
Unique reflections	1943	4140	6111	6311
Data/restraints/parameters	1943 / 1 / 175	4140 / 0 / 358	6111 / 25 / 403	6311 / 0 / 427
GOF on F^2	1.106	1.103	1.234	0.759
R_1, wR_2 [I>2σ(I)]	0.0878, 0.2591	0.0476, 0.1394	0.1377, 0.3707	0.0368, 0.1221
R_1,wR_2 (all data)	0.1070, 0.2966	0.0628, 0.1560	0.1655, 0.3935	0.0489, 0.1423
Largest diff. peak and hole [e Å^{-3}]	0.561 and -0.226	0.379 and -0.301	0.550 and -0.503	0.223 and -0.208

$\boldsymbol{R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|}$, $\boldsymbol{wR_2 = [\Sigma w(|F_o^2| - |F_c^2|)^2/\Sigma w(|F_o^2|)^2]^{1/2}}$

* **The missing water molecules decided by element analysis and TGA method were not added**

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for L1·3H$_2$O. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	10000	5619(1)	1719(6)	72(1)
C(1)	8215(1)	5003(1)	1720(4)	55(1)
N(1)	8289(1)	6779(1)	1734(5)	82(1)
O(3)	8186(1)	5614(1)	1713(4)	64(1)
C(3)	7428(1)	4037(1)	1724(6)	72(1)
O(2)	10000	3195(1)	1957(9)	148(2)
C(2)	7387(1)	4658(1)	1705(5)	66(1)
N(2)	10000	7337(2)	2895(7)	105(1)
O(4)	6728(1)	6904(1)	1785(5)	108(1)
C(4)	8284(1)	3745(1)	1803(5)	70(1)
C(7)	10000	5070(1)	1692(6)	55(1)
O(7)	5000	4380(2)	3543(13)	196(3)
C(6)	9096(1)	4720(1)	1699(4)	51(1)
O(6)	5000	5559(2)	4740(8)	161(2)
C(5)	9109(1)	4082(1)	1772(5)	61(1)
O(5)	5000	6391(1)	1785(8)	109(1)
C(8)	10000	3750(1)	1859(8)	76(1)
C(9)	7288(1)	5900(1)	1733(6)	66(1)
C(10)	7431(1)	6574(1)	1767(6)	73(1)
C(11A)	8471(3)	7437(1)	1464(9)	134(2)
C(12A)	9247(3)	7633(2)	1234(14)	205(3)
C(11B)	8433(8)	7430(5)	2028(18)	31(2)
C(12B)	9144(7)	7595(5)	3198(17)	26(2)

Table S3. Bond lengths [Å] and angles [deg] for L1·3H$_2$O.

O(1)-C(7)	1.214(3)	C(9)-H(9B)	0.9900
C(1)-O(3)	1.3533(19)	C(11A)-C(12A)	1.198(6)
C(1)-C(6)	1.401(2)	C(11B)-C(12B)	1.348(16)
C(1)-C(2)	1.405(2)	O(3)-C(1)-C(6)	118.28(14)
N(1)-C(10)	1.304(3)	O(3)-C(1)-C(2)	121.08(15)
N(1)-C(11A)	1.492(3)	C(6)-C(1)-C(2)	120.62(15)
N(1)-C(11B)	1.469(11)	C(10)-N(1)-C(11A)	120.4(2)
N(1)-H(1)	0.8800	C(10)-N(1)-C(11B)	118.1(5)
O(3)-C(9)	1.427(2)	C(10)-N(1)-H(1)	119.8
C(3)-C(2)	1.378(3)	C(11A)-N(1)-H(1)	119.8
C(3)-C(4)	1.382(3)	C(1)-O(3)-C(9)	118.15(13)
C(3)-H(3)	0.9500	C(2)-C(3)-C(4)	120.34(18)
O(2)-C(8)	1.231(3)	C(2)-C(3)-H(3)	119.8

C(2)-H(2)	0.9500	C(4)-C(3)-H(3)	119.8
N(2)-C(12B)#1	1.363(11)	C(3)-C(2)-C(1)	120.43(17)
N(2)-C(12B)	1.363(11)	C(3)-C(2)-H(2)	119.8
N(2)-C(12A)#1	1.703(8)	C(1)-C(2)-H(2)	119.8
N(2)-C(12A)	1.703(8)	C(12B)#1-N(2)-C(12B)	127.0(9)
N(2)-H(2A)	0.8800	C(12A)#1-N(2)-C(12A)	78.1(5)
O(4)-C(10)	1.240(3)	C(12A)#1-N(2)-H(2A)	140.9
C(4)-C(5)	1.391(3)	C(12A)-N(2)-H(2A)	140.9
C(4)-H(4)	0.9500	C(3)-C(4)-C(5)	119.59(17)
C(7)-C(6)	1.5040(19)	C(3)-C(4)-H(4)	120.2
C(7)-C(6)#1	1.5040(19)	C(5)-C(4)-H(4)	120.2
C(6)-C(5)	1.415(2)	O(1)-C(7)-C(6)	121.05(9)
C(5)-C(8)	1.468(2)	O(1)-C(7)-C(6)#1	121.05(9)
C(9)-C(10)	1.506(3)	C(6)-C(7)-C(6)#1	117.89(18)
C(9)-H(9A)	0.9900	C(1)-C(6)-C(5)	117.23(15)
C(1)-C(6)-C(7)	122.43(14)	O(3)-C(9)-H(9B)	110.0
C(5)-C(6)-C(7)	120.28(15)	C(10)-C(9)-H(9B)	110.0
C(4)-C(5)-C(6)	121.68(16)	H(9A)-C(9)-H(9B)	108.3
C(4)-C(5)-C(8)	117.46(16)	O(4)-C(10)-N(1)	123.38(18)
C(6)-C(5)-C(8)	120.84(16)	O(4)-C(10)-C(9)	118.44(17)
O(2)-C(8)-C(5)#1	120.11(10)	N(1)-C(10)-C(9)	118.17(17)
O(2)-C(8)-C(5)	120.11(10)	C(12A)-C(11A)-N(1)	122.0(3)
C(5)#1-C(8)-C(5)	119.8(2)	C(11A)-C(12A)-N(2)	110.7(6)
O(3)-C(9)-C(10)	108.63(14)	C(12B)-C(11B)-N(1)	117.0(9)
O(3)-C(9)-H(9A)	110.0	C(11B)-C(12B)-N(2)	117.8(10)
C(10)-C(9)-H(9A)	110.0		

Table S4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for L1·3H_2O. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a* b* U_{12}]

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O(1)	46(1)	37(1)	134(2)	6(1)	0	0
C(1)	52(1)	41(1)	71(1)	2(1)	-10(1)	-3(1)
N(1)	64(1)	42(1)	140(2)	12(1)	-21(1)	1(1)
O(3)	45(1)	40(1)	107(1)	-10(1)	-2(1)	1(1)
C(3)	60(1)	53(1)	104(1)	-13(2)	1(2)	-14(1)
O(2)	79(2)	32(1)	333(5)	-4(2)	0	0
C(2)	50(1)	52(1)	95(1)	10(1)	17(2)	-7(1)
N(2)	105(2)	53(2)	158(3)	3(2)	0	0
O(4)	65(1)	58(1)	200(2)	0(2)	4(2)	18(1)
C(4)	67(1)	44(1)	98(1)	3(2)	8(2)	-11(1)
C(7)	54(1)	33(1)	77(2)	-14(2)	0	0
O(7)	173(5)	115(3)	299(7)	47(3)	0	0

C(6)	49(1)	40(1)	64(1)	-4(1)	-3(1)	-4(1)
O(6)	156(4)	103(2)	223(4)	73(2)	0	0
C(5)	62(1)	38(1)	82(1)	-4(1)	5(2)	-5(1)
O(5)	70(1)	71(1)	187(3)	-11(2)	0	0
C(8)	65(2)	38(1)	125(2)	25(2)	0	0
C(9)	46(1)	52(1)	99(1)	-9(2)	6(2)	6(1)
C(10)	57(1)	51(1)	111(2)	-9(2)	-2(2)	6(1)
C(11A)	139(2)	42(1)	219(4)	4(2)	-77(3)	-24(1)
C(12A)	95(2)	48(1)	473(10)	19(4)	65(5)	4(2)

Table S5. Hydrogen coordinates (× 10^4) and isotropic displacement parameters (Å^2 × 10^3) for L1·3H_2O.

	x	y	z	U(eq)
H(1)	8763	6528	1873	99
H(3)	6865	3808	1683	86
H(2)	6795	4856	1681	79
H(2A)	10000	7141	3999	126
H(4)	8310	3317	1878	83
H(9A)	6930	5771	2888	79
H(9B)	6928	5783	569	79

Table S6. Torsion angles [deg] for L1·3H_2O.

C(6)-C(1)-O(3)-C(9)	179.9(3)	C(7)-C(6)-C(5)-C(8)	0.5(5)
C(2)-C(1)-O(3)-C(9)	1.4(4)	C(4)-C(5)-C(8)-O(2)	-0.1(7)
C(4)-C(3)-C(2)-C(1)	1.5(6)	C(6)-C(5)-C(8)-O(2)	178.7(5)
O(3)-C(1)-C(2)-C(3)	-179.6(3)	C(4)-C(5)-C(8)-C(5)#1	178.2(3)
C(6)-C(1)-C(2)-C(3)	1.9(5)	C(6)-C(5)-C(8)-C(5)#1	-3.0(7)
C(2)-C(3)-C(4)-C(5)	-3.0(6)	C(1)-O(3)-C(9)-C(10)	178.7(3)
O(3)-C(1)-C(6)-C(5)	177.9(3)	C(11A)-N(1)-C(10)-O(4)	-7.8(7)
C(2)-C(1)-C(6)-C(5)	-3.5(4)	C(11B)-N(1)-C(10)-O(4)	9.5(8)
O(3)-C(1)-C(6)-C(7)	0.7(5)	C(11A)-N(1)-C(10)-C(9)	170.7(4)
C(2)-C(1)-C(6)-C(7)	179.3(3)	C(11B)-N(1)-C(10)-C(9)	-172.0(6)
O(1)-C(7)-C(6)-C(1)	0.5(6)	O(3)-C(9)-C(10)-O(4)	179.9(4)
C(6)#1-C(7)-C(6)-C(1)	179.1(2)	O(3)-C(9)-C(10)-N(1)	1.3(5)
O(1)-C(7)-C(6)-C(5)	-176.6(4)	C(10)-N(1)-C(11A)-C(12A)	-172.4(7)
C(6)#1-C(7)-C(6)-C(5)	2.0(5)	N(1)-C(11A)-C(12A)-N(2)	-47.3(8)
C(3)-C(4)-C(5)-C(6)	1.2(5)	C(12A)#1-N(2)-C(12A)-C(11A)	164.6(4)
C(3)-C(4)-C(5)-C(8)	-180.0(4)	C(10)-N(1)-C(11B)-C(12B)	137.0(9)
C(1)-C(6)-C(5)-C(4)	2.0(5)	N(1)-C(11B)-C(12B)-N(2)	48.9(14)
C(7)-C(6)-C(5)-C(4)	179.2(3)	C(12B)#1-N(2)-C(12B)-C(11B)	147.9(8)
C(1)-C(6)-C(5)-C(8)	-176.8(4)		

Table S7. Hydrogen bonds for L1·3H_2O.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2A)…O(2)	0.88	2.18	3.050	170.33

Table S8. Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters ($Å^2$ ×10^3) for HL1 • NO_3 • 2H_2O. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	6579(1)	4984(2)	1760(1)	30(1)
C(1)	4151(2)	5861(3)	2262(1)	18(1)
N(1)	1588(2)	4453(3)	3146(1)	29(1)
O(2)	2435(1)	6223(2)	2450(1)	28(1)
C(2)	3081(2)	6184(3)	2077(1)	21(1)
N(2)	1889(2)	5740(3)	4307(1)	30(1)
O(5)	-61(1)	5303(3)	2789(1)	39(1)
C(5)	4509(2)	6143(3)	1362(1)	23(1)
O(4)	5338(1)	6513(2)	3863(1)	24(1)
C(4)	3460(2)	6530(3)	1195(1)	25(1)
N(4)	922(2)	864(3)	5483(1)	41(1)
O(3)	3967(1)	4896(2)	3130(1)	23(1)
C(3)	2743(2)	6539(3)	1550(1)	24(1)
N(3)	3866(1)	8158(3)	4294(1)	24(1)
O(6)	4705(1)	7594(2)	5113(1)	33(1)
C(6)	4851(2)	5835(3)	1893(1)	20(1)
O(8)	522(2)	2458(3)	5581(1)	49(1)
C(8)	6384(2)	5821(3)	2633(1)	19(1)
O(7)	552(2)	-678(3)	5639(1)	55(1)
C(7)	5988(2)	5484(3)	2068(1)	21(1)
O(9)	1688(2)	839(3)	5241(1)	56(1)
C(9)	5672(2)	5920(3)	2999(1)	18(1)
O(10)	3665(1)	3610(3)	4168(1)	32(1)
C(10)	4539(2)	5519(3)	2825(1)	19(1)
O(11)	1542(2)	5902(3)	5322(1)	41(1)
C(12)	7133(2)	6570(3)	3680(1)	23(1)
C(13)	7820(2)	6404(3)	3313(1)	24(1)
C(14)	7454(2)	6036(3)	2790(1)	23(1)
C(15)	1326(2)	6118(4)	2310(1)	28(1)
C(16)	888(2)	5260(3)	2777(1)	28(1)
C(17)	1277(2)	3342(4)	3582(1)	33(1)
C(18)	995(2)	4560(4)	4032(1)	36(1)
C(19)	1943(2)	7794(3)	4128(1)	31(1)
C(20)	2878(2)	8840(3)	4437(1)	28(1)
C(21)	4684(2)	7615(3)	4632(1)	23(1)
C(22)	5658(2)	7005(3)	4399(1)	24(1)

C(11)	6064(2)	6326(3)	3527(1)	19(1)

Table S9. Bond lengths [Å] and angles [deg] for HL1•NO_3•$2H_2O$.

O(1)-C(7)	1.224(2)	N(3)-C(20)	1.453(3)
C(1)-C(6)	1.400(3)	N(3)-H(3A)	0.8800
C(1)-C(2)	1.410(3)	O(6)-C(21)	1.233(2)
C(1)-C(10)	1.481(3)	C(6)-C(7)	1.491(3)
N(1)-C(16)	1.334(3)	C(8)-C(14)	1.389(3)
N(1)-C(17)	1.461(3)	C(8)-C(9)	1.407(3)
N(1)-H(1)	0.8800	C(8)-C(7)	1.486(3)
O(2)-C(2)	1.358(2)	C(9)-C(11)	1.407(3)
O(2)-C(15)	1.425(3)	C(9)-C(10)	1.491(3)
C(2)-C(3)	1.385(3)	O(10)-H(9)	0.95(4)
N(2)-C(19)	1.494(3)	O(10)-H(10)	0.83(4)
N(2)-C(18)	1.503(3)	O(11)-H(8)	0.86(3)
N(2)-H(2)	1.02(3)	O(11)-H(7)	0.98(4)
N(2)-H(6)	1.04(4)	C(12)-C(11)	1.388(3)
O(5)-C(16)	1.228(3)	C(12)-C(13)	1.390(3)
C(5)-C(4)	1.385(3)	C(12)-H(12)	0.9500
C(5)-C(6)	1.389(3)	C(13)-C(14)	1.381(3)
C(5)-H(5)	0.9500	C(13)-H(13)	0.9500
O(4)-C(11)	1.366(2)	C(14)-H(14)	0.9500
O(4)-C(22)	1.421(2)	C(15)-C(16)	1.518(3)
C(4)-C(3)	1.388(3)	C(15)-H(15A)	0.9900
C(4)-H(4)	0.9500	C(15)-H(15B)	0.9900
N(4)-O(9)	1.240(3)	C(17)-C(18)	1.514(3)
N(4)-O(8)	1.255(3)	C(17)-H(17A)	0.9900
N(4)-O(7)	1.255(3)	C(17)-H(17B)	0.9900
O(3)-C(10)	1.227(2)	C(18)-H(18A)	0.9900
C(3)-H(3)	0.9500	C(18)-H(18B)	0.9900
N(3)-C(21)	1.321(3)	C(19)-C(20)	1.527(3)
C(19)-H(19A)	0.9900	C(3)-C(4)-H(4)	119.7
C(19)-H(19B)	0.9900	O(9)-N(4)-O(8)	119.5(2)
C(20)-H(20A)	0.9900	O(9)-N(4)-O(7)	121.0(2)
C(20)-H(20B)	0.9900	O(8)-N(4)-O(7)	119.5(2)
C(21)-C(22)	1.526(3)	C(2)-C(3)-C(4)	119.8(2)
C(22)-H(22A)	0.9900	C(2)-C(3)-H(3)	120.1
C(22)-H(22B)	0.9900	C(4)-C(3)-H(3)	120.1
C(6)-C(1)-C(2)	117.83(19)	C(21)-N(3)-C(20)	124.83(18)
C(6)-C(1)-C(10)	119.99(19)	C(21)-N(3)-H(3A)	117.6
C(2)-C(1)-C(10)	122.17(18)	C(20)-N(3)-H(3A)	117.6
C(16)-N(1)-C(17)	122.2(2)	C(5)-C(6)-C(1)	121.3(2)

C(16)-N(1)-H(1)	118.9	C(5)-C(6)-C(7)	118.88(18)
C(17)-N(1)-H(1)	118.9	C(1)-C(6)-C(7)	119.84(19)
C(2)-O(2)-C(15)	120.96(17)	C(14)-C(8)-C(9)	121.01(19)
O(2)-C(2)-C(3)	123.3(2)	C(14)-C(8)-C(7)	119.30(17)
O(2)-C(2)-C(1)	115.70(19)	C(9)-C(8)-C(7)	119.69(18)
C(3)-C(2)-C(1)	120.93(19)	O(1)-C(7)-C(8)	121.14(19)
C(19)-N(2)-C(18)	115.7(2)	O(1)-C(7)-C(6)	121.69(19)
C(19)-N(2)-H(2)	110.6(15)	C(8)-C(7)-C(6)	117.15(17)
C(18)-N(2)-H(2)	109.0(15)	C(8)-C(9)-C(11)	118.42(18)
C(19)-N(2)-H(6)	105(2)	C(8)-C(9)-C(10)	119.61(18)
C(18)-N(2)-H(6)	109(2)	C(11)-C(9)-C(10)	121.93(17)
H(2)-N(2)-H(6)	107(3)	H(9)-O(10)-H(10)	112(3)
C(4)-C(5)-C(6)	119.53(19)	O(3)-C(10)-C(1)	121.97(19)
C(4)-C(5)-H(5)	120.2	O(3)-C(10)-C(9)	121.66(19)
C(6)-C(5)-H(5)	120.2	C(1)-C(10)-C(9)	116.36(17)
C(11)-O(4)-C(22)	120.28(16)	H(8)-O(11)-H(7)	111(3)
C(5)-C(4)-C(3)	120.6(2)	C(11)-C(12)-C(13)	120.0(2)
C(5)-C(4)-H(4)	119.7	C(11)-C(12)-H(12)	120.0
C(13)-C(12)-H(12)	120.0	C(17)-C(18)-H(18B)	108.7
C(14)-C(13)-C(12)	120.9(2)	H(18A)-C(18)-H(18B)	107.6
C(14)-C(13)-H(13)	119.6	N(2)-C(19)-C(20)	110.81(19)
C(12)-C(13)-H(13)	119.6	N(2)-C(19)-H(19A)	109.5
C(13)-C(14)-C(8)	119.36(19)	C(20)-C(19)-H(19A)	109.5
C(13)-C(14)-H(14)	120.3	N(2)-C(19)-H(19B)	109.5
C(8)-C(14)-H(14)	120.3	C(20)-C(19)-H(19B)	109.5
O(2)-C(15)-C(16)	107.03(18)	H(19A)-C(19)-H(19B)	108.1
O(2)-C(15)-H(15A)	110.3	N(3)-C(20)-C(19)	111.75(18)
C(16)-C(15)-H(15A)	110.3	N(3)-C(20)-H(20A)	109.3
O(2)-C(15)-H(15B)	110.3	C(19)-C(20)-H(20A)	109.3
C(16)-C(15)-H(15B)	110.3	N(3)-C(20)-H(20B)	109.3
H(15A)-C(15)-H(15B)	108.6	C(19)-C(20)-H(20B)	109.3
O(5)-C(16)-N(1)	124.6(2)	H(20A)-C(20)-H(20B)	107.9
O(5)-C(16)-C(15)	119.6(2)	O(6)-C(21)-N(3)	124.4(2)
N(1)-C(16)-C(15)	115.76(19)	O(6)-C(21)-C(22)	119.28(19)
N(1)-C(17)-C(18)	114.6(2)	N(3)-C(21)-C(22)	116.36(18)
N(1)-C(17)-H(17A)	108.6	O(4)-C(22)-C(21)	107.76(17)
C(18)-C(17)-H(17A)	108.6	O(4)-C(22)-H(22A)	110.2
N(1)-C(17)-H(17B)	108.6	C(21)-C(22)-H(22A)	110.2
C(18)-C(17)-H(17B)	108.6	O(4)-C(22)-H(22B)	110.2
H(17A)-C(17)-H(17B)	107.6	C(21)-C(22)-H(22B)	110.2
N(2)-C(18)-C(17)	114.05(19)	H(22A)-C(22)-H(22B)	108.5
N(2)-C(18)-H(18A)	108.7	O(4)-C(11)-C(12)	123.38(18)
C(17)-C(18)-H(18A)	108.7	O(4)-C(11)-C(9)	116.32(18)
N(2)-C(18)-H(18B)	108.7	C(12)-C(11)-C(9)	120.27(18)

Table S10. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $HL1 \cdot NO_3 \cdot 2H_2O$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O(1)	26(1)	45(1)	20(1)	-5(1)	7(1)	6(1)
C(1)	17(1)	16(1)	20(1)	0(1)	1(1)	0(1)
N(1)	18(1)	40(1)	30(1)	-2(1)	4(1)	0(1)
O(2)	12(1)	46(1)	24(1)	-2(1)	3(1)	0(1)
C(2)	19(1)	23(1)	20(1)	-1(1)	3(1)	-2(1)
N(2)	24(1)	38(1)	29(1)	1(1)	7(1)	-2(1)
O(5)	17(1)	51(1)	51(1)	3(1)	8(1)	1(1)
C(5)	27(1)	25(1)	18(1)	-1(1)	5(1)	-2(1)
O(4)	18(1)	39(1)	14(1)	-4(1)	4(1)	-2(1)
C(4)	30(1)	26(1)	18(1)	1(1)	-1(1)	-2(1)
N(4)	31(1)	52(1)	39(1)	-14(1)	0(1)	2(1)
O(3)	18(1)	33(1)	20(1)	2(1)	5(1)	-1(1)
C(3)	20(1)	28(1)	24(1)	2(1)	-3(1)	0(1)
N(3)	22(1)	36(1)	17(1)	1(1)	6(1)	0(1)
O(6)	34(1)	49(1)	15(1)	2(1)	4(1)	8(1)
C(6)	22(1)	19(1)	19(1)	-2(1)	2(1)	-1(1)
O(8)	38(1)	46(1)	64(1)	-14(1)	16(1)	3(1)
C(8)	19(1)	18(1)	21(1)	1(1)	4(1)	1(1)
O(7)	51(1)	50(1)	63(1)	-4(1)	4(1)	-2(1)
C(7)	20(1)	21(1)	22(1)	1(1)	6(1)	0(1)
O(9)	38(1)	78(2)	56(1)	-21(1)	18(1)	5(1)
C(9)	18(1)	19(1)	17(1)	0(1)	2(1)	0(1)
O(10)	29(1)	38(1)	30(1)	5(1)	8(1)	5(1)
C(10)	18(1)	20(1)	18(1)	-2(1)	3(1)	2(1)
O(11)	42(1)	50(1)	33(1)	4(1)	10(1)	5(1)
C(12)	20(1)	28(1)	19(1)	0(1)	0(1)	0(1)
C(13)	16(1)	30(1)	26(1)	0(1)	2(1)	0(1)
C(14)	19(1)	26(1)	24(1)	0(1)	6(1)	0(1)
C(15)	13(1)	40(1)	31(1)	0(1)	-1(1)	0(1)
C(16)	20(1)	31(1)	34(1)	-4(1)	4(1)	0(1)
C(17)	28(1)	36(1)	36(1)	1(1)	6(1)	-4(1)
C(18)	24(1)	49(1)	34(1)	-2(1)	7(1)	-6(1)
C(19)	24(1)	37(1)	32(1)	5(1)	6(1)	5(1)
C(20)	26(1)	33(1)	27(1)	2(1)	10(1)	6(1)
C(21)	26(1)	25(1)	18(1)	0(1)	5(1)	-4(1)
C(22)	23(1)	33(1)	16(1)	-1(1)	2(1)	-1(1)
C(11)	18(1)	22(1)	18(1)	0(1)	6(1)	1(1)

Table S11. Hydrogen coordinates (× 10^4) and isotropic displacement parameters ($Å^2$ × 10^3) for HL1•NO_3•$2H_2O$.

	x	y	z	U(eq)
H(1)	2259	4595	3126	35
H(2)	2570(20)	5040(40)	4280(10)	36(7)
H(5)	4991	6088	1115	28
H(4)	3229	6791	834	30
H(3)	2023	6789	1432	29
H(3A)	3924	8103	3957	29
H(6)	1820(30)	5840(50)	4703(16)	83(12)
H(8)	1230(30)	6940(50)	5400(13)	51(9)
H(7)	1100(30)	4760(60)	5344(16)	84(13)
H(9)	4190(30)	3260(50)	4448(14)	67(11)
H(10)	3920(30)	4050(50)	3912(14)	58(10)
H(12)	7394	6851	4037	27
H(13)	8552	6546	3422	29
H(14)	7929	5931	2541	27
H(15A)	1145	5287	1996	34
H(15B)	1032	7427	2229	34
H(17A)	1860	2464	3720	40
H(17B)	667	2525	3447	40
H(18A)	417	5448	3894	43
H(18B)	733	3694	4292	43
H(19A)	1287	8475	4177	37
H(19B)	2007	7818	3749	37
H(20A)	2811	10250	4369	33
H(20B)	2874	8628	4818	33
H(22A)	6171	8082	4425	29
H(22B)	5994	5875	4592	29

Table S12. Torsion angles [deg] for HL1•NO_3•$2H_2O$.

C(15)-O(2)-C(2)-C(3)	17.1(3)	C(6)-C(1)-C(10)-O(3)	-155.28(19)
C(15)-O(2)-C(2)-C(1)	-166.36(19)	C(2)-C(1)-C(10)-O(3)	23.5(3)
C(6)-C(1)-C(2)-O(2)	-179.10(18)	C(6)-C(1)-C(10)-C(9)	23.0(3)
C(10)-C(1)-C(2)-O(2)	2.0(3)	C(2)-C(1)-C(10)-C(9)	-158.13(18)
C(6)-C(1)-C(2)-C(3)	-2.5(3)	C(8)-C(9)-C(10)-O(3)	152.9(2)
C(10)-C(1)-C(2)-C(3)	178.66(19)	C(11)-C(9)-C(10)-O(3)	-24.5(3)
C(6)-C(5)-C(4)-C(3)	-2.5(3)	C(8)-C(9)-C(10)-C(1)	-25.4(3)
O(2)-C(2)-C(3)-C(4)	178.0(2)	C(11)-C(9)-C(10)-C(1)	157.14(18)
C(1)-C(2)-C(3)-C(4)	1.7(3)	C(11)-C(12)-C(13)-C(14)	1.3(3)

C(5)-C(4)-C(3)-C(2)	0.9(3)	C(12)-C(13)-C(14)-C(8)	-0.3(3)
C(4)-C(5)-C(6)-C(1)	1.6(3)	C(9)-C(8)-C(14)-C(13)	-1.7(3)
C(4)-C(5)-C(6)-C(7)	-178.02(19)	C(7)-C(8)-C(14)-C(13)	178.15(19)
C(2)-C(1)-C(6)-C(5)	0.8(3)	C(2)-O(2)-C(15)-C(16)	153.76(19)
C(10)-C(1)-C(6)-C(5)	179.72(18)	C(17)-N(1)-C(16)-O(5)	6.7(4)
C(2)-C(1)-C(6)-C(7)	-179.53(18)	C(17)-N(1)-C(16)-C(15)	-171.6(2)
C(10)-C(1)-C(6)-C(7)	-0.7(3)	O(2)-C(15)-C(16)-O(5)	168.4(2)
C(14)-C(8)-C(7)-O(1)	15.8(3)	O(2)-C(15)-C(16)-N(1)	-13.3(3)
C(9)-C(8)-C(7)-O(1)	-164.3(2)	C(16)-N(1)-C(17)-C(18)	-80.8(3)
C(14)-C(8)-C(7)-C(6)	-162.57(18)	C(19)-N(2)-C(18)-C(17)	96.1(3)
C(9)-C(8)-C(7)-C(6)	17.3(3)	N(1)-C(17)-C(18)-N(2)	-63.7(3)
C(5)-C(6)-C(7)-O(1)	-18.5(3)	C(18)-N(2)-C(19)-C(20)	179.74(18)
C(1)-C(6)-C(7)-O(1)	161.9(2)	C(21)-N(3)-C(20)-C(19)	-130.3(2)
C(5)-C(6)-C(7)-C(8)	159.86(18)	N(2)-C(19)-C(20)-N(3)	71.2(2)
C(1)-C(6)-C(7)-C(8)	-19.8(3)	C(20)-N(3)-C(21)-O(6)	1.0(4)
C(14)-C(8)-C(9)-C(11)	2.7(3)	C(20)-N(3)-C(21)-C(22)	-178.20(19)
C(7)-C(8)-C(9)-C(11)	-177.23(17)	C(11)-O(4)-C(22)-C(21)	165.56(17)
C(14)-C(8)-C(9)-C(10)	-174.88(18)	O(6)-C(21)-C(22)-O(4)	160.22(19)
C(7)-C(8)-C(9)-C(10)	5.2(3)	N(3)-C(21)-C(22)-O(4)	-20.5(3)
C(22)-O(4)-C(11)-C(12)	0.8(3)	C(8)-C(9)-C(11)-O(4)	176.53(18)
C(22)-O(4)-C(11)-C(9)	-177.29(18)	C(10)-C(9)-C(11)-O(4)	-6.0(3)
C(13)-C(12)-C(11)-O(4)	-178.35(19)	C(8)-C(9)-C(11)-C(12)	-1.6(3)
C(13)-C(12)-C(11)-C(9)	-0.4(3)	C(10)-C(9)-C(11)-C(12)	175.90(19)

Table S13. Hydrogen bonds for HL1 • NO_3 • $2H_2O$.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)…O(3)	0.88	2.21	3.09	176.28
N(2)-H(2)…O(10)	1.02	1.77	2.78	172.14
N(3)-H(3A)…O(1)	0.9	2.27	2.97	135.98
N(2)-H(6)…O(11)	1.04	1.68	2.71	172.37
O(11)-H(8)…O(7)	0.86	2.00	2.86	175.62
O(11)-H(7)…O(8)	0.98	1.89	2.841	162.58
O(10)-H(9)…O(6)	0.94	1.79	2.72	169.66
O(10)-H(10)…O(4)	0.83	2.52	3.12	130.97
O(10)-H(10)…O(3)	0.83	2.10	2.89	157.86

Table S14. Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for $H_2L•H_2O$. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	6534(3)	2620(11)	4117(2)	117(2)
C(1)	5052(3)	2345(5)	4733(2)	50(1)
N(1)	3152(5)	1859(14)	5666(2)	136(3)
O(2)	3937(2)	2220(4)	4940(1)	55(1)
C(2)	4359(3)	2181(6)	4577(2)	53(1)
N(2)	3343(3)	3374(8)	6836(2)	78(1)
O(3)	4990(2)	2782(5)	5626(1)	59(1)
C(3)	4108(3)	1938(7)	4051(2)	59(1)
N(3)	5162(2)	3629(6)	6855(2)	67(1)
O(4)	6045(2)	3016(5)	6299(1)	64(1)
C(4)	4542(3)	1790(8)	3684(2)	69(2)
O(5)	2235(3)	2090(9)	5103(2)	107(2)
C(5)	5214(3)	1960(8)	3833(2)	65(1)
O(6)	5870(2)	4101(7)	7589(1)	81(1)
C(6)	5472(3)	2277(6)	4345(2)	58(1)
O(8)	3218(2)	2722(5)	7816(1)	69(1)
C(8)	6493(3)	2724(6)	5007(2)	57(1)
O(7)	2405(2)	2843(7)	8534(2)	81(1)
C(7)	6185(3)	2517(8)	4469(2)	66(1)
C(9)	6081(2)	2756(6)	5403(2)	50(1)
C(10)	5354(2)	2643(5)	5282(2)	47(1)
C(11)	6424(3)	2973(6)	5919(2)	55(1)
C(12)	7112(3)	3059(7)	6012(2)	64(1)
C(13)	7500(3)	3007(8)	5618(2)	68(1)
C(14)	7168(3)	2823(7)	5106(2)	66(1)
C(15)	3243(3)	2129(7)	4758(2)	58(1)
C(16)	2836(4)	2079(10)	5203(3)	80(2)
C(17)	2879(9)	1190(30)	6123(4)	238(11)
C(18)	2842(5)	2360(20)	6513(4)	160(6)
C(20)	4560(3)	3844(9)	7078(2)	71(1)
C(21)	5768(3)	3766(7)	7127(2)	64(1)
C(22)	6332(3)	3471(8)	6815(2)	66(1)
C(23)	3105(3)	5312(10)	6955(2)	78(2)
C(24)	2609(3)	5279(8)	7333(2)	63(1)
C(25)	2093(3)	6620(10)	7292(2)	76(2)
C(26)	1671(3)	6730(9)	7662(3)	76(2)

C(27)	1768(3)	5454(9)	8075(2)	74(2)
C(28)	2279(3)	4108(8)	8119(2)	66(1)
C(29)	2712(3)	4001(7)	7758(2)	60(1)
C(30)	1101(3)	8308(12)	7625(3)	93(2)
C(31)	546(6)	7460(20)	7250(11)	252(14)
C(32)	1282(9)	10033(18)	7433(14)	315(18)
C(33)	905(13)	8650(50)	8117(6)	318(18)
C(19)	3994(3)	3381(10)	6653(2)	77(2)

Table S15. Bond lengths [Å] and angles [deg] for $H_2L•H_2O$.

O(1)-C(7)	1.235(7)	O(8)-C(29)	1.343(7)	C(22)-H(22B)	0.9900
C(1)-C(6)	1.408(7)	O(8)-H(8)	0.8400	C(23)-C(24)	1.501(8)
C(1)-C(2)	1.415(7)	C(8)-C(14)	1.361(8)	C(23)-H(23A)	0.9900
C(1)-C(10)	1.499(7)	C(8)-C(9)	1.415(7)	C(23)-H(23B)	0.9900
N(1)-C(16)	1.301(11)	C(8)-C(7)	1.469(8)	C(24)-C(25)	1.386(8)
N(1)-C(17)	1.454(11)	O(7)-C(28)	1.384(7)	C(24)-C(29)	1.407(7)
N(1)-H(1)	0.8800	O(7)-H(7)	0.8400	C(25)-C(26)	1.375(9)
O(2)-C(2)	1.358(6)	C(9)-C(11)	1.440(7)	C(25)-H(25)	0.9500
O(2)-C(15)	1.426(7)	C(9)-C(10)	1.470(7)	C(26)-C(27)	1.382(9)
C(2)-C(3)	1.411(7)	C(11)-C(12)	1.386(8)	C(26)-C(30)	1.576(10)
N(2)-C(18)	1.416(10)	C(12)-C(13)	1.375(8)	C(27)-C(28)	1.380(9)
N(2)-C(23)	1.460(9)	C(12)-H(12)	0.9500	C(27)-H(27)	0.9500
N(2)-C(19)	1.463(8)	C(13)-C(14)	1.423(9)	C(28)-C(29)	1.376(7)
O(3)-C(10)	1.239(6)	C(13)-H(13)	0.9500	C(30)-C(32)	1.35(2)
C(3)-C(4)	1.389(8)	C(14)-H(14)	0.9500	C(30)-C(33)	1.414(18)
C(3)-H(3)	0.9500	C(15)-C(16)	1.513(8)	C(30)-C(31)	1.508(17)
N(3)-C(21)	1.340(8)	C(15)-H(15A)	0.9900	C(31)-H(31A)	0.9800
N(3)-C(20)	1.430(8)	C(15)-H(15B)	0.9900	C(31)-H(31B)	0.9800
N(3)-H(3A)	0.8800	C(17)-C(18)	1.304(12)	C(31)-H(31C)	0.9800
O(4)-C(11)	1.336(6)	C(17)-H(17A)	0.9900	C(32)-H(32A)	0.9800
O(4)-C(22)	1.431(6)	C(17)-H(17B)	0.9900	C(32)-H(32B)	0.9800
C(4)-C(5)	1.373(9)	C(18)-H(18A)	0.9900	C(32)-H(32C)	0.9800
C(4)-H(4)	0.9500	C(18)-H(18B)	0.9900	C(33)-H(33A)	0.9800
O(5)-C(16)	1.214(9)	C(20)-C(19)	1.521(8)	C(33)-H(33B)	0.9800
C(5)-C(6)	1.388(7)	C(20)-H(20A)	0.9900	C(33)-H(33C)	0.9800
C(5)-H(5)	0.9500	C(20)-H(20B)	0.9900	C(19)-H(19A)	0.9900
O(6)-C(21)	1.219(6)	C(21)-C(22)	1.504(8)	C(19)-H(19B)	0.9900
C(6)-C(7)	1.450(9)	C(22)-H(22A)	0.9900	C(6)-C(1)-C(2)	117.6(4)
C(6)-C(1)-C(2)	117.6(4)	C(1)-C(6)-C(7)	121.2(4)	O(2)-C(15)-H(15A)	109.4
C(6)-C(1)-C(10)	118.9(5)	C(29)-O(8)-H(8)	109.5	C(16)-C(15)-H(15A)	109.4
C(2)-C(1)-C(10)	123.5(4)	C(14)-C(8)-C(9)	122.5(5)	O(2)-C(15)-H(15B)	109.4
C(16)-N(1)-C(17)	127.2(10)	C(14)-C(8)-C(7)	118.6(5)	C(16)-C(15)-H(15B)	109.4
C(16)-N(1)-H(1)	116.4	C(9)-C(8)-C(7)	118.9(5)	H(15A)-C(15)-H(15B)	108.0

C(17)-N(1)-H(1)	116.4	C(28)-O(7)-H(7)	109.5	O(5)-C(16)-N(1)	124.0(6)
C(2)-O(2)-C(15)	116.9(4)	O(1)-C(7)-C(6)	119.7(5)	O(5)-C(16)-C(15)	118.0(6)
O(2)-C(2)-C(3)	120.0(5)	O(1)-C(7)-C(8)	119.5(6)	N(1)-C(16)-C(15)	117.7(7)
O(2)-C(2)-C(1)	119.5(4)	C(6)-C(7)-C(8)	120.8(4)	C(18)-C(17)-N(1)	121.1(12)
C(3)-C(2)-C(1)	120.5(4)	C(8)-C(9)-C(11)	115.2(5)	C(18)-C(17)-H(17A)	107.1
C(18)-N(2)-C(23)	110.1(7)	C(8)-C(9)-C(10)	121.1(4)	N(1)-C(17)-H(17A)	107.1
C(18)-N(2)-C(19)	114.6(5)	C(11)-C(9)-C(10)	123.7(4)	C(18)-C(17)-H(17B)	107.1
C(23)-N(2)-C(19)	113.9(5)	O(3)-C(10)-C(9)	121.2(4)	N(1)-C(17)-H(17B)	107.1
C(4)-C(3)-C(2)	120.0(5)	O(3)-C(10)-C(1)	119.7(4)	H(17A)-C(17)-H(17B)	106.8
C(4)-C(3)-H(3)	120.0	C(9)-C(10)-C(1)	119.0(4)	C(17)-C(18)-N(2)	131.0(10)
C(2)-C(3)-H(3)	120.0	O(4)-C(11)-C(12)	122.3(5)	C(17)-C(18)-H(18A)	104.5
C(21)-N(3)-C(20)	123.4(4)	O(4)-C(11)-C(9)	116.3(5)	N(2)-C(18)-H(18A)	104.5
C(21)-N(3)-H(3A)	118.3	C(12)-C(11)-C(9)	121.4(4)	C(17)-C(18)-H(18B)	104.5
C(20)-N(3)-H(3A)	118.3	C(13)-C(12)-C(11)	121.9(5)	N(2)-C(18)-H(18B)	104.5
C(11)-O(4)-C(22)	120.2(4)	C(13)-C(12)-H(12)	119.0	H(18A)-C(18)-H(18B)	105.6
C(5)-C(4)-C(3)	119.7(5)	C(11)-C(12)-H(12)	119.0	N(3)-C(20)-C(19)	106.6(4)
C(5)-C(4)-H(4)	120.1	C(12)-C(13)-C(14)	117.4(5)	N(3)-C(20)-H(20A)	110.4
C(3)-C(4)-H(4)	120.1	C(12)-C(13)-H(13)	121.3	C(19)-C(20)-H(20A)	110.4
C(4)-C(5)-C(6)	121.3(5)	C(14)-C(13)-H(13)	121.3	N(3)-C(20)-H(20B)	110.4
C(4)-C(5)-H(5)	119.3	C(8)-C(14)-C(13)	121.5(5)	C(19)-C(20)-H(20B)	110.4
C(6)-C(5)-H(5)	119.3	C(8)-C(14)-H(14)	119.3	H(20A)-C(20)-H(20B)	108.6
C(5)-C(6)-C(1)	120.8(5)	C(13)-C(14)-H(14)	119.3	O(6)-C(21)-N(3)	124.3(5)
C(5)-C(6)-C(7)	118.0(5)	O(2)-C(15)-C(16)	111.1(5)	O(6)-C(21)-C(22)	121.2(5)
N(3)-C(21)-C(22)	114.5(4)	C(25)-C(26)-C(27)	118.3(6)	C(30)-C(31)-H(31B)	109.5
O(4)-C(22)-C(21)	107.1(4)	C(25)-C(26)-C(30)	121.0(6)	H(31A)-C(31)-H(31B)	109.5
O(4)-C(22)-H(22A)	110.3	C(27)-C(26)-C(30)	120.6(6)	C(30)-C(31)-H(31C)	109.5
C(21)-C(22)-H(22A)	110.3	C(28)-C(27)-C(26)	121.1(5)	H(31A)-C(31)-H(31C)	109.5
O(4)-C(22)-H(22B)	110.3	C(28)-C(27)-H(27)	119.4	H(31B)-C(31)-H(31C)	109.5
C(21)-C(22)-H(22B)	110.3	C(26)-C(27)-H(27)	119.4	C(30)-C(32)-H(32A)	109.5
H(22A)-C(22)-H(22B)	108.5	C(29)-C(28)-C(27)	121.2(5)	C(30)-C(32)-H(32B)	109.5
N(2)-C(23)-C(24)	113.3(5)	C(29)-C(28)-O(7)	115.7(5)	H(32A)-C(32)-H(32B)	109.5
N(2)-C(23)-H(23A)	108.9	C(27)-C(28)-O(7)	123.0(5)	C(30)-C(32)-H(32C)	109.5
C(24)-C(23)-H(23A)	108.9	O(8)-C(29)-C(28)	120.3(4)	H(32A)-C(32)-H(32C)	109.5
N(2)-C(23)-H(23B)	108.9	O(8)-C(29)-C(24)	121.9(4)	H(32B)-C(32)-H(32C)	109.5
C(24)-C(23)-H(23B)	108.9	C(28)-C(29)-C(24)	117.8(5)	C(30)-C(33)-H(33A)	109.5
H(23A)-C(23)-H(23B)	107.7	C(32)-C(30)-C(33)	108.5(19)	C(30)-C(33)-H(33B)	109.5
C(25)-C(24)-C(29)	120.4(5)	C(32)-C(30)-C(31)	108.0(17)	H(33A)-C(33)-H(33B)	109.5
C(25)-C(24)-C(23)	120.3(5)	C(33)-C(30)-C(31)	112.2(18)	C(30)-C(33)-H(33C)	109.5
C(29)-C(24)-C(23)	119.0(5)	C(32)-C(30)-C(26)	112.9(8)	H(33A)-C(33)-H(33C)	109.5
C(26)-C(25)-C(24)	121.1(5)	C(33)-C(30)-C(26)	110.4(8)	H(33B)-C(33)-H(33C)	109.5
C(26)-C(25)-H(25)	119.4	C(31)-C(30)-C(26)	104.9(7)	N(2)-C(19)-C(20)	113.0(4)
C(24)-C(25)-H(25)	119.4	C(30)-C(31)-H(31A)	109.5	N(2)-C(19)-H(19A)	109.0
C(20)-C(19)-H(19A)	109.0	N(2)-C(19)-H(19B)	109.0	C(20)-C(19)-H(19B)	109.0
H(19A)-C(19)-	107.8				

H(19B)	

Table S16. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $H_2L•H_2O$. The anisotropic displacement factor exponent takes the form: $-2\ pi^2\ [\ h^2\ a^{*2}\ U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O(1)	93(3)	218(7)	45(2)	30(3)	23(2)	12(3)
C(1)	78(3)	35(2)	37(2)	3(1)	10(2)	-1(2)
N(1)	166(7)	192(7)	57(3)	-45(4)	38(4)	-104(6)
O(2)	69(2)	53(2)	44(2)	-3(1)	7(1)	0(1)
C(2)	79(3)	34(2)	45(2)	7(2)	9(2)	1(2)
N(2)	84(3)	92(3)	63(3)	-14(2)	28(2)	-15(3)
O(3)	75(2)	66(2)	37(2)	-3(1)	10(2)	1(2)
C(3)	83(3)	49(2)	46(2)	4(2)	6(2)	1(2)
N(3)	88(3)	68(3)	45(2)	-1(2)	9(2)	-6(2)
O(4)	77(2)	74(2)	40(2)	-9(1)	10(2)	-4(2)
C(4)	109(5)	60(3)	38(2)	2(2)	12(2)	4(3)
O(5)	85(4)	141(4)	101(4)	-40(3)	32(3)	-29(3)
C(5)	94(4)	61(3)	42(3)	5(2)	15(2)	2(2)
O(6)	93(3)	103(3)	45(2)	-13(2)	3(2)	3(2)
C(6)	89(4)	49(2)	38(2)	9(2)	17(2)	3(2)
O(8)	87(3)	69(2)	52(2)	10(2)	15(2)	11(2)
C(8)	73(3)	45(2)	53(3)	7(2)	10(2)	3(2)
O(7)	85(3)	102(3)	55(2)	19(2)	10(2)	-6(2)
C(7)	84(4)	72(3)	46(3)	13(2)	15(2)	5(2)
C(9)	75(3)	32(2)	43(2)	5(2)	12(2)	2(2)
C(10)	73(3)	27(2)	41(2)	4(1)	12(2)	3(2)
C(11)	76(3)	42(2)	49(2)	0(2)	14(2)	3(2)
C(12)	73(3)	58(3)	59(3)	-1(2)	-2(2)	-1(2)
C(13)	69(3)	63(3)	73(3)	-5(2)	11(3)	-4(2)
C(14)	81(4)	56(3)	62(3)	11(2)	16(3)	2(2)
C(15)	71(3)	50(2)	53(3)	0(2)	4(2)	-1(2)
C(16)	91(5)	86(4)	68(4)	-21(3)	24(3)	-23(3)
C(17)	340(20)	320(20)	73(6)	-63(9)	87(9)	-236(19)
C(18)	105(6)	258(13)	131(8)	-125(9)	69(6)	-78(7)
C(20)	84(4)	82(4)	46(3)	-5(2)	10(2)	-6(3)
C(21)	86(4)	53(3)	51(3)	-5(2)	9(2)	6(2)
C(22)	84(3)	61(3)	50(3)	-5(2)	3(2)	2(2)
C(23)	85(4)	94(4)	56(3)	20(3)	13(3)	0(3)
C(24)	64(3)	78(3)	47(2)	4(2)	4(2)	-1(2)
C(25)	75(3)	87(4)	66(3)	17(3)	4(3)	4(3)
C(26)	68(3)	74(4)	84(4)	-6(3)	1(3)	2(3)
C(27)	82(4)	77(4)	65(3)	-13(3)	16(3)	-7(3)

C(28)	85(3)	71(3)	43(2)	0(2)	10(2)	-10(3)
C(29)	71(3)	62(3)	48(2)	-4(2)	9(2)	-2(2)
C(30)	61(3)	114(6)	102(5)	11(4)	2(3)	7(3)
C(31)	95(7)	127(9)	500(40)	-104(15)	-87(13)	20(6)
C(32)	166(13)	75(7)	720(60)	-19(15)	110(20)	28(8)
C(33)	310(20)	510(40)	129(11)	-5(16)	17(13)	310(30)
C(19)	80(4)	106(4)	47(3)	-12(3)	13(2)	-18(3)

Table S 17. Hydrogen coordinates (× 10^4) and isotropic displacement parameters (Å^2 × 10^3) for $H_2L•H_2O$.

	x	y	z	U(eq)
H(1)	3578	2146	5708	163
H(3)	3642	1876	3948	71
H(3A)	5134	3394	6521	80
H(4)	4375	1572	3332	82
H(5)	5509	1858	3580	78
H(8)	3395	2679	7543	103
H(7)	2804	2483	8563	121
H(12)	7322	3156	6358	77
H(13)	7970	3091	5686	82
H(14)	7423	2767	4826	79
H(15A)	3149	945	4543	70
H(15B)	3114	3282	4539	70
H(17A)	2423	717	6007	286
H(17B)	3143	42	6257	286
H(18A)	2609	1581	6754	192
H(18B)	2524	3381	6375	192
H(20A)	4518	5195	7204	85
H(20B)	4554	2934	7371	85
H(22A)	6604	4672	6819	79
H(22B)	6621	2388	6961	79
H(23A)	2899	5934	6631	94
H(23B)	3489	6123	7098	94
H(25)	2031	7479	7004	92
H(27)	1479	5503	8332	89
H(31A)	227	8497	7133	378
H(31B)	321	6433	7421	378
H(31C)	729	6917	6952	378
H(32A)	1089	11106	7612	472
H(32B)	1120	10097	7063	472
H(32C)	1767	10145	7485	472
H(33A)	495	7926	8147	476
H(33B)	829	10044	8161	476
H(33C)	1257	8199	8385	476
H(19A)	3992	4360	6374	93
H(19B)	4074	2085	6506	93

Table S 18. Torsion angles [deg] for $H_2L \cdot H_2O$.

C(15)-O(2)-C(2)-C(3)	-3.8(5)	C(9)-C(8)-C(7)-C(6)	-2.2(7)
C(15)-O(2)-C(2)-C(1)	177.5(4)	C(14)-C(8)-C(9)-C(11)	2.2(6)
C(6)-C(1)-C(2)-O(2)	179.3(3)	C(7)-C(8)-C(9)-C(11)	-179.7(4)
C(10)-C(1)-C(2)-O(2)	-2.5(6)	C(14)-C(8)-C(9)-C(10)	-179.8(4)
C(6)-C(1)-C(2)-C(3)	0.6(6)	C(7)-C(8)-C(9)-C(10)	-1.8(6)
C(10)-C(1)-C(2)-C(3)	178.8(4)	C(8)-C(9)-C(10)-O(3)	-175.8(4)
O(2)-C(2)-C(3)-C(4)	-176.4(4)	C(11)-C(9)-C(10)-O(3)	2.0(6)
C(1)-C(2)-C(3)-C(4)	2.3(6)	C(8)-C(9)-C(10)-C(1)	4.4(5)
C(2)-C(3)-C(4)-C(5)	-2.6(7)	C(11)-C(9)-C(10)-C(1)	-177.8(3)
C(3)-C(4)-C(5)-C(6)	0.0(7)	C(6)-C(1)-C(10)-O(3)	177.2(4)
C(4)-C(5)-C(6)-C(1)	3.0(7)	C(2)-C(1)-C(10)-O(3)	-1.0(6)
C(4)-C(5)-C(6)-C(7)	-177.6(5)	C(6)-C(1)-C(10)-C(9)	-3.0(5)
C(2)-C(1)-C(6)-C(5)	-3.2(6)	C(2)-C(1)-C(10)-C(9)	178.8(3)
C(10)-C(1)-C(6)-C(5)	178.5(4)	C(22)-O(4)-C(11)-C(12)	10.2(6)
C(2)-C(1)-C(6)-C(7)	177.4(4)	C(22)-O(4)-C(11)-C(9)	-172.1(4)
C(10)-C(1)-C(6)-C(7)	-0.9(6)	C(8)-C(9)-C(11)-O(4)	179.7(4)
C(10)-C(9)-C(11)-O(4)	1.8(6)	C(17)-N(1)-C(16)-O(5)	13.9(16)
C(8)-C(9)-C(11)-C(12)	-2.6(6)	C(17)-N(1)-C(16)-C(15)	-160.0(12)
C(5)-C(6)-C(7)-O(1)	6.9(8)	O(2)-C(15)-C(16)-O(5)	176.7(6)
C(1)-C(6)-C(7)-O(1)	-173.7(5)	O(2)-C(15)-C(16)-N(1)	-9.0(8)
C(5)-C(6)-C(7)-C(8)	-175.8(4)	C(16)-N(1)-C(17)-C(18)	-113.5(16)
C(1)-C(6)-C(7)-C(8)	3.6(7)	N(1)-C(17)-C(18)-N(2)	-60(3)
C(14)-C(8)-C(7)-O(1)	-6.8(8)	C(23)-N(2)-C(18)-C(17)	141.1(18)
C(9)-C(8)-C(7)-O(1)	175.1(5)	C(9)-C(11)-C(12)-C(13)	2.2(7)
C(14)-C(8)-C(7)-C(6)	175.9(4)	C(11)-C(12)-C(13)-C(14)	-1.2(7)
C(10)-C(9)-C(11)-C(12)	179.5(4)	C(9)-C(8)-C(14)-C(13)	-1.4(7)
O(4)-C(11)-C(12)-C(13)	179.8(4)	C(7)-C(8)-C(14)-C(13)	-179.4(5)
C(12)-C(13)-C(14)-C(8)	0.8(7)	C(26)-C(27)-C(28)-C(29)	0.6(8)
C(2)-O(2)-C(15)-C(16)	177.0(4)	C(26)-C(27)-C(28)-O(7)	178.1(5)
C(19)-N(2)-C(18)-C(17)	11(2)	C(27)-C(28)-C(29)-O(8)	178.0(5)
C(21)-N(3)-C(20)-C(19)	-174.3(5)	O(7)-C(28)-C(29)-O(8)	0.3(7)
C(20)-N(3)-C(21)-O(6)	-0.6(8)	C(27)-C(28)-C(29)-C(24)	-1.5(8)
C(20)-N(3)-C(21)-C(22)	179.4(5)	O(7)-C(28)-C(29)-C(24)	-179.1(5)
C(11)-O(4)-C(22)-C(21)	169.7(4)	C(25)-C(24)-C(29)-O(8)	-178.1(5)
O(6)-C(21)-C(22)-O(4)	177.2(5)	C(23)-C(24)-C(29)-O(8)	-4.4(8)
N(3)-C(21)-C(22)-O(4)	-2.8(6)	C(25)-C(24)-C(29)-C(28)	1.4(8)
C(18)-N(2)-C(23)-C(24)	73.7(7)	C(23)-C(24)-C(29)-C(28)	175.1(5)
C(19)-N(2)-C(23)-C(24)	-156.1(5)	C(25)-C(26)-C(30)-C(32)	-36.2(18)
N(2)-C(23)-C(24)-C(25)	-145.6(6)	C(27)-C(26)-C(30)-C(32)	142.1(17)
N(2)-C(23)-C(24)-C(29)	40.7(7)	C(25)-C(26)-C(30)-C(33)	-157.8(19)

C(29)-C(24)-C(25)-C(26)	-0.3(9)	C(27)-C(26)-C(30)-C(33)	21(2)
C(23)-C(24)-C(25)-C(26)	-174.0(6)	C(25)-C(26)-C(30)-C(31)	81.2(14)
C(24)-C(25)-C(26)-C(27)	-0.6(9)	C(27)-C(26)-C(30)-C(31)	-100.5(13)
C(24)-C(25)-C(26)-C(30)	177.8(6)	C(18)-N(2)-C(19)-C(20)	-160.3(9)
C(25)-C(26)-C(27)-C(28)	0.4(9)	C(23)-N(2)-C(19)-C(20)	71.7(7)
C(30)-C(26)-C(27)-C(28)	-177.9(6)	N(3)-C(20)-C(19)-N(2)	175.0(5)

Table S 19. Hydrogen bonds for $H_2L•H_2O$.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(3)-H(3A)…O(3)	0.88	2.35	3.23	177.02
N(3)-H(3A)…O(4)	0.88	2.03	2.48	111.02
O(8)-H(8)…N(2)	0.84	1.90	2.65	147.76
O(7)-H(7)…O(8)	0.84	2.22	2.65	111.91

Table S 20. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for [Fe (HL) Cl_2]$_2$. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	5777(1)	4763(1)	4611(1)	53(1)
Cl(1)	6358(1)	6325(1)	4434(1)	79(1)
Cl(2)	6628(1)	3475(1)	5190(1)	72(1)
O(1)	4562(1)	4819(1)	4399(1)	60(1)
O(2)	5524(1)	4104(2)	3576(1)	59(1)
O(3)	5617(2)	-614(2)	4347(2)	104(1)
O(4)	7412(1)	830(2)	5030(1)	88(1)
O(5)	8074(1)	2338(2)	4268(1)	88(1)
O(6)	10109(2)	3473(3)	6848(2)	139(1)
O(7)	7807(2)	4355(2)	3869(1)	107(1)
O(8)	6645(2)	4893(2)	2012(1)	92(1)
N(1)	5546(1)	2283(2)	2643(1)	62(1)
N(2)	5906(2)	1140(2)	4252(1)	77(1)
N(3)	7108(1)	3355(2)	2665(1)	73(1)
C(1)	4188(1)	4396(2)	3699(1)	53(1)
C(2)	3363(2)	4325(2)	3425(1)	60(1)
C(3)	3052(2)	3886(2)	2685(1)	64(1)
C(4)	3595(2)	3504(2)	2250(1)	64(1)
C(5)	4426(2)	3556(2)	2527(1)	57(1)
C(6)	4724(1)	4031(2)	3254(1)	52(1)
C(7)	5015(2)	3077(2)	2098(1)	63(1)
C(8)	5050(2)	1402(2)	2930(2)	75(1)

C(9)	5115(2)	1412(2)	3804(2)	75(1)
C(10)	6072(2)	135(3)	4519(2)	79(1)
C(11)	6880(2)	-36(3)	5085(2)	86(1)
C(12)	8057(2)	1015(3)	5634(2)	82(1)
C(13)	8276(2)	294(4)	6262(2)	98(1)
C(14)	8909(2)	552(5)	6875(2)	120(2)
C(15)	9304(2)	1524(5)	6896(2)	113(1)
C(16)	9103(2)	2243(3)	6278(2)	89(1)
C(17)	9526(2)	3281(4)	6322(2)	98(1)
C(18)	9212(2)	4110(3)	5727(2)	86(1)
C(19)	9491(2)	5158(4)	5850(2)	98(1)
C(20)	9195(2)	5951(4)	5328(2)	100(1)
C(21)	8629(2)	5695(3)	4655(2)	94(1)
C(22)	8365(2)	4644(3)	4515(2)	82(1)
C(23)	8639(2)	3835(3)	5049(2)	75(1)
C(24)	8363(2)	2702(3)	4923(2)	76(1)
C(25)	7526(2)	5075(3)	3253(2)	75(1)
C(26)	7046(2)	4425(3)	2585(2)	71(1)
C(27)	8486(2)	1980(3)	5620(2)	78(1)
C(28)	6757(2)	2625(3)	2040(2)	83(1)
C(29)	6200(2)	1801(3)	2284(2)	80(1)
C(30)	2134(2)	3782(3)	2408(2)	84(1)
C(31)	1898(2)	3410(4)	1565(3)	123(2)
C(32)	1849(3)	2928(6)	2930(3)	146(2)
C(33)	1724(2)	4860(4)	2499(3)	128(2)

Table S 21. Bond lengths [Å] and angles [deg] for [Fe (HL) Cl_2]$_2$.

Fe(1)-O(2)	1.9447(14)	C(10)-C(11)	1.521(5)
Fe(1)-O(1)#1	2.0020(15)	C(11)-H(11A)	0.9700
Fe(1)-O(1)	2.0109(17)	C(11)-H(11B)	0.9700
Fe(1)-Cl(1)	2.2249(8)	C(12)-C(13)	1.401(5)
Fe(1)-Cl(2)	2.2425(7)	C(12)-C(27)	1.403(5)
O(1)-C(1)	1.355(3)	C(13)-C(14)	1.379(6)
O(2)-C(6)	1.353(3)	C(13)-H(13)	0.9300
O(3)-C(10)	1.204(4)	C(14)-C(15)	1.377(7)
O(4)-C(12)	1.366(4)	C(14)-H(14)	0.9300
O(4)-C(11)	1.420(4)	C(15)-C(16)	1.385(5)
O(5)-C(24)	1.229(3)	C(15)-H(15)	0.9300
O(6)-C(17)	1.220(4)	C(16)-C(27)	1.415(4)
O(7)-C(22)	1.355(4)	C(16)-C(17)	1.467(6)
O(7)-C(25)	1.399(4)	C(17)-C(18)	1.479(5)
O(8)-C(26)	1.228(3)	C(18)-C(19)	1.384(6)
N(1)-C(29)	1.507(4)	C(18)-C(23)	1.402(4)
N(1)-C(8)	1.526(4)	C(19)-C(20)	1.362(6)
N(1)-C(7)	1.522(3)	C(19)-H(19)	0.9300
N(1)-H(1)	0.9800	C(20)-C(21)	1.385(5)
N(2)-C(10)	1.339(4)	C(20)-H(20)	0.9300
N(2)-C(9)	1.440(4)	C(21)-C(22)	1.383(5)
N(2)-H(2)	0.8600	C(21)-H(21)	0.9300
N(3)-C(26)	1.337(4)	C(22)-C(23)	1.381(5)
N(3)-C(28)	1.445(4)	C(23)-C(24)	1.484(5)
N(3)-H(3)	0.8600	C(24)-C(27)	1.489(4)
C(1)-C(2)	1.379(3)	C(25)-C(26)	1.505(4)
C(1)-C(6)	1.390(3)	C(25)-H(25A)	0.9700
C(2)-C(3)	1.396(3)	C(25)-H(25B)	0.9700
C(2)-H(2A)	0.9300	C(28)-C(29)	1.512(5)
C(3)-C(4)	1.394(4)	C(28)-H(28A)	0.9700
C(3)-C(30)	1.531(4)	C(28)-H(28B)	0.9700
C(4)-C(5)	1.389(4)	C(29)-H(29A)	0.9700
C(4)-H(4)	0.9300	C(29)-H(29B)	0.9700
C(5)-C(6)	1.393(3)	C(30)-C(31)	1.511(5)
C(5)-C(7)	1.491(4)	C(30)-C(32)	1.541(7)
C(7)-H(7A)	0.9700	C(30)-C(33)	1.531(6)
C(7)-H(7B)	0.9700	C(31)-H(31A)	0.9600
C(8)-C(9)	1.505(4)	C(31)-H(31B)	0.9600
C(8)-H(8A)	0.9700	C(31)-H(31C)	0.9600
C(8)-H(8B)	0.9700	C(32)-H(32A)	0.9600
C(9)-H(9A)	0.9700	C(32)-H(32B)	0.9600
C(9)-H(9B)	0.9700	C(32)-H(32C)	0.9600
C(33)-H(33A)	0.9600	C(4)-C(5)-C(6)	118.7(2)

C(33)-H(33B)	0.9600	C(4)-C(5)-C(7)	122.9(2)
C(33)-H(33C)	0.9600	C(6)-C(5)-C(7)	118.3(2)
O(2)-Fe(1)-O(1)#1	149.73(7)	O(2)-C(6)-C(1)	117.50(18)
O(2)-Fe(1)-O(1)	80.21(6)	O(2)-C(6)-C(5)	122.8(2)
O(1)#1-Fe(1)-O(1)	71.34(7)	C(1)-C(6)-C(5)	119.6(2)
O(2)-Fe(1)-Cl(1)	104.71(6)	C(5)-C(7)-N(1)	108.27(19)
O(1)#1-Fe(1)-Cl(1)	96.33(6)	C(5)-C(7)-H(7A)	110.0
O(1)-Fe(1)-Cl(1)	114.16(6)	N(1)-C(7)-H(7A)	110.0
O(2)-Fe(1)-Cl(2)	96.39(5)	C(5)-C(7)-H(7B)	110.0
O(1)#1-Fe(1)-Cl(2)	94.05(5)	N(1)-C(7)-H(7B)	110.0
O(1)-Fe(1)-Cl(2)	129.84(6)	H(7A)-C(7)-H(7B)	108.4
Cl(1)-Fe(1)-Cl(2)	115.03(3)	C(9)-C(8)-N(1)	113.5(2)
C(1)-O(1)-Fe(1)#1	135.51(15)	C(9)-C(8)-H(8A)	108.9
C(1)-O(1)-Fe(1)	114.53(14)	N(1)-C(8)-H(8A)	108.9
Fe(1)#1-O(1)-Fe(1)	108.66(7)	C(9)-C(8)-H(8B)	108.9
C(6)-O(2)-Fe(1)	114.55(13)	N(1)-C(8)-H(8B)	108.9
C(12)-O(4)-C(11)	119.4(2)	H(8A)-C(8)-H(8B)	107.7
C(22)-O(7)-C(25)	122.1(3)	N(2)-C(9)-C(8)	114.0(3)
C(29)-N(1)-C(8)	110.9(2)	N(2)-C(9)-H(9A)	108.7
C(29)-N(1)-C(7)	112.7(2)	C(8)-C(9)-H(9A)	108.7
C(8)-N(1)-C(7)	112.1(2)	N(2)-C(9)-H(9B)	108.7
C(29)-N(1)-H(1)	106.9	C(8)-C(9)-H(9B)	108.7
C(8)-N(1)-H(1)	106.9	H(9A)-C(9)-H(9B)	107.6
C(7)-N(1)-H(1)	106.9	O(3)-C(10)-N(2)	123.9(3)
C(10)-N(2)-C(9)	120.5(3)	O(3)-C(10)-C(11)	119.4(3)
C(10)-N(2)-H(2)	119.7	N(2)-C(10)-C(11)	116.6(3)
C(9)-N(2)-H(2)	119.7	O(4)-C(11)-C(10)	110.2(3)
C(26)-N(3)-C(28)	122.2(2)	O(4)-C(11)-H(11A)	109.6
C(26)-N(3)-H(3)	118.9	C(10)-C(11)-H(11A)	109.6
C(28)-N(3)-H(3)	118.9	O(4)-C(11)-H(11B)	109.6
O(1)-C(1)-C(2)	125.5(2)	C(10)-C(11)-H(11B)	109.6
O(1)-C(1)-C(6)	113.2(2)	H(11A)-C(11)-H(11B)	108.1
C(2)-C(1)-C(6)	121.3(2)	O(4)-C(12)-C(13)	122.0(4)
C(1)-C(2)-C(3)	120.0(2)	O(4)-C(12)-C(27)	117.5(3)
C(1)-C(2)-H(2A)	120.0	C(13)-C(12)-C(27)	120.4(3)
C(3)-C(2)-H(2A)	120.0	C(14)-C(13)-C(12)	119.3(4)
C(4)-C(3)-C(2)	118.3(2)	C(14)-C(13)-H(13)	120.3
C(4)-C(3)-C(30)	122.8(2)	C(12)-C(13)-H(13)	120.3
C(2)-C(3)-C(30)	118.8(3)	C(15)-C(14)-C(13)	121.0(4)
C(3)-C(4)-C(5)	122.1(2)	C(15)-C(14)-H(14)	119.5
C(3)-C(4)-H(4)	118.9	C(13)-C(14)-H(14)	119.5
C(5)-C(4)-H(4)	118.9	C(14)-C(15)-C(16)	120.5(4)
C(14)-C(15)-H(15)	119.8	C(12)-C(27)-C(24)	123.0(3)
C(16)-C(15)-H(15)	119.7	C(16)-C(27)-C(24)	118.3(3)

C(15)-C(16)-C(27)	119.9(4)	N(3)-C(28)-C(29)	113.0(2)
C(15)-C(16)-C(17)	119.3(3)	N(3)-C(28)-H(28A)	109.0
C(27)-C(16)-C(17)	120.9(3)	C(29)-C(28)-H(28A)	109.0
O(6)-C(17)-C(16)	121.3(4)	N(3)-C(28)-H(28B)	109.0
O(6)-C(17)-C(18)	120.3(4)	C(29)-C(28)-H(28B)	109.0
C(16)-C(17)-C(18)	118.5(3)	H(28A)-C(28)-H(28B)	107.8
C(19)-C(18)-C(23)	120.7(3)	C(28)-C(29)-N(1)	114.0(2)
C(19)-C(18)-C(17)	119.1(3)	C(28)-C(29)-H(29A)	108.8
C(23)-C(18)-C(17)	120.2(4)	N(1)-C(29)-H(29A)	108.8
C(18)-C(19)-C(20)	120.7(3)	C(28)-C(29)-H(29B)	108.8
C(18)-C(19)-H(19)	119.6	N(1)-C(29)-H(29B)	108.8
C(20)-C(19)-H(19)	119.6	H(29A)-C(29)-H(29B)	107.7
C(19)-C(20)-C(21)	119.4(4)	C(31)-C(30)-C(32)	108.3(4)
C(19)-C(20)-H(20)	120.3	C(31)-C(30)-C(33)	109.6(3)
C(21)-C(20)-H(20)	120.3	C(32)-C(30)-C(33)	109.5(4)
C(22)-C(21)-C(20)	120.3(4)	C(31)-C(30)-C(3)	111.9(3)
C(22)-C(21)-H(21)	119.8	C(32)-C(30)-C(3)	107.2(3)
C(20)-C(21)-H(21)	119.8	C(33)-C(30)-C(3)	110.2(3)
O(7)-C(22)-C(21)	122.5(3)	C(30)-C(31)-H(31A)	109.5
O(7)-C(22)-C(23)	116.3(3)	C(30)-C(31)-H(31B)	109.5
C(21)-C(22)-C(23)	121.2(3)	H(31A)-C(31)-H(31B)	109.5
C(22)-C(23)-C(18)	117.7(3)	C(30)-C(31)-H(31C)	109.5
C(22)-C(23)-C(24)	122.7(3)	H(31A)-C(31)-H(31C)	109.5
C(18)-C(23)-C(24)	119.7(3)	H(31B)-C(31)-H(31C)	109.5
O(5)-C(24)-C(23)	122.4(3)	C(30)-C(32)-H(32A)	109.5
O(5)-C(24)-C(27)	119.7(3)	C(30)-C(32)-H(32B)	109.5
C(23)-C(24)-C(27)	117.7(3)	H(32A)-C(32)-H(32B)	109.5
O(7)-C(25)-C(26)	106.9(3)	C(30)-C(32)-H(32C)	109.5
O(7)-C(25)-H(25A)	110.3	H(32A)-C(32)-H(32C)	109.5
C(26)-C(25)-H(25A)	110.3	H(32B)-C(32)-H(32C)	109.5
O(7)-C(25)-H(25B)	110.3	C(30)-C(33)-H(33A)	109.5
C(26)-C(25)-H(25B)	110.3	C(30)-C(33)-H(33B)	109.5
H(25A)-C(25)-H(25B)	108.6	H(33A)-C(33)-H(33B)	109.5
O(8)-C(26)-N(3)	125.0(3)	C(30)-C(33)-H(33C)	109.5
O(8)-C(26)-C(25)	119.3(3)	H(33A)-C(33)-H(33C)	109.5
N(3)-C(26)-C(25)	115.7(2)	H(33B)-C(33)-H(33C)	109.5
C(12)-C(27)-C(16)	118.6(3)		

Table S 22. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $[Fe(HL)Cl_2]_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	54(1)	64(1)	37(1)	-6(1)	4(1)	3(1)
Cl(1)	94(1)	70(1)	72(1)	2(1)	18(1)	-7(1)
Cl(2)	81(1)	76(1)	55(1)	-1(1)	3(1)	19(1)
O(1)	55(1)	82(1)	40(1)	-14(1)	4(1)	2(1)
O(2)	58(1)	74(1)	41(1)	-11(1)	5(1)	4(1)
O(3)	147(2)	67(1)	84(1)	0(1)	-10(1)	-8(1)
O(4)	100(2)	97(2)	61(1)	19(1)	4(1)	5(1)
O(5)	117(2)	90(1)	56(1)	0(1)	14(1)	12(1)
O(6)	110(2)	168(3)	109(2)	8(2)	-42(2)	0(2)
O(7)	140(2)	93(2)	67(1)	16(1)	-24(1)	-25(2)
O(8)	98(2)	108(2)	64(1)	15(1)	7(1)	19(1)
N(1)	72(1)	63(1)	48(1)	-9(1)	2(1)	5(1)
N(2)	94(2)	67(1)	64(1)	7(1)	4(1)	-7(1)
N(3)	74(1)	89(2)	52(1)	-1(1)	7(1)	9(1)
C(1)	63(1)	58(1)	36(1)	-5(1)	4(1)	1(1)
C(2)	59(1)	69(2)	50(1)	-6(1)	9(1)	-1(1)
C(3)	63(1)	70(2)	52(1)	-7(1)	-1(1)	-4(1)
C(4)	72(2)	70(2)	43(1)	-11(1)	-2(1)	2(1)
C(5)	68(1)	61(1)	39(1)	-2(1)	5(1)	4(1)
C(6)	60(1)	54(1)	38(1)	-3(1)	4(1)	1(1)
C(7)	74(2)	72(2)	39(1)	-5(1)	3(1)	7(1)
C(8)	88(2)	60(2)	70(2)	-4(1)	0(1)	-5(1)
C(9)	86(2)	64(2)	74(2)	3(1)	16(1)	-2(1)
C(10)	118(2)	67(2)	48(1)	-3(1)	10(2)	-2(2)
C(11)	113(3)	81(2)	60(2)	7(1)	11(2)	9(2)
C(12)	79(2)	104(2)	61(2)	14(2)	12(1)	28(2)
C(13)	86(2)	126(3)	80(2)	34(2)	11(2)	19(2)
C(14)	87(2)	174(5)	91(3)	62(3)	3(2)	22(3)
C(15)	74(2)	173(4)	82(2)	39(3)	-5(2)	12(2)
C(16)	66(2)	130(3)	66(2)	12(2)	2(1)	22(2)
C(17)	69(2)	142(3)	76(2)	3(2)	0(2)	15(2)
C(18)	62(2)	123(3)	70(2)	-6(2)	6(1)	8(2)
C(19)	76(2)	128(3)	82(2)	-16(2)	0(2)	-5(2)
C(20)	87(2)	112(3)	98(3)	-12(2)	8(2)	-12(2)
C(21)	92(2)	98(2)	87(2)	-1(2)	7(2)	-7(2)
C(22)	83(2)	96(2)	64(2)	3(2)	7(1)	-6(2)
C(23)	66(2)	97(2)	61(2)	0(1)	10(1)	5(1)
C(24)	72(2)	101(2)	55(1)	3(1)	12(1)	22(2)
C(25)	82(2)	82(2)	62(2)	9(1)	15(1)	1(2)
C(26)	70(2)	90(2)	55(1)	6(1)	18(1)	9(2)

C(27)	69(2)	102(2)	61(2)	11(1)	10(1)	22(2)
C(28)	81(2)	106(2)	62(2)	-15(2)	18(1)	16(2)
C(29)	85(2)	80(2)	73(2)	-19(1)	9(1)	20(2)
C(30)	62(2)	104(2)	78(2)	-25(2)	-2(1)	-7(2)
C(31)	78(2)	177(4)	98(3)	-47(3)	-17(2)	-3(2)
C(32)	98(3)	202(6)	131(4)	1(4)	7(3)	-63(3)
C(33)	67(2)	153(4)	145(4)	-54(3)	-17(2)	27(2)

Table S 23. Hydrogen coordinates (× 10^4) and isotropic displacement parameters (Å^2 × 10^3) for [Fe (HL) Cl_2]$_2$.

	x	y	z	U(eq)
H(1)	5816	2689	3107	75
H(2)	6276	1626	4350	92
H(3)	7364	3092	3104	87
H(2A)	3014	4568	3733	72
H(4)	3393	3204	1759	77
H(7A)	5346	3640	1942	75
H(7B)	4730	2710	1630	75
H(8A)	4486	1488	2671	90
H(8B)	5228	706	2778	90
H(9A)	4972	2124	3959	90
H(9B)	4726	906	3932	90
H(11A)	6796	-86	5617	103
H(11B)	7118	-708	4961	103
H(13)	7998	-351	6265	118
H(14)	9071	60	7280	144
H(15)	9708	1700	7328	135
H(19)	9885	5321	6293	118
H(20)	9370	6658	5423	121
H(21)	8425	6232	4295	112
H(25A)	7977	5427	3094	90
H(25B)	7187	5622	3416	90
H(28A)	7188	2253	1861	99
H(28B)	6455	3039	1602	99
H(29A)	6521	1313	2660	96
H(29B)	5949	1382	1828	96
H(31A)	2034	3957	1227	184
H(31B)	1326	3278	1431	184
H(31C)	2183	2759	1502	184
H(32A)	1269	2913	2822	219
H(32B)	2052	3106	3472	219
H(32C)	2050	2234	2822	219

H(33A)	1864	5374	2139	191
H(33B)	1903	5118	3026	191
H(33C)	1148	4763	2388	191

Table S 24. Torsion angles [deg] for [Fe (HL) Cl_2]$_2$.

Fe(1)#1-O(1)-C(1)-C(2)	13.8(4)	C(13)-C(14)-C(15)-C(16)	-3.6(7)
Fe(1)-O(1)-C(1)-C(2)	178.9(2)	C(14)-C(15)-C(16)-C(27)	0.2(6)
Fe(1)#1-O(1)-C(1)-C(6)	-166.64(17)	C(14)-C(15)-C(16)-C(17)	179.0(4)
Fe(1)-O(1)-C(1)-C(6)	-1.6(3)	C(15)-C(16)-C(17)-O(6)	8.4(6)
O(1)-C(1)-C(2)-C(3)	178.9(2)	C(27)-C(16)-C(17)-O(6)	-172.8(4)
C(6)-C(1)-C(2)-C(3)	-0.6(4)	C(15)-C(16)-C(17)-C(18)	-169.7(3)
C(1)-C(2)-C(3)-C(4)	1.7(4)	C(27)-C(16)-C(17)-C(18)	9.1(5)
C(1)-C(2)-C(3)-C(30)	178.0(3)	O(6)-C(17)-C(18)-C(19)	-11.5(6)
C(2)-C(3)-C(4)-C(5)	-0.6(4)	C(16)-C(17)-C(18)-C(19)	166.6(3)
C(30)-C(3)-C(4)-C(5)	-176.8(3)	O(6)-C(17)-C(18)-C(23)	168.6(4)
C(3)-C(4)-C(5)-C(6)	-1.6(4)	C(16)-C(17)-C(18)-C(23)	-13.3(5)
C(3)-C(4)-C(5)-C(7)	175.2(3)	C(23)-C(18)-C(19)-C(20)	2.3(6)
Fe(1)-O(2)-C(6)-C(1)	-1.8(3)	C(17)-C(18)-C(19)-C(20)	-177.6(4)
Fe(1)-O(2)-C(6)-C(5)	-178.17(18)	C(18)-C(19)-C(20)-C(21)	-2.3(6)
O(1)-C(1)-C(6)-O(2)	2.2(3)	C(19)-C(20)-C(21)-C(22)	0.3(6)
C(2)-C(1)-C(6)-O(2)	-178.2(2)	C(25)-O(7)-C(22)-C(21)	7.3(6)
O(1)-C(1)-C(6)-C(5)	178.7(2)	C(25)-O(7)-C(22)-C(23)	-174.9(3)
C(2)-C(1)-C(6)-C(5)	-1.7(4)	C(20)-C(21)-C(22)-O(7)	179.4(4)
C(4)-C(5)-C(6)-O(2)	179.0(2)	C(20)-C(21)-C(22)-C(23)	1.8(6)
C(7)-C(5)-C(6)-O(2)	2.0(4)	O(7)-C(22)-C(23)-C(18)	-179.6(3)
C(4)-C(5)-C(6)-C(1)	2.7(4)	C(21)-C(22)-C(23)-C(18)	-1.8(5)
C(7)-C(5)-C(6)-C(1)	-174.3(2)	O(7)-C(22)-C(23)-C(24)	1.5(5)
C(4)-C(5)-C(7)-N(1)	-123.1(2)	C(21)-C(22)-C(23)-C(24)	179.3(3)
C(6)-C(5)-C(7)-N(1)	53.8(3)	C(19)-C(18)-C(23)-C(22)	-0.2(5)
C(29)-N(1)-C(7)-C(5)	-176.4(2)	C(17)-C(18)-C(23)-C(22)	179.6(3)
C(8)-N(1)-C(7)-C(5)	57.7(3)	C(19)-C(18)-C(23)-C(24)	178.7(3)
C(29)-N(1)-C(8)-C(9)	116.3(3)	C(17)-C(18)-C(23)-C(24)	-1.4(4)
C(7)-N(1)-C(8)-C(9)	-116.8(3)	C(22)-C(23)-C(24)-O(5)	22.1(5)
C(10)-N(2)-C(9)-C(8)	-97.4(3)	C(18)-C(23)-C(24)-O(5)	-156.8(3)
N(1)-C(8)-C(9)-N(2)	-66.8(3)	C(22)-C(23)-C(24)-C(27)	-161.3(3)
C(9)-N(2)-C(10)-O(3)	7.4(5)	C(18)-C(23)-C(24)-C(27)	19.8(4)
C(9)-N(2)-C(10)-C(11)	-171.3(3)	C(22)-O(7)-C(25)-C(26)	169.4(3)
C(12)-O(4)-C(11)-C(10)	159.9(3)	C(28)-N(3)-C(26)-O(8)	5.9(5)
O(3)-C(10)-C(11)-O(4)	162.8(3)	C(28)-N(3)-C(26)-C(25)	-173.0(3)
N(2)-C(10)-C(11)-O(4)	-18.5(4)	O(7)-C(25)-C(26)-O(8)	170.3(3)
C(11)-O(4)-C(12)-C(13)	8.7(5)	O(7)-C(25)-C(26)-N(3)	-10.7(4)
C(11)-O(4)-C(12)-C(27)	-169.3(3)	O(4)-C(12)-C(27)-C(16)	173.5(3)
O(4)-C(12)-C(13)-C(14)	-176.7(4)	C(13)-C(12)-C(27)-C(16)	-4.6(5)
C(27)-C(12)-C(13)-C(14)	1.3(6)	O(4)-C(12)-C(27)-C(24)	-11.0(4)

C(12)-C(13)-C(14)-C(15)	2.8(7)	C(13)-C(12)-C(27)-C(24)	170.9(3)
C(15)-C(16)-C(27)-C(12)	3.8(5)	N(3)-C(28)-C(29)-N(1)	53.4(3)
C(17)-C(16)-C(27)-C(12)	-175.0(3)	C(8)-N(1)-C(29)-C(28)	-175.8(2)
C(15)-C(16)-C(27)-C(24)	-171.9(3)	C(7)-N(1)-C(29)-C(28)	57.7(3)
C(17)-C(16)-C(27)-C(24)	9.3(5)	C(4)-C(3)-C(30)-C(31)	-10.2(5)
O(5)-C(24)-C(27)-C(12)	-22.5(4)	C(2)-C(3)-C(30)-C(31)	173.7(3)
C(23)-C(24)-C(27)-C(12)	160.8(3)	C(4)-C(3)-C(30)-C(32)	108.4(4)
O(5)-C(24)-C(27)-C(16)	153.1(3)	C(2)-C(3)-C(30)-C(32)	-67.7(4)
C(23)-C(24)-C(27)-C(16)	-23.7(4)	C(4)-C(3)-C(30)-C(33)	-132.5(4)
C(26)-N(3)-C(28)-C(29)	-125.6(3)	C(2)-C(3)-C(30)-C(33)	51.4(4)

Table S 25. Hydrogen bonds for [Fe (HL) Cl_2]$_2$.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(25)-H(25B)...Cl(1)	0.97	2.64	3.507(3)	149.6
C(11)-H(11A)...O(8)#2	0.97	2.51	3.474(4)	170.6
C(7)-H(7B)...Cl(1)#3	0.97	2.89	3.825(3)	163.1
N(3)-H(3)...O(5)	0.86	2.32	3.184(3)	178.1
N(2)-H(2)...Cl(2)	0.86	2.72	3.423(3)	139.9