Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information

Water-soluble chiral coordination polymers of Li^+, Na^+, K^+, and Ba^{2+} with an anionic Iron(III) complex of L-threonine derivative and significant red shift of visible spectra with Al^{3+} salt

Chanreingam Long [a] and Manabendra Ray *[a]

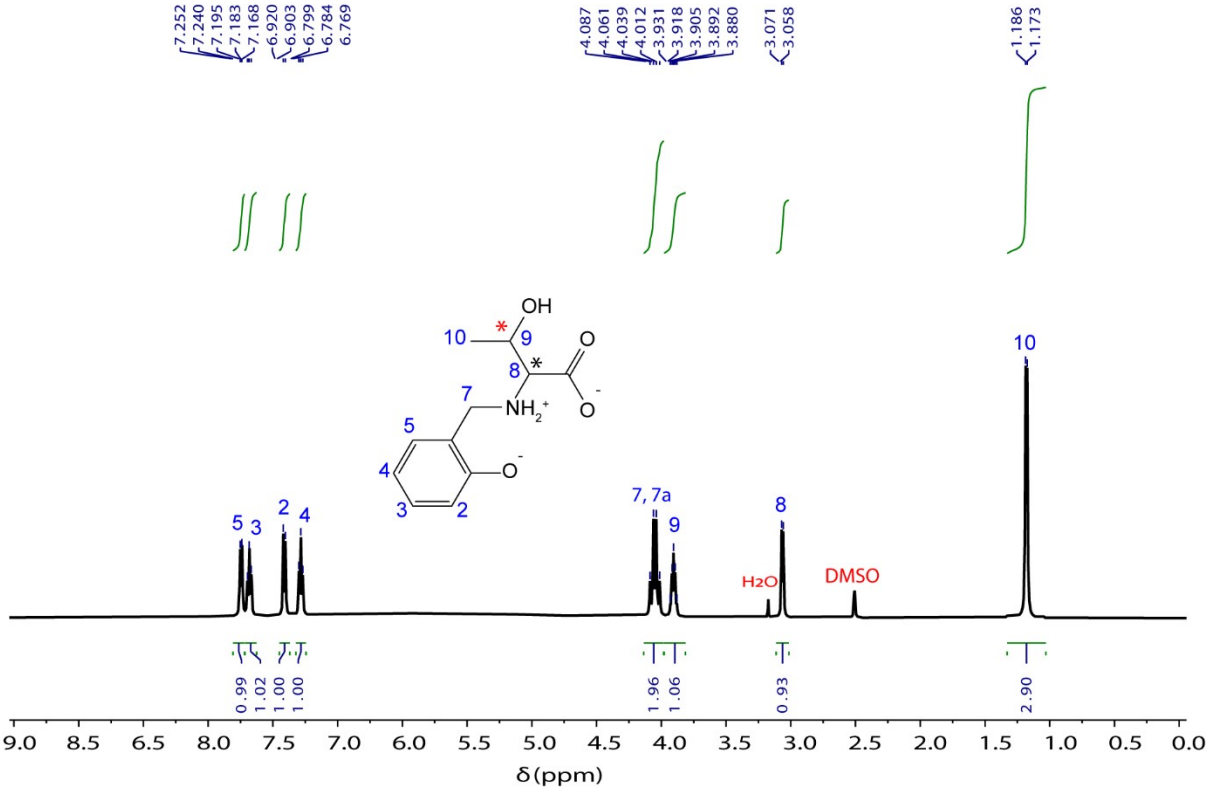

Figure S1. ^{1}H NMR of $H_2L^{L\text{-}thr}$ in d_6-DMSO recorded on a 500 MHz spectrometer.

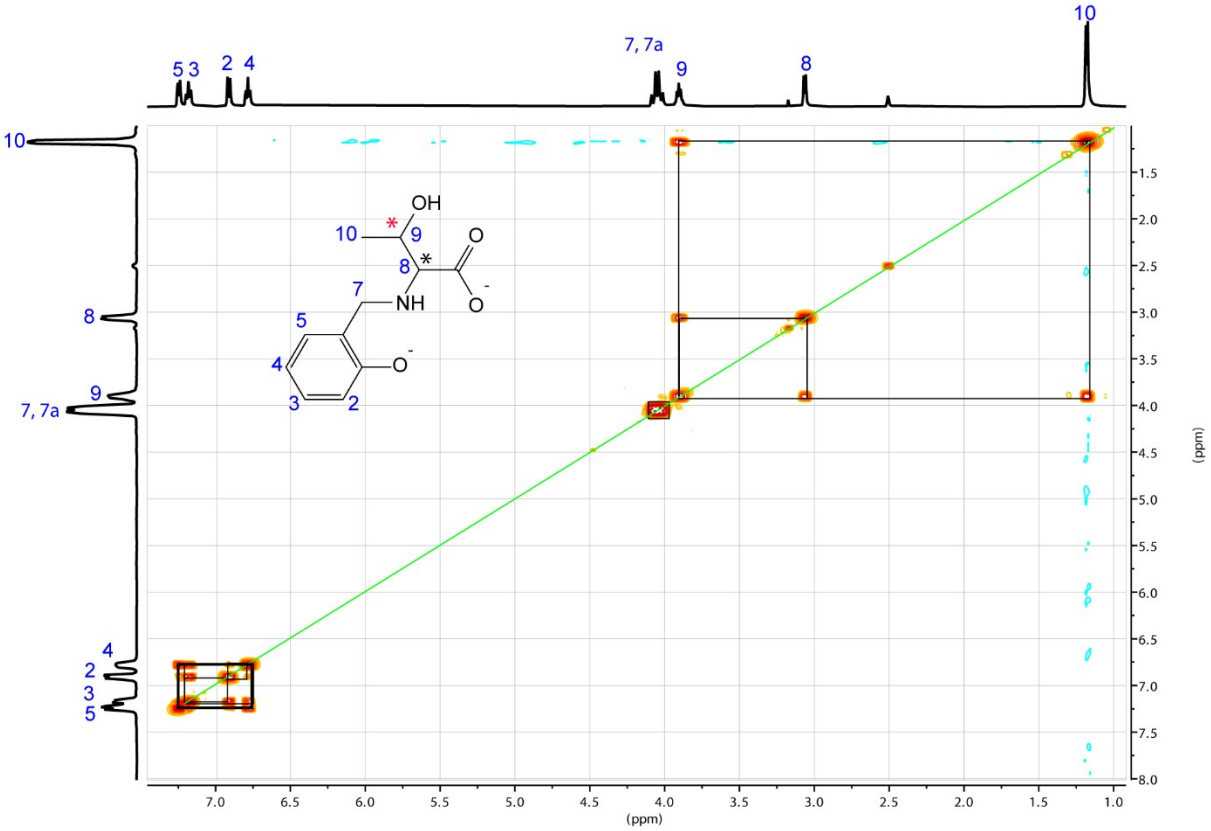

Figure S2. ^{1}H COSY spectra of $H_2L^{L\text{-}thr}$ in d_6-DMSO recorded on a 500 MHz spectrometer.

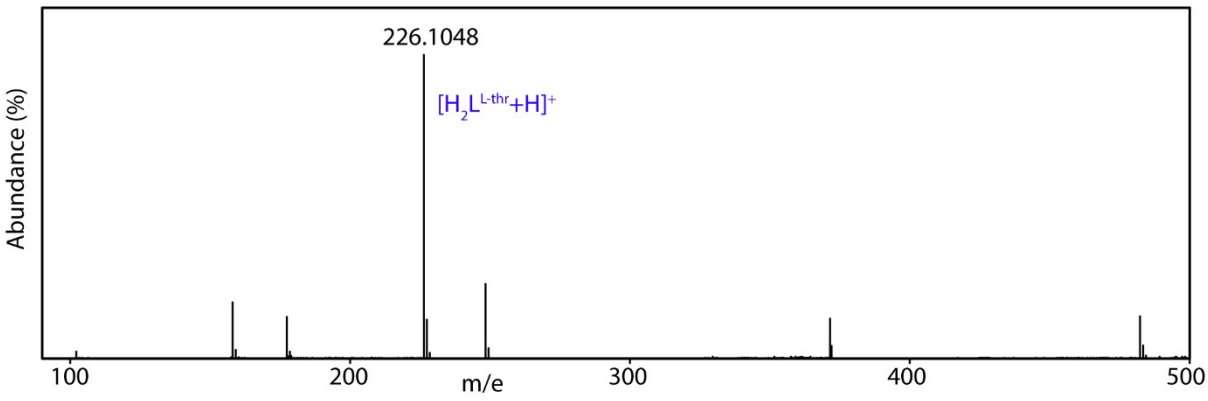

Figure S3. Positive ion mode ESI-MS spectrum of $H_2L^{L\text{-}thr}$ in MeOH.

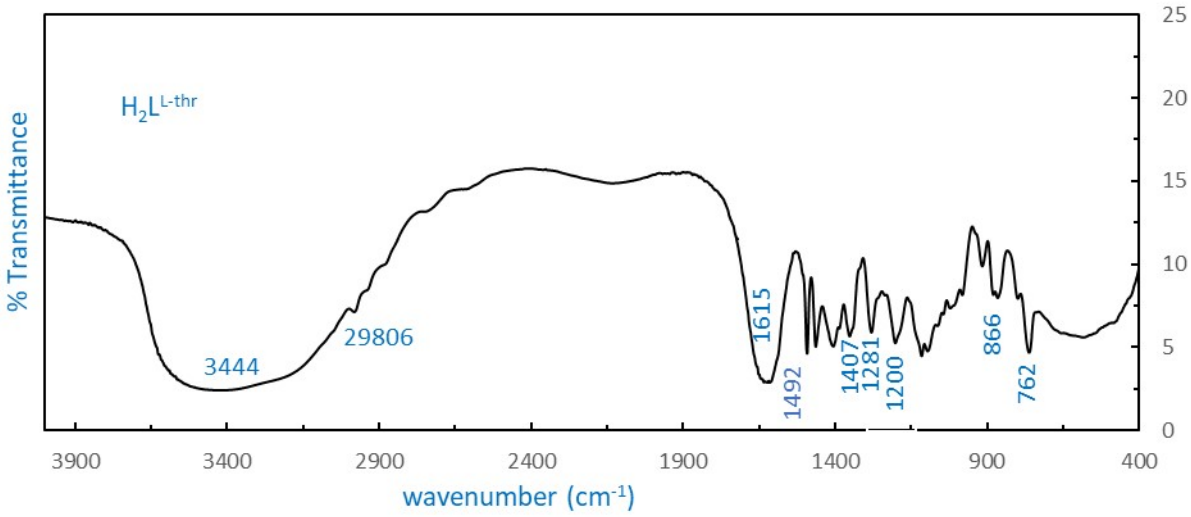

Figure S4. FTIR spectra of $H_2L^{L\text{-}thr}$.

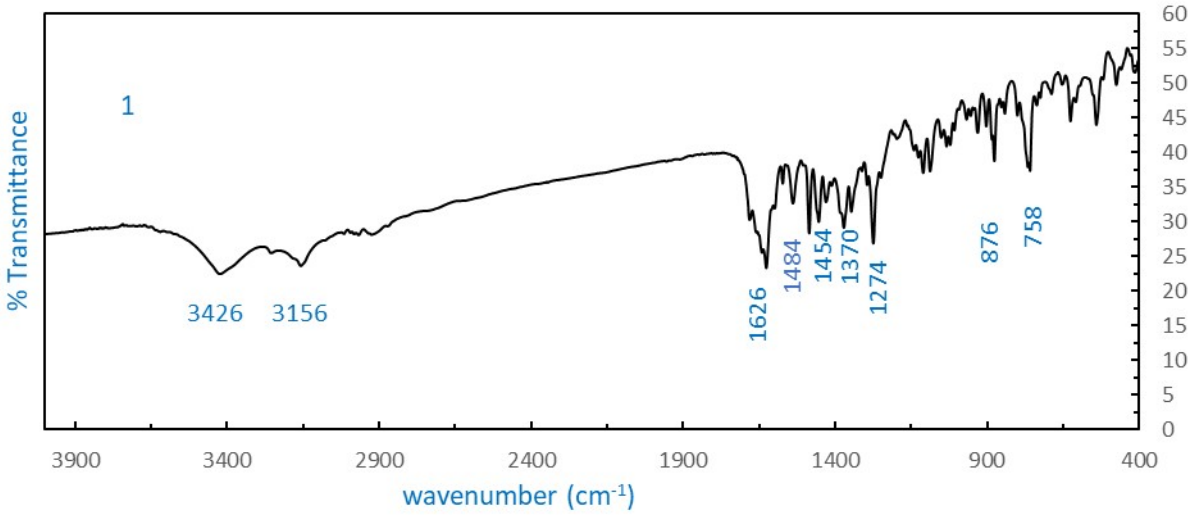

Figure S5. FTIR spectra of Complex **1**.

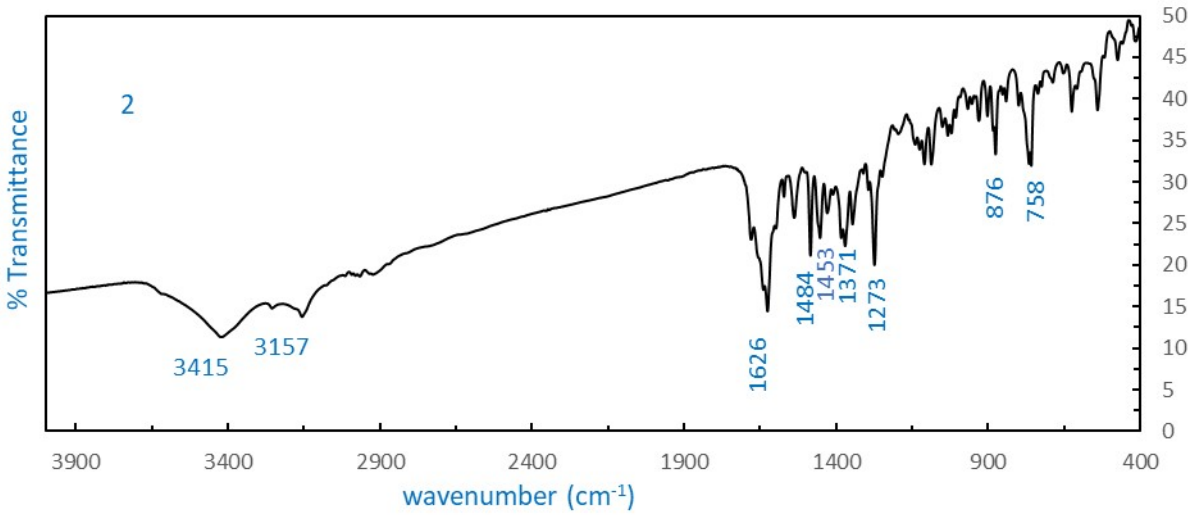

Figure S6. FTIR spectra of Complex **2** synthesized directly from $H_2L^{L\text{-}thr}$.

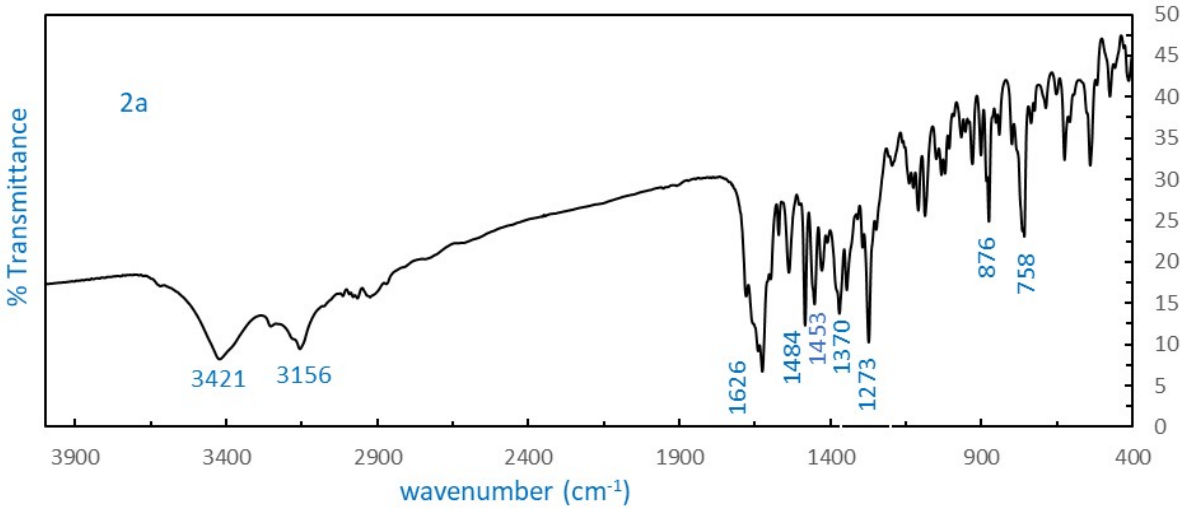

Figure S7. FTIR spectra of Complex **2** synthesized from Complex **1**.

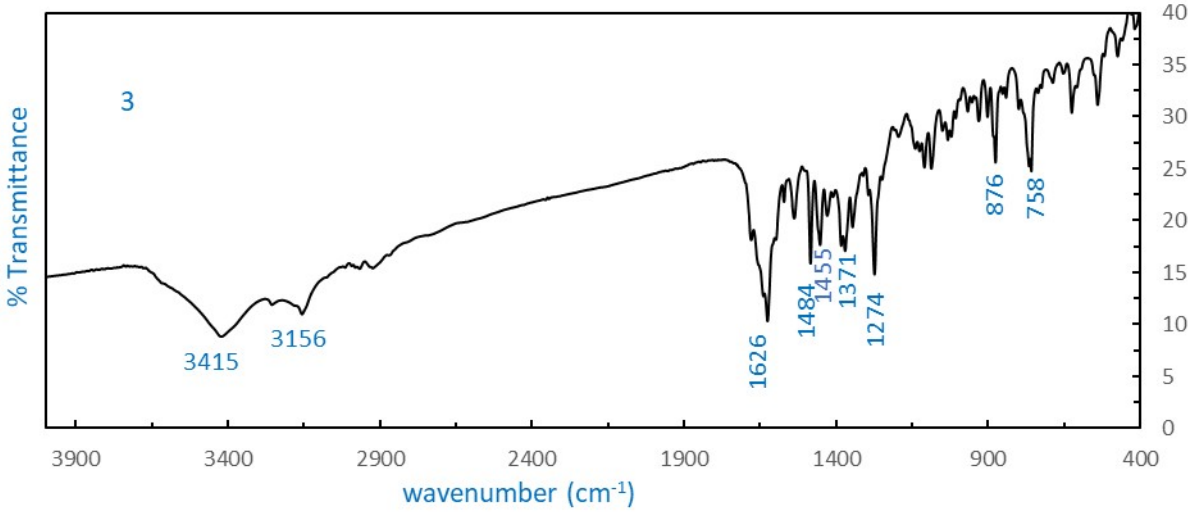

Figure S8. FTIR spectra of Complex **3** synthesized from Complex **2**.

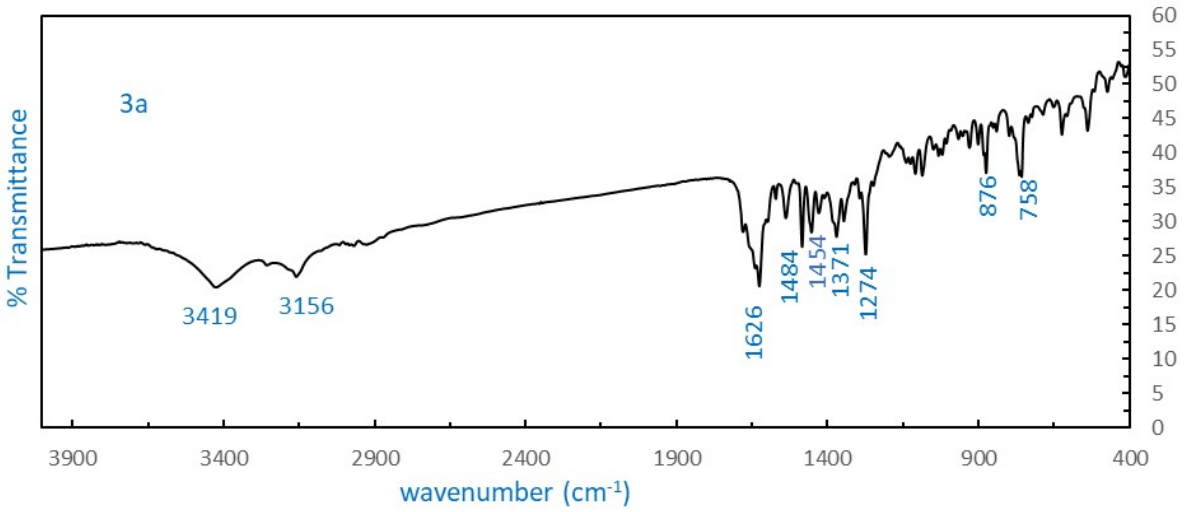

Figure S9. FTIR spectra of Complex **3** from Complex **1**.

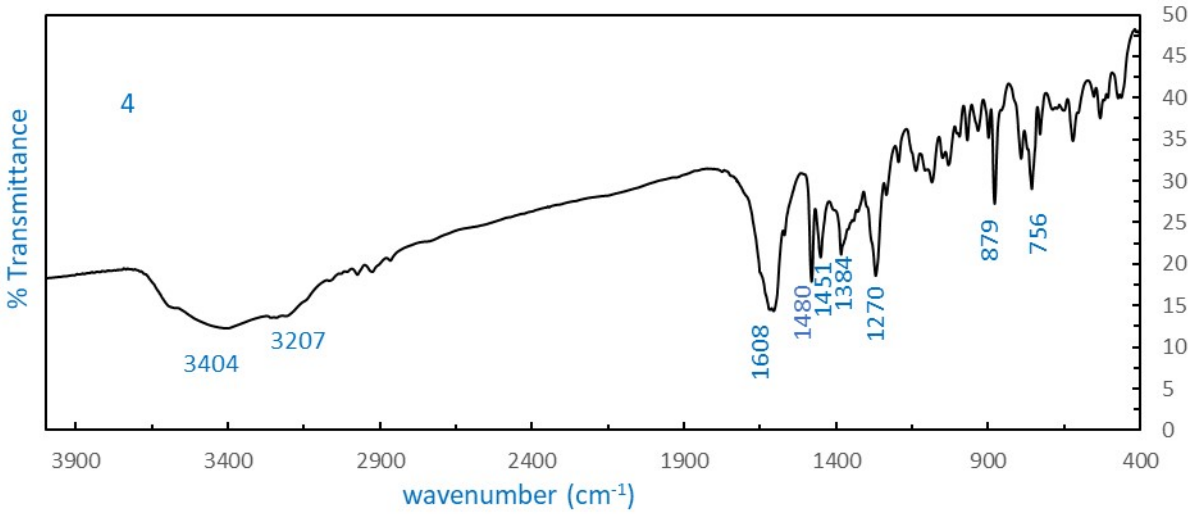

Figure S10. FTIR spectra of Complex **4** synthesized from Complex **2**.

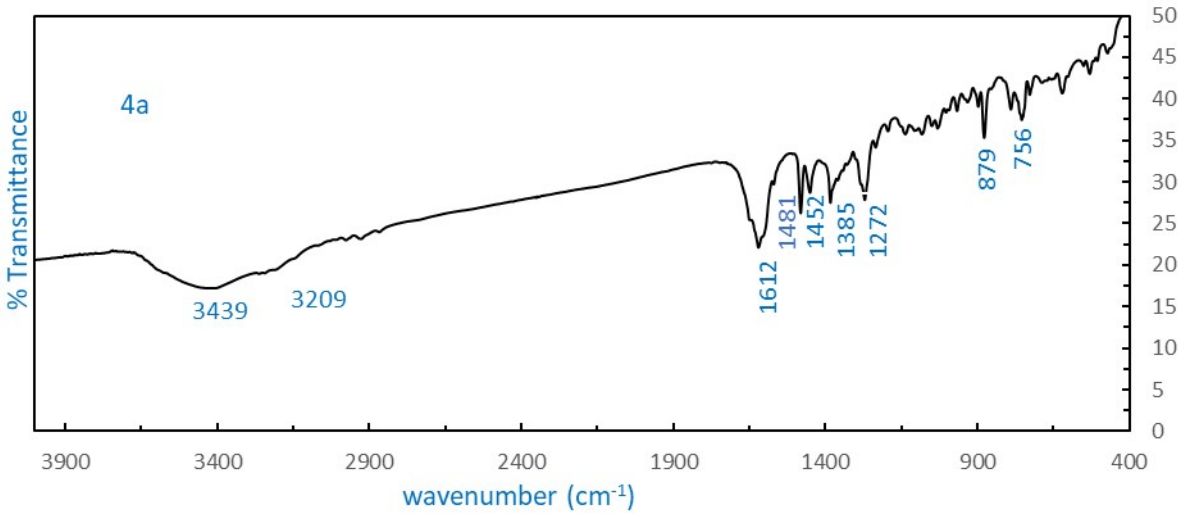

Figure S11. FTIR spectra of Complex **4** synthesized directly from $H_2L^{L\text{-}thr}$.

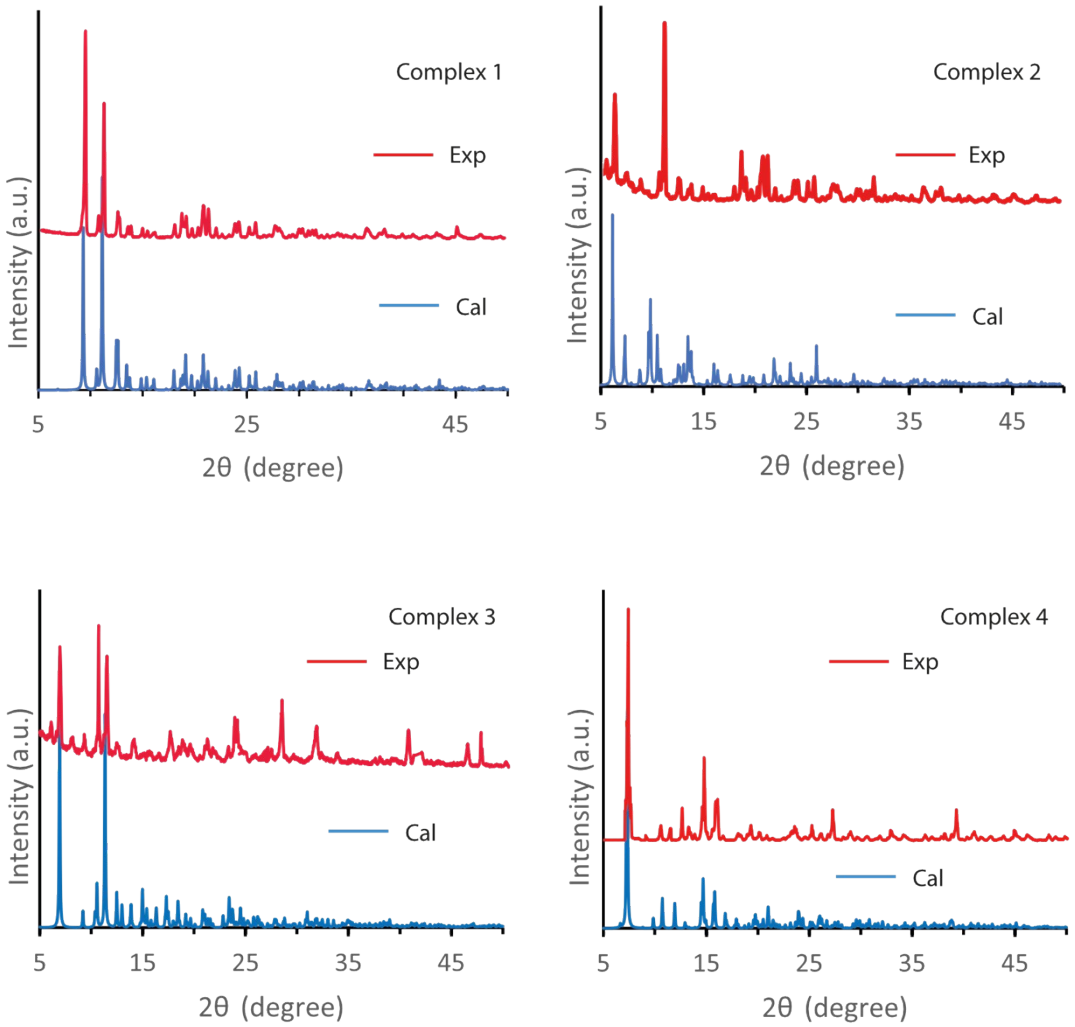

Figure S11a. Powder diffraction of the complexes along with calculated spectra from single crystal X-ray structures using Mercury software. Single crystal X-ray and bulk differ in number and type of solvent/water (Experimental section) due to desolvation and absorption of moisture, hence exp and cal plot may not match exactly.

Note on H-bonding tables. The following H-bonding tables were generated from PLATON[1]. As H's on some of the solvent molecules could not be located or refined, PLATON does not list those H-bonds. Those marked with * were determined based on the distance from Mercury software by the Cambridge Crystallographic Data Centre.

1. (a) A.L.Spek, J. Appl. Cryst. 2003, 36, 7-11. Single-crystal structure validation with the program PLATON. (b) A.L.Spek, Acta Cryst. 2009, D65, 148-155. (c) A.L.Spek, Inorg. Chim. Acta 2018, 470, 232-237. (d) A.L.Spek, Acta Cryst. 2020, E76, 1-11.

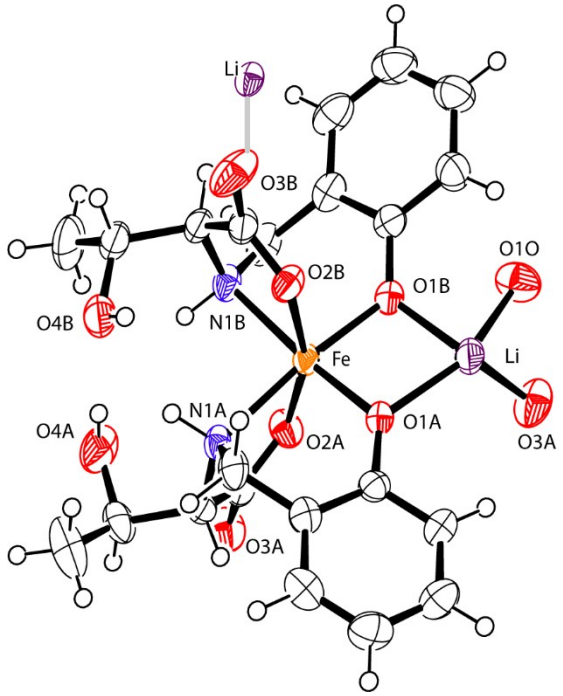

Figure S12. ORTEP diagram of Complex **1** with thermal ellipsoid set at 40% probability.

Table S1. Selected bond distance (Å) and angles (°) of Complex **1**

Fe-O1A	1.916(2)	O1A-Fe -O1B	86.04(9)
Fe-O1B	1.932(2)	O1A-Fe-O2A	100.17(9)
Fe-O2A	2.012(2)	O1A -Fe -O2B	95.87(9)
Fe-O2B	2.012(2)	O1A-Fe-N1A	89.52(9)
Fe-N1A	2.169(2)	O1A-Fe-N1B	173.17(9)
Fe-N1B	2.192(2)	O1B-Fe-O2A	97.22(9)
Li-O1A	1.999(6)	O1B-Fe-O2B	95.49(9)
Li-O1B	2.026(6)	O1B-Fe-N1A	173.36(9)
Li-O1O	1.897(6)	O1B-Fe-N1B	92.11(9)
Li-O3A	1.922(2)	O2A-Fe-O2B	160.14(9)
		O2A-Fe-N1A	78.70(9)
		O2A-Fe-N1B	86.58(9)
		O2B-Fe-N1A	89.86(9)
		O2B-Fe-N1B	77.75(9)
		N1A-Fe-N1B	92.87(9)
		Fe -O1A-Li	96.99(18)
		Fe-O1B-Li	95.56(18)

Table S2. Non-covalent interactions in Complex **1.**

D-H…A	D-H (Å)	H…A(Å)	D…A(Å)	DHA (°)
N1A- H1A…O4A	0.9800	2.3100	2.787(3)	109.00
N1A- H1A…O4B	0.9300	2.1500	3.085(3)	160.00
O4A-H4A…O4B	0.8900	2.1800	3.067(3)	175.00
O4A-H4A…N1A	0.8900	2.500	2.787(8)	100.00
O4B-H4B…O20	0.8200	1.9900	2.706(4)	145.00
C4A-H4AA…O3B	0.9300	2.5100	3.246(4)	136.00
C9A-H9A…O1A	0.9300	2.5100	3.246(4)	136.00
O2B…O4A			2.750*	
O2A…O4B			2.863*	

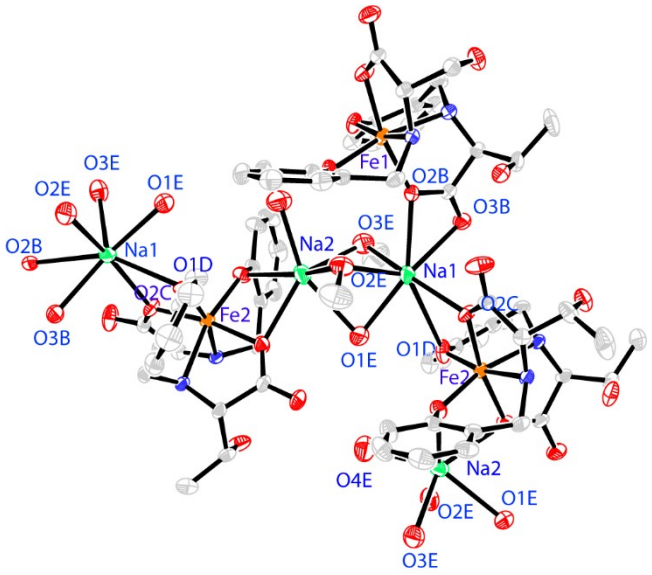

Figure S13. ORTEP diagram of Complex **2** with thermal ellipsoid set at 40% probability.

Table S3. Selected bond distance (Å) and angles (°) of Complex **2**.

Fe1-O1A	1.927(3)	O1A-Fe1 -O1B	93.60(13)
Fe1-O1B	1.902(3)	O1A-Fe1-O2A	99.02(13)
Fe1-O2A	2.034(3)	O1A -Fe1 -O2B	91.61(12)
Fe1-O2B	2.012(3)	O1A-Fe1-N1A	89.00(13)
Fe1-N1A	2.191(4)	O1A-Fe1-N1B	167.77(14)
Fe1-N1B	2.221(4)	O1B-Fe1-O2A	89.12(13)
Fe2-O1C	1.903(3)	O1B-Fe1-O2B	94.04(12)
Fe2-O1D	1.927(4)	O1B-Fe1-N1A	167.19(14)
Fe-O2C	1.991(3)	O1B-Fe1-N1B	92.47(13)
Fe-O2D	2.004(3)	O2A-Fe1-O2B	168.71(13)
Fe2-N1C	2.194(4)	O2A-Fe1-N1A	78.08(14)
Fe2-N1D	2.210(3)	O2A-Fe1-N1B	91.67(14)

Na1-O1E	2.451(5)	O2B-Fe1-N1A	98.44(14)
Na1-O2B	2.555(3)	O2B-Fe1-N1B	77.38(14)
Na1-O2C	2.332(4)	N1A-Fe1-N1B	87.42(13)
Na1-O2E	2.484(5)	O1C-Fe2-O2C	99.10(13)
Na1-O3B	2.398(4)	O1C-Fe2-O2D	89.02(13)
Na1-O3E	2.438(4)	O1C-Fe2-N1C	90.02(13)
Na2-O1E	2.544(5)	O1C-Fe2-N1D	165.82(12)
Na2-O2E	2.409(6)	O1D-Fe-O2C	89.19(15)
Na2-O3E	2.419(4)	O1D-Fe-O2D	95.70(15)
Na2-O4E	2.365(5)	O1D-Fe-N1C	167.47(15)
Na2-O1C	2.398(4)	O1D-Fe-N1D	89.98(14)
Na2-O2D	2.450(4)	O2C-Fe-O2D	170.01(13)
		O2C-Fe-N1C	79.22(14)
		O2C-Fe-N1D	93.54(13)
		O2D-Fe-N1C	95.06(14)
		O2D-Fe-N1D	77.80(13)
		N1C-Fe-N1D	86.04(13)

Table S4. Non-covalent interactions in Complex **2**.

D-H…A	D-H (Å)	H…A(Å)	D…A(Å)	DHA (°)
O1-H1... O3A	0.8200	2.0300	2.841(6)	172.00
N1A-H1…O4A	0.9800	2.4700	2.873(5)	104.00
N1A-H1A... O4B	0.9800	2.0100	2.910(5)	152.00
N1B-H1B…O4A	0.9800	2.2200	3.155(5)	159.00
N1C-H1C…O4C	0.9800	2.3700	2.809(5)	107.00
N1C-H1C...O4D	0.9800	2.1200	3.046(6)	157.00
N1D-H1D…O4C	0.9800	2.2300	3.169(5)	160.00
O4A-H4A…O7E	0.9800	2.5200	2.869(7)	101.00
N1D-H1D…O4C	0.8200	1.9700	2.782(6)	169.00
O4B-H4B…O3C	0.8200	1.9500	2.735(5)	177.00
O4C-H4C…O1	0.8200	2.4600	2.768(6)	178.00
O4D-H4D…O2A	0.8200	1.9700	3.276(5)	174.00
O6E-H6E…O3A	0.8200	1.9200	2.776(6)	165.00
O7E-H7E…O6E	0.8200	2.18	2.736(8)	172.00
O4E-H4EA …O1A	0.86	2.13	2.869(5)	137(6)
O4E-H4EB…O3D	0.85	2.4600	2.976(5)	177(13)
C1B-H1BA...O3C	0.9300	2.5700	3.136(7)	129.00
C9D-H9D…O1B	0.9800	2.4200	3.059(5)	122.00
C9D-H9D…O3D	0.9800	2.5800	2.907(6)	100.00
C7D-H7DB…O3B	0.9700	2.5300	3.488(5)	170.00
O4A…O7E			2.740*	

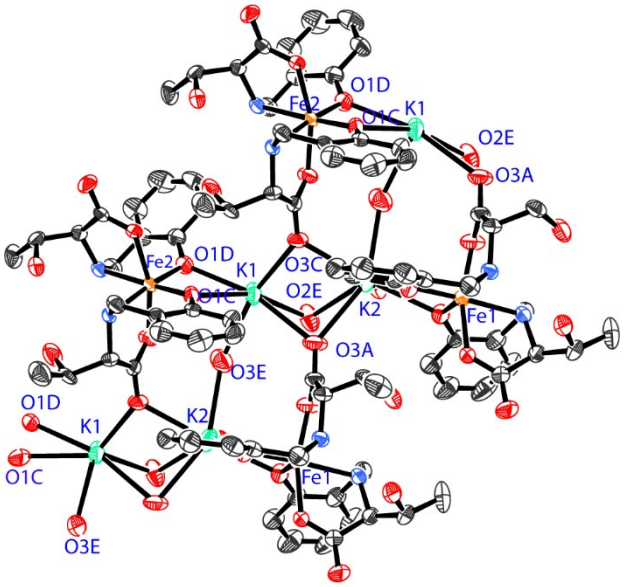

Figure S14. ORTEP diagram of Complex **3** with thermal ellipsoid set at 40% probability.

Table S5. Selected bond distance (Å) and angles (°) of the Complex **3**.

Fe1-O1A	1.902(5)	O1A-Fe1 -O1B	95.02(2)
Fe1-O1B	1.908(5)	O1A-Fe1-O2A	96.14(19)
Fe1-O2A	2.022(6)	O1A -Fe1 -O2B	97.07(19)
Fe1-O2B	2.019(4)	O1A-Fe1-N1A	87.4(2)
Fe1-N1A	2.165(5)	O1A-Fe1-N1B	172.9(2)
Fe1-N1B	2.210(5)	O1B-Fe1-O2A	91.95(18)
Fe2-O1C	1.908 (4)	O1B-Fe1-O2B	95.98(18)
Fe2-O1D	1.915(5)	O1B-Fe1-N1A	171.22(19)
Fe-O2C	2.017(4)	O1B-Fe1-N1B	90.64(19)
Fe-O2D	2.021(5)	O2A-Fe1-O2B	163.93(19)
Fe2-N1C	2.168(5)	O2A-Fe1-N1A	79.4(2)
Fe2-N1D	2.201(4)	O2A-Fe1-N1B	88.07(19)
K1-O1C	2.696(5)	O2B-Fe1-N1A	92.1(2)
K1-O1D	2.693(6)	O2B-Fe1-N1B	77.92(19)
K1-O2E	2.721(5)	N1A-Fe1-N1B	87.70(19)
K1-O3E	2.840(5)	O1C-Fe2-O2C	94.45(19)
K1-O3A	2.849(6)	O1C-Fe2-O2D	97.26(19)
K2-O3D	2.805(6)	O1C-Fe2-N1C	96.04(19)
K2-O1A	2.679(6)	O1C-Fe2-N1D	87.5(2)
K2-O1B	2.717(6)	O1D-Fe-O2C	172.5(2)
K2-O3A	2.825(6)	O1D-Fe-O2D	93.3(19)
K2-O3C	2.838(6)	O1D-Fe-N1C	96.04(19)
K2-O3E	2.803(6)	O1D-Fe-N1D	172.0(2)
		O2C-Fe-O2D	90.8(18)
		O2C-Fe-N1C	162.93(17)
		O2C-Fe-N1D	78.76(19)
		O2D-Fe-N1C	87.84(17)
		O2D-Fe-N1D	91.2(19)

		N1C-Fe-N1D	88.1(19)

Table S6. Non-covalent interactions in the Complex **3**.

D-H…A	D-H (Å)	H…A(Å)	D…A(Å)	DHA (°)
O00C-H00C…O2E	0.8200	1.900	2.708(6)	170.00
N1A-H1…O4A	0.9800	2.3100	2.792(6)	109.00
N1A-H1A…O4B	0.9800	2.0300	2.940(7)	154.00
N1B-H1B…O4A	0.9800	2.5100	3.419(6)	155.00
N1B-H1B…O4B	0.9800	2.5300	2.877(7)	100.00
N1C-H1C…O00C	0.9800	2.0700	3.001(7)	158.00
N1C-H1C…O4C	0.9800	2.3600	2.822(8)	108.00
N1D-H1D…O00C	0.9800	2.5200	2.869(7)	101.00
N1D-H1D…O4C	0.9800	2.5500	3.461(7)	155.00
O4A-H4A…O2B	0.8200	2.1000	2.904(6)	166.00
O4B-H4B…O1E	0.8200	1. 9000	2.712(8)	172.00
O4C-H4C…O2D	0.8200	2.1500	2.952(6)	167.00
C9A-H9A…O1A	0.9800	2.5000	3.354 (8)	146.00
C9A-H9A…O3A	0.9800	2.5300	2.879(7)	101.00
C9C-H9C…O1C	0.9800	2.4300	3.257(8)	142.00
C9C-H9C…O3C	0.9800	2.5800	2.906(9)	100.00

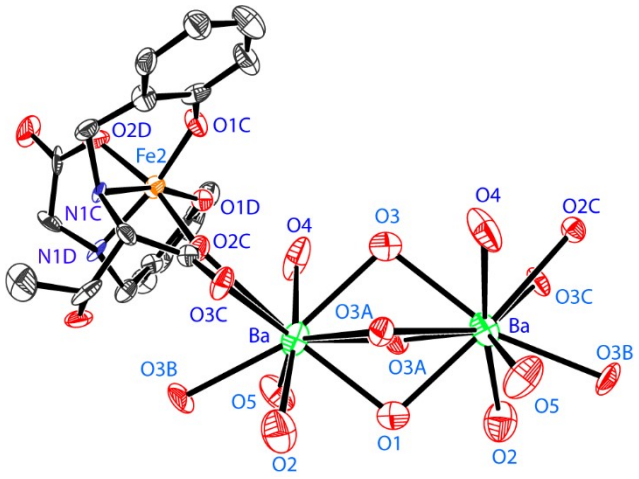

Figure S15. ORTEP diagram of the Complex **4** with thermal ellipsoid set at 40% probability.

Table S7. Selected bond distance (Å) and angles (°) of the Complex **4**.

Fe1-O1A	1.888(16)	O1A-Fe1 -O2A	99.7(7)
Fe1-O2A	2.036(17)	O1A-Fe1-N1A	89.6(6)
Fe1-N1A	2.197(17)	O1A-Fe1-O1A_b	98.0(7)
Fe1-O1A_b	1.888(16)	O1A-Fe1-O2A_b	87.8(7)
Fe1-O2A_b	2.036(17)	O1A-Fe1-N1A_b	165.0(7)
Fe1-N1A_b	2.197(17)	O2A-Fe1-N1A	78.1(7)
Fe2-O1C	1.903(16)	O2A-Fe1-O2A_b	168.3(7)
Fe2-O2C	2.033(18)	O2A-Fe1-N1A_b	93.3(7)
Fe2-N1C	2.208(17)	N1A-Fe1-N1A_b	86.2(6)
Fe-O1B_d	1.924(15)	O1C-Fe2-O2C	93.9(7)
Fe2-O2B_d	2.024(18)	O1C-Fe2-O1B_b	97.8(7)
Fe2-N1B_d	2.201(19)	O1C-Fe2-N1C	89.9(7)
Ba-O1	2.815(17)	O2C-Fe2-N1C	78.6(7)
Ba-O2	2.76(2)	N1C-Fe2-O2B_d	91.7(7)
Ba-O3B	2.956(19)	N1C-Fe1-N1B_d	84.3(7)
Ba-O2C	3.018(17)	O2C-Fe-N1B_d	92.1(7)
Ba-O3	2.91(3)	O1B_d-Fe2-O2B-d	98.0(7)
Ba-O3A	3.052(17)	O1B_d-Fe2-N1B_d	89.2(7)
Ba-O3C	2.788(17)	O2B_d-Fe-N1B_d	77.5(7)
Ba-O4	2.89(2)	O2C-Ba-O3C	44.6(5)
Ba-O5	2.76(2)	O3B-Ba-O3A	124.2(5)
		O3B-Ba-O3C	72.4(5)
		O2C-Ba-O3A	113.7(5)
		O2C-Ba-O3B	70.7(5)
		O3A-Ba-O3C	76.5(5)

Table S8. Non-covalent interactions in the Complex **4**.

D-H…A	D-H (Å)	H…A(Å)	D…A(Å)	DHA (°)
N1C-H1C...O4C	0.9800	2.4800	2.86(2)	102.00
N1C-H1C...O4B	0.9800	2.1100	3.03(2)	155.00
O4C-H4C…O3B	0.8200	2.1800	3.00(2)	176.00
O4C-H4C…O2B	0.8200	2.5300	3.12(2)	130.00
N1B-H1B…O4B	0.9800	2.5200	2.90(2)	103.00
N1B-H1B…O4C	0.9800	2.0500	2.95(2)	153.00
O4B-H4B…O7	0.8200	2.090	2.84(3)	152.00
N1A-H1A…O4A	0.9800	2.5200	2.89(2)	102.00
N1A-H1A…O4A	0.9800	2.2300	3.15(2)	156.00
C4C-H4CA…Cl	0.8200	2.8100	3.69(4)	157.00

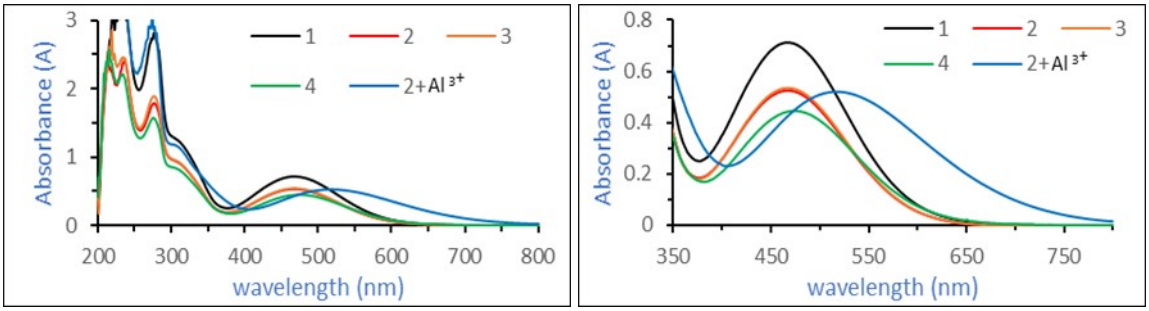

Figure S16. UV-Visible spectra of the complexes in Water.

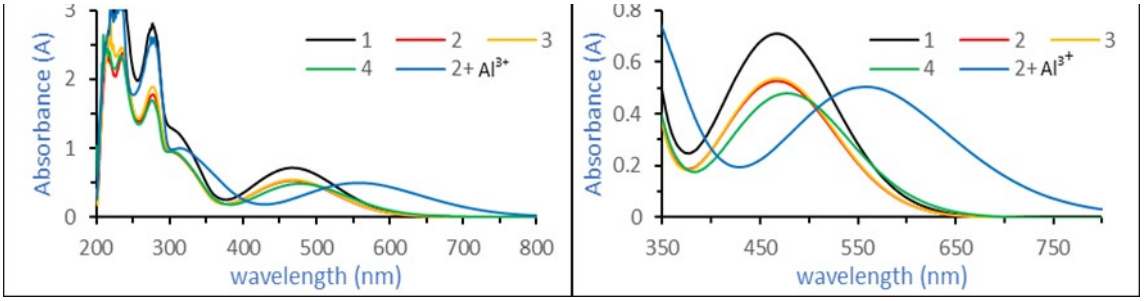

Figure S17. UV-Visible spectra of the complexes in MeOH.

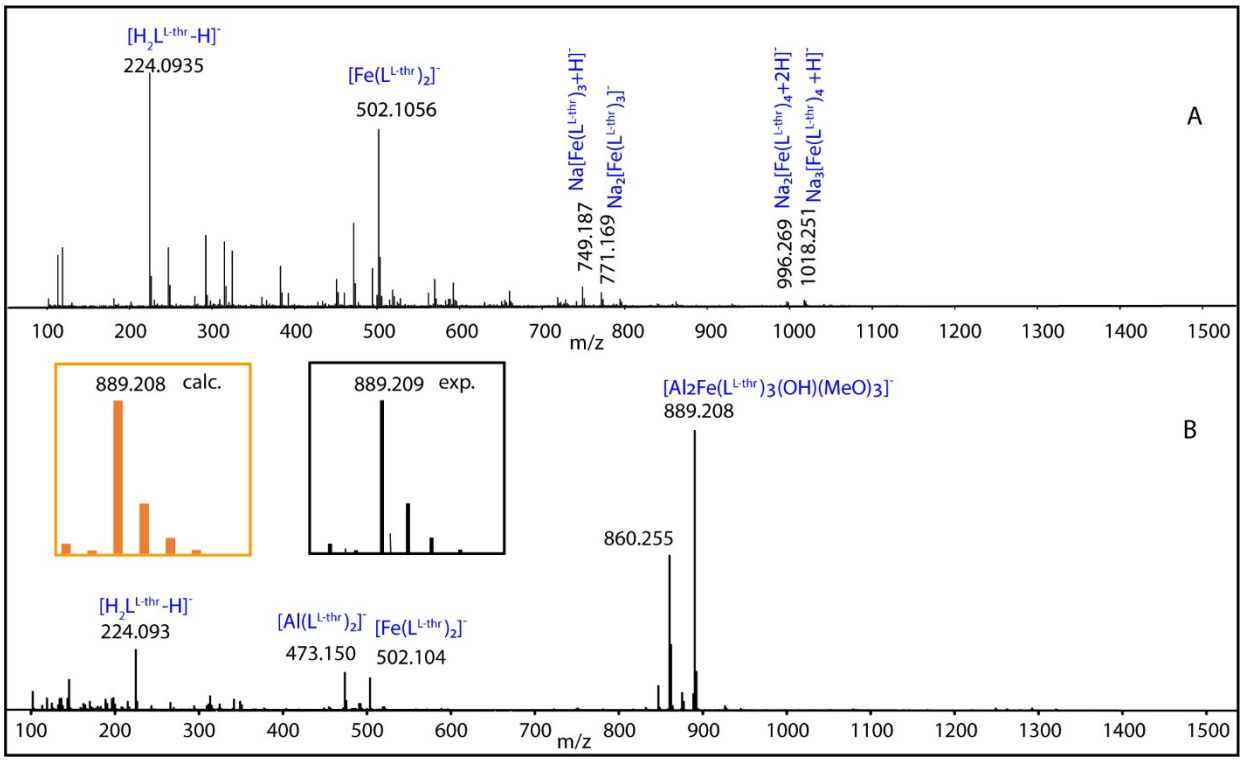

Figure S18. ESI-Mass spectra of the Complex **2** (A) before and (B) after addition of aluminium salt in MeOH.