Electronic Supplementary Information

Design and Synthesis of a Dinucleating Ligand System with Varying Terminal Donor Functions that Provides no Bridging Donor and its Application to the Synthesis of a Series of Fe^{III}-μ-O-Fe^{III} Complexes

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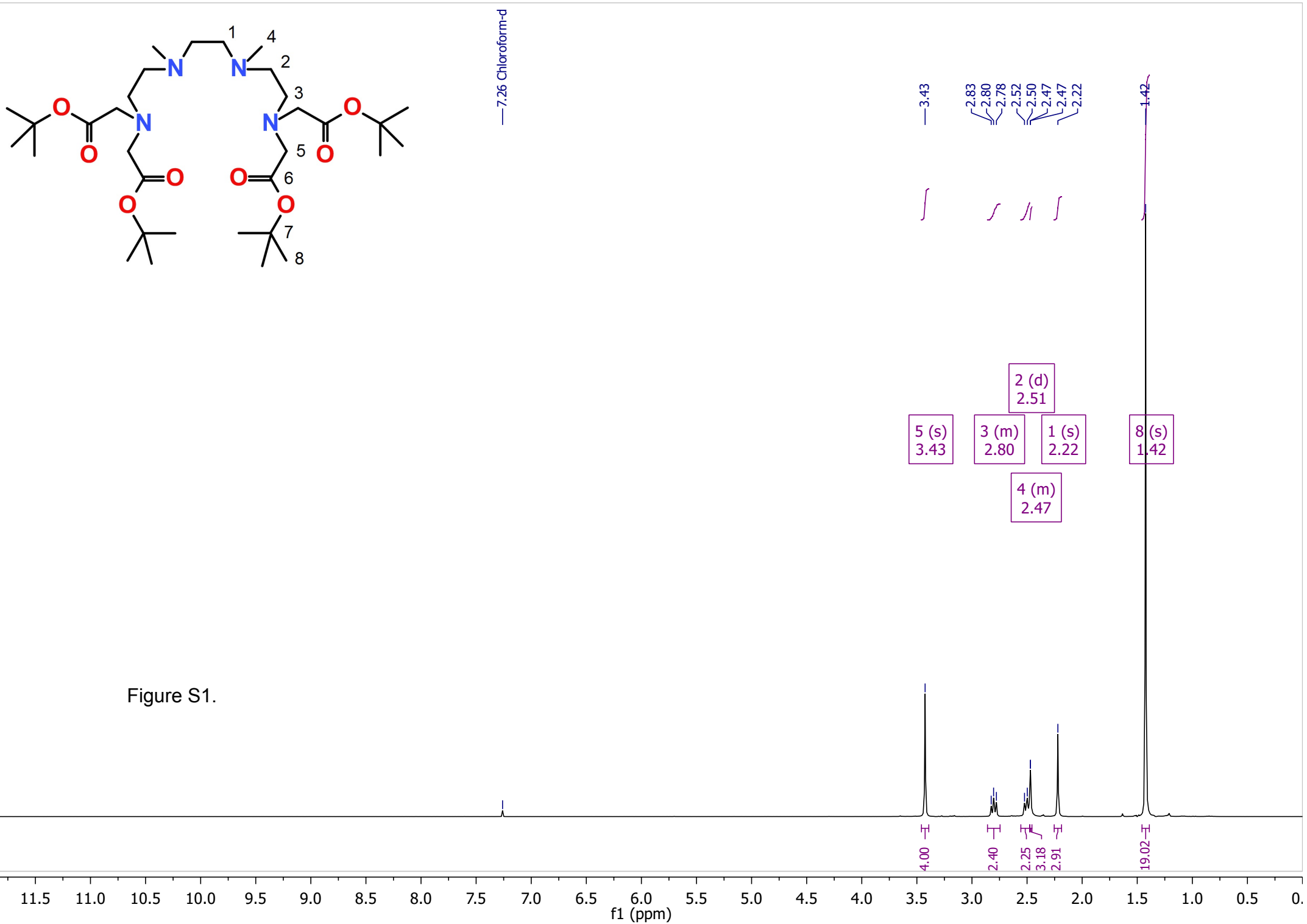

7.26 Chloroform-d
3.43
2.83
2.80
2.78
2.52
2.50
2.47
2.47
2.22
1.42
2 (d)
2.51
5 (s)
3.43
3 (m)
2.80
1 (s)
2.22
8 (s)
1.42
4 (m)
2.47
4.00
2.40
2.25
3.18
2.91
19.02
f1 (ppm)

Figure S1.

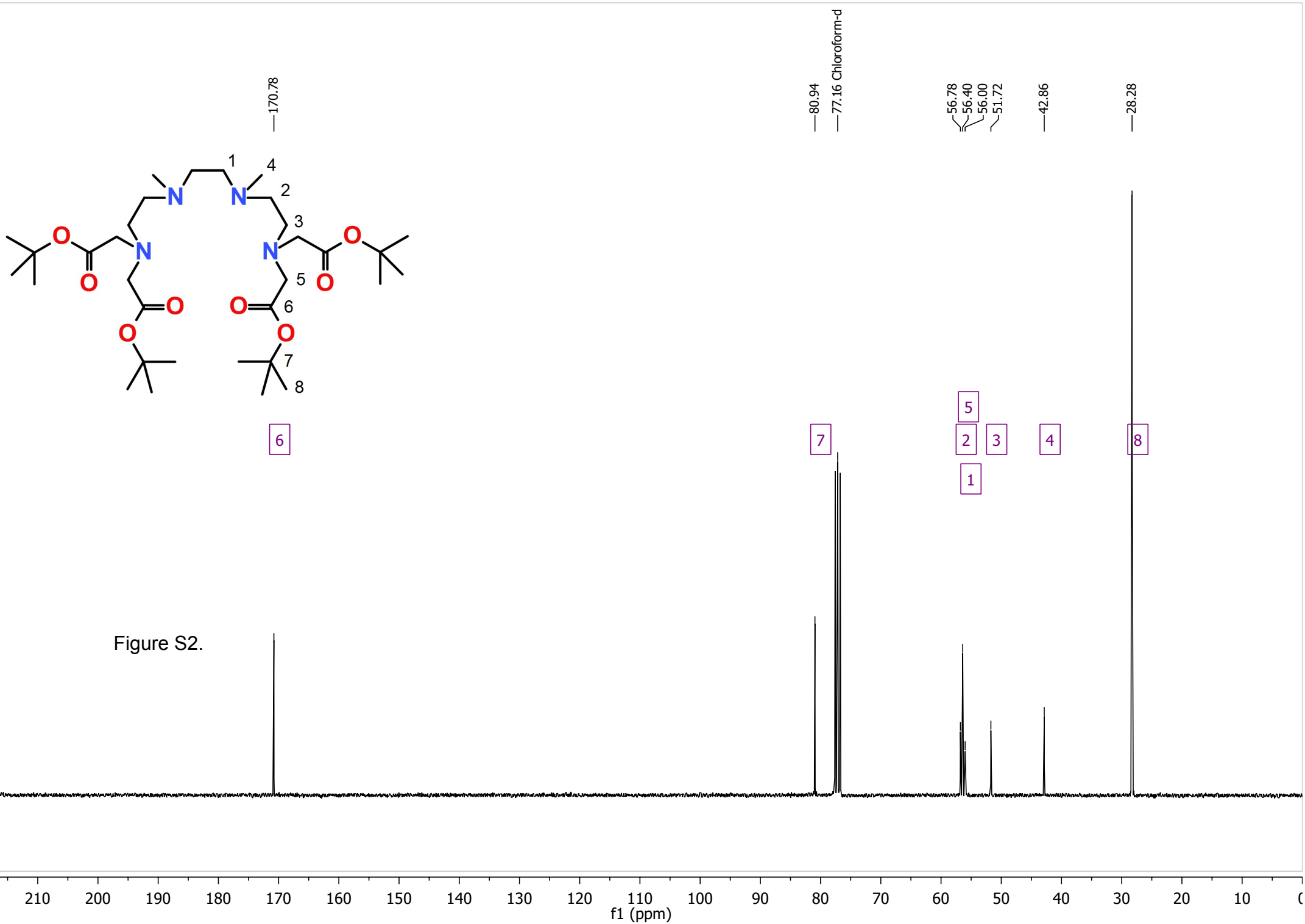
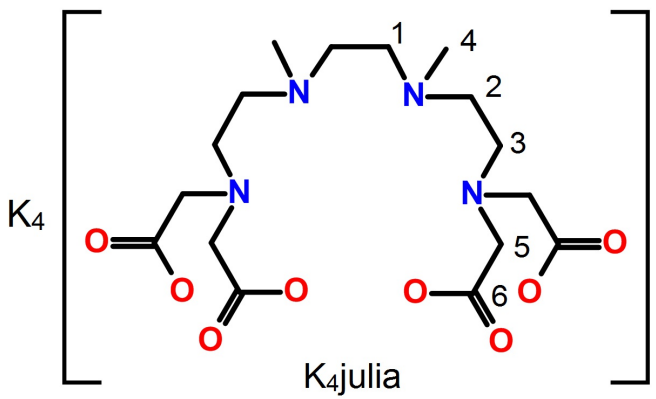

170.78
80.94
77.16 Chloroform-d
56.78
56.40
56.00
51.72
42.86
28.28
1
2
3
4
5
6
7
8
6
7
5
2
3
4
1
8
f1 (ppm)

Figure S2.


K4
1
2
3
4
5
6
K4julia

4.81 HDO
3.66 EtOH/D2O
3.65 EtOH/D2O
3.63 EtOH/D2O
3.62 EtOH/D2O
3.22
2.75
2.74
2.74
2.73
2.72
2.59
2.58
2.57
2.56
2.23
1.18 EtOH/D2O
1.17 EtOH/D2O
1.16 EtOH/D2O
2, 1 (m)
2.58
5 (s)
3.22
3 (m)
2.73
4 (s)
2.23
4.00
1.99
3.81
2.87
f1 (ppm)

Figure S3.

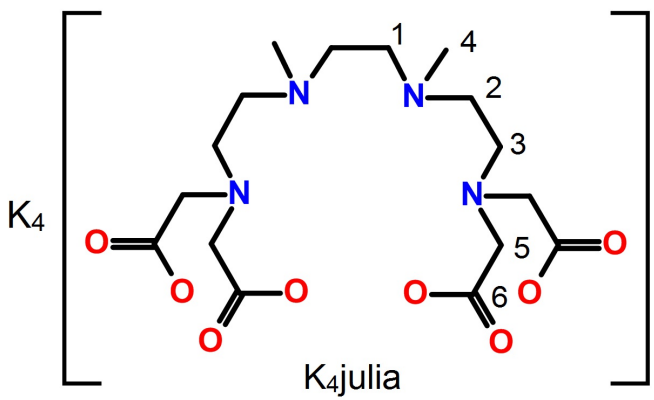
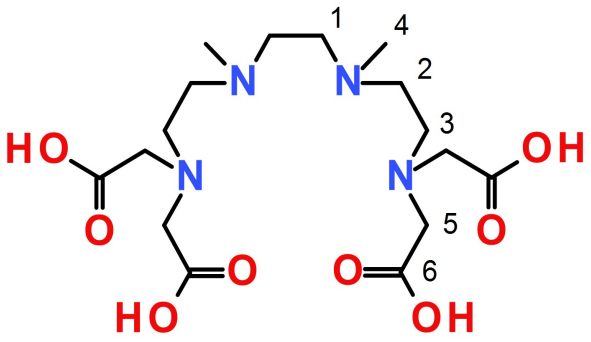

K4
1
4
2
3
5
6
K4julia

Figure S4.

180.07
59.23
58.08 EtOH/D2O
54.85
54.27
51.59
42.07
17.47 EtOH/D2O
6
5
1
3
2
4
f1 (ppm)


1
4
2
3
5
6
HO
OH
HO
OH
O
O
O
O
N
N
N
N

4.83 HDO
3.81
3.77
3.48
3.47
3.46
3.32
3.31
3.29
3.03
2.22 Aceton/D2O
5 (s)
3.77
3 (t)
3.31
1 (s)
3.81
2 (t)
3.47
4 (s)
3.03
1.00
2.10
1.12
1.11
1.51
f1 (ppm)

Figure S5.

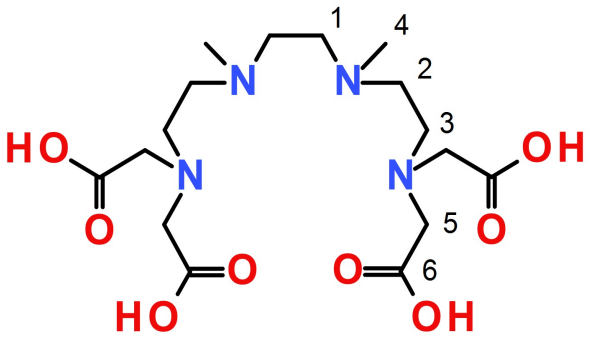

HO
O
N
N
N
N
OH
O
O
O
HO
OH
1
2
3
4
5
6

Figure S6.

216.02 Aceton
175.13
56.56
56.14
51.36
50.49
41.36
30.89 Aceton/D2O
2
3
5
1
4
6
f1 (ppm)

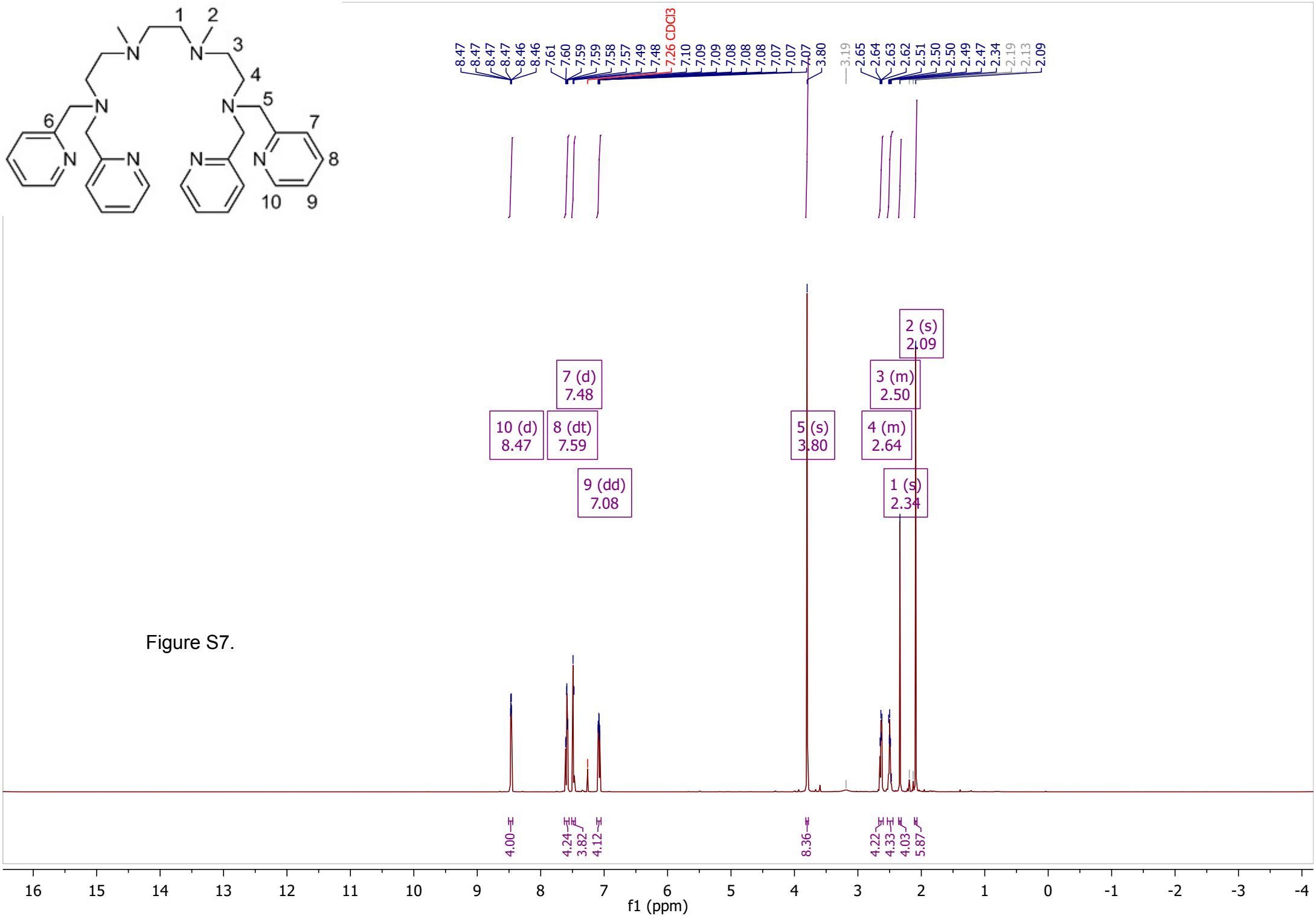

1
2
3
4
5
6
7
8
9
10
N
8.47
8.47
8.47
8.46
8.46
7.61
7.60
7.59
7.59
7.58
7.57
7.49
7.48
7.26 CDCl3
7.10
7.09
7.09
7.08
7.08
7.08
7.07
7.07
7.07
3.80
3.19
2.65
2.64
2.63
2.62
2.51
2.50
2.50
2.49
2.47
2.34
2.19
2.13
2.09
2 (s)
2.09
7 (d)
7.48
3 (m)
2.50
10 (d)
8.47
8 (dt)
7.59
5 (s)
3.80
4 (m)
2.64
9 (dd)
7.08
1 (s)
2.34
4.00
4.24
3.82
4.12
8.36
4.22
4.33
4.03
5.87
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)

Figure S7.

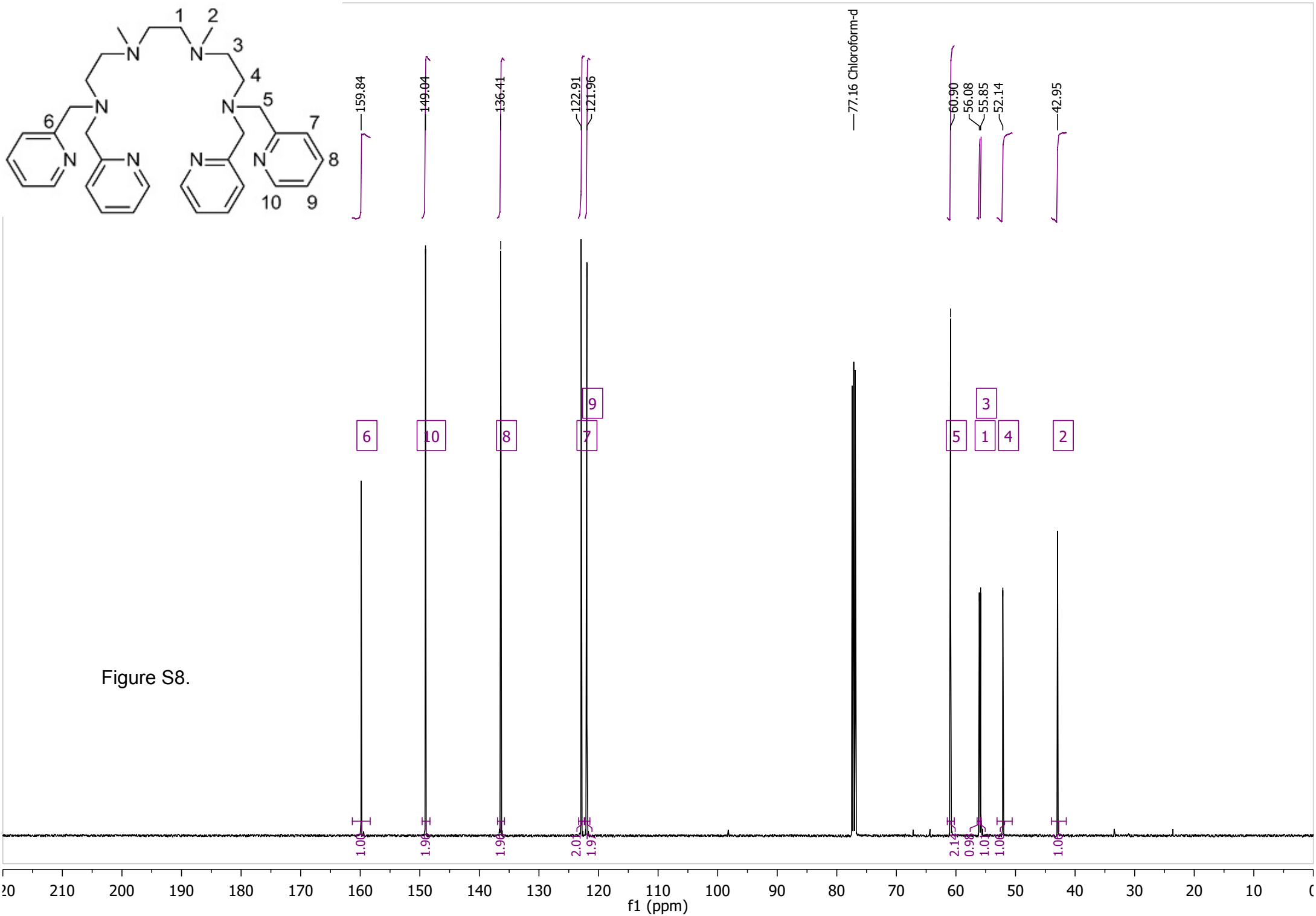

159.84
149.04
136.41
122.91
121.96
77.16 Chloroform-d
60.90
56.08
55.85
52.14
42.95
6
10
8
9
7
3
5
1
4
2
f1 (ppm)

Figure S8.

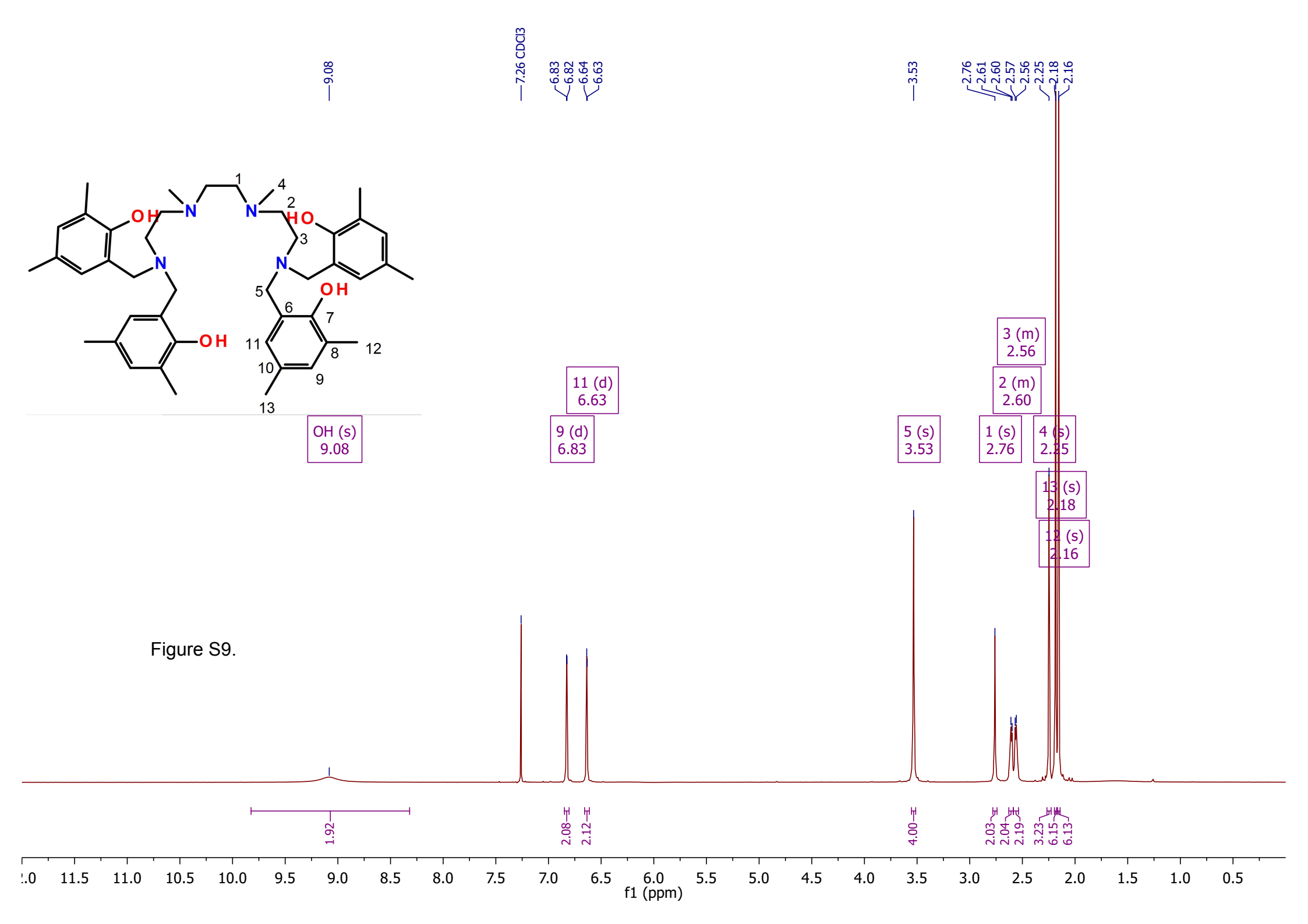

9.08
7.26 CDCl3
6.83
6.82
6.64
6.63
3.53
2.76
2.61
2.60
2.57
2.56
2.25
2.18
2.16
OH
N
N
HO
N
N
OH
OH
1
2
3
4
5
6
7
8
9
10
11
12
13
OH (s)
9.08
9 (d)
6.83
11 (d)
6.63
5 (s)
3.53
1 (s)
2.76
2 (m)
2.60
3 (m)
2.56
4 (s)
2.25
13 (s)
2.18
12 (s)
2.16
1.92
2.08
2.12
4.00
2.03
2.04
2.19
3.23
6.15
6.13
f1 (ppm)

Figure S9.

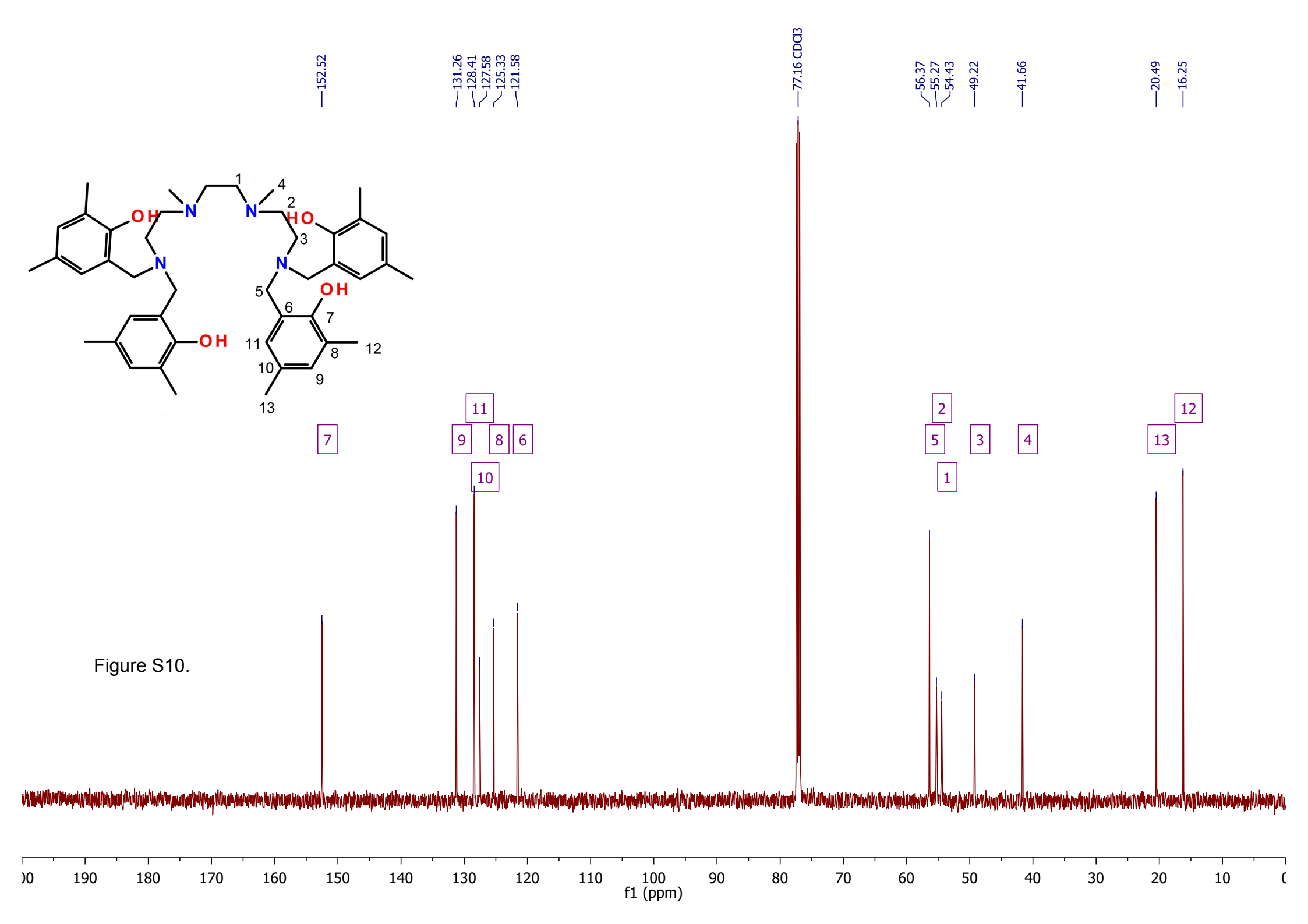

152.52
131.26
128.41
127.58
125.33
121.58
77.16 CDCl3
56.37
55.27
54.43
49.22
41.66
20.49
16.25
OH
N
N
HO
N
N
OH
OH
1
2
3
4
5
6
7
8
9
10
11
12
13
7
11
9
8
6
10
2
5
3
4
1
12
13
f1 (ppm)

Figure S10.

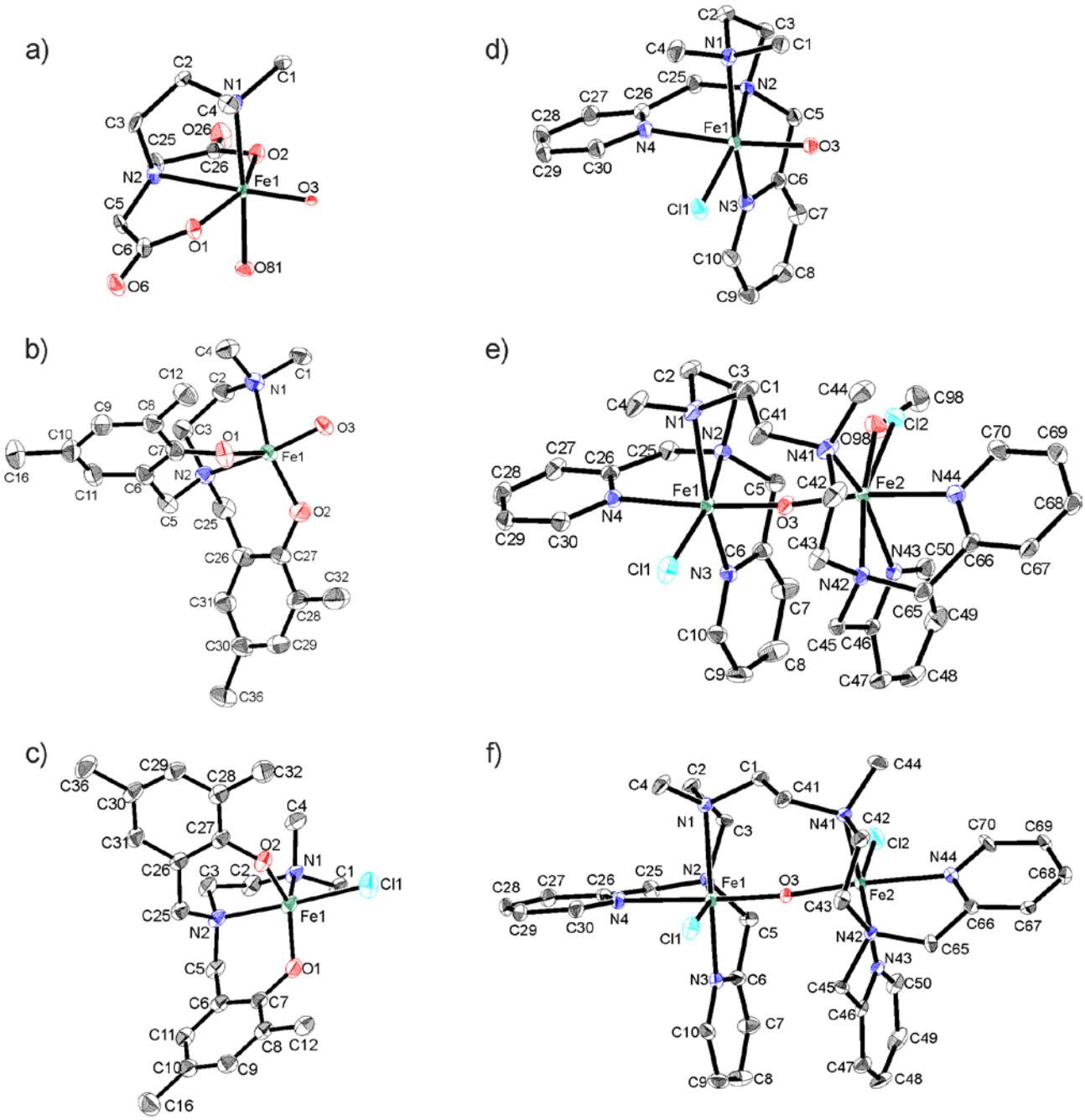


Fig. S11. Thermal ellipsoid plots of the asymmetric units in crystals of a) [(julia){Fe(OH_2)(μ-O)Fe(OH_2)}]•7H_2O, b) [(hilde^{Me_2}){Fe(μ-O)Fe}]•CH_2Cl_2, c) [(hilde^{Me_2}){$FeCl_2$}]•2CH_2Cl_2, d) [(susan){FeCl(μ-O)FeCl}]Cl_2•2H_2O, e) [(susan){FeCl(μ-O)$FeCl_{0.75}(OCH_3)_{0.25}$}]-$(ClO_4)_2$•0.5MeOH, and f) [(susan){FeCl(μ-O)FeCl}]$(ClO_4)_2$•0.5EtOH with the numbering scheme used. Thermal ellipsoids are drawn at the 50 % probability level; non-coordinating solvent molecules and hydrogen atoms are omitted for clarity.

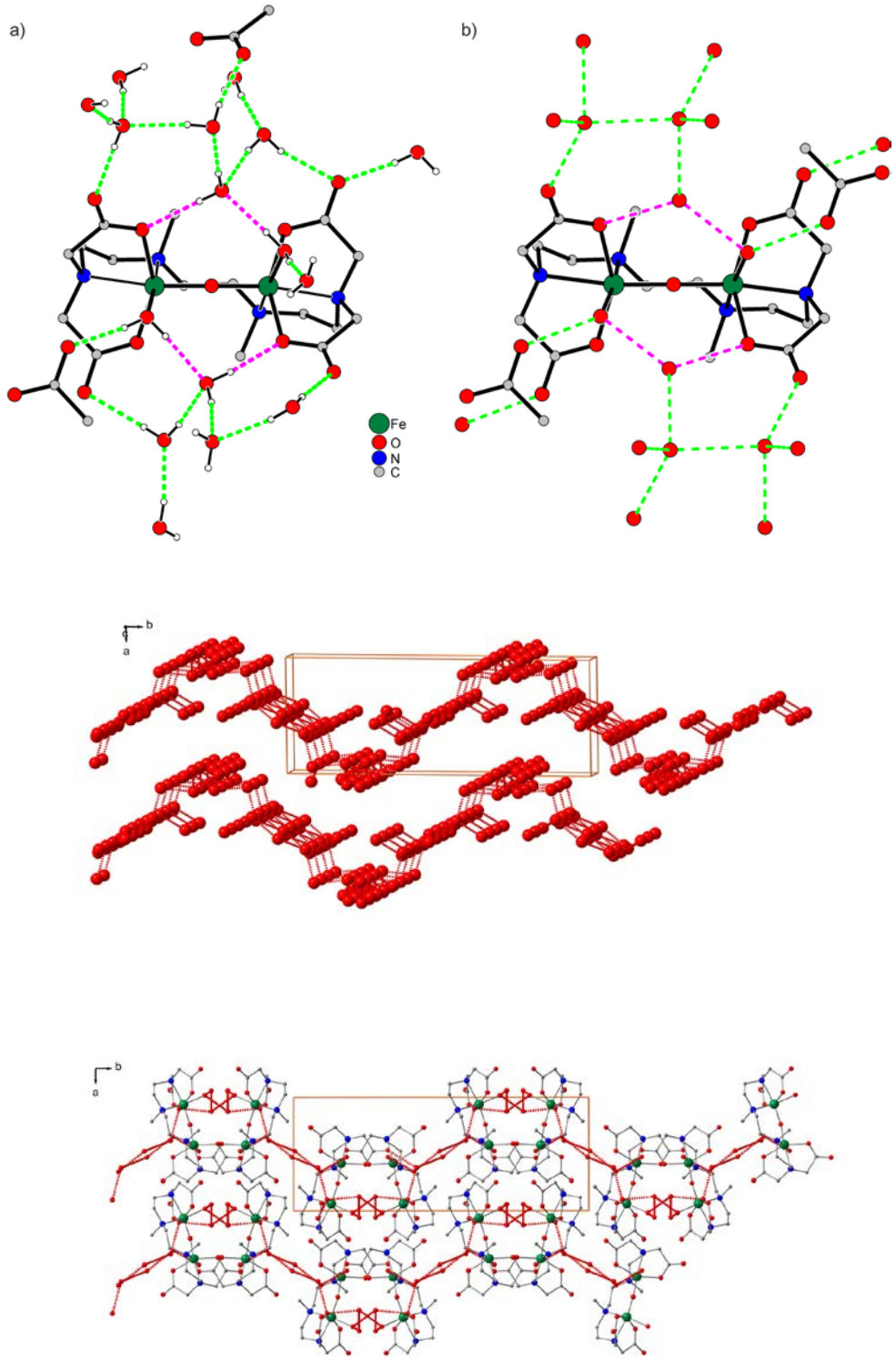


Fig. S12. Sections of the hydrogen bonding networks around the [(julia){Fe(OH_2)(μ-O)Fe(OH_2)}] complexes in crystals of a) [(julia){Fe(OH_2)(μ-O)Fe(OH_2)}]•6H_2O and b) [(julia){Fe(OH_2)(μ-O)Fe(OH_2)}]•7H_2O. c) Curled layers of water molecules in the crystals structure of [(julia){Fe(OH_2)(μ-O)Fe(OH_2)}]•6H_2O and d) including the dinuclear complexes appended to these layers.

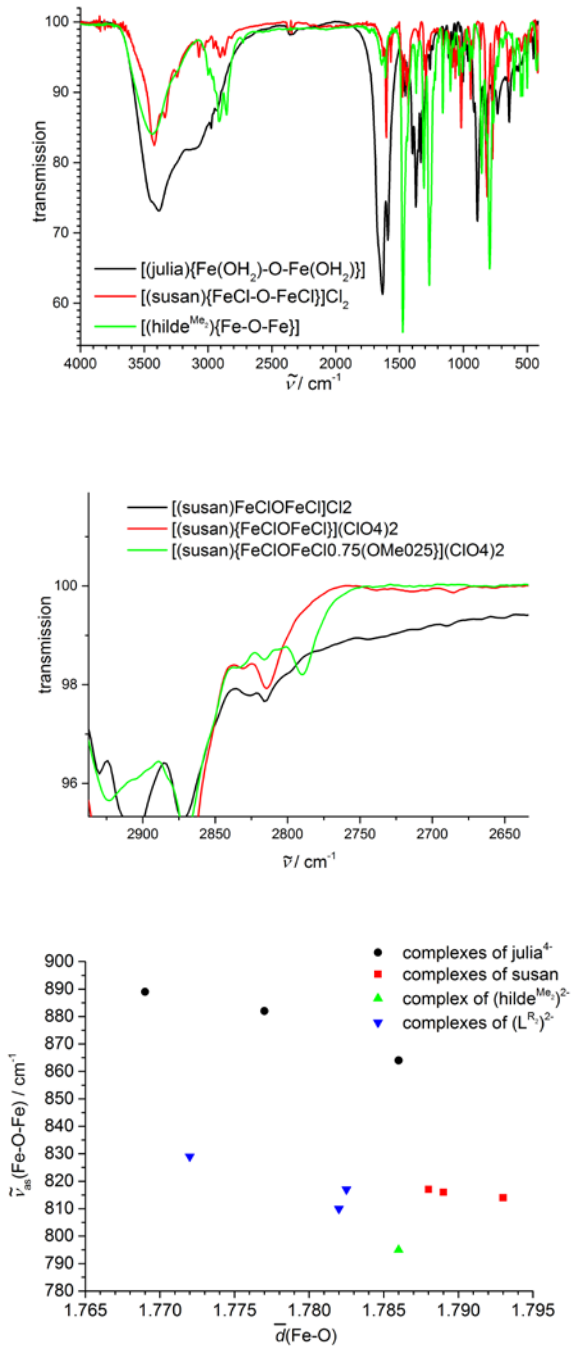


Fig. S13. a) FTIR spectra of three selected dinuclear complexes as representative examples for each dinucleating ligand. b) Section of the FTIR spectra of the three different [(susan){FeCl(μ-O)FeCl}]Cl_2 complexes demonstrating the appearance of the ν(C-H) stretch at 2790 cm^{-1} of the 25 % coordinated methanolate in [(susan){FeCl(μ-O)$FeCl_{0.75}(OCH_3)_{0.25}$}]$(ClO_4)_2$, which is absent in the spectra of the pure complexes $[(susan)\{FeCl(\mu\text{-}O)FeCl\}]^{2+}$. c) Dependence of the ν_{as}(Fe-O-Fe) stretch from the mean bond length $\bar{d}$(Fe-O) for dinuclear complexes with a central $\{Fe^{III}(\mu\text{-}O)Fe^{III}\}$ core.

Figure S14. Temperature-dependence of the effective magnetic moment, μ_{eff}, of the complexes indicated in the figure at 1 T. The solid lines are the fits to the experimental data (black dots), while the dashed lines correspond to paramagnetic S = 5/2 impurities.

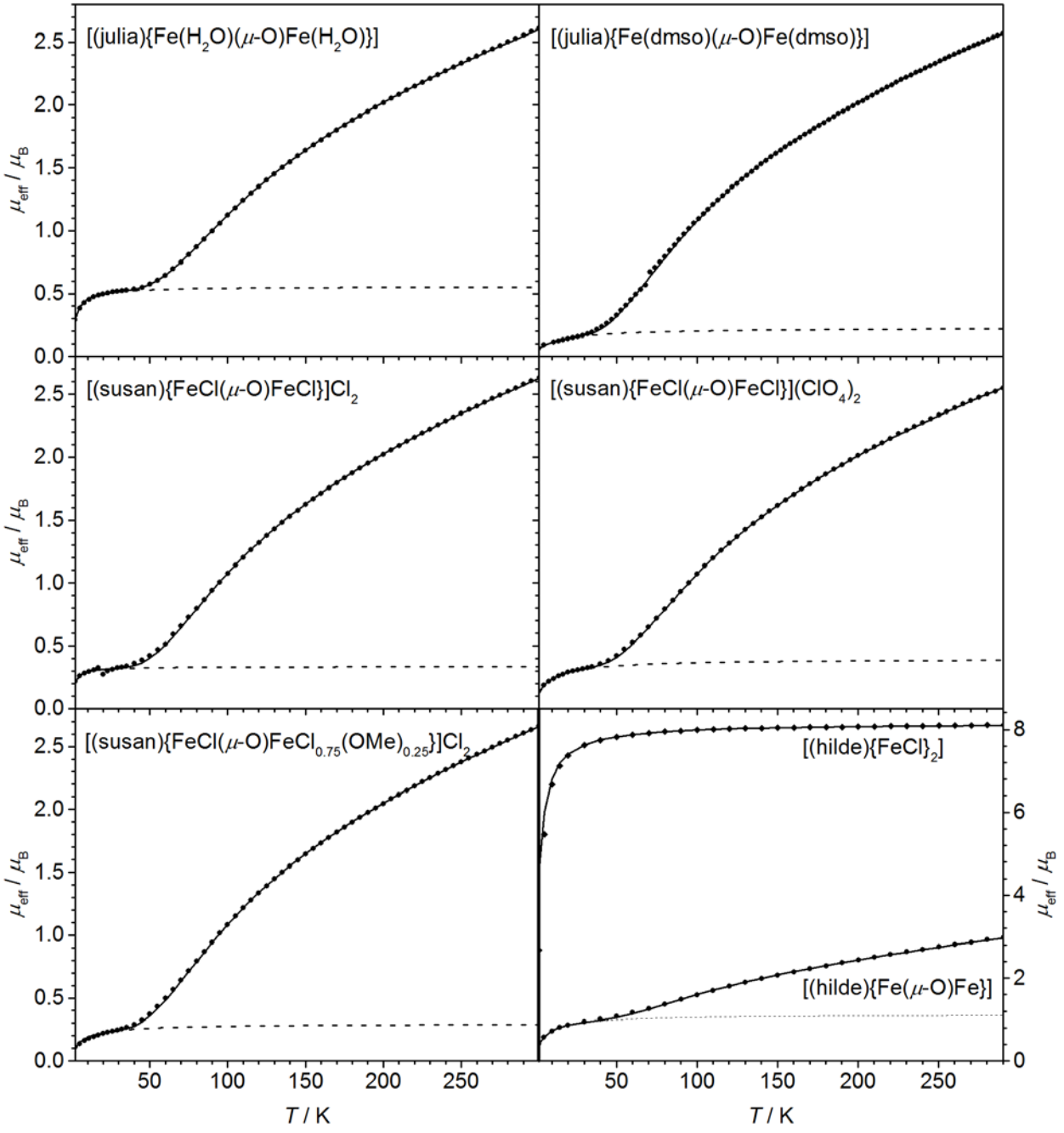


Figure S15. ^{57}Fe Mössbauer spectra of the complexes indicated in the figure at 80 K. The solid lines correspond to the fit of the experimental spectra given as dots.

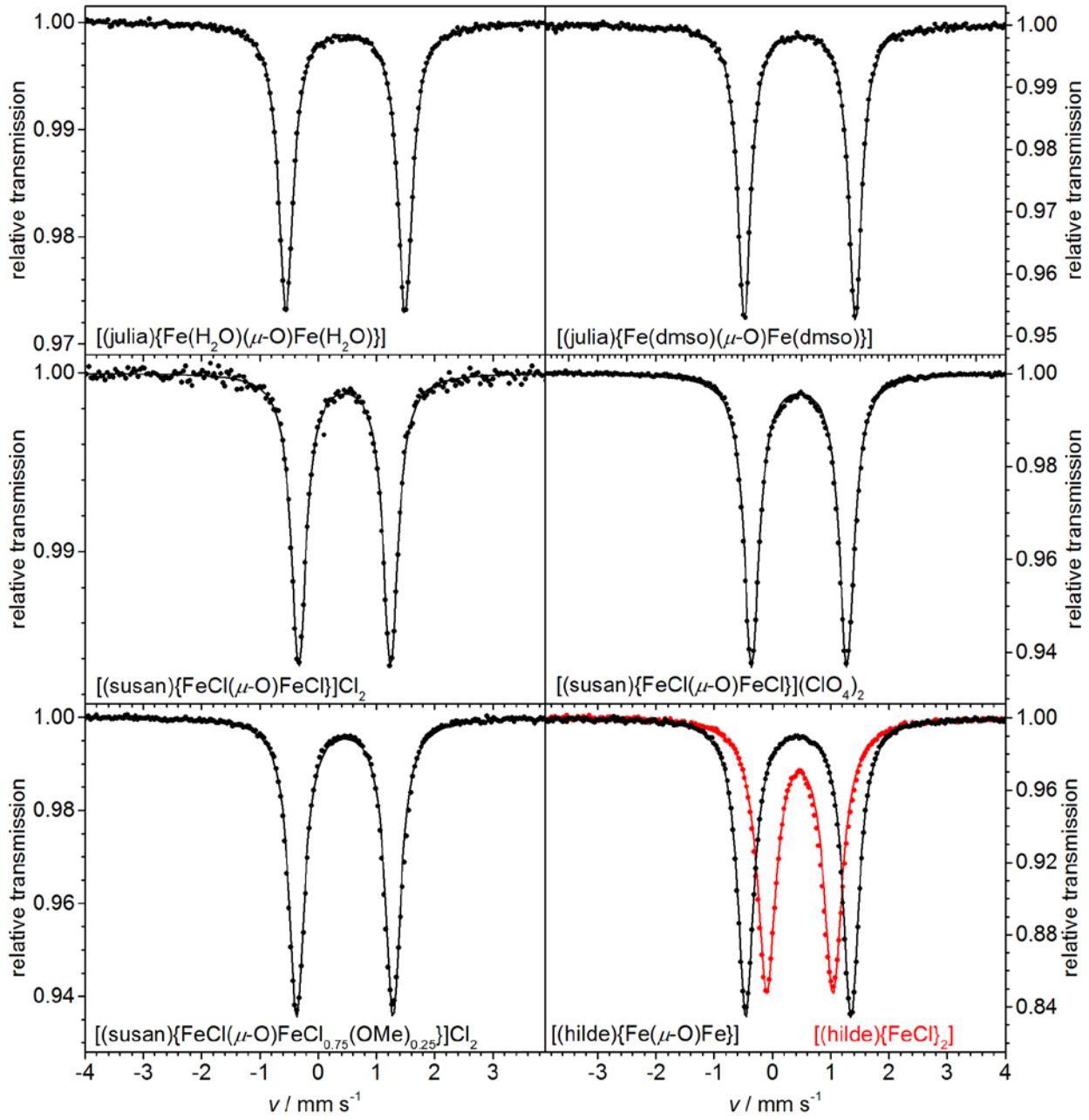


Table S1. Bond lengths [Å] and angles [°] for [(julia){Fe(OH_2)(μ-O)Fe(OH_2)}]•7H_2O.

Fe1-O3	1.7769(8)		O2-Fe1-N2	78.29(13)
Fe1-N1	2.190(4)		O1-Fe1-N2	75.77(13)
Fe1-N2	2.223(4)		O81-Fe1-N2	90.86(13)
Fe1-O1	2.033(3)		N1-Fe1-N2	82.43(14)
Fe1-O2	2.032(3)		O3-Fe1-Fe1#1	145.42(3)
Fe1-O81	2.085(3)		O2-Fe1-Fe1#1	46.08(9)
Fe1-Fe1#1	36.343(2)		O1-Fe1-Fe1#1	108.10(9)
O1-C6	1.295(6)		O81-Fe1-Fe1#1	65.40(9)
O2-C26	1.273(6)		N1-Fe1-Fe1#1	104.96(10)
O3-Fe1#2	1.7770(8)		N2-Fe1-Fe1#1	42.51(9)
N1-C2	1.490(6)		C6-O1-Fe1	117.7(3)
N1-C4	1.492(5)		C26-O2-Fe1	119.6(3)
N1-C1	1.501(6)		Fe1-O3-Fe1#2	164.6(3)
N2-C5	1.468(6)		C2-N1-C4	109.3(4)
N2-C25	1.485(6)		C2-N1-C1	105.1(4)
N2-C3	1.486(6)		C4-N1-C1	109.8(4)
O6-C6	1.236(6)		C2-N1-Fe1	106.2(3)
O26-C26	1.239(6)		C4-N1-Fe1	109.5(3)
C1-C1#2	1.510(9)		C1-N1-Fe1	116.5(3)
C1-H1A	0.9900		C5-N2-C25	115.1(4)
C1-H1B	0.9900		C5-N2-C3	109.8(4)
C2-C3	1.513(7)		C25-N2-C3	112.2(4)
C2-H2A	0.9900		C5-N2-Fe1	106.2(3)
C2-H2B	0.9900		C25-N2-Fe1	108.0(3)
C3-H3A	0.9900		C3-N2-Fe1	104.9(3)
C3-H3B	0.9900		N1-C1-C1#2	121.1(4)
C4-H4A	0.9800		N1-C1-H1A	107.0
C4-H4B	0.9800		C1#2-C1-H1A	107.0
C4-H4C	0.9800		N1-C1-H1B	107.0
C5-C6	1.520(6)		C1#2-C1-H1B	107.0
C5-H5A	0.9900		H1A-C1-H1B	106.8
C5-H5B	0.9900		N1-C2-C3	111.1(4)
C25-C26	1.517(6)		N1-C2-H2A	109.4
C25-H25A	0.9900		C3-C2-H2A	109.4
C25-H25B	0.9900		N1-C2-H2B	109.4
			C3-C2-H2B	109.4
O3-Fe1-O2	107.77(10)		H2A-C2-H2B	108.0
O3-Fe1-O1	98.68(11)		N2-C3-C2	111.0(4)
O2-Fe1-O1	153.24(13)		N2-C3-H3A	109.4
O3-Fe1-O81	94.70(15)		C2-C3-H3A	109.4
O2-Fe1-O81	85.72(14)		N2-C3-H3B	109.4
O1-Fe1-O81	88.19(13)		C2-C3-H3B	109.4
O3-Fe1-N1	92.72(15)		H3A-C3-H3B	108.0
O2-Fe1-N1	85.89(14)		N1-C4-H4A	109.5
O1-Fe1-N1	97.05(14)		N1-C4-H4B	109.5
O81-Fe1-N1	170.17(13)		H4A-C4-H4B	109.5
O3-Fe1-N2	172.03(11)		N1-C4-H4C	109.5
H4A-C4-H4C	109.5			
H4B-C4-H4C	109.5			
N2-C5-C6	110.0(4)			
N2-C5-H5A	109.7			
C6-C5-H5A	109.7			

N2-C5-H5B	109.7			
C6-C5-H5B	109.7			
H5A-C5-H5B	108.2			
O6-C6-O1	125.2(4)			
O6-C6-C5	118.6(4)			
O1-C6-C5	116.2(4)			
N2-C25-C26	112.3(4)			
N2-C25-H25A	109.1			
C26-C25-H25A	109.1			
N2-C25-H25B	109.1			
C26-C25-H25B	109.1			
H25A-C25-H25B	107.9			
O26-C26-O2	123.7(4)			
O26-C26-C25	118.4(4)			
O2-C26-C25	117.9(4)			

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+1 #2 -x+2,y,-z+1

Table S2. Bond lengths [Å] and angles [°] for [(susan){FeCl(μ-O)FeCl}]Cl_2•$2H_2O$.

Fe1-O3	1.7932(3)		O99-H99A	0.99(3)
Fe1-N1	2.2330(13)		O99-H99B	1.04(4)
Fe1-N2	2.2019(13)			
Fe1-N3	2.1741(14)		O3-Fe1-N3	90.55(6)
Fe1-N4	2.2278(13)		O3-Fe1-N2	93.48(3)
Fe1-Cl1	2.3099(4)		N3-Fe1-N2	74.48(5)
O3-Fe1#1	1.7932(3)		O3-Fe1-N4	170.27(4)
N1-C4	1.483(2)		N3-Fe1-N4	87.15(5)
N1-C2	1.491(2)		N2-Fe1-N4	76.79(5)
N1-C1	1.498(2)		O3-Fe1-N1	90.16(5)
N2-C5	1.4860(19)		N3-Fe1-N1	156.44(5)
N2-C3	1.487(2)		N2-Fe1-N1	81.98(5)
N2-C25	1.4891(19)		N4-Fe1-N1	88.21(5)
N3-C10	1.344(2)		O3-Fe1-Cl1	100.719(14)
N3-C6	1.347(2)		N3-Fe1-Cl1	97.39(4)
N4-C26	1.342(2)		N2-Fe1-Cl1	163.78(4)
N4-C30	1.353(2)		N4-Fe1-Cl1	88.96(4)
C1-C1#1	1.535(3)		N1-Fe1-Cl1	105.60(4)
C1-H1A	0.9900		Fe1#1-O3-Fe1	171.47(9)
C1-H1B	0.9900		C4-N1-C2	109.20(12)
C2-C3	1.514(2)		C4-N1-C1	108.56(12)
C2-H2A	0.9900		C2-N1-C1	109.12(12)
C2-H2B	0.9900		C4-N1-Fe1	112.89(10)
C3-H3A	0.9900		C2-N1-Fe1	105.00(9)
C3-H3B	0.9900		C1-N1-Fe1	111.96(9)
C4-H4A	0.9800		C5-N2-C3	112.38(12)
C4-H4B	0.9800		C5-N2-C25	109.44(12)
C4-H4C	0.9800		C3-N2-C25	112.25(12)
C5-C6	1.509(2)		C5-N2-Fe1	104.34(9)
C5-H5A	0.9900		C3-N2-Fe1	105.11(9)
C5-H5B	0.9900		C25-N2-Fe1	113.03(9)
C6-C7	1.389(2)		C10-N3-C6	119.24(14)
C7-C8	1.385(2)		C10-N3-Fe1	126.91(11)
C7-H7A	0.9500		C6-N3-Fe1	113.35(10)
C8-C9	1.388(2)		C26-N4-C30	118.46(13)
C8-H8A	0.9500		C26-N4-Fe1	114.52(10)
C9-C10	1.385(2)		C30-N4-Fe1	125.47(11)
C9-H9A	0.9500		N1-C1-C1#1	112.53(15)
C10-H10A	0.9500		N1-C1-H1A	109.1
C25-C26	1.508(2)		C1#1-C1-H1A	109.1
C25-H25A	0.9900		N1-C1-H1B	109.1
C25-H25B	0.9900		C1#1-C1-H1B	109.1
C26-C27	1.395(2)		H1A-C1-H1B	107.8
C27-C28	1.380(2)		N1-C2-C3	111.43(13)
C27-H27A	0.9500		N1-C2-H2A	109.3
C28-C29	1.388(3)		C3-C2-H2A	109.3
C28-H28A	0.9500		N1-C2-H2B	109.3
C29-C30	1.383(2)		C3-C2-H2B	109.3
C29-H29A	0.9500		H2A-C2-H2B	108.0
C30-H30A	0.9500		N2-C3-C2	109.17(12)
N2-C3-H3A	109.8		C9-C8-H8A	120.2
C2-C3-H3A	109.8		C10-C9-C8	118.48(15)
N2-C3-H3B	109.8		C10-C9-H9A	120.8
C2-C3-H3B	109.8		C8-C9-H9A	120.8

H3A-C3-H3B	108.3		N3-C10-C9	122.17(15)
N1-C4-H4A	109.5		N3-C10-H10A	118.9
N1-C4-H4B	109.5		C9-C10-H10A	118.9
H4A-C4-H4B	109.5		N2-C25-C26	113.96(12)
N1-C4-H4C	109.5		N2-C25-H25A	108.8
H4A-C4-H4C	109.5		C26-C25-H25A	108.8
H4B-C4-H4C	109.5		N2-C25-H25B	108.8
N2-C5-C6	108.06(12)		C26-C25-H25B	108.8
N2-C5-H5A	110.1		H25A-C25-H25B	107.7
C6-C5-H5A	110.1		N4-C26-C27	121.98(14)
N2-C5-H5B	110.1		N4-C26-C25	117.85(13)
C6-C5-H5B	110.1		C27-C26-C25	120.12(14)
H5A-C5-H5B	108.4		C28-C27-C26	118.97(15)
N3-C6-C7	121.68(14)		C28-C27-H27A	120.5
N3-C6-C5	115.87(13)		C26-C27-H27A	120.5
C7-C6-C5	122.45(14)		C27-C28-C29	119.38(15)
C8-C7-C6	118.77(15)		C27-C28-H28A	120.3
C8-C7-H7A	120.6		C29-C28-H28A	120.3
C6-C7-H7A	120.6		C30-C29-C28	118.57(16)
C7-C8-C9	119.62(16)		C30-C29-H29A	120.7
C7-C8-H8A	120.2		C28-C29-H29A	120.7
			N4-C30-C29	122.52(15)
			N4-C30-H30A	118.7
			C29-C30-H30A	118.7
			H99A-O99-H99B	102(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+3/2

Table S3. Bond lengths [Å] and angles [°] for [(susan){FeCl(μ-O)FeCl$_{0.75}$(OCH$_3$)$_{0.25}$}](ClO$_4$)$_2$•0.5MeOH.

Fe1-O3	1.7786(10)		C5-C6	1.505(2)
Fe2-O3	1.7974(10)		C5-H5A	0.9900
Fe1-N1	2.2614(13)		C5-H5B	0.9900
Fe2-N41	2.2501(14)		C6-C7	1.385(2)
Fe1-N2	2.2052(13)		C7-C8	1.383(3)
Fe2-N42	2.2204(13)		C7-H7	0.9500
Fe1-N3	2.1653(12)		C8-C9	1.375(3)
Fe1-N4	2.2559(13)		C8-H8	0.9500
Fe2-N43	2.1608(13)		C9-C10	1.382(2)
Fe2-N44	2.2011(13)		C9-H9	0.9500
Fe1-Cl1	2.2982(5)		C10-H10	0.9500
Fe2-Cl2	2.3311(11)		C25-C26	1.496(2)
Fe2-O98	1.745(6)		C25-H25A	0.9900
Fe1-Fe2	3.5693(4)		C25-H25B	0.9900
O98-C98	1.416(10)		C26-C27	1.392(2)
C98-H98A	0.9800		C27-C28	1.377(2)
C98-H98B	0.9800		C27-H27	0.9500
C98-H98C	0.9800		C28-C29	1.382(3)
N1-C4	1.484(2)		C28-H28	0.9500
N1-C2	1.489(2)		C29-C30	1.372(2)
N1-C1	1.493(2)		C29-H29	0.9500
N2-C5	1.4772(19)		C30-H30	0.9500
N2-C3	1.4817(19)		C41-H41A	0.9900
N2-C25	1.4825(19)		C41-H41B	0.9900
N3-C10	1.3435(19)		C42-C43	1.512(2)
N3-C6	1.344(2)		C42-H42A	0.9900
N4-C26	1.3387(19)		C42-H42B	0.9900
N4-C30	1.349(2)		C43-H43A	0.9900
N41-C44	1.485(2)		C43-H43B	0.9900
N41-C41	1.495(2)		C44-H44A	0.9800
N41-C42	1.495(2)		C44-H44B	0.9800
N44-C66	1.338(2)		C44-H44C	0.9800
N44-C70	1.350(2)		C45-C46	1.507(2)
N42-C43	1.4823(19)		C45-H45A	0.9900
N42-C45	1.4841(18)		C45-H45B	0.9900
N42-C65	1.4844(18)		C46-C47	1.387(2)
N43-C46	1.3434(19)		C47-C48	1.387(2)
N43-C50	1.346(2)		C47-H47	0.9500
C1-C41	1.527(2)		C48-C49	1.385(3)
C1-H1A	0.9900		C48-H48	0.9500
C1-H1B	0.9900		C49-C50	1.379(2)
C2-C3	1.516(2)		C49-H49	0.9500
C2-H2A	0.9900		C50-H50	0.9500
C2-H2B	0.9900		C65-C66	1.501(2)
C3-H3A	0.9900		C65-H65A	0.9900
C3-H3B	0.9900		C65-H65B	0.9900
C4-H4A	0.9800		C66-C67	1.387(2)
C4-H4B	0.9800		C67-C68	1.376(3)
C4-H4C	0.9800		C67-H67	0.9500
C68-C69	1.380(3)		N43-Fe2-N44	87.31(5)
C68-H68	0.9500		O98-Fe2-N42	169.78(19)
C69-C70	1.373(2)		O3-Fe2-N42	94.60(5)
C69-H69	0.9500		N43-Fe2-N42	74.17(5)

C70-H70	0.9500		N44-Fe2-N42	76.57(5)
Cl3-O33	1.4310(14)		O98-Fe2-N41	95.7(2)
Cl3-O32	1.4368(13)		O3-Fe2-N41	90.14(5)
Cl3-O34	1.4370(15)		N43-Fe2-N41	154.94(5)
Cl3-O31	1.4384(14)		N44-Fe2-N41	88.16(5)
Cl4-O42	1.4323(12)		N42-Fe2-N41	80.81(5)
Cl4-O41	1.4392(13)		O98-Fe2-Cl2	12.7(2)
Cl4-O43	1.4445(11)		O3-Fe2-Cl2	99.62(4)
Cl4-O44	1.4447(12)		N43-Fe2-Cl2	97.18(4)
C1M-C1MB#1	0.40(2)		N44-Fe2-Cl2	89.15(4)
C1M-O1MB	0.988(17)		N42-Fe2-Cl2	163.46(4)
C1M-O1MB#1	0.988(17)		N41-Fe2-Cl2	107.39(4)
C1M-O1M	1.477(4)		O98-Fe2-Fe1	92.67(19)
C1M-O1M#1	1.477(4)		O3-Fe2-Fe1	3.49(3)
O1M-C1MB#1	1.149(19)		N43-Fe2-Fe1	93.80(3)
O1M-O1MB	1.519(17)		N44-Fe2-Fe1	172.72(4)
O1M-C1MB	1.84(2)		N42-Fe2-Fe1	96.79(3)
O1MB-C1MB#1	0.79(2)		N41-Fe2-Fe1	87.81(4)
O1MB-C1MB	1.29(3)		Cl2-Fe2-Fe1	97.846(19)
C1MB-O1MB#1	0.79(2)		C98-O98-Fe2	142.1(6)
C1MB-C1MB#1	0.80(4)		O98-C98-H98A	109.5
C1MB-O1M#1	1.149(19)		O98-C98-H98B	109.5
			H98A-C98-H98B	109.5
O3-Fe1-N3	90.94(5)		O98-C98-H98C	109.5
O3-Fe1-N2	95.88(5)		H98A-C98-H98C	109.5
N3-Fe1-N2	75.09(5)		H98B-C98-H98C	109.5
O3-Fe1-N4	171.18(5)		Fe1-O3-Fe2	172.98(7)
N3-Fe1-N4	86.89(5)		C4-N1-C2	109.45(12)
N2-Fe1-N4	75.31(5)		C4-N1-C1	108.76(12)
O3-Fe1-N1	90.29(5)		C2-N1-C1	107.71(13)
N3-Fe1-N1	156.18(5)		C4-N1-Fe1	113.97(11)
N2-Fe1-N1	81.12(5)		C2-N1-Fe1	104.66(9)
N4-Fe1-N1	88.28(5)		C1-N1-Fe1	112.02(9)
O3-Fe1-Cl1	98.95(4)		C5-N2-C3	112.57(12)
N3-Fe1-Cl1	99.89(4)		C5-N2-C25	109.76(12)
N2-Fe1-Cl1	164.44(4)		C3-N2-C25	111.21(12)
N4-Fe1-Cl1	89.84(3)		C5-N2-Fe1	103.29(9)
N1-Fe1-Cl1	103.41(4)		C3-N2-Fe1	105.10(9)
O3-Fe1-Fe2	3.53(3)		C25-N2-Fe1	114.67(9)
N3-Fe1-Fe2	93.92(3)		C10-N3-C6	119.03(13)
N2-Fe1-Fe2	94.82(3)		C10-N3-Fe1	126.84(11)
N4-Fe1-Fe2	169.55(3)		C6-N3-Fe1	113.63(10)
N1-Fe1-Fe2	86.80(3)		C26-N4-C30	117.58(13)
Cl1-Fe1-Fe2	100.262(14)		C26-N4-Fe1	116.92(10)
O98-Fe2-O3	95.02(19)		C30-N4-Fe1	125.31(10)
O98-Fe2-N43	109.1(2)		C44-N41-C41	108.54(13)
O3-Fe2-N43	90.59(5)		C44-N41-C42	108.91(13)
O98-Fe2-N44	93.77(19)		C41-N41-C42	107.88(14)
O3-Fe2-N44	171.17(5)		C44-N41-Fe2	113.54(12)
C41-N41-Fe2	111.92(9)		C7-C8-H8	120.2
C42-N41-Fe2	105.86(9)		C8-C9-C10	118.94(15)
C66-N44-C70	118.38(14)		C8-C9-H9	120.5
C66-N44-Fe2	117.03(10)		C10-C9-H9	120.5
C70-N44-Fe2	124.46(11)		N3-C10-C9	121.89(15)
C43-N42-C45	112.66(12)		N3-C10-H10	119.1
C43-N42-C65	111.33(12)		C9-C10-H10	119.1
C45-N42-C65	110.21(11)		N2-C25-C26	113.75(12)

C43-N42-Fe2	105.26(9)		N2-C25-H25A	108.8
C45-N42-Fe2	104.32(8)		C26-C25-H25A	108.8
C65-N42-Fe2	112.80(9)		N2-C25-H25B	108.8
C46-N43-C50	119.07(13)		C26-C25-H25B	108.8
C46-N43-Fe2	114.55(10)		H25A-C25-H25B	107.7
C50-N43-Fe2	125.80(11)		N4-C26-C27	122.32(14)
N1-C1-C41	113.50(14)		N4-C26-C25	117.58(13)
N1-C1-H1A	108.9		C27-C26-C25	120.01(14)
C41-C1-H1A	108.9		C28-C27-C26	118.97(15)
N1-C1-H1B	108.9		C28-C27-H27	120.5
C41-C1-H1B	108.9		C26-C27-H27	120.5
H1A-C1-H1B	107.7		C27-C28-C29	119.21(15)
N1-C2-C3	110.21(12)		C27-C28-H28	120.4
N1-C2-H2A	109.6		C29-C28-H28	120.4
C3-C2-H2A	109.6		C30-C29-C28	118.43(15)
N1-C2-H2B	109.6		C30-C29-H29	120.8
C3-C2-H2B	109.6		C28-C29-H29	120.8
H2A-C2-H2B	108.1		N4-C30-C29	123.48(15)
N2-C3-C2	108.66(13)		N4-C30-H30	118.3
N2-C3-H3A	110.0		C29-C30-H30	118.3
C2-C3-H3A	110.0		N41-C41-C1	112.18(15)
N2-C3-H3B	110.0		N41-C41-H41A	109.2
C2-C3-H3B	110.0		C1-C41-H41A	109.2
H3A-C3-H3B	108.3		N41-C41-H41B	109.2
N1-C4-H4A	109.5		C1-C41-H41B	109.2
N1-C4-H4B	109.5		H41A-C41-H41B	107.9
H4A-C4-H4B	109.5		N41-C42-C43	109.93(12)
N1-C4-H4C	109.5		N41-C42-H42A	109.7
H4A-C4-H4C	109.5		C43-C42-H42A	109.7
H4B-C4-H4C	109.5		N41-C42-H42B	109.7
N2-C5-C6	108.89(12)		C43-C42-H42B	109.7
N2-C5-H5A	109.9		H42A-C42-H42B	108.2
C6-C5-H5A	109.9		N42-C43-C42	109.58(14)
N2-C5-H5B	109.9		N42-C43-H43A	109.8
C6-C5-H5B	109.9		C42-C43-H43A	109.8
H5A-C5-H5B	108.3		N42-C43-H43B	109.8
N3-C6-C7	121.93(15)		C42-C43-H43B	109.8
N3-C6-C5	115.21(13)		H43A-C43-H43B	108.2
C7-C6-C5	122.82(15)		N41-C44-H44A	109.5
C8-C7-C6	118.54(17)		N41-C44-H44B	109.5
C8-C7-H7	120.7		H44A-C44-H44B	109.5
C6-C7-H7	120.7		N41-C44-H44C	109.5
C9-C8-C7	119.66(16)		H44A-C44-H44C	109.5
C9-C8-H8	120.2		H44B-C44-H44C	109.5
N42-C45-C46	108.33(12)		O33-Cl3-O31	109.38(10)
C46-C45-H45A	110.0		O32-Cl3-O31	109.33(9)
N42-C45-H45B	110.0		O34-Cl3-O31	109.09(9)
C46-C45-H45B	110.0		O42-Cl4-O41	109.89(8)
H45A-C45-H45B	108.4		O42-Cl4-O43	109.82(7)
N43-C46-C47	121.63(14)		O41-Cl4-O43	109.56(8)
N43-C46-C45	115.49(12)		O42-Cl4-O44	109.26(8)
C47-C46-C45	122.87(13)		O41-Cl4-O44	109.24(8)
C46-C47-C48	118.82(15)		O43-Cl4-O44	109.05(7)
C46-C47-H47	120.6		N42-C45-H45A	110.0
C48-C47-H47	120.6		C1MB#1-C1M-O1MB	49(2)
C49-C48-C47	119.59(15)		C1MB#1-C1M-O1MB#1	131(2)

C49-C48-H48	120.2		O1MB-C1M-O1MB#1	180.0(11)
C47-C48-H48	120.2		C1MB#1-C1M-O1M	30(2)
C50-C49-C48	118.35(15)		O1MB-C1M-O1M	73.0(10)
C50-C49-H49	120.8		O1MB#1-C1M-O1M	107.0(10)
C48-C49-H49	120.8		C1MB#1-C1M-O1M#1	150(2)
N43-C50-C49	122.52(15)		O1MB-C1M-O1M#1	107.0(10)
N43-C50-H50	118.7		O1MB#1-C1M-O1M#1	73.0(10)
C49-C50-H50	118.7		O1M-C1M-O1M#1	180.0(3)
N42-C65-C66	113.69(12)		C1MB#1-O1M-C1M	10.2(9)
N42-C65-H65A	108.8		C1MB#1-O1M-O1MB	30.4(11)
C66-C65-H65A	108.8		C1M-O1M-O1MB	38.5(7)
N42-C65-H65B	108.8		C1MB#1-O1M-C1MB	16.6(14)
C66-C65-H65B	108.8		C1M-O1M-C1MB	6.4(5)
H65A-C65-H65B	107.7		O1MB-O1M-C1MB	43.9(9)
N44-C66-C67	121.75(15)		C1MB#1-O1MB-C1M	22.7(18)
N44-C66-C65	118.12(13)		C1MB#1-O1MB-C1MB	36(3)
C67-C66-C65	120.12(14)		C1M-O1MB-C1MB	13.6(9)
C68-C67-C66	119.15(16)		C1MB#1-O1MB-O1M	47.8(19)
C68-C67-H67	120.4		C1M-O1MB-O1M	68.5(10)
C66-C67-H67	120.4		C1MB-O1MB-O1M	81.2(13)
C67-C68-C69	119.46(15)		O1MB#1-C1MB-C1MB#1	108(3)
C67-C68-H68	120.3		O1MB#1-C1MB-O1M#1	102(3)
C69-C68-H68	120.3		C1MB#1-C1MB-O1M#1	139(3)
C70-C69-C68	118.44(16)		O1MB#1-C1MB-O1MB	144(3)
C70-C69-H69	120.8		C1MB#1-C1MB-O1MB	35.4(17)
C68-C69-H69	120.8		O1M#1-C1MB-O1MB	110.4(15)
N44-C70-C69	122.80(16)		O1MB#1-C1MB-O1M	90(2)
N44-C70-H70	118.6		C1MB#1-C1MB-O1M	24.0(18)
C69-C70-H70	118.6		O1M#1-C1MB-O1M	163.4(14)
O33-Cl3-O32	109.33(8)		O1MB-C1MB-O1M	54.9(9)
O33-Cl3-O34	110.64(10)			
O32-Cl3-O34	109.05(10)			

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z+1

Table S4. Bond lengths [Å] and angles [°] for [(susan){FeCl(μ-O)FeCl}]$(ClO_4)_2$•0.5EtOH.

Fe1-O3	1.780(2)		C8-C9	1.370(6)
Fe2-O3	1.798(2)		C8-H8	0.9500
Fe1-N1	2.255(3)		C9-C10	1.384(5)
Fe2-N41	2.249(3)		C9-H9	0.9500
Fe1-N2	2.201(3)		C10-H10	0.9500
Fe2-N42	2.217(3)		C25-C26	1.502(5)
Fe1-N3	2.157(3)		C25-H25A	0.9900
Fe1-N4	2.259(3)		C25-H25B	0.9900
Fe2-N43	2.155(3)		C26-C27	1.391(5)
Fe2-N44	2.202(3)		C27-C28	1.374(5)
Fe1-Cl1	2.2961(10)		C27-H27	0.9500
Fe2-Cl2	2.3166(11)		C28-C29	1.394(6)
Fe1-Fe2	3.5721(7)		C28-H28	0.9500
N1-C4	1.478(4)		C29-C30	1.378(5)
N1-C1	1.491(4)		C29-H29	0.9500
N1-C2	1.493(5)		C30-H30	0.9500
N2-C5	1.478(4)		C41-H41A	0.9900
N2-C25	1.480(4)		C41-H41B	0.9900
N2-C3	1.483(4)		C42-C43	1.512(5)
N3-C10	1.344(4)		C42-H42A	0.9900
N3-C6	1.353(4)		C42-H42B	0.9900
N4-C26	1.334(4)		C43-H43A	0.9900
N4-C30	1.349(4)		C43-H43B	0.9900
N41-C41	1.491(4)		C44-H44A	0.9800
N41-C44	1.493(5)		C44-H44B	0.9800
N41-C42	1.495(5)		C44-H44C	0.9800
N42-C65	1.479(4)		C45-C46	1.513(4)
N42-C43	1.486(4)		C45-H45A	0.9900
N42-C45	1.490(4)		C45-H45B	0.9900
N43-C50	1.343(4)		C46-C47	1.371(5)
N43-C46	1.352(4)		C47-C48	1.393(5)
N44-C66	1.338(5)		C47-H47	0.9500
N44-C70	1.350(4)		C48-C49	1.373(6)
C1-C41	1.524(5)		C48-H48	0.9500
C1-H1A	0.9900		C49-C50	1.375(6)
C1-H1B	0.9900		C49-H49	0.9500
C2-C3	1.515(5)		C50-H50	0.9500
C2-H2A	0.9900		C65-C66	1.505(5)
C2-H2B	0.9900		C65-H65A	0.9900
C3-H3A	0.9900		C65-H65B	0.9900
C3-H3B	0.9900		C66-C67	1.390(5)
C4-H4A	0.9800		C67-C68	1.379(6)
C4-H4B	0.9800		C67-H67	0.9500
C4-H4C	0.9800		C68-C69	1.371(6)
C5-C6	1.508(5)		C68-H68	0.9500
C5-H5A	0.9900		C69-C70	1.373(5)
C5-H5B	0.9900		C69-H69	0.9500
C6-C7	1.368(5)		C70-H70	0.9500
C7-C8	1.395(6)		Cl3-O34	1.430(3)
C7-H7	0.9500		Cl3-O31	1.440(3)
Cl3-O33	1.446(3)		N41-Fe2-Fe1	87.67(7)
Cl4-O41	1.428(3)		Cl2-Fe2-Fe1	97.69(3)
Cl3-O32	1.443(3)		Fe1-O3-Fe2	173.51(15)
Cl4-O44	1.436(3)		C4-N1-C1	108.9(3)

Cl4-O43	1.439(3)		C4-N1-C2	109.6(3)
Cl4-O42	1.443(3)		C1-N1-C2	107.8(3)
O1S-C1S	1.194(11)		C4-N1-Fe1	113.5(2)
O1S-C2S	1.626(7)		C1-N1-Fe1	112.3(2)
C1S-C2S	0.775(10)		C2-N1-Fe1	104.5(2)
C1S-C1S#1	1.55(2)		C5-N2-C25	110.1(3)
C2S-C1S#1	0.775(10)		C5-N2-C3	112.3(3)
C2S-O1S#1	1.626(7)		C25-N2-C3	111.0(3)
			C5-N2-Fe1	103.3(2)
O3-Fe1-N3	91.16(11)		C25-N2-Fe1	114.86(19)
O3-Fe1-N2	95.62(10)		C3-N2-Fe1	105.1(2)
N3-Fe1-N2	75.10(10)		C10-N3-C6	118.8(3)
O3-Fe1-N1	90.17(11)		C10-N3-Fe1	126.8(2)
N3-Fe1-N1	156.41(11)		C6-N3-Fe1	113.9(2)
N2-Fe1-N1	81.33(11)		C26-N4-C30	117.7(3)
O3-Fe1-N4	170.87(11)		C26-N4-Fe1	117.1(2)
N3-Fe1-N4	86.95(10)		C30-N4-Fe1	125.1(2)
N2-Fe1-N4	75.25(10)		C41-N41-C44	108.8(3)
N1-Fe1-N4	88.03(10)		C41-N41-C42	108.1(3)
O3-Fe1-Cl1	99.42(8)		C44-N41-C42	108.7(3)
N3-Fe1-Cl1	99.97(8)		C41-N41-Fe2	111.9(2)
N2-Fe1-Cl1	164.29(8)		C44-N41-Fe2	113.2(2)
N1-Fe1-Cl1	103.04(8)		C42-N41-Fe2	105.9(2)
N4-Fe1-Cl1	89.71(8)		C65-N42-C43	111.6(3)
O3-Fe1-Fe2	3.26(8)		C65-N42-C45	110.1(2)
N3-Fe1-Fe2	94.22(7)		C43-N42-C45	112.3(3)
N2-Fe1-Fe2	95.32(7)		C65-N42-Fe2	113.0(2)
N1-Fe1-Fe2	86.91(7)		C43-N42-Fe2	105.3(2)
N4-Fe1-Fe2	169.89(8)		C45-N42-Fe2	104.37(19)
Cl1-Fe1-Fe2	99.96(3)		C50-N43-C46	118.5(3)
O3-Fe2-N43	90.44(11)		C50-N43-Fe2	126.2(2)
O3-Fe2-N44	172.00(11)		C46-N43-Fe2	114.7(2)
N43-Fe2-N44	87.28(11)		C66-N44-C70	118.6(3)
O3-Fe2-N42	95.17(10)		C66-N44-Fe2	116.4(2)
N43-Fe2-N42	74.38(10)		C70-N44-Fe2	124.9(2)
N44-Fe2-N42	76.83(11)		N1-C1-C41	113.5(3)
O3-Fe2-N41	90.28(11)		N1-C1-H1A	108.9
N43-Fe2-N41	155.07(11)		C41-C1-H1A	108.9
N44-Fe2-N41	88.57(11)		N1-C1-H1B	108.9
N42-Fe2-N41	80.74(11)		C41-C1-H1B	108.9
O3-Fe2-Cl2	98.75(8)		H1A-C1-H1B	107.7
N43-Fe2-Cl2	97.78(8)		N1-C2-C3	110.3(3)
N44-Fe2-Cl2	89.16(8)		N1-C2-H2A	109.6
N42-Fe2-Cl2	164.10(7)		C3-C2-H2A	109.6
N41-Fe2-Cl2	106.73(9)		N1-C2-H2B	109.6
O3-Fe2-Fe1	3.23(8)		C3-C2-H2B	109.6
N43-Fe2-Fe1	93.61(7)		H2A-C2-H2B	108.1
N44-Fe2-Fe1	172.90(8)		N2-C3-C2	108.5(3)
N42-Fe2-Fe1	96.61(7)		N2-C3-H3A	110.0
C2-C3-H3A	110.0		N41-C41-H41A	109.0
N2-C3-H3B	110.0		C1-C41-H41A	109.0
C2-C3-H3B	110.0		N41-C41-H41B	109.0
H3A-C3-H3B	108.4		C1-C41-H41B	109.0
N1-C4-H4A	109.5		H41A-C41-H41B	107.8
N1-C4-H4B	109.5		N41-C42-C43	109.6(3)
H4A-C4-H4B	109.5		N41-C42-H42A	109.7
N1-C4-H4C	109.5		C43-C42-H42A	109.7

H4A-C4-H4C	109.5		N41-C42-H42B	109.7
H4B-C4-H4C	109.5		C43-C42-H42B	109.7
N2-C5-C6	108.7(3)		H42A-C42-H42B	108.2
N2-C5-H5A	109.9		N42-C43-C42	109.3(3)
C6-C5-H5A	109.9		N42-C43-H43A	109.8
N2-C5-H5B	109.9		C42-C43-H43A	109.8
C6-C5-H5B	109.9		N42-C43-H43B	109.8
H5A-C5-H5B	108.3		C42-C43-H43B	109.8
N3-C6-C7	122.2(3)		H43A-C43-H43B	108.3
N3-C6-C5	114.6(3)		N41-C44-H44A	109.5
C7-C6-C5	123.1(3)		N41-C44-H44B	109.5
C6-C7-C8	118.6(3)		H44A-C44-H44B	109.5
C6-C7-H7	120.7		N41-C44-H44C	109.5
C8-C7-H7	120.7		H44A-C44-H44C	109.5
C9-C8-C7	119.4(4)		H44B-C44-H44C	109.5
C9-C8-H8	120.3		N42-C45-C46	108.2(3)
C7-C8-H8	120.3		N42-C45-H45A	110.1
C8-C9-C10	119.2(4)		C46-C45-H45A	110.1
C8-C9-H9	120.4		N42-C45-H45B	110.1
C10-C9-H9	120.4		C46-C45-H45B	110.1
N3-C10-C9	121.7(3)		H45A-C45-H45B	108.4
N3-C10-H10	119.1		N43-C46-C47	122.2(3)
C9-C10-H10	119.1		N43-C46-C45	115.2(3)
N2-C25-C26	113.6(3)		C47-C46-C45	122.6(3)
N2-C25-H25A	108.8		C46-C47-C48	118.4(3)
C26-C25-H25A	108.8		C46-C47-H47	120.8
N2-C25-H25B	108.8		C48-C47-H47	120.8
C26-C25-H25B	108.8		C49-C48-C47	119.6(3)
H25A-C25-H25B	107.7		C49-C48-H48	120.2
N4-C26-C27	122.7(3)		C47-C48-H48	120.2
N4-C26-C25	117.3(3)		C48-C49-C50	118.8(3)
C27-C26-C25	119.9(3)		C48-C49-H49	120.6
C28-C27-C26	119.0(3)		C50-C49-H49	120.6
C28-C27-H27	120.5		N43-C50-C49	122.4(3)
C26-C27-H27	120.5		N43-C50-H50	118.8
C27-C28-C29	119.0(3)		C49-C50-H50	118.8
C27-C28-H28	120.5		N42-C65-C66	113.3(3)
C29-C28-H28	120.5		N42-C65-H65A	108.9
C30-C29-C28	118.3(3)		C66-C65-H65A	108.9
C30-C29-H29	120.8		N42-C65-H65B	108.9
C28-C29-H29	120.8		C66-C65-H65B	108.9
N4-C30-C29	123.3(3)		H65A-C65-H65B	107.7
N4-C30-H30	118.4		N44-C66-C67	121.4(3)
C29-C30-H30	118.4		N44-C66-C65	118.7(3)
N41-C41-C1	112.8(3)		C67-C66-C65	119.9(3)
C68-C67-C66	119.1(4)		O32-Cl3-O33	109.12(16)
C68-C67-H67	120.4		O41-Cl4-O44	109.44(19)
C66-C67-H67	120.4		O41-Cl4-O43	109.5(2)
C69-C68-C67	119.6(3)		O44-Cl4-O43	109.5(2)
C69-C68-H68	120.2		O41-Cl4-O42	110.7(2)
C67-C68-H68	120.2		O44-Cl4-O42	108.8(2)
C68-C69-C70	118.6(3)		O43-Cl4-O42	108.9(2)
C68-C69-H69	120.7		C1S-O1S-C2S	26.7(5)
C70-C69-H69	120.7		C2S-C1S-O1S	109.5(11)
N44-C70-C69	122.7(4)		C2S-C1S-C1S#1	0.0(6)
N44-C70-H70	118.7		O1S-C1S-C1S#1	109.5(11)
C69-C70-H70	118.7		C1S#1-C2S-C1S	180.0(19)

O34-Cl3-O31	109.41(18)		C1S#1-C2S-O1S#1	43.8(8)
O34-Cl3-O32	110.05(17)		C1S-C2S-O1S#1	136.2(8)
O31-Cl3-O32	109.65(17)		C1S#1-C2S-O1S	136.2(8)
O34-Cl3-O33	109.05(18)		C1S-C2S-O1S	43.8(8)
O31-Cl3-O33	109.54(18)		O1S#1-C2S-O1S	179.998(1)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1

Table S5. Bond lengths [Å] and angles [°] for [(hilde^{Me2}){Fe(μ-O)Fe}]•CH_2Cl_2.

Fe1-O3	1.7858(7)		C27-C28	1.405(5)
Fe1-N1	2.242(3)		C28-C29	1.385(5)
Fe1-N2	2.294(3)		C28-C32	1.503(5)
Fe1-O1	1.877(2)		C29-C30	1.394(5)
Fe1-O2	1.892(2)		C29-H29A	0.9500
Fe1-Fe1#1	3.5215(9)		C30-C31	1.385(5)
O1-C7	1.338(4)		C30-C36	1.514(5)
O2-C27	1.349(4)		C31-H31A	0.9500
O3-Fe1#1	1.7858(7)		C32-H32A	0.9800
N1-C2	1.484(4)		C32-H32B	0.9800
N1-C1	1.488(4)		C32-H32C	0.9800
N1-C4	1.490(4)		C36-H36A	0.9800
N2-C3	1.484(4)		C36-H36B	0.9800
N2-C5	1.496(4)		C36-H36C	0.9800
N2-C25	1.501(4)		C100-Cl1	1.773(5)
C1-C1#1	1.524(7)		C100-Cl1#1	1.773(5)
C1-H1A	0.9900		C100-H10A	0.9602
C1-H1B	0.9900			
C2-C3	1.520(4)		O3-Fe1-O1	104.62(10)
C2-H2A	0.9900		O3-Fe1-O2	95.25(8)
C2-H2B	0.9900		O1-Fe1-O2	119.76(11)
C3-H3A	0.9900		O3-Fe1-N1	89.49(11)
C3-H3B	0.9900		O1-Fe1-N1	106.61(10)
C4-H4A	0.9800		O2-Fe1-N1	130.18(11)
C4-H4B	0.9800		O3-Fe1-N2	164.15(11)
C4-H4C	0.9800		O1-Fe1-N2	88.28(9)
C5-C6	1.504(5)		O2-Fe1-N2	85.98(10)
C5-H5A	0.9900		N1-Fe1-N2	77.83(9)
C5-H5B	0.9900		O3-Fe1-Fe1#1	9.61(10)
C6-C11	1.396(5)		O1-Fe1-Fe1#1	111.49(7)
C6-C7	1.409(4)		O2-Fe1-Fe1#1	96.96(7)
C7-C8	1.405(5)		N1-Fe1-Fe1#1	81.14(7)
C8-C9	1.387(5)		N2-Fe1-Fe1#1	154.58(6)
C8-C12	1.507(5)		C7-O1-Fe1	132.0(2)
C9-C10	1.393(5)		C27-O2-Fe1	130.7(2)
C9-H9A	0.9500		Fe1#1-O3-Fe1	160.78(19)
C10-C11	1.375(5)		C2-N1-C1	109.7(3)
C10-C16	1.520(5)		C2-N1-C4	110.5(3)
C11-H11A	0.9500		C1-N1-C4	107.6(2)
C12-H12A	0.9800		C2-N1-Fe1	109.88(18)
C12-H12B	0.9800		C1-N1-Fe1	113.10(19)
C12-H12C	0.9800		C4-N1-Fe1	105.87(19)
C16-H16A	0.9800		C3-N2-C5	111.0(3)
C16-H16B	0.9800		C3-N2-C25	109.8(2)
C16-H16C	0.9800		C5-N2-C25	107.8(2)
C25-C26	1.508(5)		C3-N2-Fe1	109.23(18)
C25-H25A	0.9900		C5-N2-Fe1	109.10(19)
C25-H25B	0.9900		C25-N2-Fe1	109.85(19)
C26-C27	1.394(5)		N1-C1-C1#1	112.4(3)
C26-C31	1.401(4)		N1-C1-H1A	109.1
C1#1-C1-H1A	109.1		C8-C12-H12C	109.5
N1-C1-H1B	109.1		H12A-C12-H12C	109.5
C1#1-C1-H1B	109.1		H12B-C12-H12C	109.5
H1A-C1-H1B	107.9		C10-C16-H16A	109.5

N1-C2-C3	110.8(3)		C10-C16-H16B	109.5
N1-C2-H2A	109.5		H16A-C16-H16B	109.5
C3-C2-H2A	109.5		C10-C16-H16C	109.5
N1-C2-H2B	109.5		H16A-C16-H16C	109.5
C3-C2-H2B	109.5		H16B-C16-H16C	109.5
H2A-C2-H2B	108.1		N2-C25-C26	112.1(3)
N2-C3-C2	109.9(3)		N2-C25-H25A	109.2
N2-C3-H3A	109.7		C26-C25-H25A	109.2
C2-C3-H3A	109.7		N2-C25-H25B	109.2
N2-C3-H3B	109.7		C26-C25-H25B	109.2
C2-C3-H3B	109.7		H25A-C25-H25B	107.9
H3A-C3-H3B	108.2		C27-C26-C31	119.6(3)
N1-C4-H4A	109.5		C27-C26-C25	118.9(3)
N1-C4-H4B	109.5		C31-C26-C25	121.5(3)
H4A-C4-H4B	109.5		O2-C27-C26	120.1(3)
N1-C4-H4C	109.5		O2-C27-C28	119.9(3)
H4A-C4-H4C	109.5		C26-C27-C28	120.0(3)
H4B-C4-H4C	109.5		C29-C28-C27	118.5(3)
N2-C5-C6	114.2(3)		C29-C28-C32	121.8(3)
N2-C5-H5A	108.7		C27-C28-C32	119.7(3)
C6-C5-H5A	108.7		C28-C29-C30	122.9(3)
N2-C5-H5B	108.7		C28-C29-H29A	118.6
C6-C5-H5B	108.7		C30-C29-H29A	118.6
H5A-C5-H5B	107.6		C31-C30-C29	117.6(3)
C11-C6-C7	119.2(3)		C31-C30-C36	122.0(3)
C11-C6-C5	120.4(3)		C29-C30-C36	120.4(3)
C7-C6-C5	120.2(3)		C30-C31-C26	121.5(3)
O1-C7-C8	119.1(3)		C30-C31-H31A	119.3
O1-C7-C6	121.5(3)		C26-C31-H31A	119.3
C8-C7-C6	119.4(3)		C28-C32-H32A	109.5
C9-C8-C7	118.6(3)		C28-C32-H32B	109.5
C9-C8-C12	122.5(3)		H32A-C32-H32B	109.5
C7-C8-C12	118.9(3)		C28-C32-H32C	109.5
C8-C9-C10	122.9(3)		H32A-C32-H32C	109.5
C8-C9-H9A	118.5		H32B-C32-H32C	109.5
C10-C9-H9A	118.5		C30-C36-H36A	109.5
C11-C10-C9	117.4(3)		C30-C36-H36B	109.5
C11-C10-C16	121.3(4)		H36A-C36-H36B	109.5
C9-C10-C16	121.2(4)		C30-C36-H36C	109.5
C10-C11-C6	122.2(3)		H36A-C36-H36C	109.5
C10-C11-H11A	118.9		H36B-C36-H36C	109.5
C6-C11-H11A	118.9		Cl1-C100-Cl1#1	109.2(4)
C8-C12-H12A	109.5		Cl1-C100-H10A	110.0
C8-C12-H12B	109.5		Cl1#1-C100-H10A	109.5
H12A-C12-H12B	109.5			

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+1/2

Table S6. Bond lengths [Å] and angles [°] for [(hilde^{Me2}){FeCl}$_2$]•2CH_2Cl_2.

Fe1-O2	1.833(2)		C27-C28	1.392(4)
Fe1-O1	1.862(2)		C28-C29	1.396(4)
Fe1-N2	2.220(3)		C28-C32	1.504(5)
Fe1-N1	2.223(2)		C29-C30	1.391(5)
Fe1-Cl1	2.3202(10)		C29-H29A	0.9500
Fe1-Fe1#1	6.3799(8)		C30-C31	1.388(5)
O1-C7	1.352(3)		C30-C36	1.518(4)
O2-C27	1.358(3)		C31-H31A	0.9500
N2-C3	1.485(4)		C32-H32A	0.9800
N2-C25	1.497(4)		C32-H32B	0.9800
N2-C5	1.497(4)		C32-H32C	0.9800
N1-C2	1.490(4)		C36-H36A	0.9800
N1-C1	1.494(3)		C36-H36B	0.9800
N1-C4	1.498(4)		C36-H36C	0.9800
C1-C1#1	1.527(6)		C101-Cl12	1.764(4)
C1-H1A	0.9900		C101-Cl11	1.769(4)
C1-H1B	0.9900		C101-H10A	0.9900
C2-C3	1.526(4)		C101-H10B	0.9900
C2-H2A	0.9900			
C2-H2B	0.9900		O2-Fe1-O1	120.18(10)
C3-H3A	0.9900		O2-Fe1-N2	88.58(9)
C3-H3B	0.9900		O1-Fe1-N2	88.63(9)
C4-H4A	0.9800		O2-Fe1-N1	111.08(9)
C4-H4B	0.9800		O1-Fe1-N1	126.65(10)
C4-H4C	0.9800		N2-Fe1-N1	78.46(9)
C5-C6	1.502(4)		O2-Fe1-Cl1	98.22(7)
C5-H5A	0.9900		O1-Fe1-Cl1	97.11(7)
C5-H5B	0.9900		N2-Fe1-Cl1	167.27(7)
C6-C11	1.383(4)		N1-Fe1-Cl1	89.03(7)
C6-C7	1.399(4)		O2-Fe1-Fe1#1	143.46(7)
C7-C8	1.405(4)		O1-Fe1-Fe1#1	96.22(7)
C8-C9	1.390(4)		N2-Fe1-Fe1#1	95.87(6)
C8-C12	1.503(4)		N1-Fe1-Fe1#1	36.11(6)
C9-C10	1.397(5)		Cl1-Fe1-Fe1#1	72.28(2)
C9-H9A	0.9500		C7-O1-Fe1	130.45(17)
C10-C11	1.388(4)		C27-O2-Fe1	135.3(2)
C10-C16	1.515(5)		C3-N2-C25	109.7(2)
C11-H11A	0.9500		C3-N2-C5	109.3(2)
C12-H12A	0.9800		C25-N2-C5	109.2(2)
C12-H12B	0.9800		C3-N2-Fe1	109.38(18)
C12-H12C	0.9800		C25-N2-Fe1	111.31(19)
C16-H16A	0.9800		C5-N2-Fe1	107.94(17)
C16-H16B	0.9800		C2-N1-C1	110.1(2)
C16-H16C	0.9800		C2-N1-C4	108.9(2)
C25-C26	1.503(4)		C1-N1-C4	107.7(2)
C25-H25A	0.9900		C2-N1-Fe1	111.20(18)
C25-H25B	0.9900		C1-N1-Fe1	115.32(17)
C26-C31	1.396(4)		C4-N1-Fe1	103.21(18)
C26-C27	1.404(5)		N1-C1-C1#1	111.8(3)
N1-C1-H1A	109.3		H12A-C12-H12C	109.5
C1#1-C1-H1A	109.3		H12B-C12-H12C	109.5
N1-C1-H1B	109.3		C10-C16-H16A	109.5

C1#1-C1-H1B	109.3		C10-C16-H16B	109.5
H1A-C1-H1B	107.9		H16A-C16-H16B	109.5
N1-C2-C3	109.9(2)		C10-C16-H16C	109.5
N1-C2-H2A	109.7		H16A-C16-H16C	109.5
C3-C2-H2A	109.7		H16B-C16-H16C	109.5
N1-C2-H2B	109.7		N2-C25-C26	114.0(2)
C3-C2-H2B	109.7		N2-C25-H25A	108.8
H2A-C2-H2B	108.2		C26-C25-H25A	108.8
N2-C3-C2	109.5(2)		N2-C25-H25B	108.8
N2-C3-H3A	109.8		C26-C25-H25B	108.8
C2-C3-H3A	109.8		H25A-C25-H25B	107.7
N2-C3-H3B	109.8		C31-C26-C27	118.9(3)
C2-C3-H3B	109.8		C31-C26-C25	119.9(3)
H3A-C3-H3B	108.2		C27-C26-C25	121.1(3)
N1-C4-H4A	109.5		O2-C27-C28	119.1(3)
N1-C4-H4B	109.5		O2-C27-C26	120.3(3)
H4A-C4-H4B	109.5		C28-C27-C26	120.7(3)
N1-C4-H4C	109.5		C27-C28-C29	118.6(3)
H4A-C4-H4C	109.5		C27-C28-C32	120.3(3)
H4B-C4-H4C	109.5		C29-C28-C32	121.2(3)
N2-C5-C6	112.4(2)		C30-C29-C28	122.1(3)
N2-C5-H5A	109.1		C30-C29-H29A	118.9
C6-C5-H5A	109.1		C28-C29-H29A	118.9
N2-C5-H5B	109.1		C31-C30-C29	118.2(3)
C6-C5-H5B	109.1		C31-C30-C36	120.8(3)
H5A-C5-H5B	107.9		C29-C30-C36	120.9(3)
C11-C6-C7	119.8(3)		C30-C31-C26	121.5(3)
C11-C6-C5	121.4(3)		C30-C31-H31A	119.3
C7-C6-C5	118.8(3)		C26-C31-H31A	119.3
O1-C7-C6	119.5(3)		C28-C32-H32A	109.5
O1-C7-C8	120.4(3)		C28-C32-H32B	109.5
C6-C7-C8	120.1(3)		H32A-C32-H32B	109.5
C9-C8-C7	118.1(3)		C28-C32-H32C	109.5
C9-C8-C12	121.6(3)		H32A-C32-H32C	109.5
C7-C8-C12	120.3(3)		H32B-C32-H32C	109.5
C8-C9-C10	122.8(3)		C30-C36-H36A	109.5
C8-C9-H9A	118.6		C30-C36-H36B	109.5
C10-C9-H9A	118.6		H36A-C36-H36B	109.5
C11-C10-C9	117.4(3)		C30-C36-H36C	109.5
C11-C10-C16	121.5(3)		H36A-C36-H36C	109.5
C9-C10-C16	121.1(3)		H36B-C36-H36C	109.5
C6-C11-C10	121.8(3)		Cl12-C101-Cl11	111.1(2)
C6-C11-H11A	119.1		Cl12-C101-H10A	109.4
C10-C11-H11A	119.1		Cl11-C101-H10A	109.4
C8-C12-H12A	109.5		Cl12-C101-H10B	109.4
C8-C12-H12B	109.5		Cl11-C101-H10B	109.4
H12A-C12-H12B	109.5		H10A-C101-H10B	108.0
C8-C12-H12C	109.5			

Symmetry transformations used to generate equivalent atoms:

Table S7. Parameters obtained from fitting of the experimental magnetic data

	J / cm^{-1}	$g_1=g_2$	Θ_W / K	TIP / 10^6 cm^3mol^{-1}	*p.i.* / %	Θ_W *(p.i.)* / K
[(julia){Fe(H_2O)(μ-O)Fe(H_2O)}]·6H_2O	-108	2.03		100	0.9	-5
[(julia){Fe(dmso)(μ-O)Fe(dmso)}]	-102	2.00			0.1	-29
[(susan){FeCl(μ-O)FeCl}]Cl_2	-106	2.05			0.3	-3
[(susan){FeCl(μ-O)FeCl$_{0.75}$(OMe)$_{0.25}$}](ClO_4)$_2$	-105	2.07			0.3	-15
[(susan){FeCl(μ-O)FeCl}](ClO_4)$_2$	-108	2.05			0.4	-18
[(hilde^{Me2}){Fe(μ-O)Fe}]	-93.5	2.09			3.6	-14
[(hilde^{Me2}){FeCl}$_2$]		1.95	-4.3			