Electronic Supplementary Information (ESI)

Transition metal complexes of a versatile polyalkoxy oxazolidine-based ligand derived from *in-situ* cyclization

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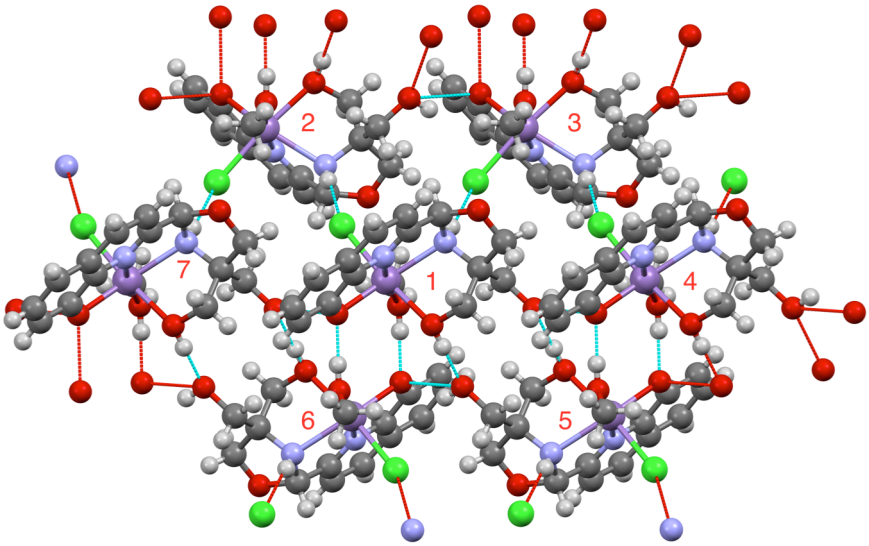
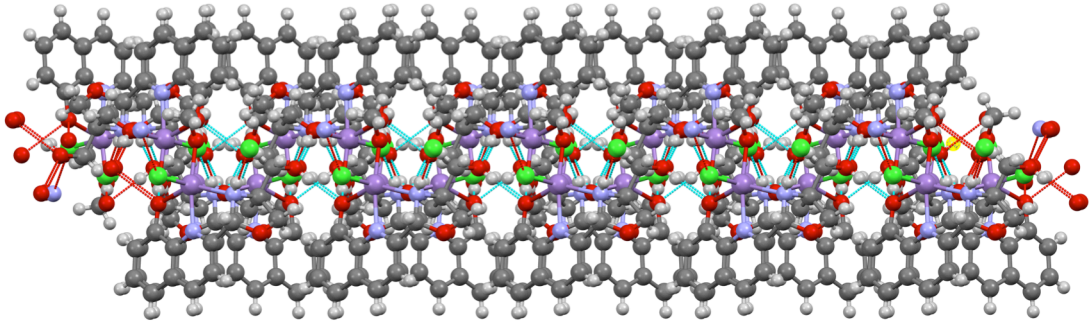


(a)



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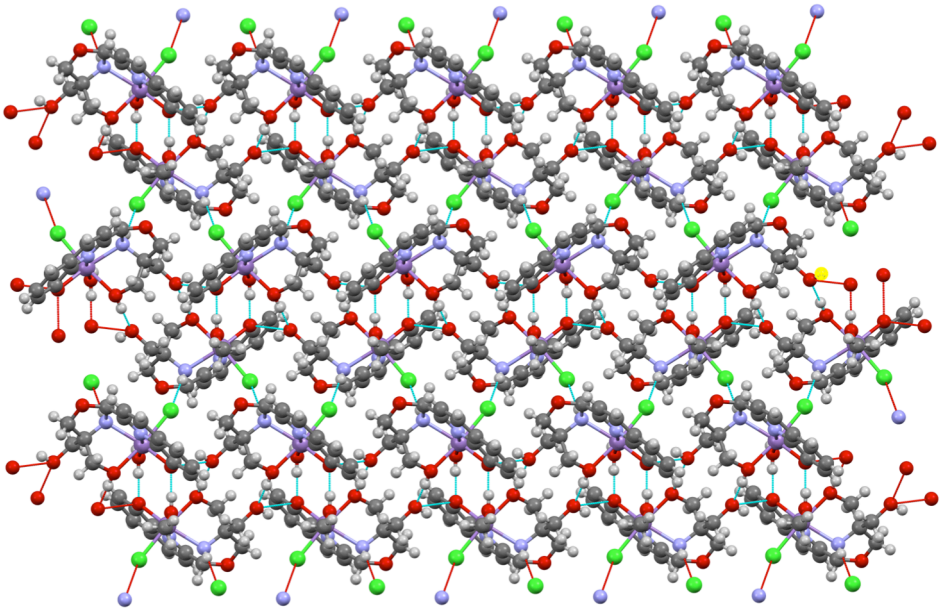

(c)

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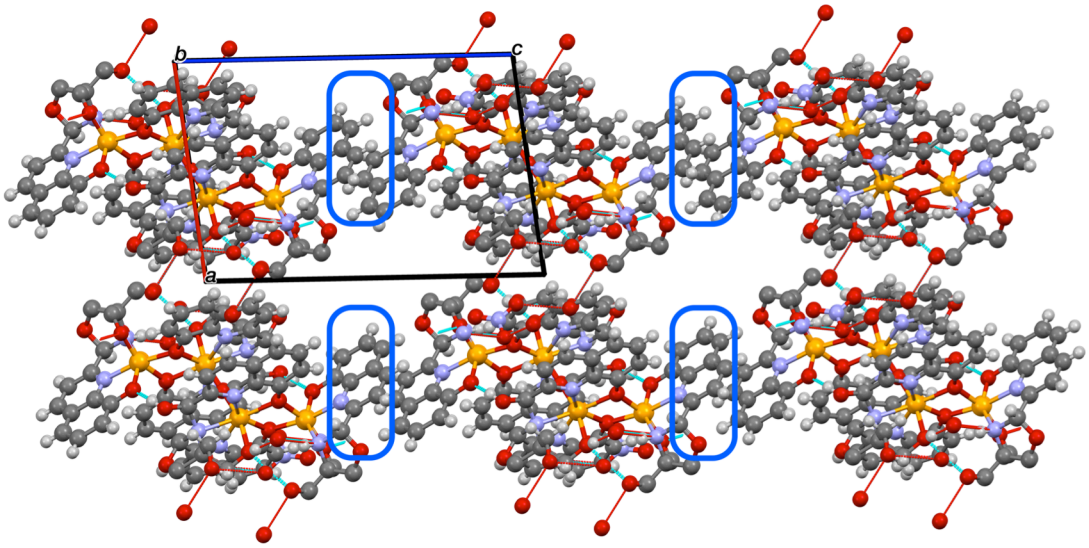
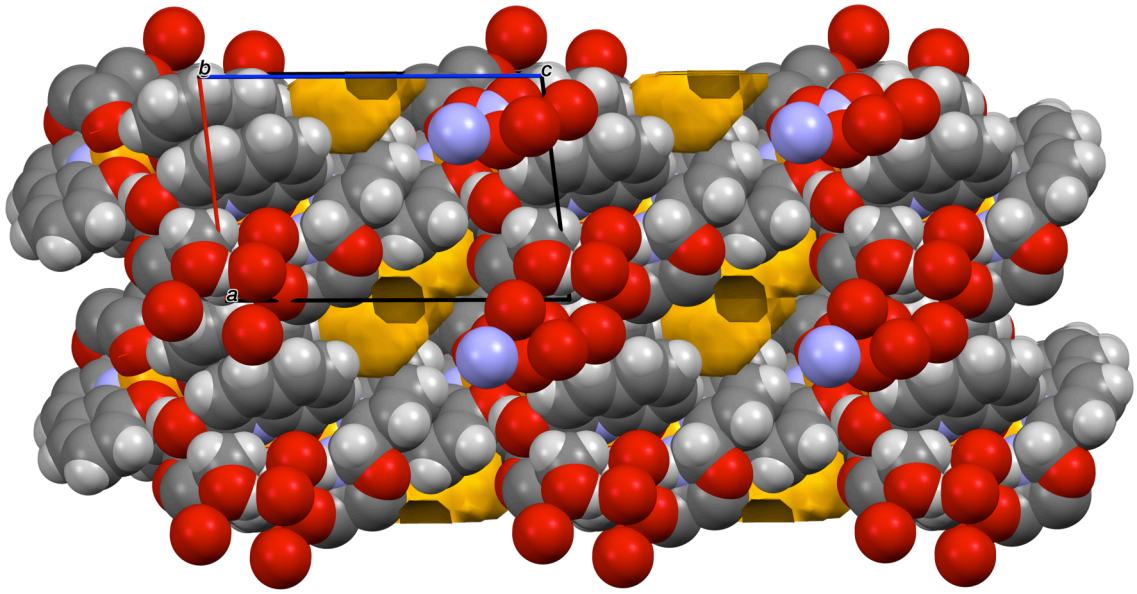


(a)



(b)

Figure S2. (a) The packing diagram of compound 5 showing intermolecular **π- π** interaction along c axis forming a chain-like structure, with hydrogen bonding interaction between the neighboring chains (elongated red bonds). (b) The three-dimensional supramolecular interaction results into a porous structure with 5.9 % solvent accessible pore volume for a probe of 1.2 **Å** radius. *Colour code for the atoms: Blue (N), gray (C), red (O), orange (Fe).*

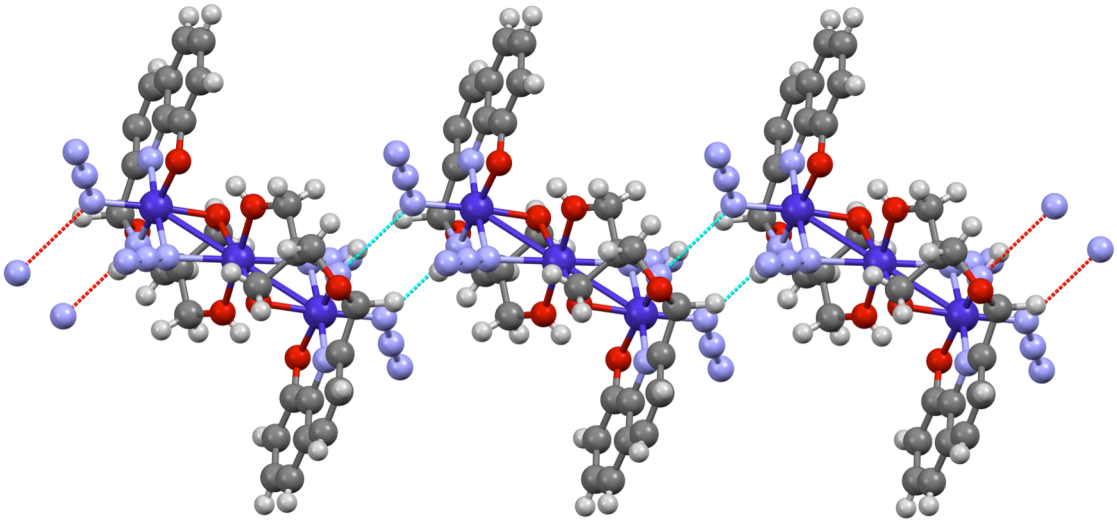


Figure S3. The hydrogen bonding interactions between the neighboring units through the terminal azide units and the N-H group of the oxazolidine ring.

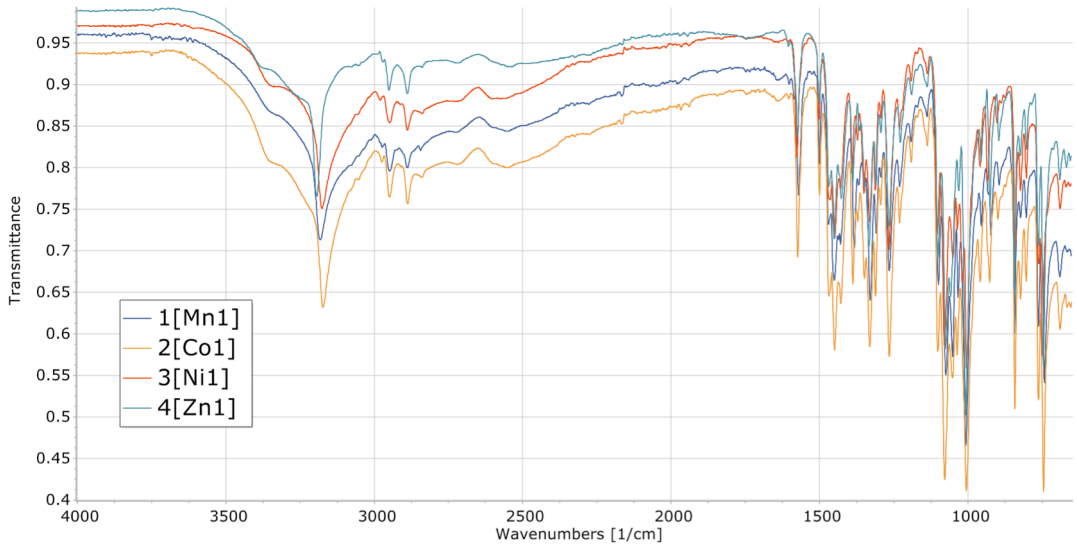


Figure S4. Overlay of the infrared spectra for the isostructural compounds **1** - **4**

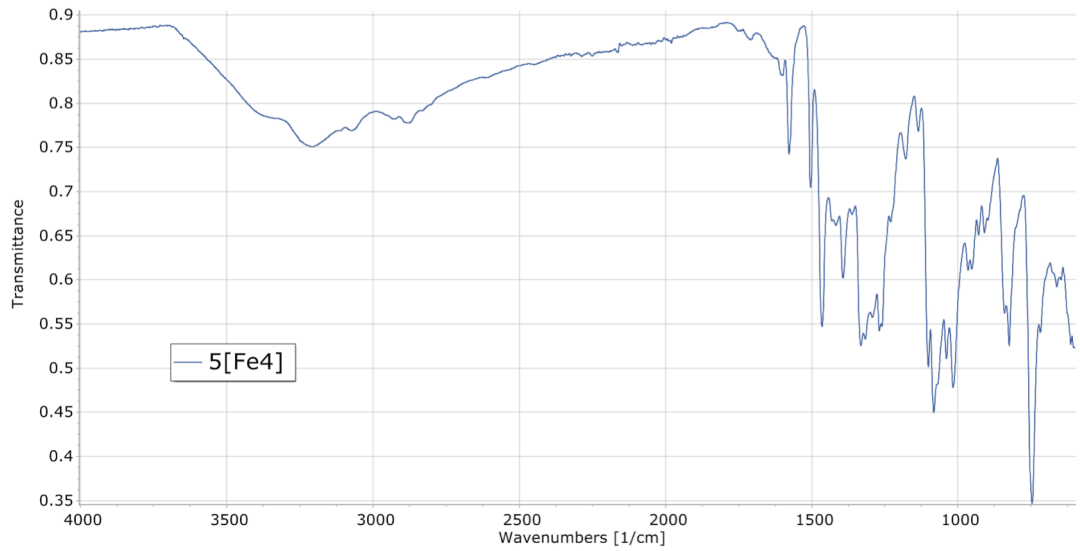


Figure S5. Infrared spectrum of Compound **5**.

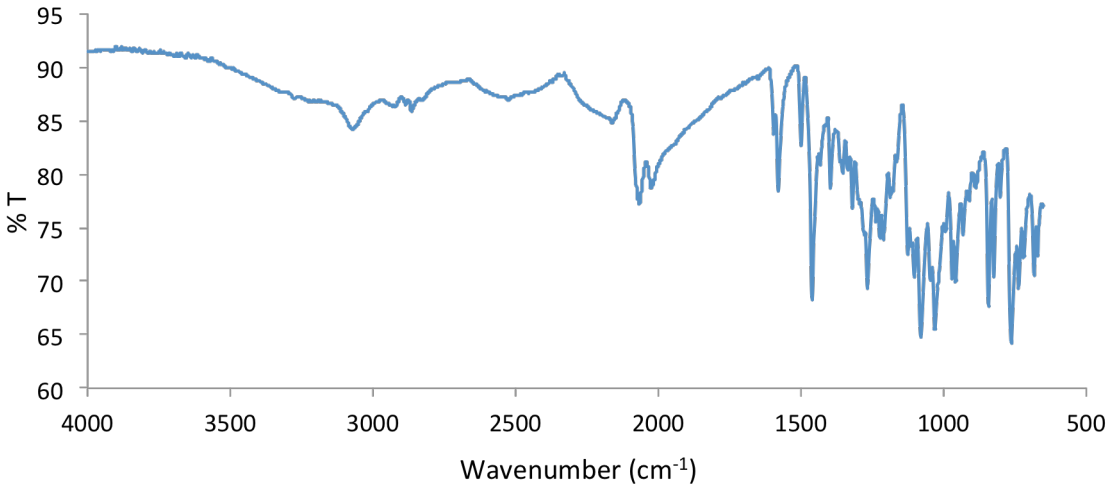


Figure S6. Infrared spectrum of Compound **6**.

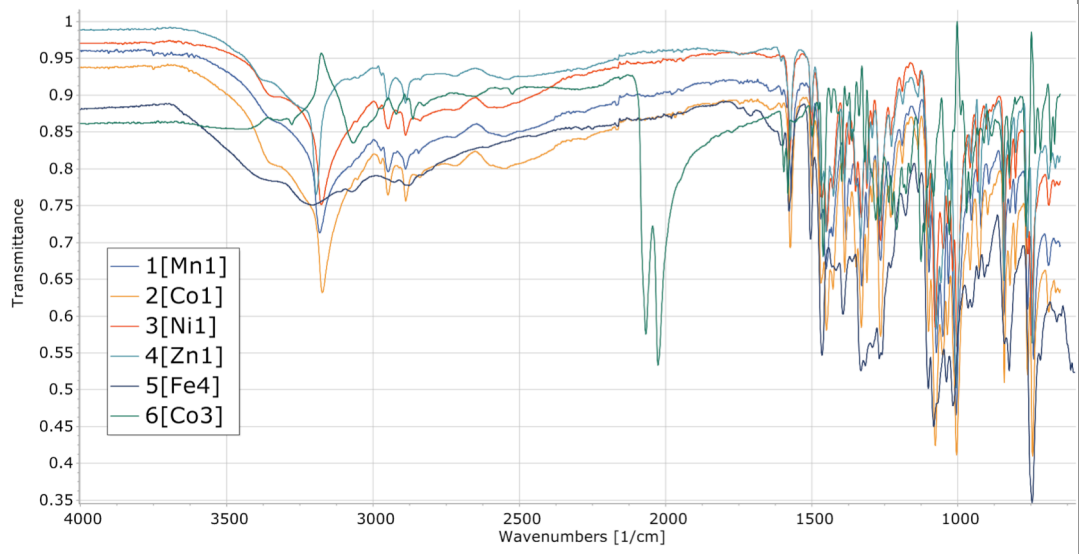


Figure S7. Overlay of the infrared spectra for compounds **1** – **6.**

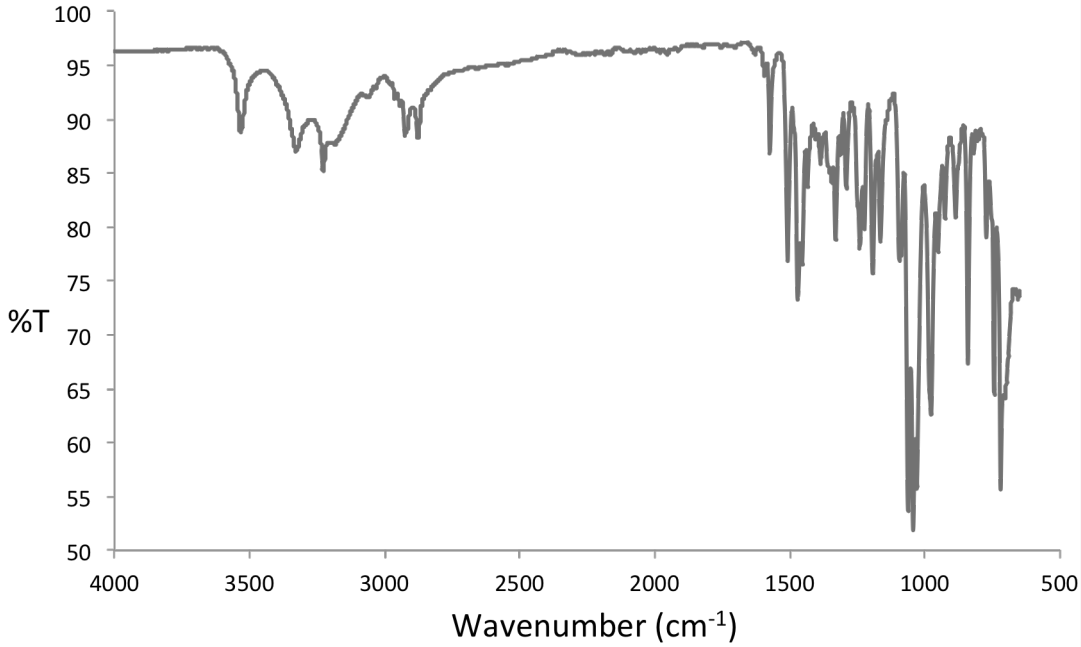


Figure S8. Infrared spectrum of isolated $\mathbf{L_2H_3}$ is shown.

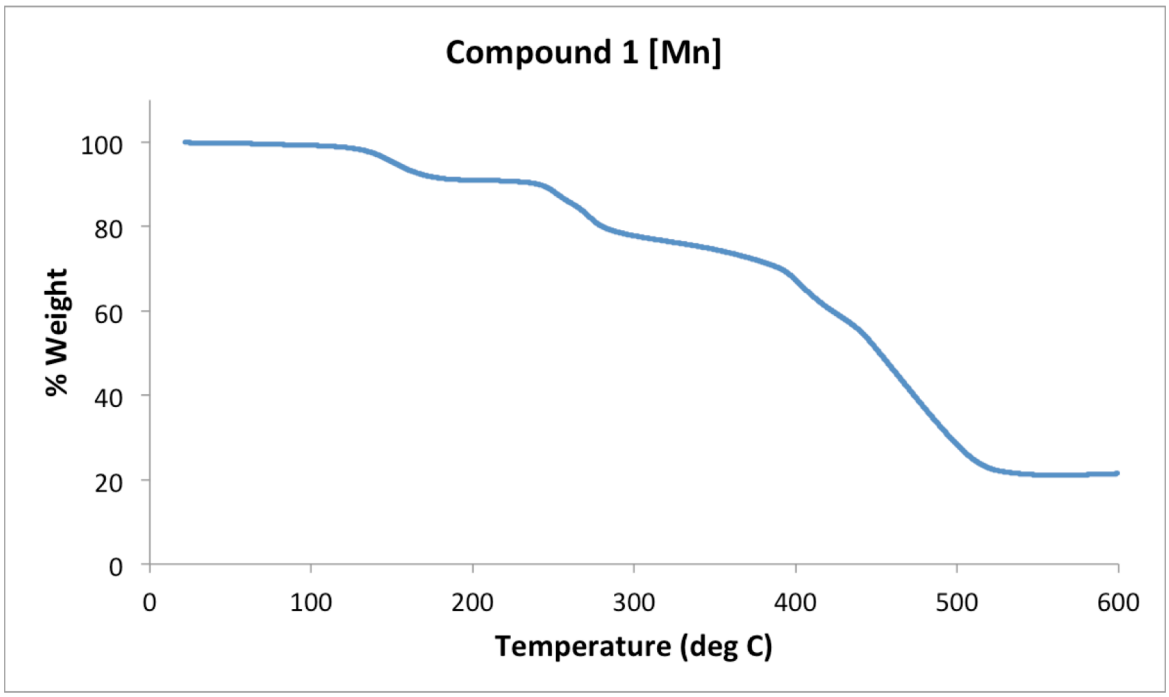


Figure S9. Thermogravimetric analysis (TGA) of Compound **1** is presented.

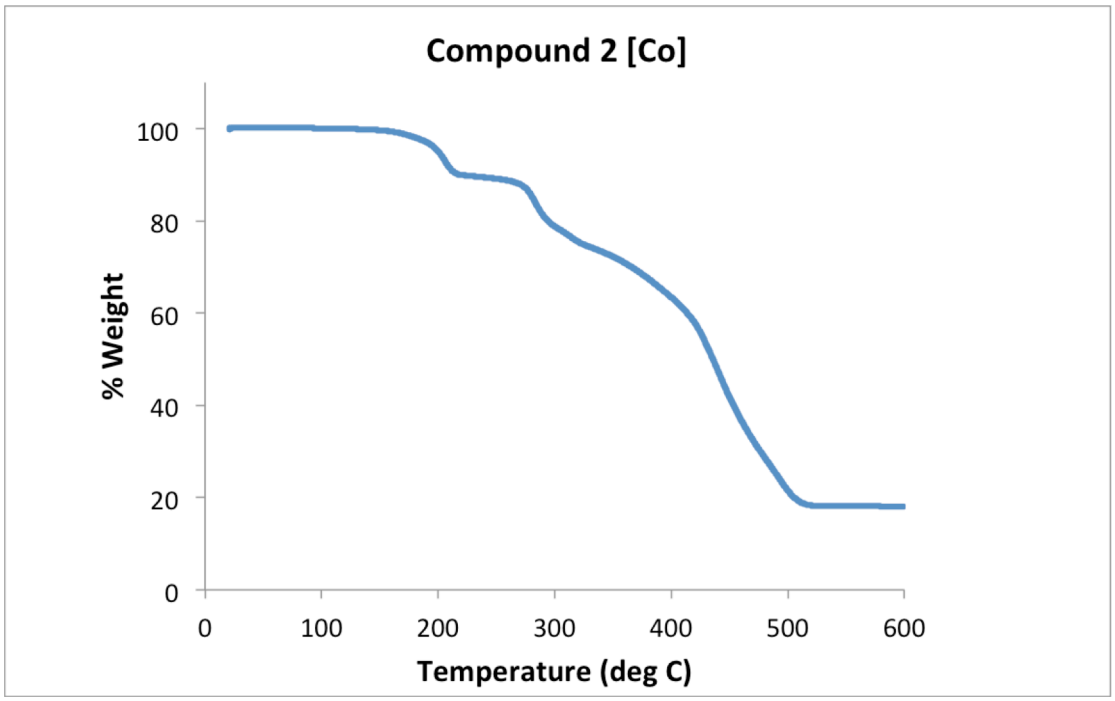


Figure S10. Thermogravimetric analysis (TGA) of Compound **2** is presented.

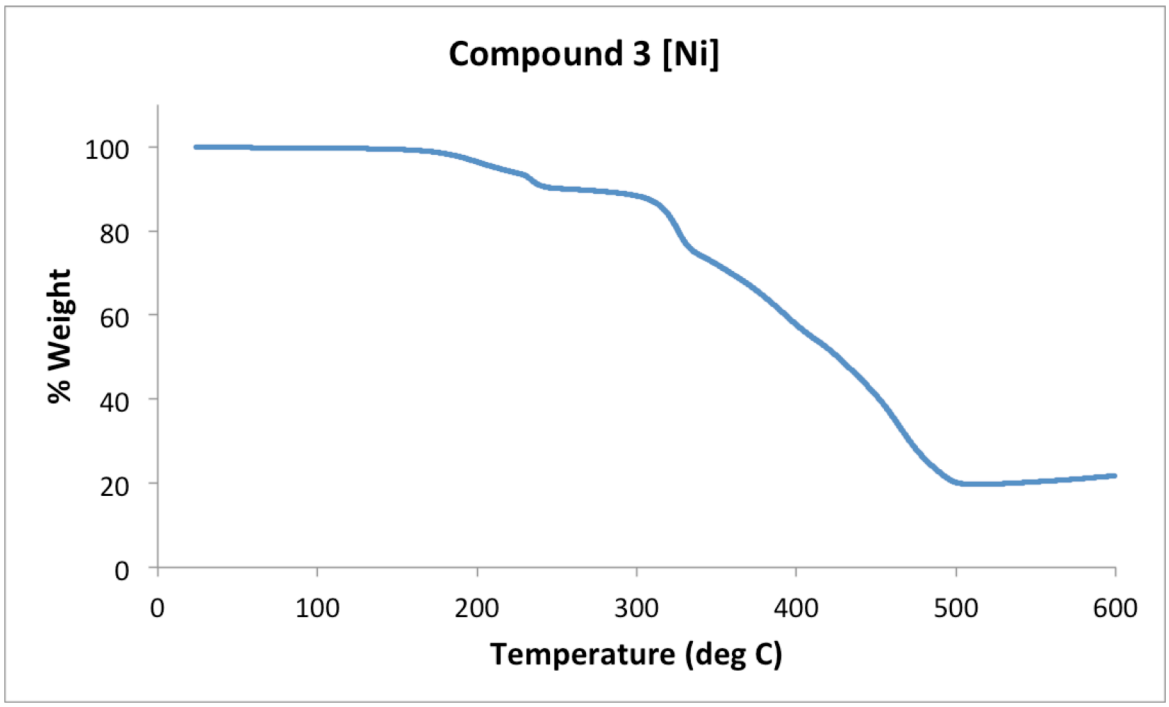


Figure S11. Thermogravimetric analysis (TGA) of Compound **3** is presented.

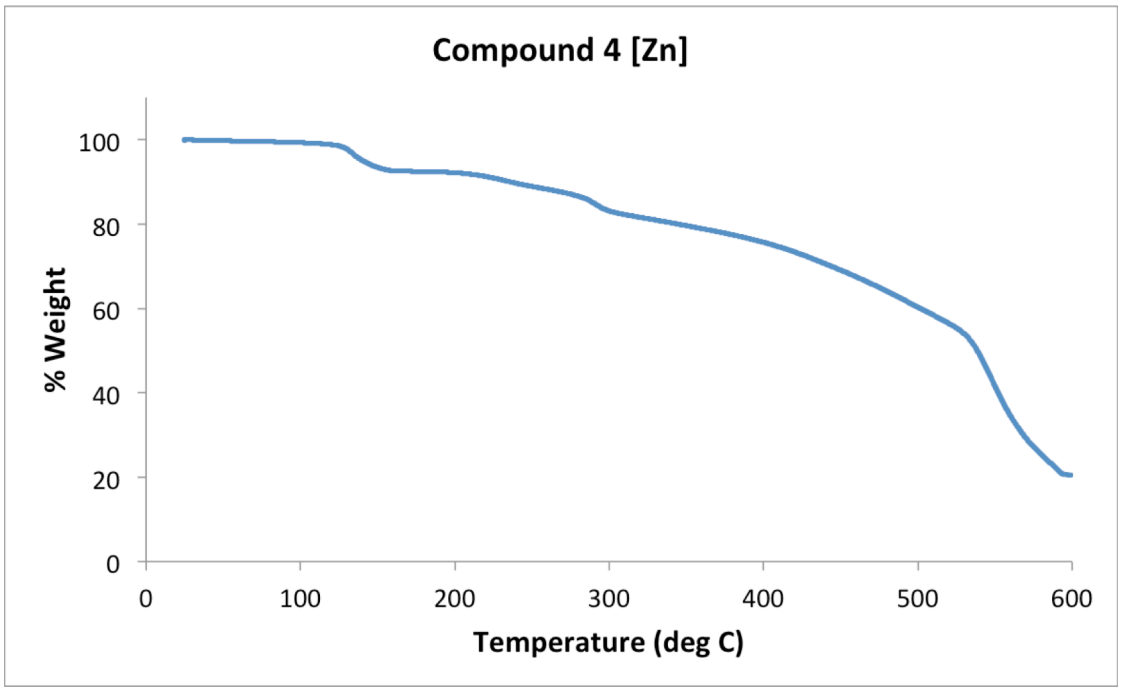


Figure S12. Thermogravimetric analysis (TGA) of Compound **4** is presented.

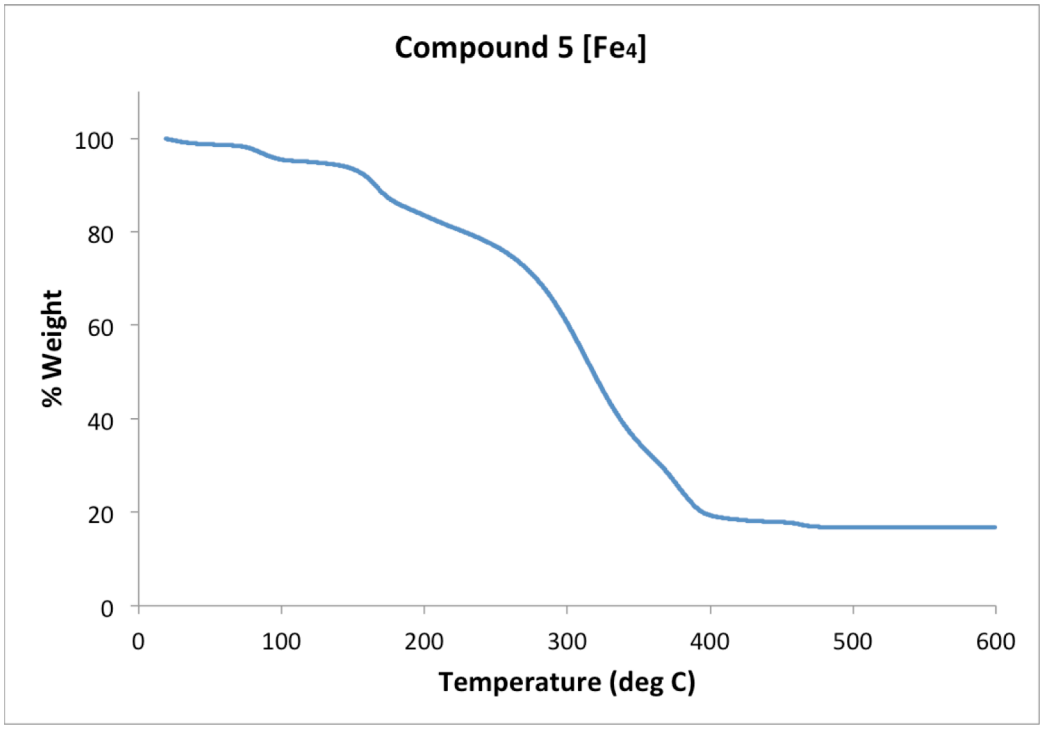


Figure S13. Thermogravimetric analysis (TGA) of Compound **5** is presented.

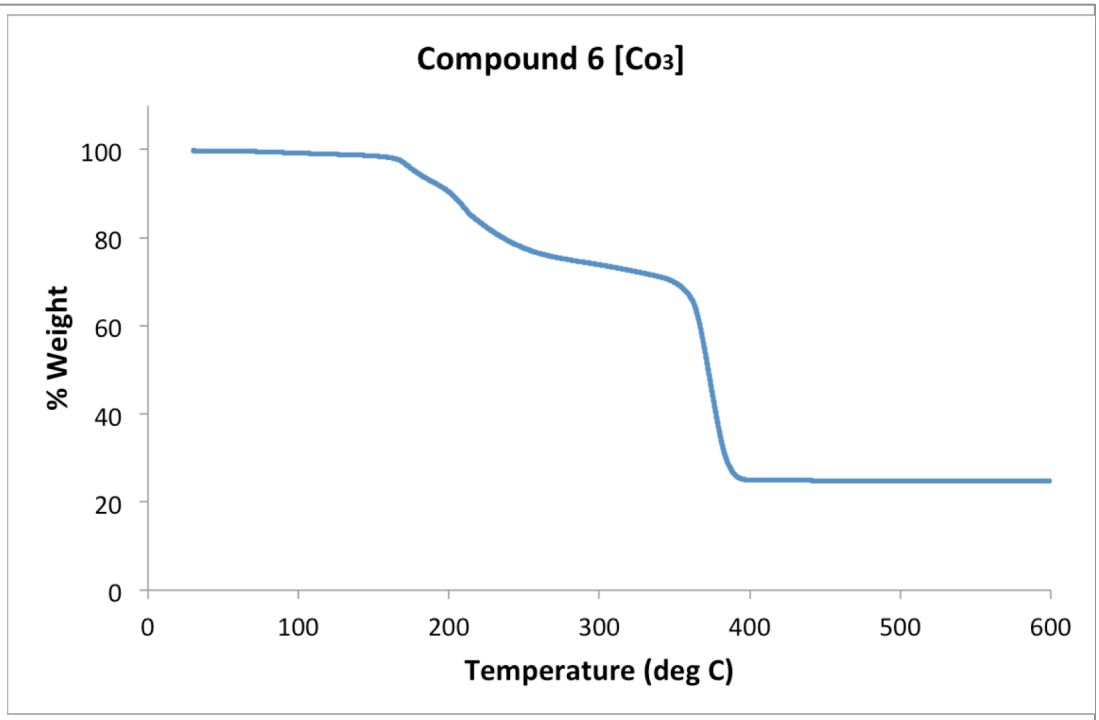


Figure S14. Thermogravimetric analysis (TGA) of Compound **5** is presented.

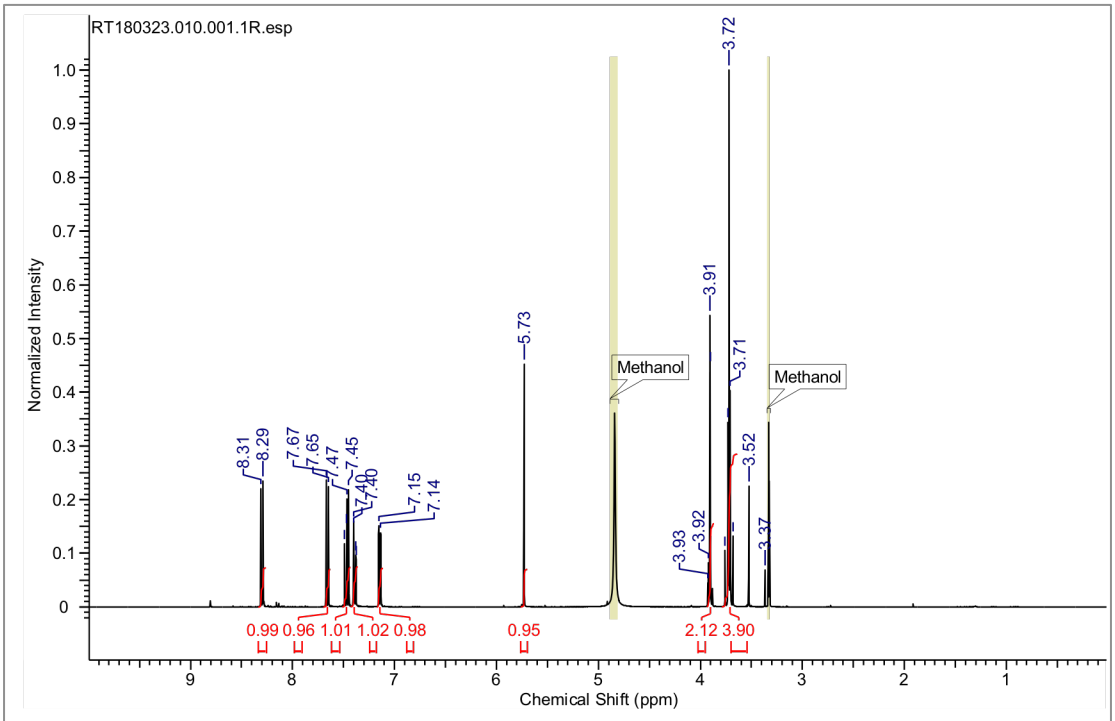


Figure S15. ^{1}H NMR spectra of $\mathbf{L_2H_3}$ in CH_3OD.

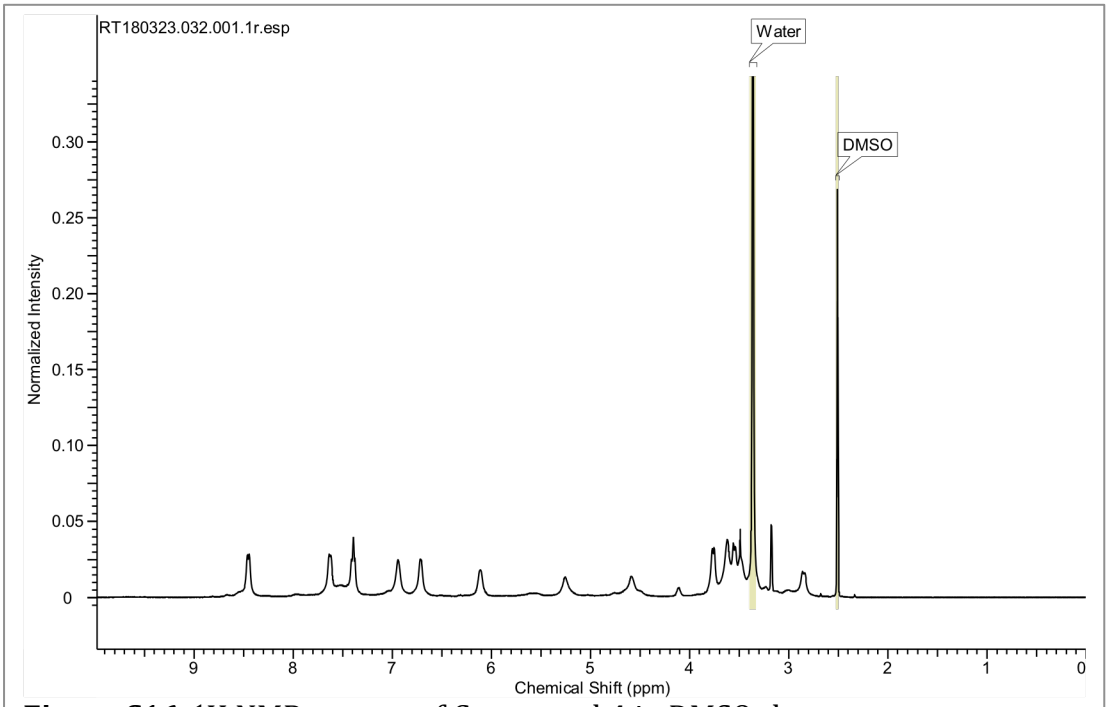


Figure S16. ^{1}H NMR spectra of Compound **4** in DMSO-d_6.

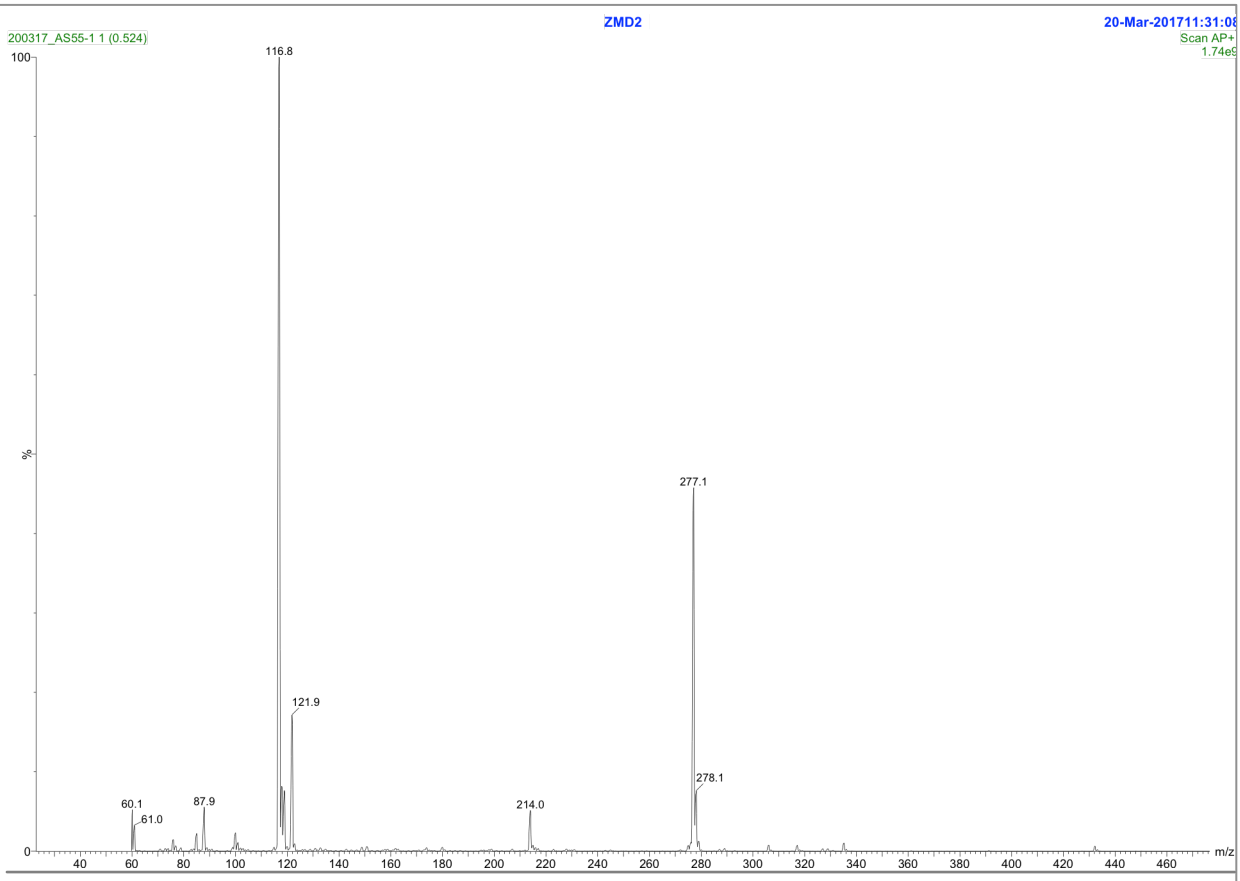


Figure S17. ESI-MS of the isolated ligand **H_3L_2** is shown. The peak at 277($^m/_z$) corresponds to $[H_3L_2 + H^+]^+$.

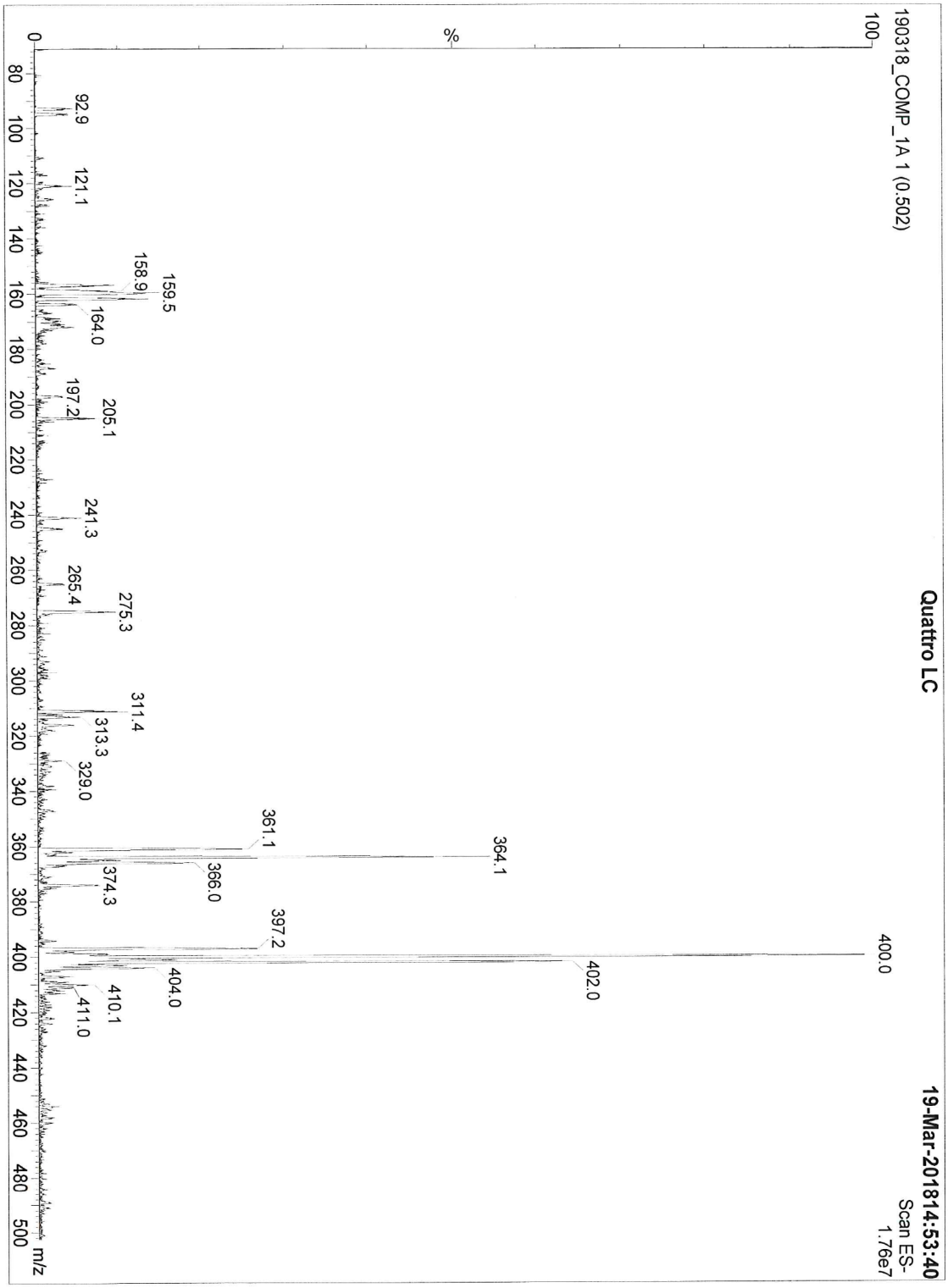


Figure S18. ESI-MS of Compound **1** is shown. The peak at 400($^{m}/_{z}$) corresponds to the [1+H^+]$^+$ fragment and the peak at 364($^{m}/_{z}$) corresponds to the [**1**-Cl^-]$^+$ fragment.

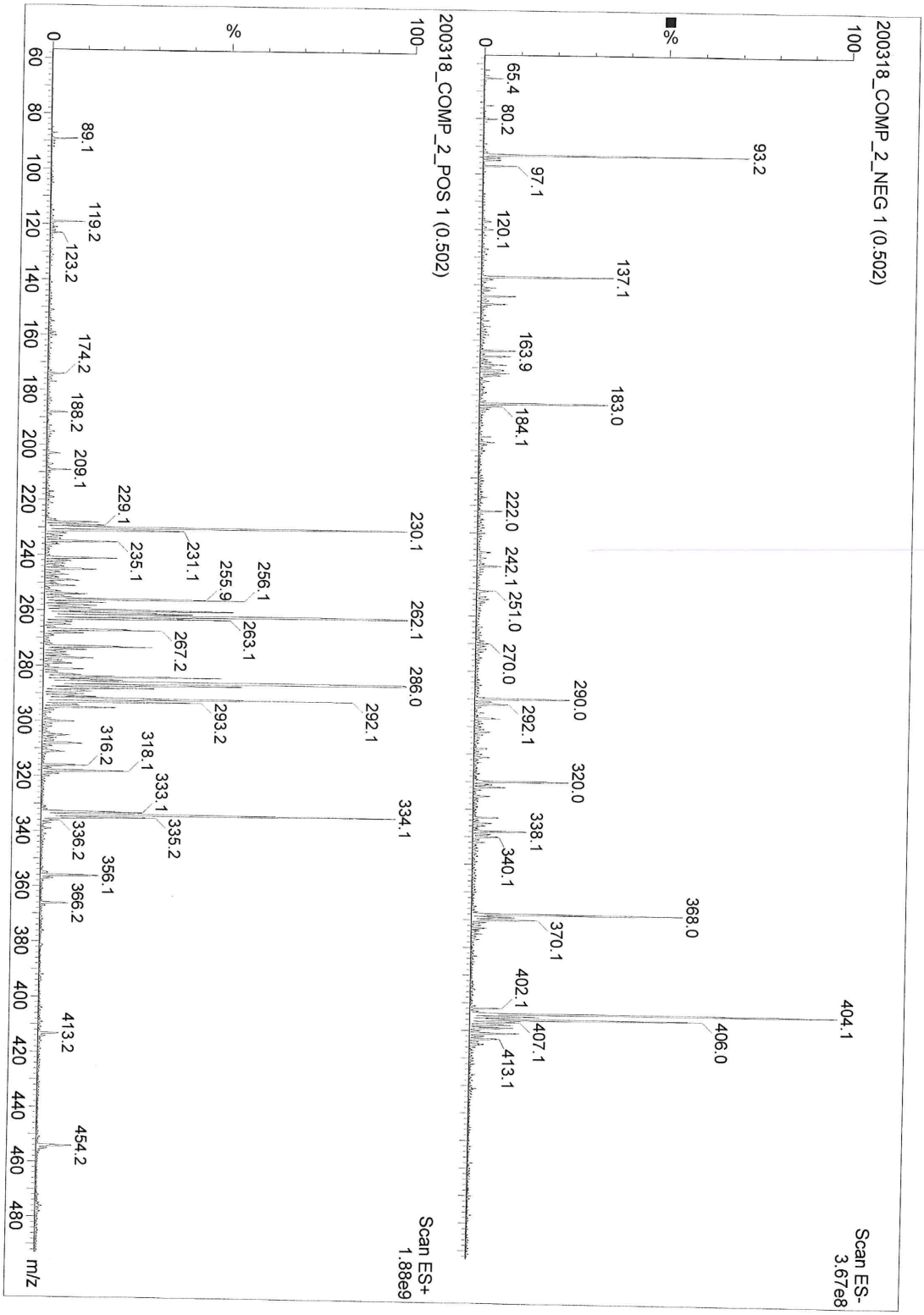


Figure S19. ESI-MS of Compound **2** is shown. The peak at 404($^{m}/_{z}$) corresponds to the [**2**+H^{+}]$^{+}$ fragment and the peak at 368($^{m}/_{z}$) corresponds to the [**2**-Cl^{-}]$^{+}$ fragment.

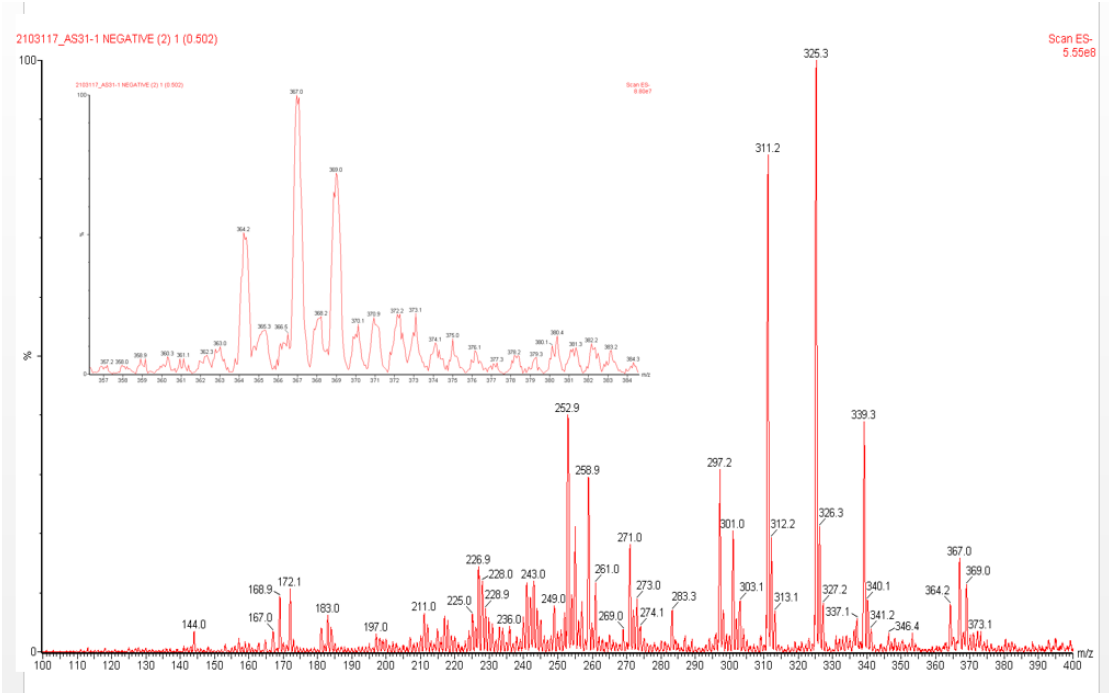


Figure S20. ESI-MS of Compound **3** is shown. The peak at 369($^{m}/_{z}$) corresponds to the [**3**-Cl^{-}]$^{+}$ fragment.

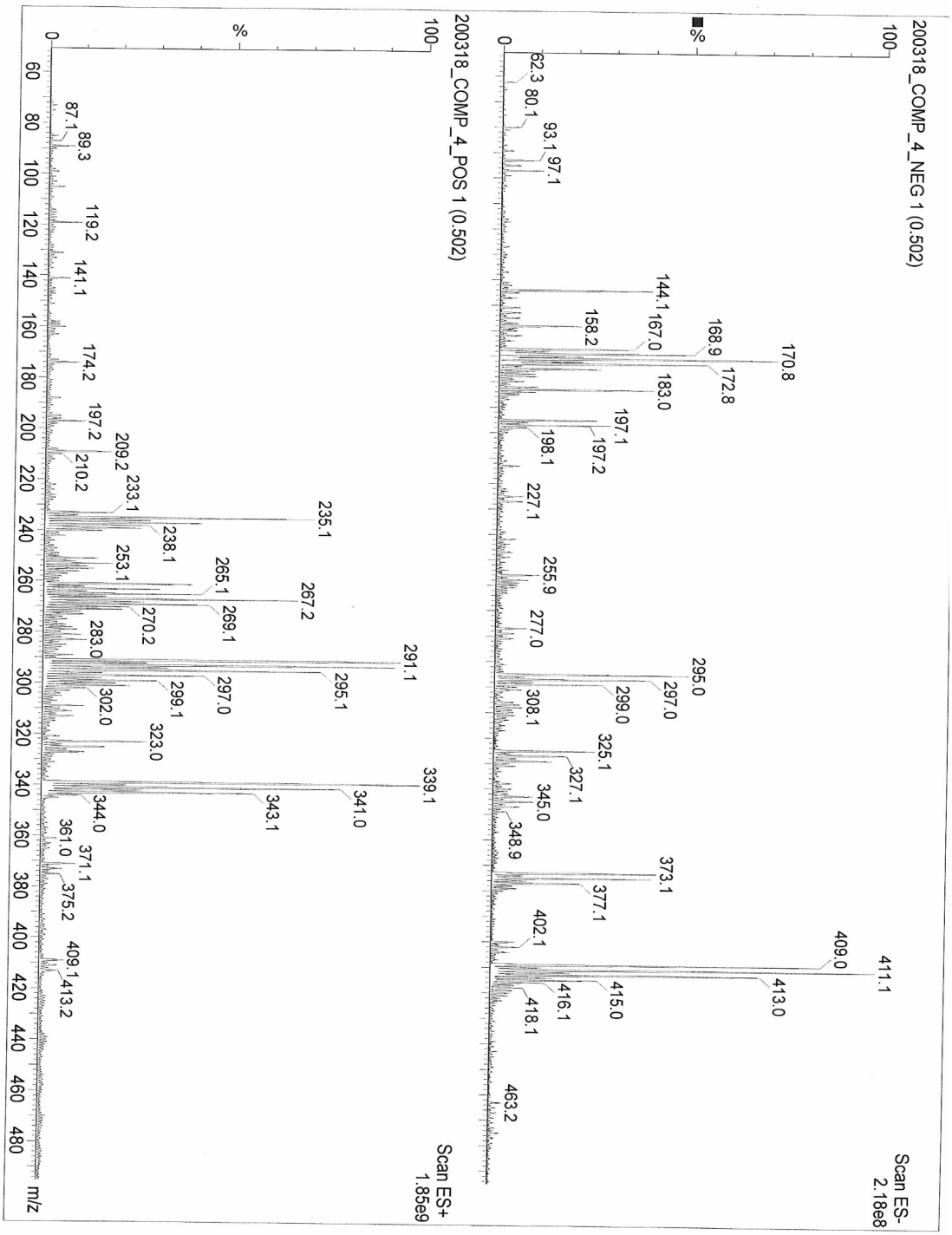


Figure S21. ESI-MS of Compound **4** is shown. The peak at 339($^{m}/_{z}$) corresponds to the [**4** - Cl^{-}]$^{+}$ fragment.

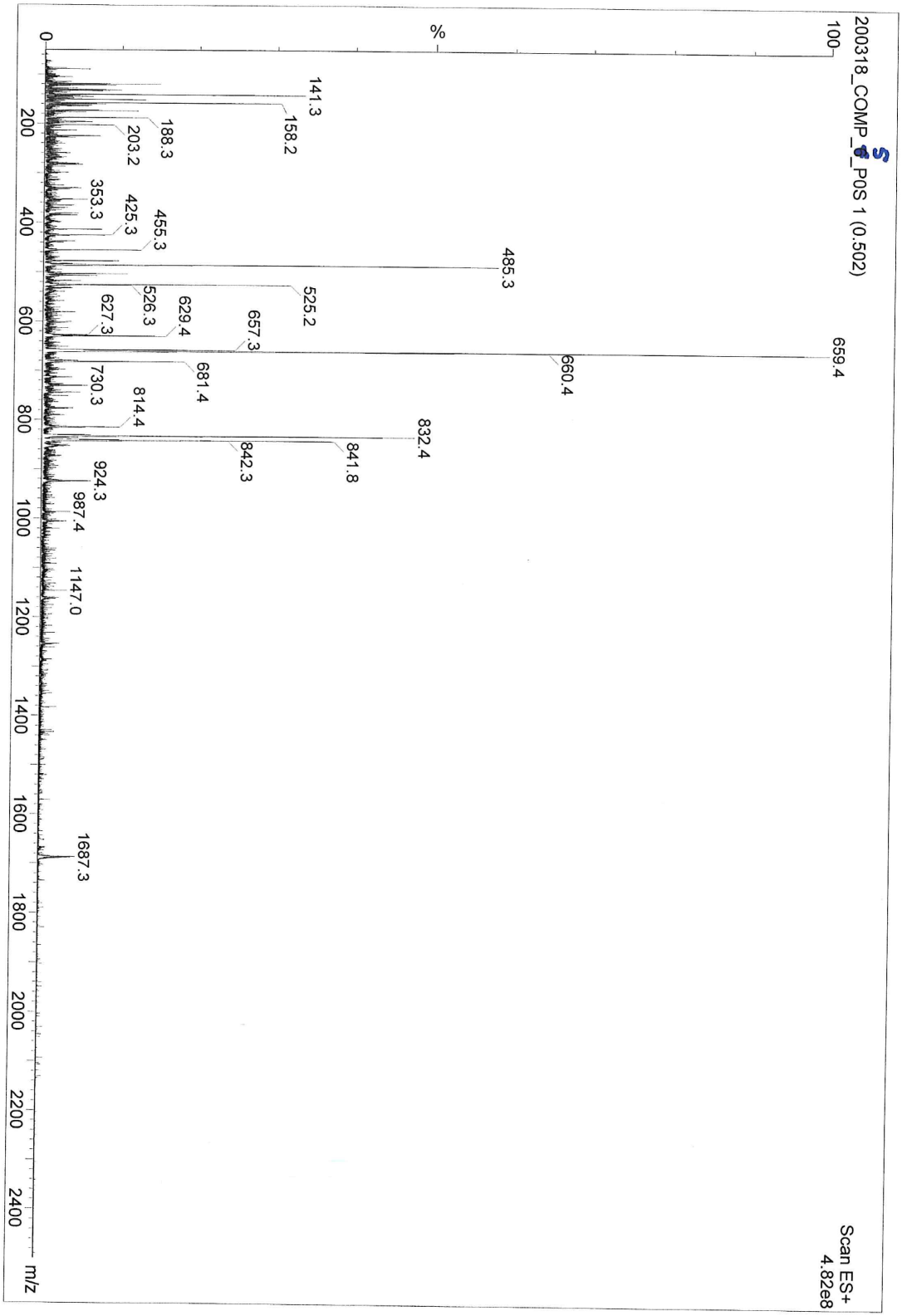


Figure S22. ESI-MS of Compound **5** is shown. The peak at 841($^{m}/_{z}$) corresponds to the $[Fe_4O(HL_2)_2(H_3L_3)_2]^{2+}$ fragment.

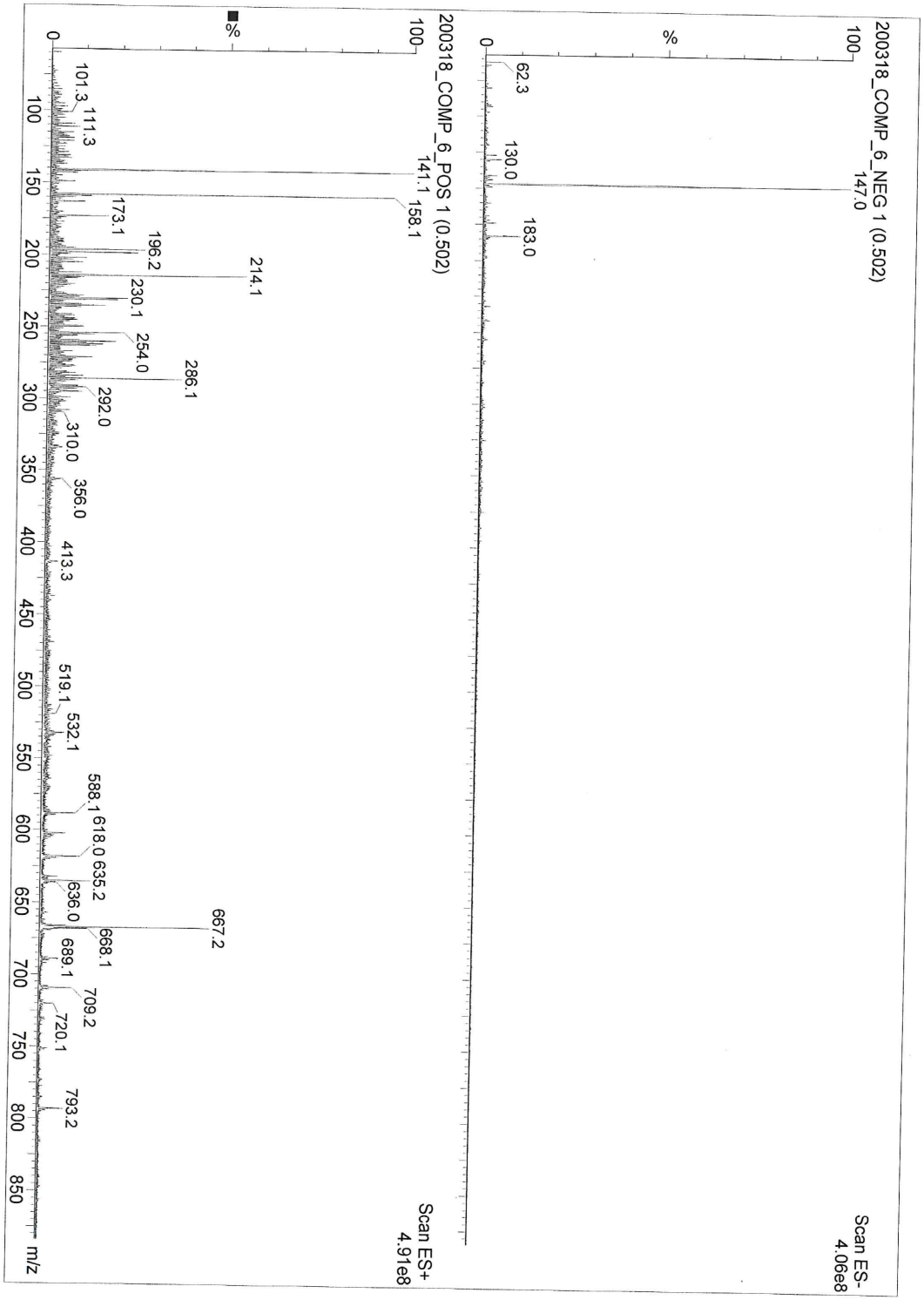


Figure S23. ESI-MS of Compound **6** is shown. The compound seems unstable at the ESI conditions like many polynuclear complexes, and only shows a minor peak at 793($^{m}/_{z}$) which might arise from [**6** - OH]$^{+}$.

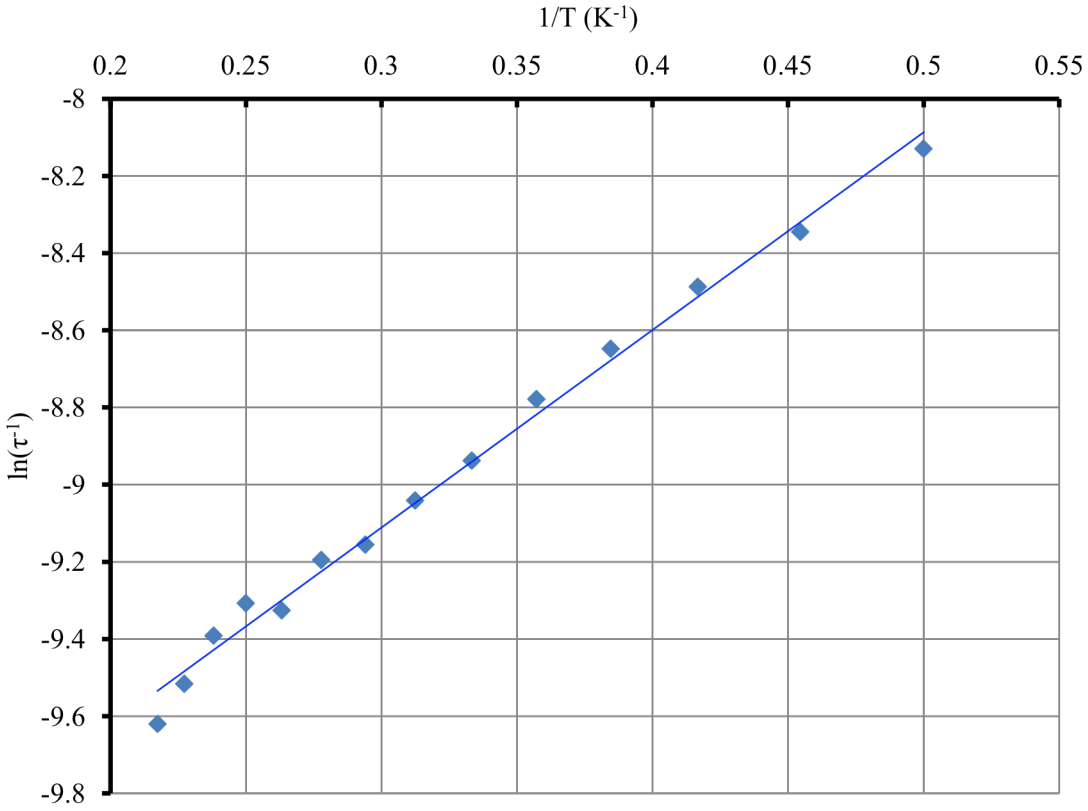


Figure S24. Arrhenius plot for Compound **6**.

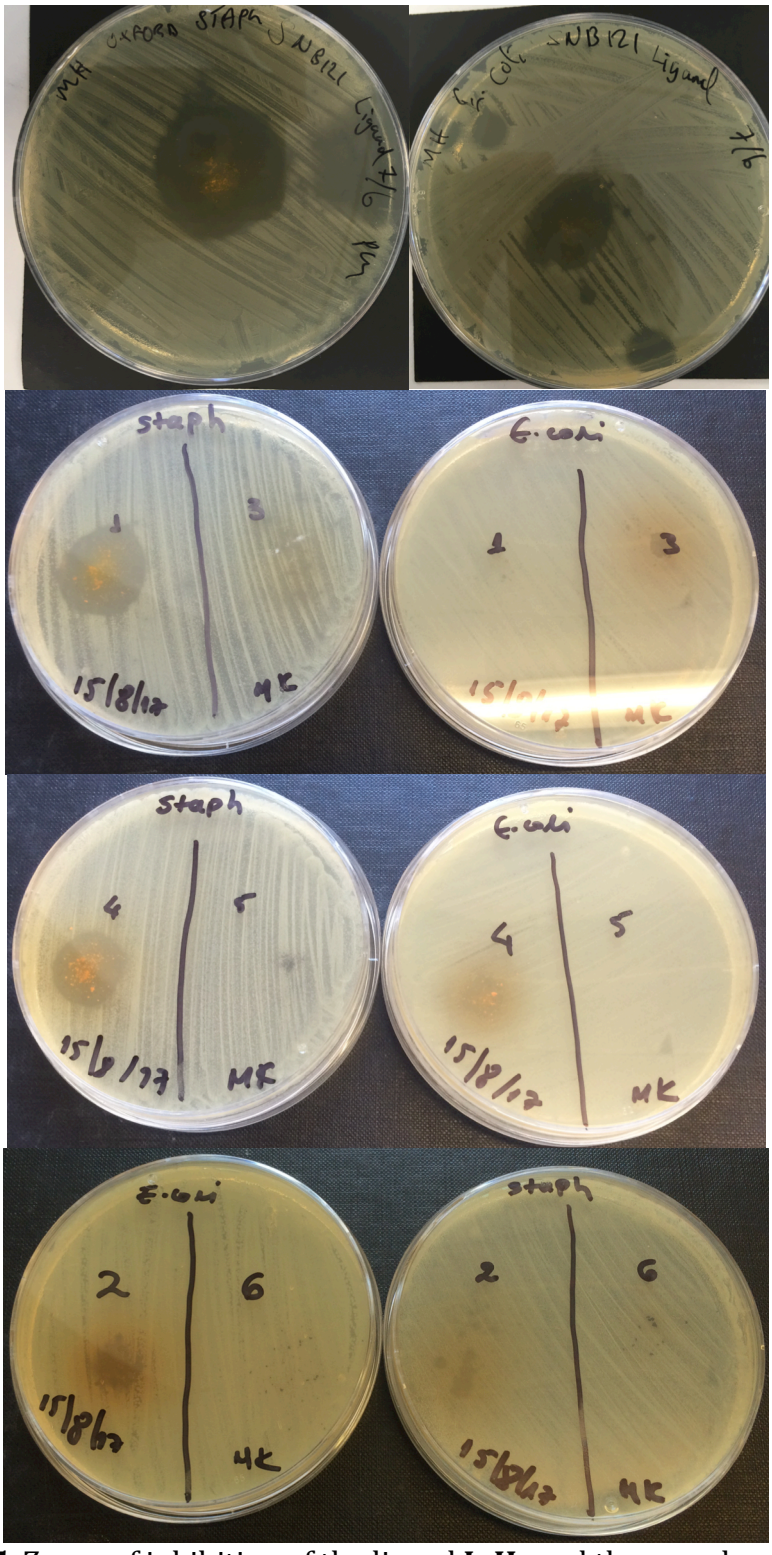


Figure S25. Zones of inhibition of the ligand L_2H_3 and the complexes **1-6**, against *S. aureus* (a) and *E.coli* (b).

Single-crystal X-ray analysis of Compound 1:

Data was collected with an Bruker D8 QUEST area detector diffractometer equipped with with MoK$_\alpha$ radiation, a graded multilayer mirror monochromator (λ = 0.71073 Å) and a PHOTON-100 CMOS detector using an oil-coated shock-cooled crystal at 100(2) K. Absorption effects were corrected semi-empirical using multiscanned reflexions (SADABS (Bruker AXS Inc., 2016)). Cell constants were refined using 9973 of observed reflections of the data collection. The structure was solved by direct methods by using the program XT V2014/1 (Bruker AXS Inc., 2014) and refined by full matrix least squares procedures on F^2 using SHELXL-2018/1 (Sheldrick, 2018). The non-hydrogen atoms have been refined anisotropically, carbon bonded hydrogen atoms were included at calculated positions and refined using the 'riding model' with isotropic temperature factors at 1.2 times (for CH_3 groups 1.5 times) that of the preceding carbon atom. CH_3 groups were allowed to rotate about the bond to their next atom to fit the electron density. Nitrogen or oxygen bonded hydrogen atoms were located and allowed to refine isotropically.

Table S1. Bond lengths [Å] and angles [°] for Compound 1.

Mn1-O2	2.1417(13)	C6-H6	0.9500
Mn1-N1	2.1808(14)	C7-C8	1.424(3)
Mn1-O1	2.1953(12)	C8-C9	1.370(3)
Mn1-O3	2.2695(13)	C8-H8	0.9500
Mn1-N2	2.3468(14)	C9-C10	1.410(2)
Mn1-Cl1	2.4551(5)	C9-H9	0.9500
O1-C3	1.334(2)	C10-C11	1.527(2)
O2-C16	1.432(2)	C11-H11	1.0000
O2-H2	0.88(3)	C12-C13	1.544(2)
O3-C14	1.427(2)	C12-H12A	0.9900
O3-H3A	0.84(2)	C12-H12B	0.9900
O4-C12	1.410(2)	C13-C15	1.526(3)
O4-C11	1.418(2)	C13-C14	1.532(2)
N1-C10	1.316(2)	C14-H14A	0.9900
N1-C2	1.357(2)	C14-H14B	0.9900
N2-C11	1.466(2)	C15-O5A	1.328(11)
N2-C13	1.491(2)	C15-O5	1.440(3)
N2-H3	0.83(2)	C15-H15A	0.9900
C2-C7	1.415(2)	C15-H15B	0.9900
C2-C3	1.434(2)	C15-H15C	0.9900
C3-C4	1.388(2)	C15-H15D	0.9900
C4-C5	1.409(3)	C16-H16A	0.9800
C4-H4	0.9500	C16-H16B	0.9800
C5-C6	1.372(3)	C16-H16C	0.9800
C5-H5	0.9500	O5-H5A	0.8400
C6-C7	1.414(3)	O5A-H5A1	0.8400
O2-Mn1-N1	170.09(5)	Mn1-O2-H2	122.6(16)
O2-Mn1-O1	109.92(5)	C14-O3-Mn1	112.07(10)
N1-Mn1-O1	74.98(5)	C14-O3-H3A	107.9(17)
O2-Mn1-O3	85.88(5)	Mn1-O3-H3A	125.0(16)
N1-Mn1-O3	85.52(5)	C12-O4-C11	109.48(13)
O1-Mn1-O3	89.87(5)	C10-N1-C2	120.77(14)
O2-Mn1-N2	101.14(5)	C10-N1-Mn1	123.42(11)
N1-Mn1-N2	71.82(5)	C2-N1-Mn1	115.80(11)
O1-Mn1-N2	144.28(5)	C11-N2-C13	104.66(13)
O3-Mn1-N2	74.91(5)	C11-N2-Mn1	111.93(10)
O2-Mn1-Cl1	94.85(4)	C13-N2-Mn1	111.52(10)
N1-Mn1-Cl1	93.27(4)	C11-N2-H3	108.8(14)
O1-Mn1-Cl1	94.83(4)	C13-N2-H3	108.2(15)
O3-Mn1-Cl1	174.68(3)	Mn1-N2-H3	111.4(15)
N2-Mn1-Cl1	99.79(4)	N1-C2-C7	121.84(15)
C3-O1-Mn1	114.82(10)	N1-C2-C3	115.89(15)
C16-O2-Mn1	122.88(11)	C7-C2-C3	122.26(15)
C16-O2-H2	110.1(16)	O1-C3-C4	124.62(16)

O1-C3-C2	118.48(15)	H12A-C12-H12B	108.6
C4-C3-C2	116.90(16)	N2-C13-C15	109.22(15)
C3-C4-C5	120.82(17)	N2-C13-C14	109.72(14)
C3-C4-H4	119.6	C15-C13-C14	111.09(15)
C5-C4-H4	119.6	N2-C13-C12	103.30(14)
C6-C5-C4	122.29(17)	C15-C13-C12	113.67(16)
C6-C5-H5	118.9	C14-C13-C12	109.53(15)
C4-C5-H5	118.9	O3-C14-C13	111.45(14)
C5-C6-C7	119.32(16)	O3-C14-H14A	109.3
C5-C6-H6	120.3	C13-C14-H14A	109.3
C7-C6-H6	120.3	O3-C14-H14B	109.3
C6-C7-C2	118.39(16)	C13-C14-H14B	109.3
C6-C7-C8	125.39(16)	H14A-C14-H14B	108.0
C2-C7-C8	116.21(16)	O5A-C15-C13	133.2(8)
C9-C8-C7	120.64(16)	O5-C15-C13	109.76(19)
C9-C8-H8	119.7	O5-C15-H15A	109.7
C7-C8-H8	119.7	C13-C15-H15A	109.7
C8-C9-C10	118.97(16)	O5-C15-H15B	109.7
C8-C9-H9	120.5	C13-C15-H15B	109.7
C10-C9-H9	120.5	H15A-C15-H15B	108.2
N1-C10-C9	121.54(16)	O5A-C15-H15C	103.9
N1-C10-C11	115.19(14)	C13-C15-H15C	103.9
C9-C10-C11	123.26(15)	O5A-C15-H15D	103.9
O4-C11-N2	107.50(13)	C13-C15-H15D	103.9
O4-C11-C10	111.12(14)	H15C-C15-H15D	105.4
N2-C11-C10	110.99(13)	O2-C16-H16A	109.5
O4-C11-H11	109.1	O2-C16-H16B	109.5
N2-C11-H11	109.1	H16A-C16-H16B	109.5
C10-C11-H11	109.1	O2-C16-H16C	109.5
O4-C12-C13	106.98(14)	H16A-C16-H16C	109.5
O4-C12-H12A	110.3	H16B-C16-H16C	109.5
C13-C12-H12A	110.3	C15-O5-H5A	109.5
O4-C12-H12B	110.3	C15-O5A-H5A1	109.5
C13-C12-H12B	110.3		

Single-crystal X-ray analysis of compound 2:

Data was collected with an Bruker D8 QUEST area detector diffractometer equipped with with MoK$_\alpha$ radiation, a graded multilayer mirror monochromator (λ = 0.71073 Å) and a PHOTON-100 CMOS detector using an oil-coated shock-cooled crystal at 100(2) K. Absorption effects were corrected semi-empirical using multiscanned reflexions (SADABS (Bruker AXS Inc., 2016)). Cell constants were refined using 9972 of observed reflections of the data collection. The structure was solved by direct methods by using the program XT V2014/1 (Bruker AXS Inc., 2014) and refined by full matrix least squares procedures on F^2 using SHELXL-2018/1 (Sheldrick, 2018). The non-hydrogen atoms have been refined anisotropically, carbon bonded hydrogen atoms were included at calculated positions and refined using the 'riding model' with isotropic temperature factors at 1.2 times (for CH_3 groups 1.5 times) that of the preceding carbon atom. CH_3 groups were allowed to rotate about the bond to their next atom to fit the electron density. Nitrogen or oxygen bonded hydrogen atoms were located and allowed to refine isotropically.

Table S2 Bond lengths [Å] and angles [°] for Compound 2.

Co1-N1	2.0474(14)	C4-H4	0.9500
Co1-O2	2.0528(13)	C5-C6	1.374(3)
Co1-O1	2.1189(12)	C5-H5	0.9500
Co1-O3	2.1708(13)	C6-C7	1.418(3)
Co1-N2	2.2100(15)	C6-H6	0.9500
Co1-Cl1	2.4150(5)	C7-C8	1.421(3)
O1-C3	1.333(2)	C8-C9	1.371(3)
O2-C16	1.428(2)	C8-H8	0.9500
O2-H2	0.86(3)	C9-C10	1.413(2)
O3-C14	1.428(2)	C9-H9	0.9500
O3-H3A	0.78(3)	C10-C11	1.521(2)
O4-C12	1.409(2)	C11-H11	1.0000
O4-C11	1.414(2)	C12-C13	1.541(2)
O5-C15	1.420(3)	C12-H12A	0.9900
O5-H5A	0.70(4)	C12-H12B	0.9900
N1-C10	1.314(2)	C13-C14	1.528(3)
N1-C2	1.356(2)	C13-C15	1.528(3)
N2-C11	1.476(2)	C14-H14A	0.9900
N2-C13	1.489(2)	C14-H14B	0.9900
N2-H3	0.83(2)	C15-H15A	0.9900
C2-C7	1.411(2)	C15-H15B	0.9900
C2-C3	1.434(2)	C16-H16A	0.9800
C3-C4	1.387(2)	C16-H16B	0.9800
C4-C5	1.410(3)	C16-H16C	0.9800
N1-Co1-O2	174.99(6)	N2-Co1-Cl1	99.37(4)
N1-Co1-O1	78.32(5)	C3-O1-Co1	112.74(10)
O2-Co1-O1	103.41(5)	C16-O2-Co1	124.41(11)
N1-Co1-O3	88.72(5)	C16-O2-H2	111.3(18)
O2-Co1-O3	86.63(5)	Co1-O2-H2	118.5(18)
O1-Co1-O3	88.54(5)	C14-O3-Co1	111.39(10)
N1-Co1-N2	75.59(5)	C14-O3-H3A	108.5(19)
O2-Co1-N2	101.58(5)	Co1-O3-H3A	125.6(19)
O1-Co1-N2	150.85(5)	C12-O4-C11	109.91(13)
O3-Co1-N2	78.15(5)	C15-O5-H5A	113(3)
N1-Co1-Cl1	90.85(4)	C10-N1-C2	120.91(15)
O2-Co1-Cl1	93.71(4)	C10-N1-Co1	123.07(12)
O1-Co1-Cl1	93.77(4)	C2-N1-Co1	115.96(11)
O3-Co1-Cl1	177.52(4)	C11-N2-C13	104.61(13)

C11-N2-Co1	111.38(10)	N2-C11-C10	110.14(13)
C13-N2-Co1	111.59(10)	O4-C11-H11	109.3
C11-N2-H3	107.3(15)	N2-C11-H11	109.3
C13-N2-H3	108.6(16)	C10-C11-H11	109.3
Co1-N2-H3	112.9(16)	O4-C12-C13	107.03(15)
N1-C2-C7	121.83(16)	O4-C12-H12A	110.3
N1-C2-C3	114.94(15)	C13-C12-H12A	110.3
C7-C2-C3	123.22(16)	O4-C12-H12B	110.3
O1-C3-C4	125.59(16)	C13-C12-H12B	110.3
O1-C3-C2	117.97(15)	H12A-C12-H12B	108.6
C4-C3-C2	116.43(16)	N2-C13-C14	109.37(15)
C3-C4-C5	120.71(17)	N2-C13-C15	109.06(15)
C3-C4-H4	119.6	C14-C13-C15	111.27(15)
C5-C4-H4	119.6	N2-C13-C12	103.37(14)
C6-C5-C4	122.58(17)	C14-C13-C12	109.88(16)
C6-C5-H5	118.7	C15-C13-C12	113.55(16)
C4-C5-H5	118.7	O3-C14-C13	110.82(14)
C5-C6-C7	119.18(17)	O3-C14-H14A	109.5
C5-C6-H6	120.4	C13-C14-H14A	109.5
C7-C6-H6	120.4	O3-C14-H14B	109.5
C2-C7-C6	117.82(16)	C13-C14-H14B	109.5
C2-C7-C8	116.28(16)	H14A-C14-H14B	108.1
C6-C7-C8	125.89(17)	O5-C15-C13	111.02(17)
C9-C8-C7	120.82(16)	O5-C15-H15A	109.4
C9-C8-H8	119.6	C13-C15-H15A	109.4
C7-C8-H8	119.6	O5-C15-H15B	109.4
C8-C9-C10	118.61(16)	C13-C15-H15B	109.4
C8-C9-H9	120.7	H15A-C15-H15B	108.0
C10-C9-H9	120.7	O2-C16-H16A	109.5
N1-C10-C9	121.51(16)	O2-C16-H16B	109.5
N1-C10-C11	114.17(14)	H16A-C16-H16B	109.5
C9-C10-C11	124.32(15)	O2-C16-H16C	109.5
O4-C11-N2	107.82(13)	H16A-C16-H16C	109.5
O4-C11-C10	111.02(15)	H16B-C16-H16C	109.5

Symmetry transformations used to generate equivalent atoms:

Single-crystal X-ray analysis of Compound 3:

Data was collected with an Bruker D8 QUEST area detector diffractometer equipped with with MoK_a radiation, a graded multilayer mirror monochromator (l = 0.71073 Å) and a PHOTON-100 CMOS detector using an oil-coated shock-cooled crystal at 100(2) K. Absorption effects were corrected semi-empirical using multiscanned reflexions (SADABS (Bruker AXS Inc., 2016)). Cell constants were refined using 9901 of observed reflections of the data collection. The structure was solved by direct methods by using the program XT V2014/1 (Bruker AXS Inc., 2014) and refined by full matrix least squares procedures on F^2 using SHELXL-2018/1 (Sheldrick, 2018). The non-hydrogen atoms have been refined anisotropically, carbon bonded hydrogen atoms were included at calculated positions and refined using the 'riding model' with isotropic temperature factors at 1.2 times (for CH_3 groups 1.5 times) that of the preceding carbon atom. CH_3 groups were allowed to rotate about the bond to their next atom to fit the electron density. Nitrogen or oxygen bonded hydrogen atoms were located and allowed to refine isotropically.

Table S3. Bond lengths [Å] and angles [°] for Compound 3.

Ni1-N1	1.9792(14)	C4-H4	0.9500
Ni1-O2	2.0475(13)	C5-C6	1.376(3)
Ni1-O1	2.1066(12)	C5-H5	0.9500
Ni1-O3	2.1127(12)	C6-C7	1.419(2)
Ni1-N2	2.1672(14)	C6-H6	0.9500
Ni1-Cl1	2.3883(5)	C7-C8	1.425(2)
O1-C3	1.333(2)	C8-C9	1.374(3)
O2-C16	1.428(2)	C8-H8	0.9500
O2-H2	0.80(3)	C9-C10	1.409(2)
O3-C14	1.428(2)	C9-H9	0.9500
O3-H3A	0.82(3)	C10-C11	1.524(2)
O4-C11	1.416(2)	C11-H11	1.0000
O4-C12	1.416(2)	C12-C13	1.538(2)
O5-C15	1.421(2)	C12-H12A	0.9900
O5-H5A	0.67(3)	C12-H12B	0.9900
N1-C10	1.311(2)	C13-C15	1.529(3)
N1-C2	1.355(2)	C13-C14	1.532(2)
N2-C11	1.475(2)	C14-H14A	0.9900
N2-C13	1.494(2)	C14-H14B	0.9900
N2-H3	0.81(2)	C15-H15A	0.9900
C2-C7	1.411(2)	C15-H15B	0.9900
C2-C3	1.433(2)	C16-H16A	0.9800
C3-C4	1.389(2)	C16-H16B	0.9800
C4-C5	1.411(3)	C16-H16C	0.9800
N1-Ni1-O2	175.45(6)	C14-O3-H3A	109.0(17)
N1-Ni1-O1	80.16(5)	Ni1-O3-H3A	124.5(17)
O2-Ni1-O1	101.36(5)	C11-O4-C12	109.80(13)
N1-Ni1-O3	88.54(5)	C15-O5-H5A	115(3)
O2-Ni1-O3	87.19(5)	C10-N1-C2	121.54(15)
O1-Ni1-O3	89.59(5)	C10-N1-Ni1	122.54(12)
N1-Ni1-N2	78.00(6)	C2-N1-Ni1	115.88(11)
O2-Ni1-N2	99.72(5)	C11-N2-C13	104.27(13)
O1-Ni1-N2	156.10(5)	C11-N2-Ni1	110.19(10)
O3-Ni1-N2	80.29(5)	C13-N2-Ni1	110.43(10)
N1-Ni1-Cl1	90.91(4)	C11-N2-H3	108.8(16)
O2-Ni1-Cl1	93.31(4)	C13-N2-H3	107.0(16)
O1-Ni1-Cl1	92.35(4)	Ni1-N2-H3	115.5(16)
O3-Ni1-Cl1	177.86(4)	N1-C2-C7	121.46(15)
N2-Ni1-Cl1	97.57(4)	N1-C2-C3	115.09(15)
C3-O1-Ni1	110.92(10)	C7-C2-C3	123.44(15)
C16-O2-Ni1	123.70(12)	O1-C3-C4	125.79(16)
C16-O2-H2	109.2(17)	O1-C3-C2	117.94(15)
Ni1-O2-H2	118.8(17)	C4-C3-C2	116.27(16)
C14-O3-Ni1	111.31(10)	C3-C4-C5	120.74(17)

C3-C4-H4	119.6	C13-C12-H12A	110.4
C5-C4-H4	119.6	O4-C12-H12B	110.4
C6-C5-C4	122.70(17)	C13-C12-H12B	110.4
C6-C5-H5	118.7	H12A-C12-H12B	108.6
C4-C5-H5	118.7	N2-C13-C15	109.22(14)
C5-C6-C7	119.02(17)	N2-C13-C14	109.30(14)
C5-C6-H6	120.5	C15-C13-C14	111.57(15)
C7-C6-H6	120.5	N2-C13-C12	103.02(14)
C2-C7-C6	117.81(16)	C15-C13-C12	113.19(15)
C2-C7-C8	116.45(16)	C14-C13-C12	110.16(15)
C6-C7-C8	125.73(16)	O3-C14-C13	110.91(14)
C9-C8-C7	120.36(16)	O3-C14-H14A	109.5
C9-C8-H8	119.8	C13-C14-H14A	109.5
C7-C8-H8	119.8	O3-C14-H14B	109.5
C8-C9-C10	119.04(16)	C13-C14-H14B	109.5
C8-C9-H9	120.5	H14A-C14-H14B	108.0
C10-C9-H9	120.5	O5-C15-C13	111.10(16)
N1-C10-C9	121.13(16)	O5-C15-H15A	109.4
N1-C10-C11	114.13(14)	C13-C15-H15A	109.4
C9-C10-C11	124.74(15)	O5-C15-H15B	109.4
O4-C11-N2	108.10(13)	C13-C15-H15B	109.4
O4-C11-C10	110.42(14)	H15A-C15-H15B	108.0
N2-C11-C10	110.36(13)	O2-C16-H16A	109.5
O4-C11-H11	109.3	O2-C16-H16B	109.5
N2-C11-H11	109.3	H16A-C16-H16B	109.5
C10-C11-H11	109.3	O2-C16-H16C	109.5
O4-C12-C13	106.61(14)	H16A-C16-H16C	109.5
O4-C12-H12A	110.4	H16B-C16-H16C	109.5

Single-crystal X-ray analysis of Compound 4:

Data was collected with an Bruker D8 QUEST area detector diffractometer equipped with with MoK$_\alpha$ radiation, a graded multilayer mirror monochromator (λ = 0.71073 Å) and a PHOTON-100 CMOS detector using an oil-coated shock-cooled crystal at 100(2) K. Absorption effects were corrected semi-empirical using multiscanned reflexions (SADABS (Bruker AXS Inc., 2016)). Cell constants were refined using 8865 of observed reflections of the data collection. The structure was solved by direct methods by using the program XT V2014/1 (Bruker AXS Inc., 2014) and refined by full matrix least squares procedures on F^2 using SHELXL-2018/1 (Sheldrick, 2018). The non-hydrogen atoms have been refined anisotropically, carbon bonded hydrogen atoms were included at calculated positions and refined using the 'riding model' with isotropic temperature factors at 1.2 times (for CH_3 groups 1.5 times) that of the preceding carbon atom. CH_3 groups were allowed to rotate about the bond to their next atom to fit the electron density. Nitrogen or oxygen bonded hydrogen atoms were located and allowed to refine isotropically.

Table S4. Bond lengths [Å] and angles [°] for Compound 4:

Zn1-O3	2.0015(14)	C4-H4	0.9500
Zn1-N1	2.0389(16)	C5-C6	1.373(3)
Zn1-O1	2.0706(13)	C5-H5	0.9500
Zn1-Cl1	2.2449(5)	C6-C7	1.421(3)
Zn1-N2	2.2730(16)	C6-H6	0.9500
O1-C3	1.334(2)	C7-C8	1.420(3)
O3-C14	1.429(2)	C8-C9	1.375(3)
O3-H3A	0.85(3)	C8-H8	0.9500
O4-C11	1.431(2)	C9-C10	1.411(3)
O4-C12	1.438(2)	C9-H9	0.9500
O5-C15	1.419(3)	C10-C11	1.519(3)
O5-H5A	0.90(3)	C11-H11	1.0000
N1-C10	1.318(2)	C12-C13	1.523(3)
N1-C2	1.356(2)	C12-H12A	0.9900
N2-C11	1.471(2)	C12-H12B	0.9900
N2-C13	1.487(2)	C13-C14	1.531(3)
N2-H2A	0.90(3)	C13-C15	1.535(3)
C2-C7	1.411(3)	C14-H14A	0.9900
C2-C3	1.433(3)	C14-H14B	0.9900
C3-C4	1.383(3)	C15-H15A	0.9900
C4-C5	1.411(3)	C15-H15B	0.9900

O3-Zn1-N1	111.71(6)	C2-C7-C6	118.27(18)
O3-Zn1-O1	102.71(6)	C8-C7-C6	125.49(19)
N1-Zn1-O1	79.68(6)	C9-C8-C7	120.76(18)
O3-Zn1-Cl1	117.56(5)	C9-C8-H8	119.6
N1-Zn1-Cl1	128.08(5)	C7-C8-H8	119.6
O1-Zn1-Cl1	103.76(4)	C8-C9-C10	118.99(18)
O3-Zn1-N2	78.93(6)	C8-C9-H9	120.5
N1-Zn1-N2	75.01(6)	C10-C9-H9	120.5
O1-Zn1-N2	153.17(6)	N1-C10-C9	120.94(18)
Cl1-Zn1-N2	98.82(5)	N1-C10-C11	115.70(17)
C3-O1-Zn1	112.70(11)	C9-C10-C11	123.35(17)
C14-O3-Zn1	112.78(12)	O4-C11-N2	107.20(15)
C14-O3-H3A	114.2(18)	O4-C11-C10	107.94(15)
Zn1-O3-H3A	129.6(18)	N2-C11-C10	111.31(15)
C11-O4-C12	107.05(14)	O4-C11-H11	110.1
C15-O5-H5A	109(2)	N2-C11-H11	110.1
C10-N1-C2	121.24(17)	C10-C11-H11	110.1
C10-N1-Zn1	124.69(13)	O4-C12-C13	104.28(15)
C2-N1-Zn1	114.06(12)	O4-C12-H12A	110.9
C11-N2-C13	107.39(15)	C13-C12-H12A	110.9
C11-N2-Zn1	113.12(12)	O4-C12-H12B	110.9
C13-N2-Zn1	107.73(11)	C13-C12-H12B	110.9
C11-N2-H2A	107.5(18)	H12A-C12-H12B	108.9
C13-N2-H2A	108.2(17)	N2-C13-C12	102.24(15)
Zn1-N2-H2A	112.7(17)	N2-C13-C14	108.92(15)
N1-C2-C7	121.80(17)	C12-C13-C14	110.66(16)
N1-C2-C3	115.47(17)	N2-C13-C15	110.60(16)
C7-C2-C3	122.71(17)	C12-C13-C15	114.60(16)
O1-C3-C4	125.69(18)	C14-C13-C15	109.52(16)
O1-C3-C2	117.52(17)	O3-C14-C13	108.62(16)
C4-C3-C2	116.79(18)	O3-C14-H14A	110.0
C3-C4-C5	120.75(19)	C13-C14-H14A	110.0
C3-C4-H4	119.6	O3-C14-H14B	110.0
C5-C4-H4	119.6	C13-C14-H14B	110.0
C6-C5-C4	122.67(19)	H14A-C14-H14B	108.3
C6-C5-H5	118.7	O5-C15-C13	113.13(17)
C4-C5-H5	118.7	O5-C15-H15A	109.0
C5-C6-C7	118.79(19)	C13-C15-H15A	109.0
C5-C6-H6	120.6	O5-C15-H15B	109.0
C7-C6-H6	120.6	C13-C15-H15B	109.0
C2-C7-C8	116.23(18)	H15A-C15-H15B	107.8

Single-crystal X-ray analysis of Compound 5:

Data was collected with an BRUKER APEX2 diffractometer equipped with with CuK_α radiation, a graphite monochromator (λ = 1.54184 Å) and a APEX2 detector using an oil-coated shock-cooled crystal at 173(2) K. Absorption effects were corrected semi-empirical using multiscanned reflexions (TWINABS - Bruker AXS scaling for twinned crystals - Version 2012/1). Cell constants were refined using 4782 of observed reflections of the data collection. The structure was solved by direct methods by using the program SHELXT 2014/5 (Sheldrick, 2014) and refined by full matrix least squares procedures on F^2 using SHELXL-2018/3 (Sheldrick, 2018). The non-hydrogen atoms have been refined anisotropically, carbon bonded hydrogen atoms were included at calculated positions and refined using the 'riding model' with isotropic temperature factors at 1.2 times (for CH_3 groups 1.5 times) that of the preceding carbon atom. CH_3 groups were allowed to rotate about the bond to their next atom to fit the electron density. Nitrogen or oxygen bonded hydrogen atoms were located and allowed to refine isotropically. Disorder was refined using restraints for both the geometry and thermal parameters. Heavily disordered solvent was treated by using the PLATON/SQUEEZE (Spek, 2015) procedure.

Table S5. Bond lengths [Å] and angles [°] for Compound 5.

Fe1-O1	1.7912(7)	C23-C24	1.389(7)
Fe1-O30	2.129(3)	C23-C32	1.509(7)
Fe1-N1	2.138(4)	C24-C25	1.367(8)
Fe1-O38	2.153(3)	C24-H24	0.9500
Fe1-N22	2.164(4)	C25-C26	1.408(8)
Fe1-O9	2.182(3)	C25-H25	0.9500
Fe1-N33	2.431(4)	C26-C31	1.402(7)
Fe2-O100	1.889(4)	C26-C27	1.412(7)
Fe2-O309	1.998(4)	C27-C28	1.360(8)
Fe2-O30	2.023(3)	C27-H27	0.9500
Fe2-O9	2.052(3)	C28-C29	1.419(8)
Fe2-N301	2.056(14)	C28-H28	0.9500
Fe2-N401	2.155(18)	C29-C30	1.376(7)
Fe2-N312	2.296(4)	C29-H29	0.9500
N1-C2	1.325(6)	C30-O30	1.355(6)
N1-C10	1.348(6)	C30-C31	1.407(7)
C2-C3	1.408(7)	C32-O36	1.432(6)
C2-C11	1.498(7)	C32-N33	1.495(6)
C3-C4	1.357(8)	C32-H32	1.0000
C3-H3	0.9500	N33-C34	1.520(6)
C4-C5	1.412(8)	C34-C39	1.521(7)
C4-H4	0.9500	C34-C35	1.524(7)
C5-C6	1.412(8)	C34-C37	1.533(7)
C5-C10	1.416(7)	C35-O36	1.441(6)
C6-C7	1.354(9)	C35-H35A	0.9900
C6-H6	0.9500	C35-H35B	0.9900
C7-C8	1.408(8)	C37-O38	1.438(6)
C7-H7	0.9500	C37-H37A	0.9900
C8-C9	1.375(7)	C37-H37B	0.9900
C8-H01F	0.9500	O38-H38	0.8402
O9-C9	1.343(6)	C39-O40	1.432(6)
C9-C10	1.435(7)	C39-H39A	0.9900
C11-O11	1.392(6)	C39-H39B	0.9900
C11-N33	1.484(6)	O40-H40	0.8400
C11-H11A	1.0000	C101-O100	1.447(11)
O11-H11	0.8400	C101-C313	1.491(12)
N22-C23	1.317(6)	C101-H10A	0.9900
N22-C31	1.372(6)	C101-H10B	0.9900

O101-C102	1.410(18)	C305-C310	1.405(11)
O101-H101	0.8400	C305-C306	1.434(12)
C102-C313	1.492(12)	C306-C307	1.366(13)
C102-H10C	0.9900	C306-H306	0.9500
C102-H10D	0.9900	C307-C308	1.408(13)
C103-O315	1.386(12)	C307-H307	0.9500
C103-C313	1.562(12)	C308-C309	1.376(11)
C103-H10E	0.9900	C308-H308	0.9500
C103-H10F	0.9900	C309-C310	1.413(11)
O100-C201	1.296(13)	N401-C402	1.319(13)
C201-C313	1.619(15)	N401-C410	1.355(13)
C201-H20A	0.9900	C402-C403	1.416(14)
C201-H20B	0.9900	C403-C404	1.365(15)
O201-C202	1.42(2)	C403-H403	0.9500
O201-H201	0.8400	C404-C405	1.415(14)
C202-C313	1.499(15)	C404-H404	0.9500
C202-H20C	0.9900	C405-C410	1.415(13)
C202-H20D	0.9900	C405-C406	1.435(14)
C203-C313	1.500(14)	C406-C407	1.354(15)
C203-O315	1.527(16)	C406-H406	0.9500
C203-H20E	0.9900	C407-C408	1.396(15)
C203-H20F	0.9900	C407-H407	0.9500
O309-C309	1.294(12)	C408-C409	1.387(14)
O309-C409	1.453(16)	C408-H408	0.9500
C311-O315	1.410(7)	C409-C410	1.414(14)
C311-C402	1.418(18)	N501-C502	1.171(14)
C311-N312	1.494(7)	C502-C503	1.447(17)
C311-C302	1.582(14)	C503-H50A	0.9800
C311-H311	1.0000	C503-H50B	0.9800
C311-H411	1.0000	C503-H50C	0.9800
N312-C313	1.491(7)	N601-C602	1.181(19)
N312-H312	1.0000	C602-C603	1.46(2)
N301-C302	1.317(11)	C603-H60A	0.9800
N301-C310	1.362(10)	C603-H60B	0.9800
C302-C303	1.412(11)	C603-H60C	0.9800
C303-C304	1.356(12)	N900-O903	1.222(7)
C303-H303	0.9500	N900-O902	1.259(7)
C304-C305	1.417(12)	N900-O901	1.262(6)
C304-H304	0.9500		

O1-Fe1-O30	104.08(9)	O100-Fe2-O30	95.45(15)
O1-Fe1-N1	87.80(10)	O309-Fe2-O30	95.84(14)
O30-Fe1-N1	142.90(14)	O100-Fe2-O9	156.94(15)
O1-Fe1-O38	163.52(9)	O309-Fe2-O9	100.79(15)
O30-Fe1-O38	88.36(13)	O30-Fe2-O9	73.21(13)
N1-Fe1-O38	88.60(14)	O100-Fe2-N301	92.4(7)
O1-Fe1-N22	88.85(10)	O309-Fe2-N301	76.8(3)
O30-Fe1-N22	74.72(14)	O30-Fe2-N301	170.1(6)
N1-Fe1-N22	141.51(15)	O9-Fe2-N301	101.4(7)
O38-Fe1-N22	84.00(13)	O100-Fe2-N401	96.5(10)
O1-Fe1-O9	104.39(9)	O309-Fe2-N401	80.9(4)
O30-Fe1-O9	68.61(12)	O30-Fe2-N401	168.0(10)
N1-Fe1-O9	74.44(14)	O9-Fe2-N401	95.9(10)
O38-Fe1-O9	90.09(12)	O100-Fe2-N312	79.19(16)
N22-Fe1-O9	143.00(14)	O309-Fe2-N312	151.63(15)
O1-Fe1-N33	90.98(9)	O30-Fe2-N312	112.49(14)
O30-Fe1-N33	142.09(13)	O9-Fe2-N312	86.62(15)
N1-Fe1-N33	70.77(14)	N301-Fe2-N312	74.9(3)
O38-Fe1-N33	72.67(12)	N401-Fe2-N312	71.1(4)
N22-Fe1-N33	70.96(14)	Fe1#1-O1-Fe1	180.0
O9-Fe1-N33	141.22(13)	C2-N1-C10	120.5(4)
O100-Fe2-O309	100.30(16)	C2-N1-Fe1	121.6(3)

C10-N1-Fe1	117.4(3)	O30-C30-C29	125.4(5)
N1-C2-C3	121.1(5)	O30-C30-C31	116.2(4)
N1-C2-C11	114.4(5)	C29-C30-C31	118.4(5)
C3-C2-C11	124.2(5)	C30-O30-Fe2	132.6(3)
C4-C3-C2	119.0(5)	C30-O30-Fe1	117.0(3)
C4-C3-H3	120.5	Fe2-O30-Fe1	109.81(15)
C2-C3-H3	120.5	N22-C31-C26	121.5(4)
C3-C4-C5	121.3(5)	N22-C31-C30	116.0(4)
C3-C4-H4	119.4	C26-C31-C30	122.6(5)
C5-C4-H4	119.4	O36-C32-N33	107.6(4)
C4-C5-C6	126.0(5)	O36-C32-C23	108.4(4)
C4-C5-C10	115.9(5)	N33-C32-C23	112.0(4)
C6-C5-C10	118.1(5)	O36-C32-H32	109.6
C7-C6-C5	119.4(6)	N33-C32-H32	109.6
C7-C6-H6	120.3	C23-C32-H32	109.6
C5-C6-H6	120.3	C11-N33-C32	111.1(4)
C6-C7-C8	122.7(6)	C11-N33-C34	117.4(4)
C6-C7-H7	118.6	C32-N33-C34	104.9(4)
C8-C7-H7	118.6	C11-N33-Fe1	101.9(3)
C9-C8-C7	120.6(6)	C32-N33-Fe1	110.1(3)
C9-C8-H01F	119.7	C34-N33-Fe1	111.5(3)
C7-C8-H01F	119.7	N33-C34-C39	113.4(4)
C9-O9-Fe2	136.4(3)	N33-C34-C35	102.9(4)
C9-O9-Fe1	116.0(3)	C39-C34-C35	111.8(4)
Fe2-O9-Fe1	106.72(15)	N33-C34-C37	106.3(4)
O9-C9-C8	126.9(5)	C39-C34-C37	110.8(4)
O9-C9-C10	115.9(4)	C35-C34-C37	111.3(4)
C8-C9-C10	117.0(5)	O36-C35-C34	106.8(4)
N1-C10-C5	122.0(5)	O36-C35-H35A	110.4
N1-C10-C9	116.0(4)	C34-C35-H35A	110.4
C5-C10-C9	121.9(5)	O36-C35-H35B	110.4
O11-C11-N33	115.5(4)	C34-C35-H35B	110.4
O11-C11-C2	112.3(4)	H35A-C35-H35B	108.6
N33-C11-C2	108.5(4)	C32-O36-C35	109.9(4)
O11-C11-H11A	106.7	O38-C37-C34	110.3(4)
N33-C11-H11A	106.7	O38-C37-H37A	109.6
C2-C11-H11A	106.7	C34-C37-H37A	109.6
C11-O11-H11	109.5	O38-C37-H37B	109.6
C23-N22-C31	119.5(4)	C34-C37-H37B	109.6
C23-N22-Fe1	124.6(3)	H37A-C37-H37B	108.1
C31-N22-Fe1	115.2(3)	C37-O38-Fe1	117.6(3)
N22-C23-C24	122.2(5)	C37-O38-H38	109.3
N22-C23-C32	116.5(4)	Fe1-O38-H38	114.4
C24-C23-C32	121.3(4)	O40-C39-C34	108.7(4)
C25-C24-C23	119.7(5)	O40-C39-H39A	110.0
C25-C24-H24	120.2	C34-C39-H39A	110.0
C23-C24-H24	120.2	O40-C39-H39B	110.0
C24-C25-C26	119.7(5)	C34-C39-H39B	110.0
C24-C25-H25	120.1	H39A-C39-H39B	108.3
C26-C25-H25	120.1	C39-O40-H40	109.5
C31-C26-C25	117.4(5)	O100-C101-C313	111.3(8)
C31-C26-C27	117.6(5)	O100-C101-H10A	109.4
C25-C26-C27	124.9(5)	C313-C101-H10A	109.4
C28-C27-C26	120.0(5)	O100-C101-H10B	109.4
C28-C27-H27	120.0	C313-C101-H10B	109.4
C26-C27-H27	120.0	H10A-C101-H10B	108.0
C27-C28-C29	122.0(5)	C102-O101-H101	109.5
C27-C28-H28	119.0	O101-C102-C313	110.7(10)
C29-C28-H28	119.0	O101-C102-H10C	109.5
C30-C29-C28	119.4(5)	C313-C102-H10C	109.5
C30-C29-H29	120.3	O101-C102-H10D	109.5
C28-C29-H29	120.3	C313-C102-H10D	109.5

H10C-C102-H10D	108.1	C302-N301-Fe2	125.2(8)
O315-C103-C313	105.1(7)	C310-N301-Fe2	114.1(8)
O315-C103-H10E	110.7	N301-C302-C303	120.8(10)
C313-C103-H10E	110.7	N301-C302-C311	116.1(9)
O315-C103-H10F	110.7	C303-C302-C311	123.1(9)
C313-C103-H10F	110.7	C304-C303-C302	120.1(10)
H10E-C103-H10F	108.8	C304-C303-H303	119.9
C201-O100-Fe2	115.2(7)	C302-C303-H303	119.9
C101-O100-Fe2	118.9(5)	C303-C304-C305	119.7(9)
O100-C201-C313	112.1(9)	C303-C304-H304	120.2
O100-C201-H20A	109.2	C305-C304-H304	120.2
C313-C201-H20A	109.2	C310-C305-C304	117.2(8)
O100-C201-H20B	109.2	C310-C305-C306	116.5(8)
C313-C201-H20B	109.2	C304-C305-C306	126.2(9)
H20A-C201-H20B	107.9	C307-C306-C305	119.8(9)
C202-O201-H201	109.5	C307-C306-H306	120.1
O201-C202-C313	110.3(13)	C305-C306-H306	120.1
O201-C202-H20C	109.6	C306-C307-C308	122.2(9)
C313-C202-H20C	109.6	C306-C307-H307	118.9
O201-C202-H20D	109.6	C308-C307-H307	118.9
C313-C202-H20D	109.6	C309-C308-C307	120.2(9)
H20C-C202-H20D	108.1	C309-C308-H308	119.9
C313-C203-O315	101.4(9)	C307-C308-H308	119.9
C313-C203-H20E	111.5	O309-C309-C308	128.0(9)
O315-C203-H20E	111.5	O309-C309-C310	114.0(8)
C313-C203-H20F	111.5	C308-C309-C310	117.7(9)
O315-C203-H20F	111.5	N301-C310-C305	121.4(9)
H20E-C203-H20F	109.3	N301-C310-C309	115.0(9)
C309-O309-Fe2	119.2(5)	C305-C310-C309	123.5(8)
C409-O309-Fe2	111.6(6)	C402-N401-C410	121.2(13)
O315-C311-C402	110.9(13)	C402-N401-Fe2	125.7(11)
O315-C311-N312	107.4(4)	C410-N401-Fe2	113.1(10)
C402-C311-N312	114.0(8)	N401-C402-C403	120.9(13)
O315-C311-C302	107.7(9)	N401-C402-C311	115.0(13)
N312-C311-C302	108.4(6)	C403-C402-C311	124.1(13)
O315-C311-H311	111.1	C404-C403-C402	119.2(13)
N312-C311-H311	111.1	C404-C403-H403	120.4
C302-C311-H311	111.1	C402-C403-H403	120.4
O315-C311-H411	108.1	C403-C404-C405	120.5(12)
C402-C311-H411	108.1	C403-C404-H404	119.7
N312-C311-H411	108.1	C405-C404-H404	119.7
C313-N312-C311	105.9(4)	C410-C405-C404	116.7(10)
C313-N312-Fe2	106.5(3)	C410-C405-C406	115.2(11)
C311-N312-Fe2	114.0(3)	C404-C405-C406	128.0(11)
C313-N312-H312	110.1	C407-C406-C405	119.6(11)
C311-N312-H312	110.1	C407-C406-H406	120.2
Fe2-N312-H312	110.1	C405-C406-H406	120.2
N312-C313-C101	107.8(6)	C406-C407-C408	124.7(12)
N312-C313-C102	110.2(6)	C406-C407-H407	117.6
C101-C313-C102	114.3(7)	C408-C407-H407	117.6
N312-C313-C202	115.0(8)	C409-C408-C407	118.2(12)
N312-C313-C203	104.8(7)	C409-C408-H408	120.9
C202-C313-C203	111.3(8)	C407-C408-H408	120.9
N312-C313-C103	100.2(6)	C408-C409-C410	117.8(12)
C101-C313-C103	111.7(7)	C408-C409-O309	122.3(11)
C102-C313-C103	111.6(7)	C410-C409-O309	119.8(10)
N312-C313-C201	106.8(6)	N401-C410-C409	114.4(11)
C202-C313-C201	108.9(10)	N401-C410-C405	121.3(11)
C203-C313-C201	109.9(9)	C409-C410-C405	124.3(11)
C103-O315-C311	109.8(5)	N501-C502-C503	166.4(19)
C311-O315-C203	103.8(6)	C502-C503-H50A	109.5
C302-N301-C310	120.6(10)	C502-C503-H50B	109.5

H50A-C503-H50B	109.5	H60A-C603-H60B	109.5
C502-C503-H50C	109.5	C602-C603-H60C	109.5
H50A-C503-H50C	109.5	H60A-C603-H60C	109.5
H50B-C503-H50C	109.5	H60B-C603-H60C	109.5
N601-C602-C603	170(4)	O903-N900-O902	121.0(5)
C602-C603-H60A	109.5	O903-N900-O901	118.6(6)
C602-C603-H60B	109.5	O902-N900-O901	120.2(5)

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+1,-z+1

Single-crystal X-ray analysis of Compound 6:

Data was collected with an Bruker D8 QUEST area detector diffractometer equipped with with MoK$_\alpha$ radiation, a graded multilayer mirror monochromator (λ = 0.71073 Å) and a PHOTON-100 CMOS detector using an oil-coated shock-cooled crystal at 100(2) K. Absorption effects were corrected semi-empirical using multiscanned reflexions (SADABS-2016/2 - Bruker AXS area detector scaling and absorption correction). Cell constants were refined using 8108 of observed reflections of the data collection. The structure was solved by direct methods by using the program XT V2014/1 (Bruker AXS Inc., 2014) and refined by full matrix least squares procedures on F^2 using SHELXL-2018/1 (Sheldrick, 2018). The non-hydrogen atoms have been refined anisotropically, carbon bonded hydrogen atoms were included at calculated positions and refined using the 'riding model' with isotropic temperature factors at 1.2 times (for CH_3 groups 1.5 times) that of the preceding carbon atom. CH_3 groups were allowed to rotate about the bond to their next atom to fit the electron density. Nitrogen or oxygen bonded hydrogen atoms were located and allowed to refine isotropically.

Table S6. Bond lengths [Å] and angles [°] for Compound 6.

Co1-N7	1.839(2)	C1-C2	1.417(4)
Co1-O3	1.9207(18)	C1-C10	1.524(4)
Co1-O1	1.9434(17)	C2-C3	1.368(4)
Co1-N1	1.947(2)	C2-H2	0.9500
Co1-N2	1.951(2)	C3-C4	1.425(4)
Co1-N8	1.961(2)	C3-H3	0.9500
Co1-Co2	2.9652(4)	C4-C9	1.401(4)
Co2-O3	2.0086(17)	C4-C5	1.418(4)
Co2-O3#1	2.0086(17)	C5-C6	1.366(4)
Co2-O4	2.0913(19)	C5-H5	0.9500
Co2-O4#1	2.0913(19)	C6-C7	1.415(4)
Co2-N2#1	2.117(2)	C6-H6	0.9500
Co2-N2	2.117(2)	C7-C8	1.381(4)
O1-C8	1.337(3)	C7-H7	0.9500
O2-C10	1.413(3)	C8-C9	1.419(4)
O2-C12	1.422(4)	C10-H10	1.0000
O3-C13	1.420(3)	C11-C12	1.524(4)
O4-C14	1.419(3)	C11-C13	1.529(4)
O4-H4A	0.800(18)	C11-C14	1.535(4)
N1-N3A	1.223(3)	C12-H12A	0.9900
N1-N3B	1.244(14)	C12-H12B	0.9900
N2-N5	1.206(3)	C13-H13A	0.9900
N5-N6	1.142(3)	C13-H13B	0.9900
N7-C1	1.309(3)	C14-H14A	0.9900
N7-C9	1.351(3)	C14-H14B	0.9900
N8-C10	1.505(4)	N3A-N4A	1.151(4)
N8-C11	1.512(4)	N3B-N4B	1.148(16)
N8-H8A	0.85(3)		
N7-Co1-O3	89.07(9)	O1-Co1-Co2	84.65(6)
N7-Co1-O1	85.66(9)	N1-Co1-Co2	137.33(7)
O3-Co1-O1	89.32(8)	N2-Co1-Co2	45.45(7)
N7-Co1-N1	92.11(10)	N8-Co1-Co2	98.20(7)
O3-Co1-N1	175.88(8)	O3-Co2-O3#1	180.0
O1-Co1-N1	94.71(9)	O3-Co2-O4	87.01(7)
N7-Co1-N2	175.63(9)	O3#1-Co2-O4	92.99(7)
O3-Co1-N2	86.67(8)	O3-Co2-O4#1	92.99(7)
O1-Co1-N2	93.26(8)	O3#1-Co2-O4#1	87.01(7)
N1-Co1-N2	92.21(10)	O4-Co2-O4#1	180.0
N7-Co1-N8	83.64(10)	O3-Co2-N2#1	99.85(7)
O3-Co1-N8	85.18(9)	O3#1-Co2-N2#1	80.15(7)
O1-Co1-N8	168.05(9)	O4-Co2-N2#1	93.10(8)
N1-Co1-N8	91.02(10)	O4#1-Co2-N2#1	86.90(8)
N2-Co1-N8	97.00(9)	O3-Co2-N2	80.15(7)
N7-Co1-Co2	130.18(7)	O3#1-Co2-N2	99.85(7)
O3-Co1-Co2	42.13(5)	O4-Co2-N2	86.90(8)

O4#1-Co2-N2	93.10(8)	C5-C4-C3	128.3(3)
N2#1-Co2-N2	180.0	C6-C5-C4	119.0(3)
O3-Co2-Co1#1	140.10(5)	C6-C5-H5	120.5
O3#1-Co2-Co1#1	39.91(5)	C4-C5-H5	120.5
O4-Co2-Co1#1	87.69(6)	C5-C6-C7	124.0(3)
O4#1-Co2-Co1#1	92.31(6)	C5-C6-H6	118.0
N2#1-Co2-Co1#1	41.06(6)	C7-C6-H6	118.0
N2-Co2-Co1#1	138.94(6)	C8-C7-C6	118.7(3)
O3-Co2-Co1	39.90(5)	C8-C7-H7	120.7
O3#1-Co2-Co1	140.09(5)	C6-C7-H7	120.7
O4-Co2-Co1	92.31(6)	O1-C8-C7	126.2(2)
O4#1-Co2-Co1	87.69(6)	O1-C8-C9	116.8(2)
N2#1-Co2-Co1	138.94(6)	C7-C8-C9	117.0(2)
N2-Co2-Co1	41.06(6)	N7-C9-C4	121.1(2)
Co1#1-Co2-Co1	180.0	N7-C9-C8	114.1(2)
C8-O1-Co1	109.38(15)	C4-C9-C8	124.8(2)
C10-O2-C12	109.3(2)	O2-C10-N8	107.7(2)
C13-O3-Co1	112.11(15)	O2-C10-C1	111.0(2)
C13-O3-Co2	115.85(16)	N8-C10-C1	109.0(2)
Co1-O3-Co2	97.96(7)	O2-C10-H10	109.7
C14-O4-Co2	129.50(17)	N8-C10-H10	109.7
C14-O4-H4A	119(3)	C1-C10-H10	109.7
Co2-O4-H4A	111(3)	N8-C11-C12	100.9(2)
N3A-N1-Co1	115.39(19)	N8-C11-C13	104.9(2)
N3B-N1-Co1	110.2(12)	C12-C11-C13	111.7(2)
N5-N2-Co1	118.97(19)	N8-C11-C14	113.3(2)
N5-N2-Co2	130.73(18)	C12-C11-C14	111.7(2)
Co1-N2-Co2	93.49(9)	C13-C11-C14	113.5(2)
N6-N5-N2	177.3(3)	O2-C12-C11	106.3(2)
C1-N7-C9	123.8(2)	O2-C12-H12A	110.5
C1-N7-Co1	122.07(19)	C11-C12-H12A	110.5
C9-N7-Co1	113.73(18)	O2-C12-H12B	110.5
C10-N8-C11	104.1(2)	C11-C12-H12B	110.5
C10-N8-Co1	110.51(16)	H12A-C12-H12B	108.7
C11-N8-Co1	110.37(16)	O3-C13-C11	109.3(2)
C10-N8-H8A	112(2)	O3-C13-H13A	109.8
C11-N8-H8A	108(2)	C11-C13-H13A	109.8
Co1-N8-H8A	112(2)	O3-C13-H13B	109.8
N7-C1-C2	119.1(3)	C11-C13-H13B	109.8
N7-C1-C10	111.8(2)	H13A-C13-H13B	108.3
C2-C1-C10	129.1(2)	O4-C14-C11	111.7(2)
C3-C2-C1	118.7(3)	O4-C14-H14A	109.3
C3-C2-H2	120.7	C11-C14-H14A	109.3
C1-C2-H2	120.7	O4-C14-H14B	109.3
C2-C3-C4	122.0(3)	C11-C14-H14B	109.3
C2-C3-H3	119.0	H14A-C14-H14B	107.9
C4-C3-H3	119.0	N4A-N3A-N1	176.4(3)
C9-C4-C5	116.4(3)	N4B-N3B-N1	175(3)
C9-C4-C3	115.3(3)		

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1