Electronic Supplementary Material (ESI) for Dalton Transactions.

Homoleptic Quasilinear Metal(I/II) Silylamides of Cr – Co with Phenyl and Allyl Functions – Impact of Oxidation State on Secondary Ligand Interactions

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1 NMR Spectra

−N(Dipp)Si(Me$_2$Ph) (L^1) containing compounds

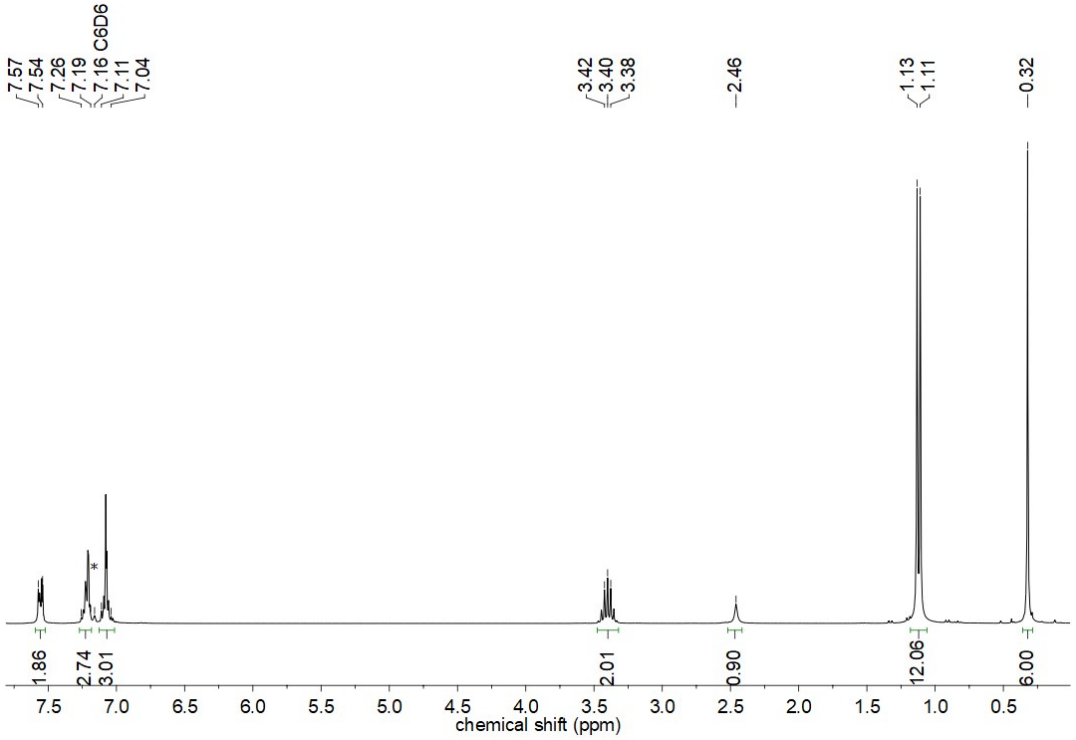

Figure S1. ^{1}H NMR spectrum (300.2 MHz, 300 K) of **HL^1** in C_6D_6. (* solvent)

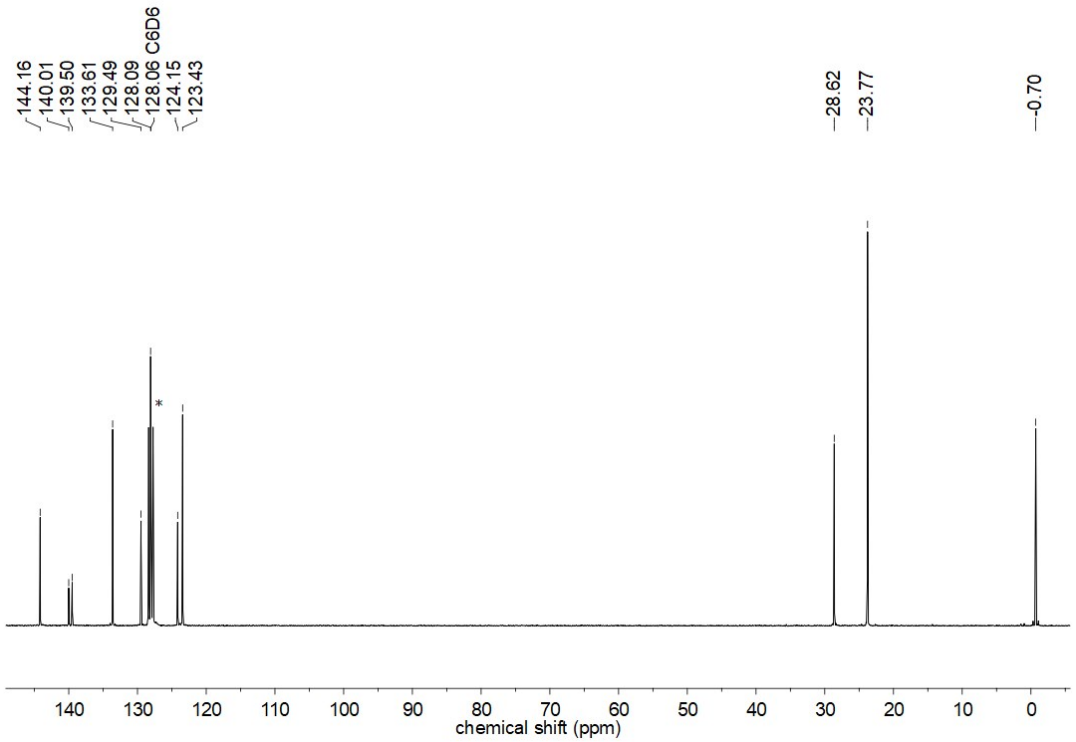

Figure S2. ^{13}C NMR spectrum (75.5 MHz, 300 K) of **HL^1** in C_6D_6. (* solvent)

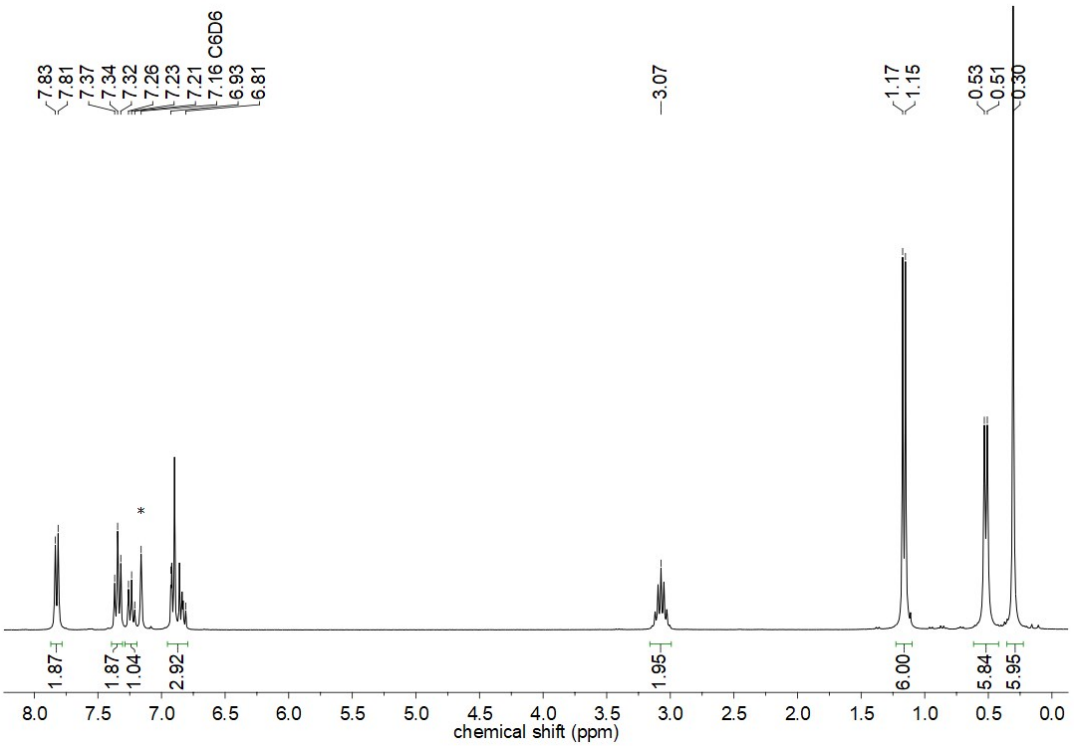

Figure S3. ^{1}H NMR spectrum (300.2 MHz, 300 K) of **LiL^{1}** in C_6D_6. (* solvent)

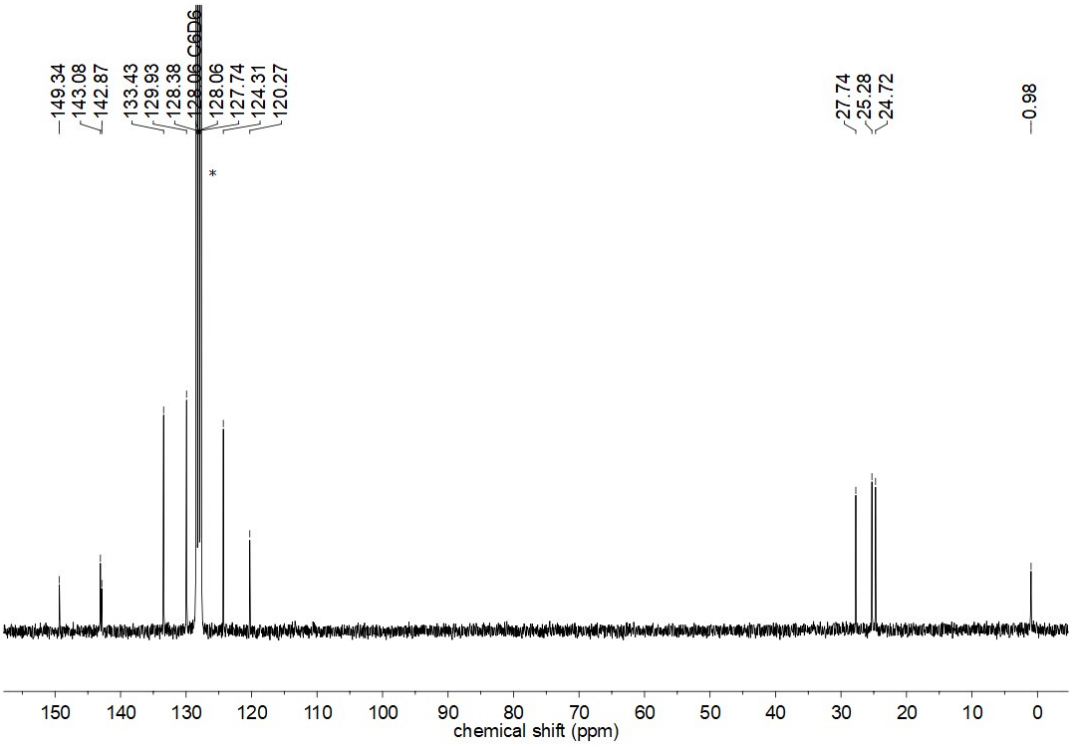

Figure S4. ^{13}C NMR spectrum (75.5 MHz, 300 K) of **LiL^{1}** in C_6D_6. (* solvent)

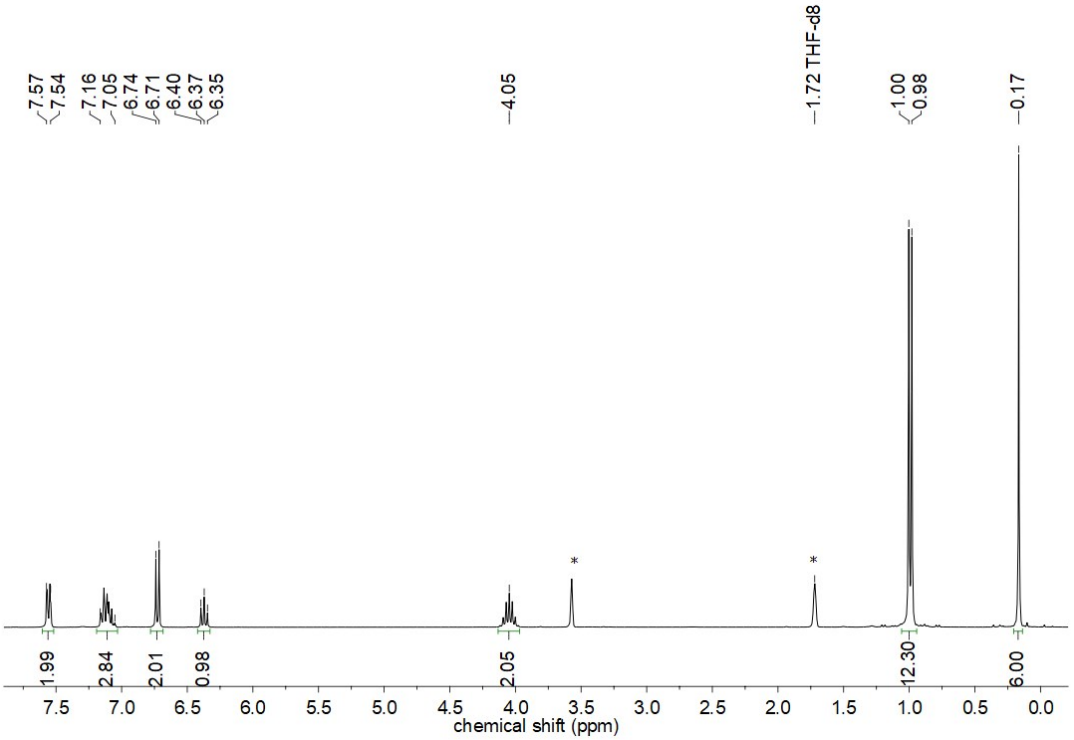

Figure S5. ^{1}H NMR spectrum (300.2 MHz, 300 K) of **LiL^{1}** in THF-d_8. (* solvent)

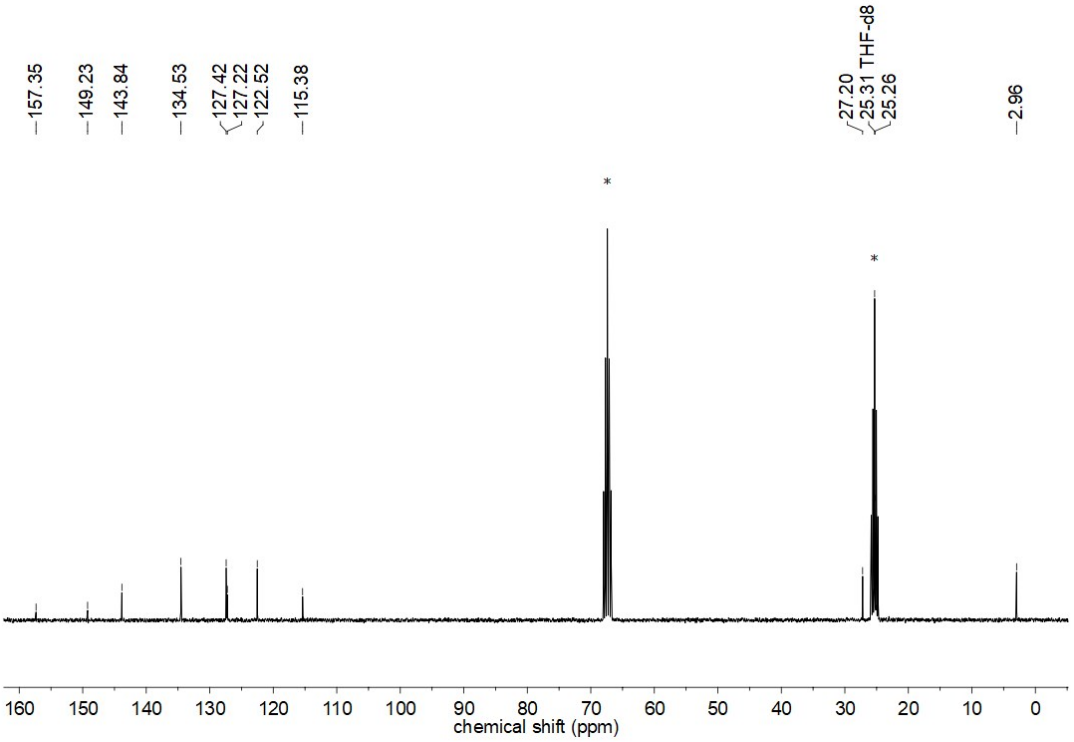

Figure S6. ^{13}C NMR spectrum (75.5 MHz, 300 K) of **LiL^{1}** in THF-d_8. (* solvent)

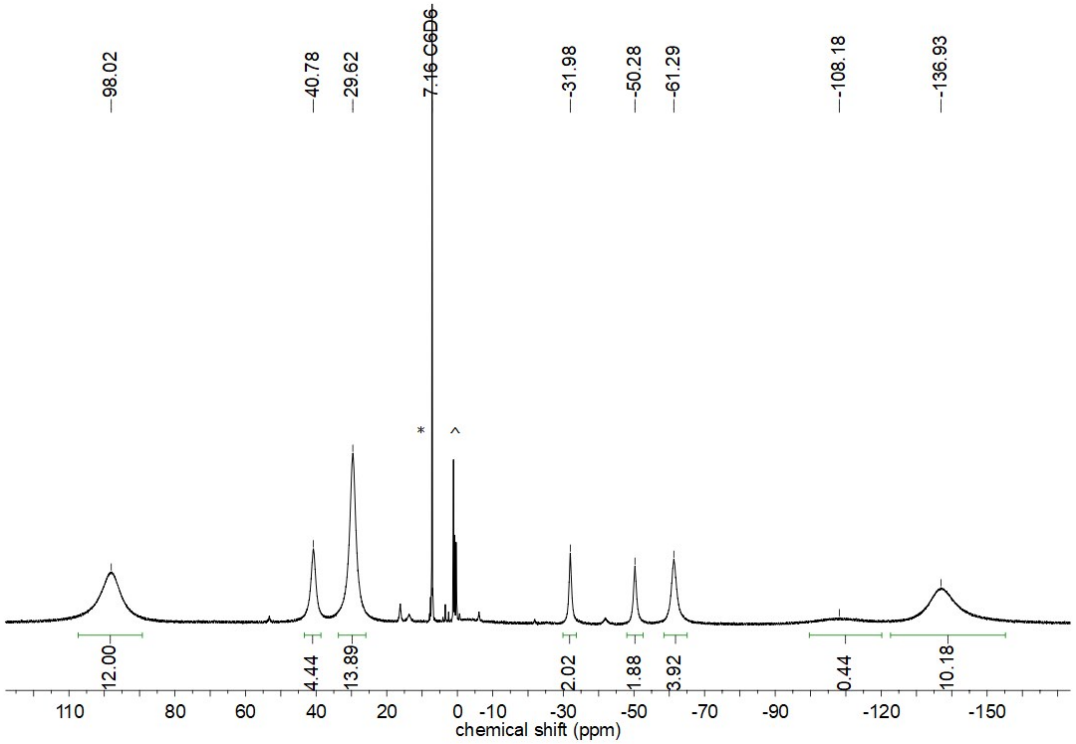

Figure S7. ^{1}H NMR spectrum (300.2 MHz, 300 K) of **[FeL$^1_2$]** in C_6D_6. (* solvent, ^ impurities)

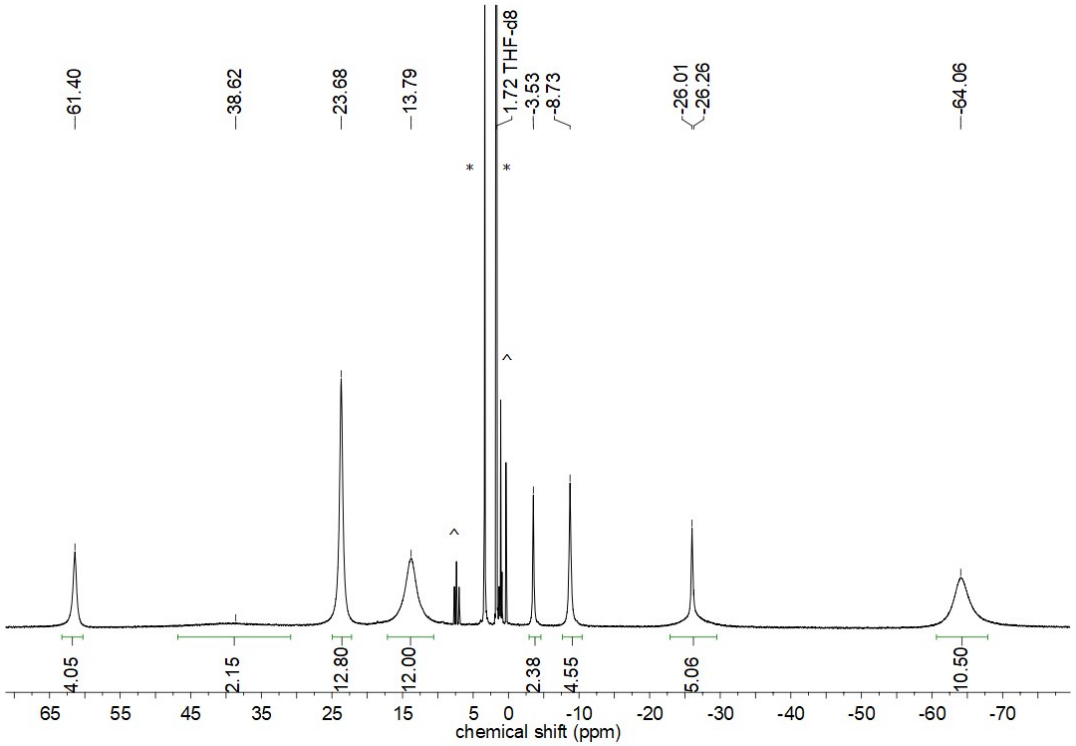

Figure S8. ^{1}H NMR spectrum (300.2 MHz, 300 K) of **[FeL$^1_2$]** in THF-d_8. (* solvent, ^ impurities)

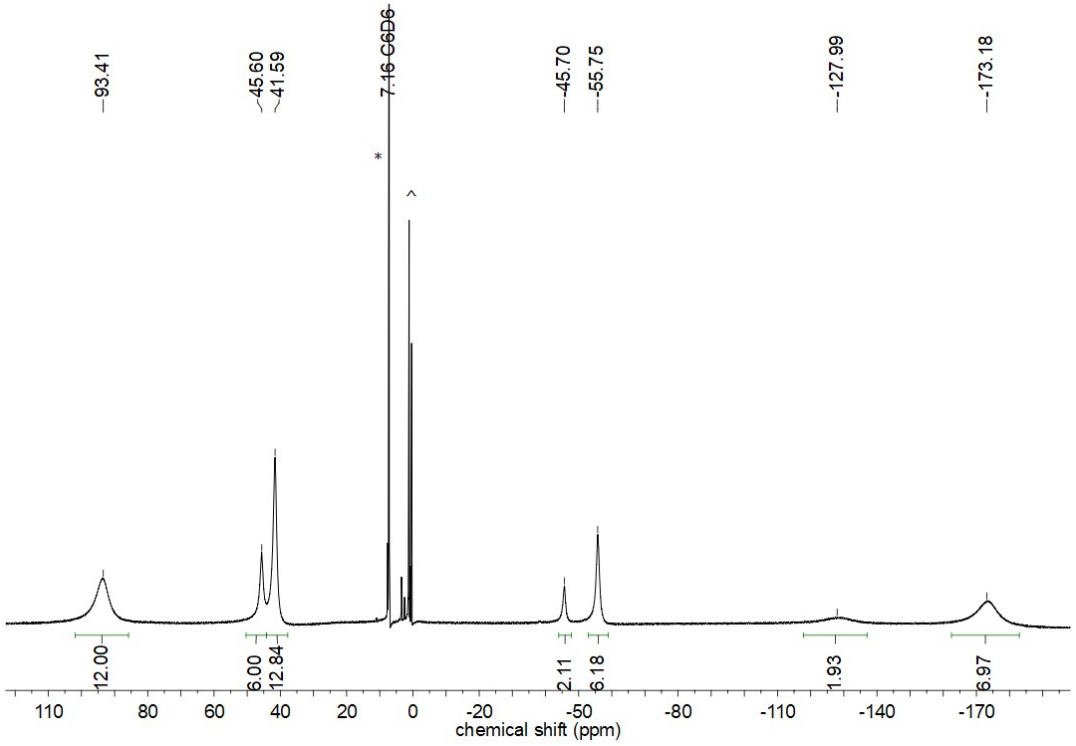

Figure S9. ^{1}H NMR spectrum (300.2 MHz, 300 K) of **[CoL$^1_2$]** in C_6D_6. (* solvent, ^ impurities)

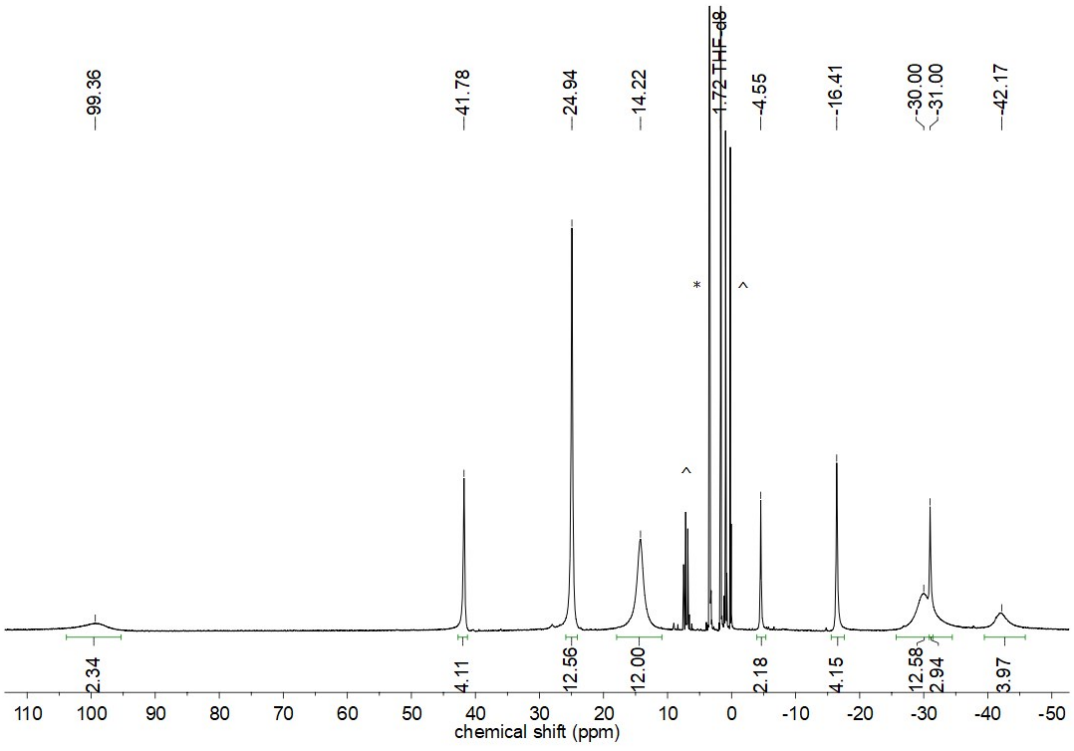

Figure S10. ^{1}H NMR spectrum (300.2 MHz, 300 K) of **[CoL$^1_2$]** in THF-d_8. (* solvent, ^ impurities)

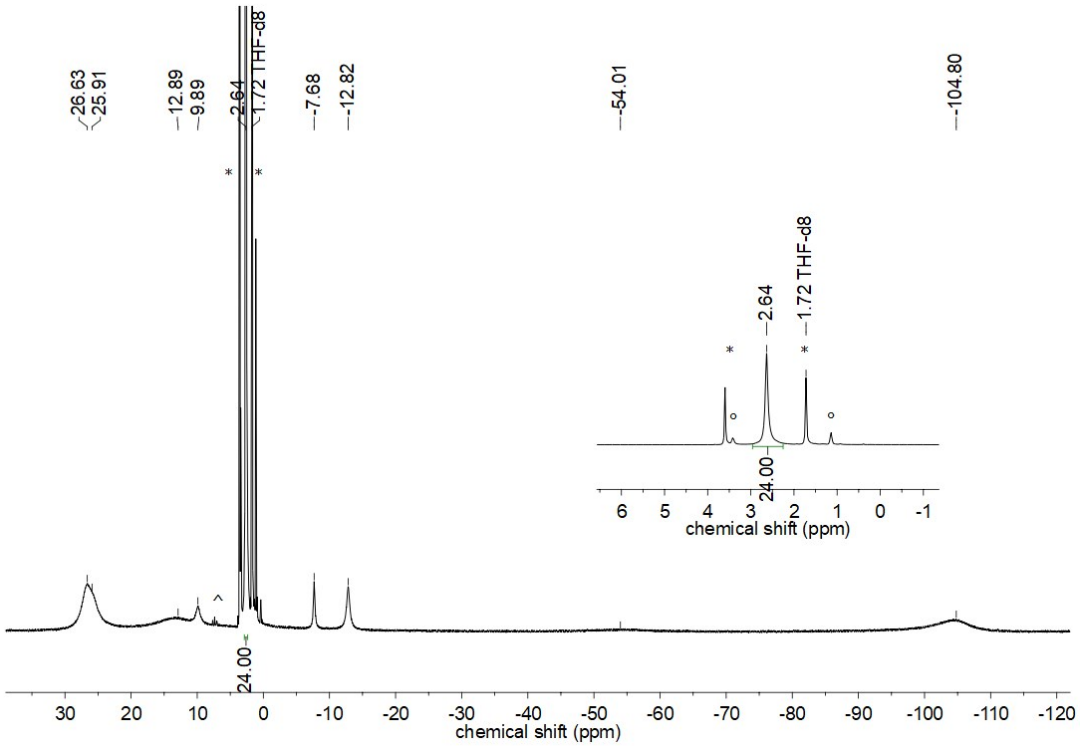

Figure S11. ^{1}H NMR spectrum (300.2 MHz, 300 K) of K{18c6}**[FeL$^{1}_{2}$]** in THF-d_8. (* solvent, ° diethyl ether)

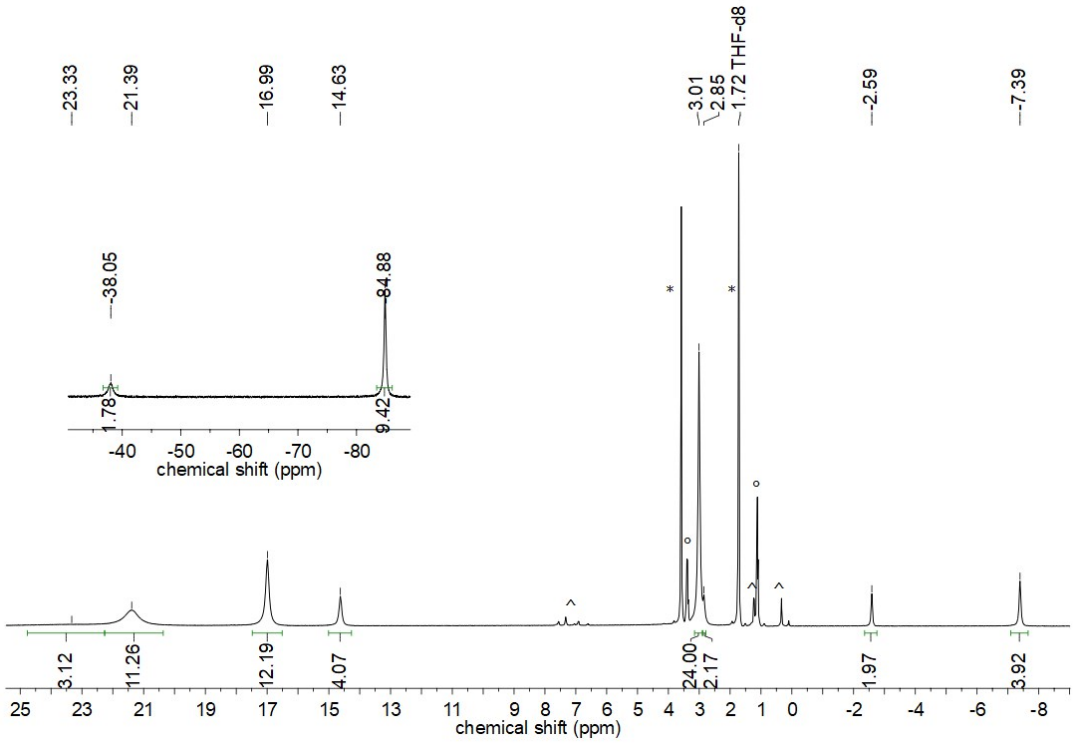

Figure S12. ^{1}H NMR spectrum (300.2 MHz, 300 K) of K{18c6}**[CoL$^{1}_{2}$]** in THF-d_8. (* solvent, ^ impurities, ° diethyl ether)

−N(Dipp)SiMePh$_2$ (L^2) containing compounds

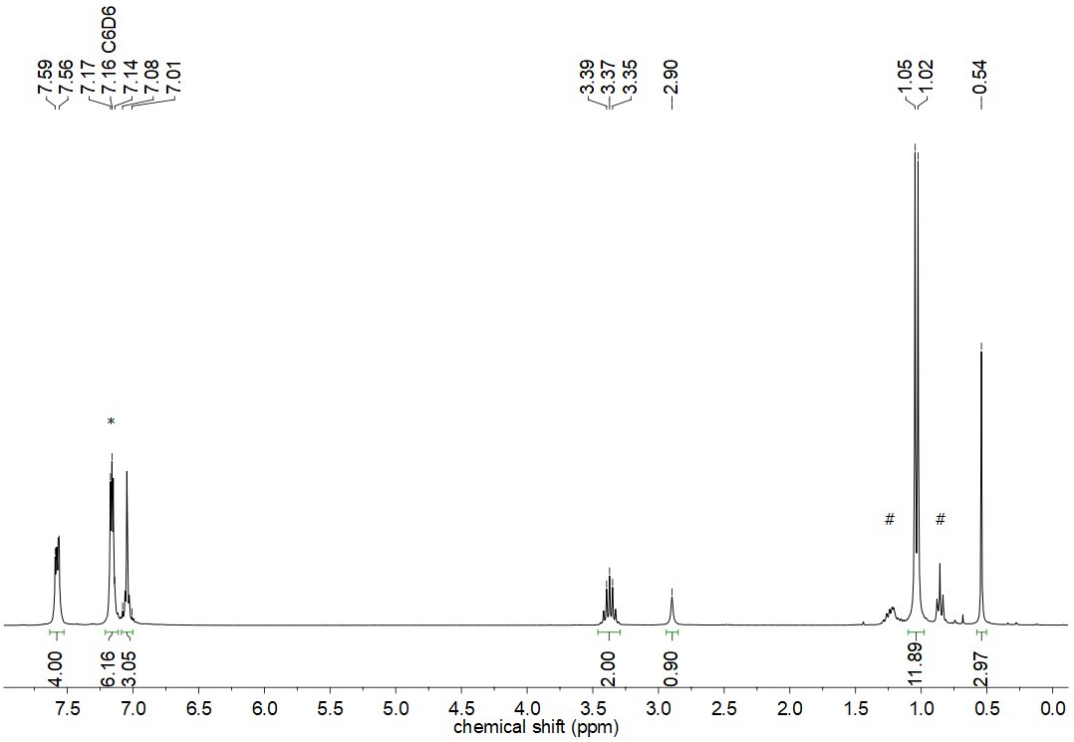

Figure S13. ^{1}H NMR spectrum (300.2 MHz, 300 K) of **HL^2** in C_6D_6. (* solvent, # *n*-pentane)

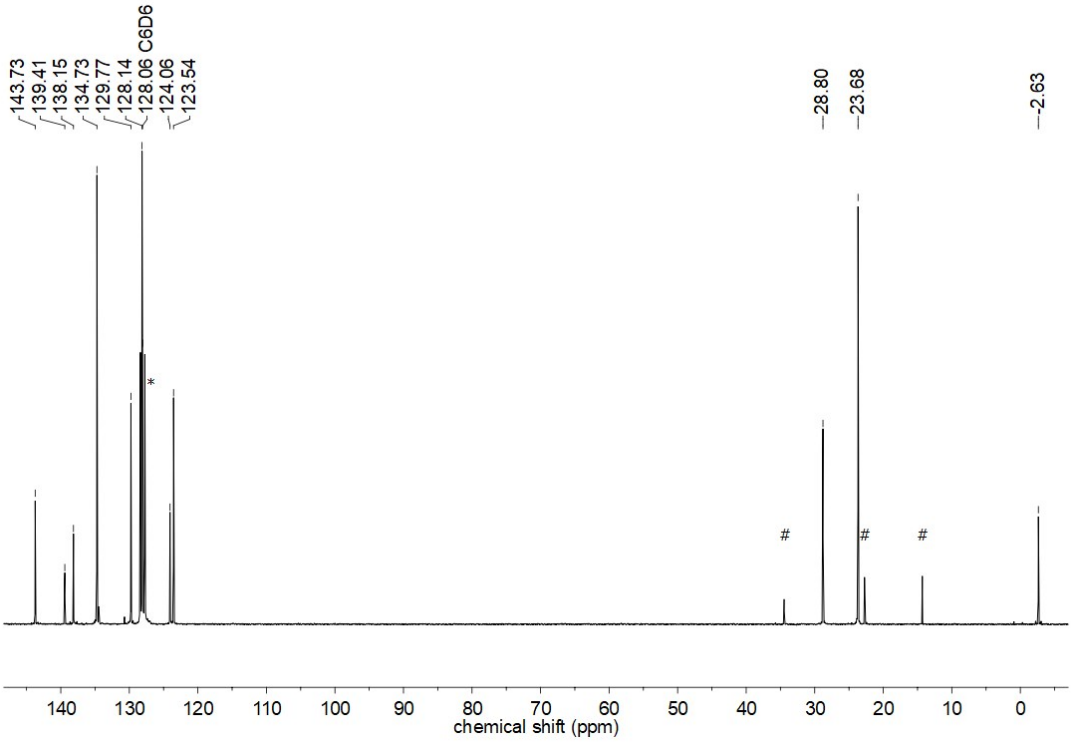

Figure S14. ^{13}C NMR spectrum (300.2 MHz, 300 K) of **HL^2** in C_6D_6. (* solvent, # *n*-pentane)

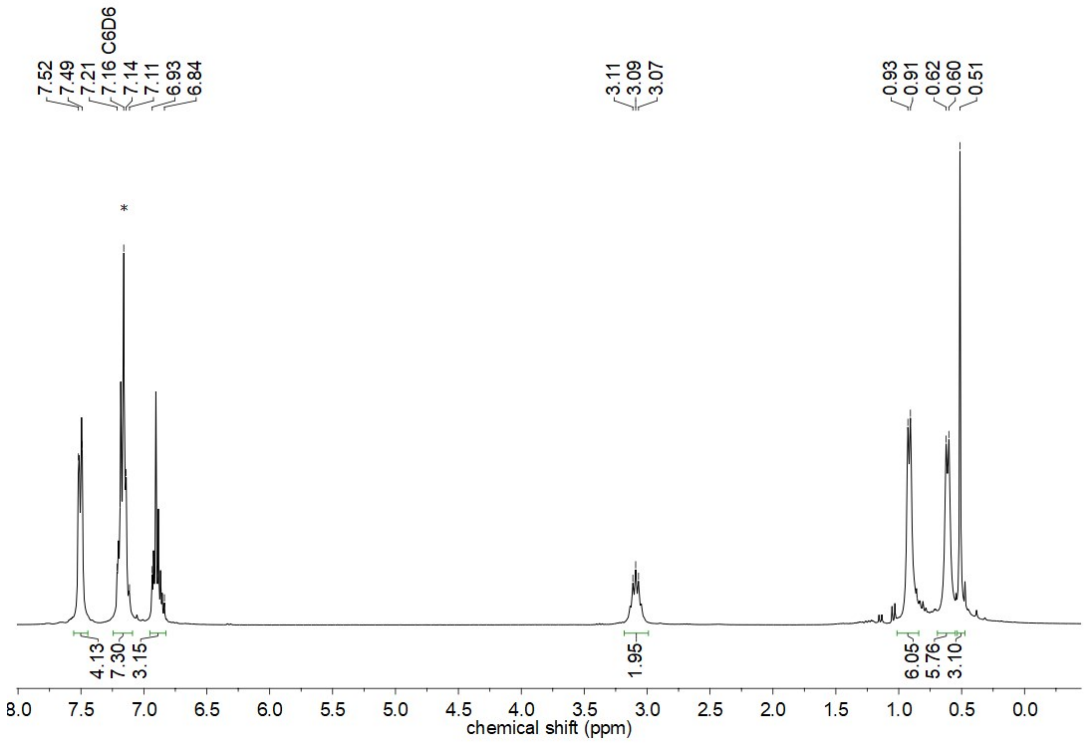

Figure S15. ^{1}H NMR spectrum (300.2 MHz, 300 K) of **LiL²** in C_6D_6. (* solvent)

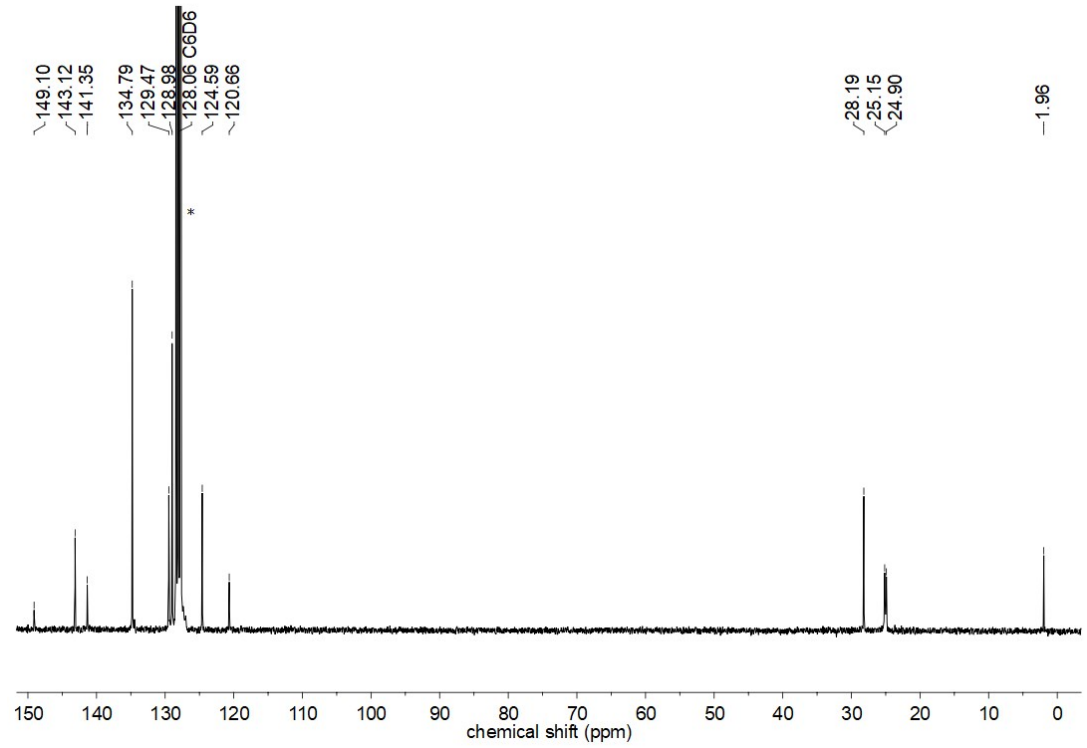

Figure S16. ^{13}C NMR spectrum (75.5 MHz, 300 K) of **LiL²** in C_6D_6. (* solvent)

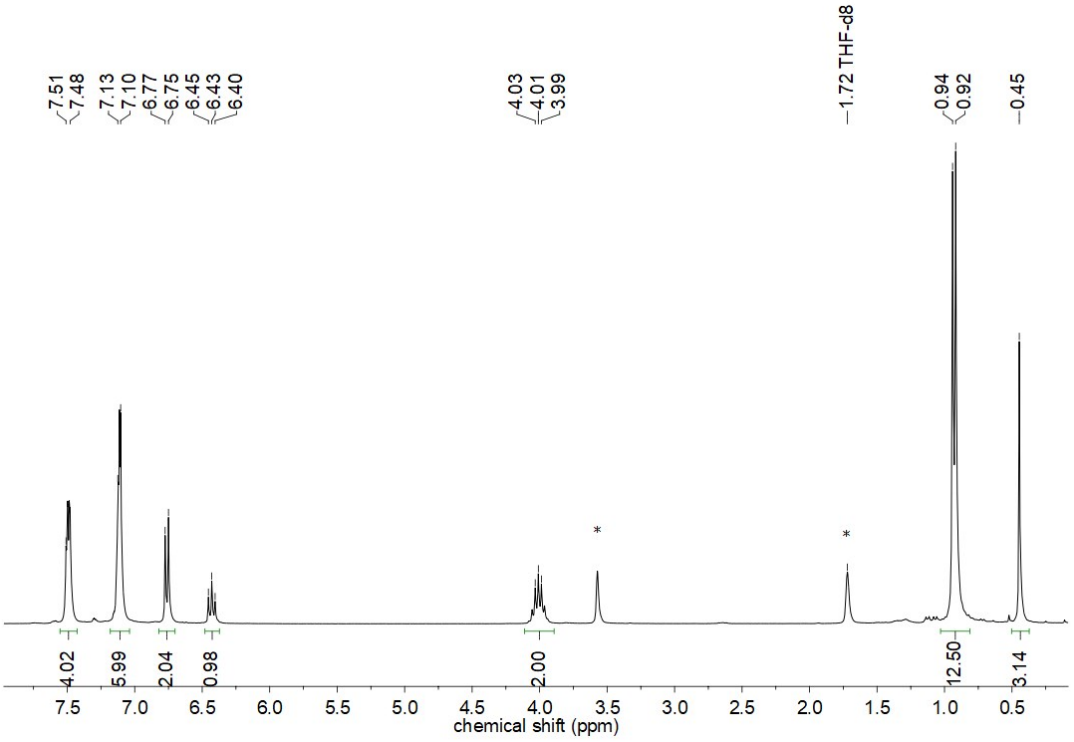

Figure S17. ^{1}H NMR spectrum (300.2 MHz, 300 K) of **LiL^{2}** in THF-d_8. (* solvent)

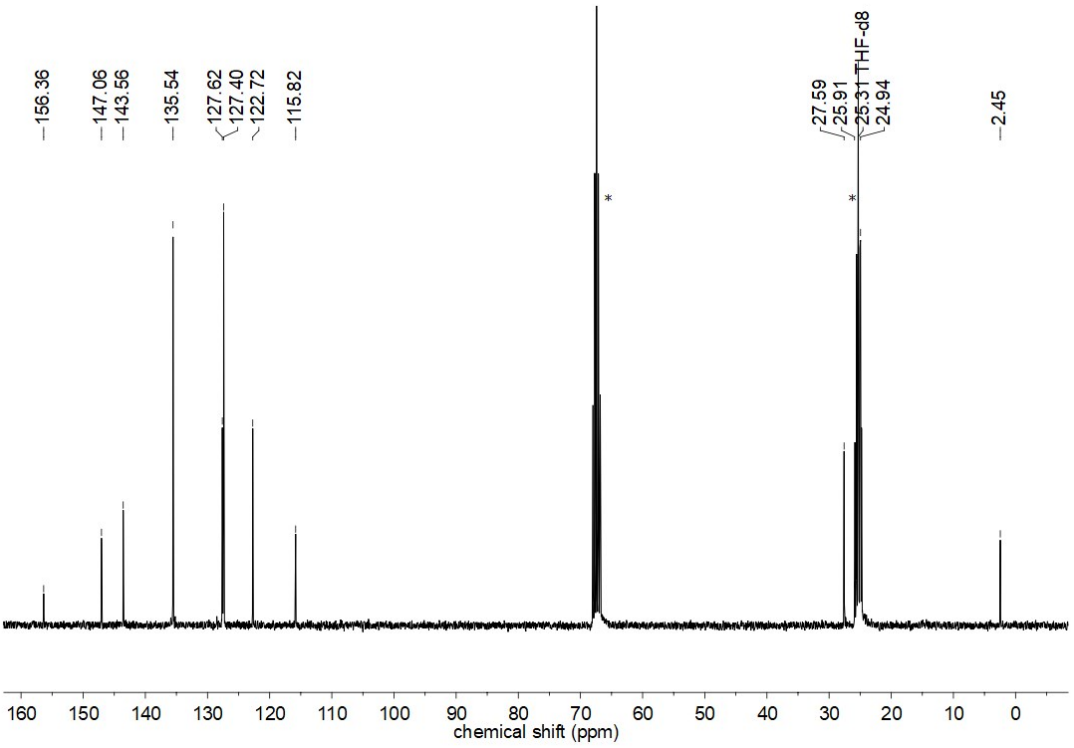

Figure S18. ^{13}C NMR spectrum (75.5 MHz, 300 K) of **LiL^{2}** in THF-d_8. (* solvent)

−N(Dipp)SiPh$_3$ (L^3) containing compounds

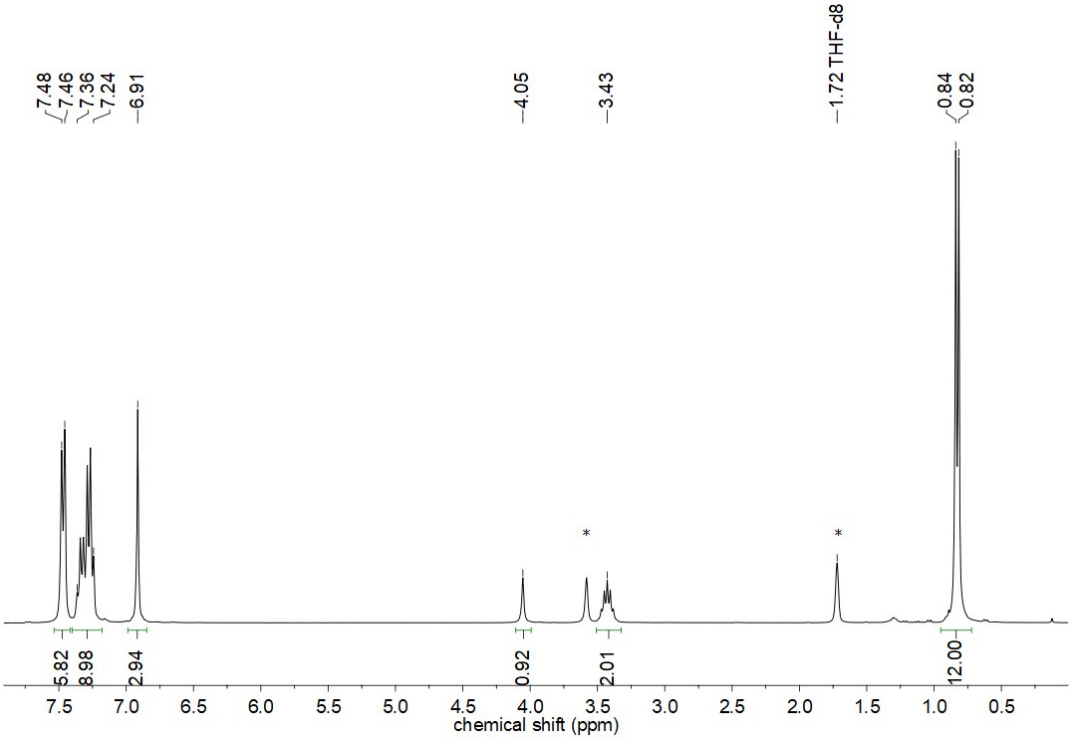

Figure S19. ^{1}H NMR spectrum (300.2 MHz, 300 K) of **HL^3** in THF-d_8. (* solvent)

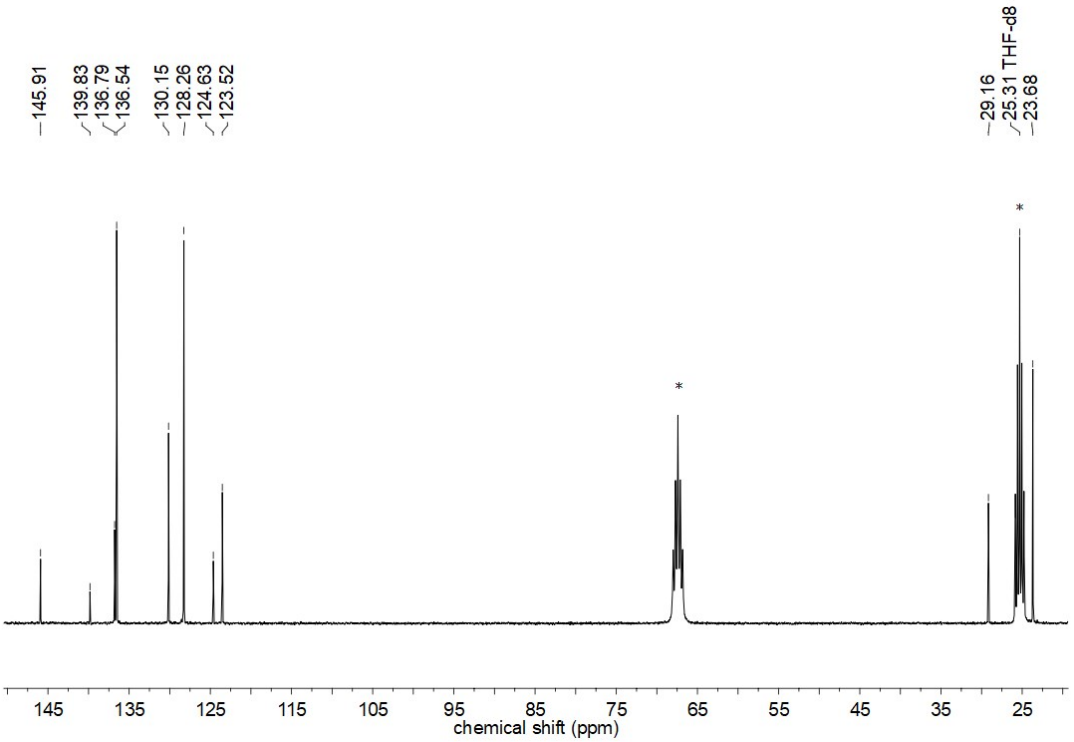

Figure S20. ^{13}C NMR spectrum (75.5 MHz, 300 K) of **HL^3** in THF-d_8. (* solvent)

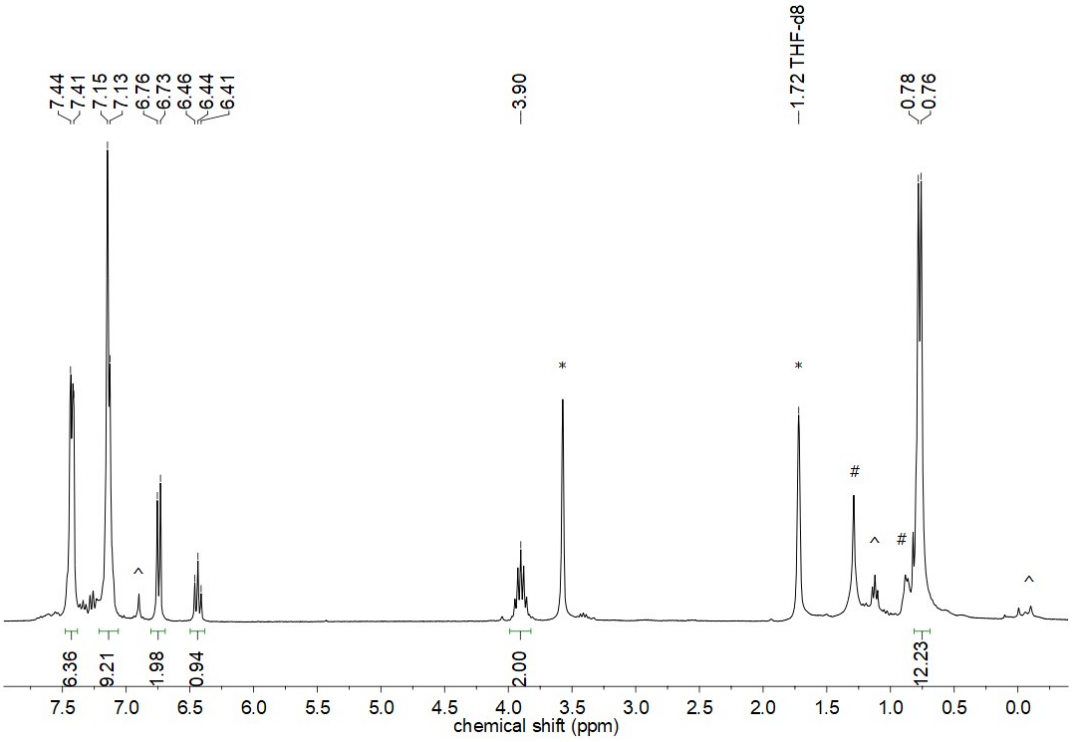

Figure S21. ^{1}H NMR spectrum (300.2 MHz, 300 K) of **LiL^{3}** in THF-d_8. (* solvent, # *n*-pentane, ^ impurities)

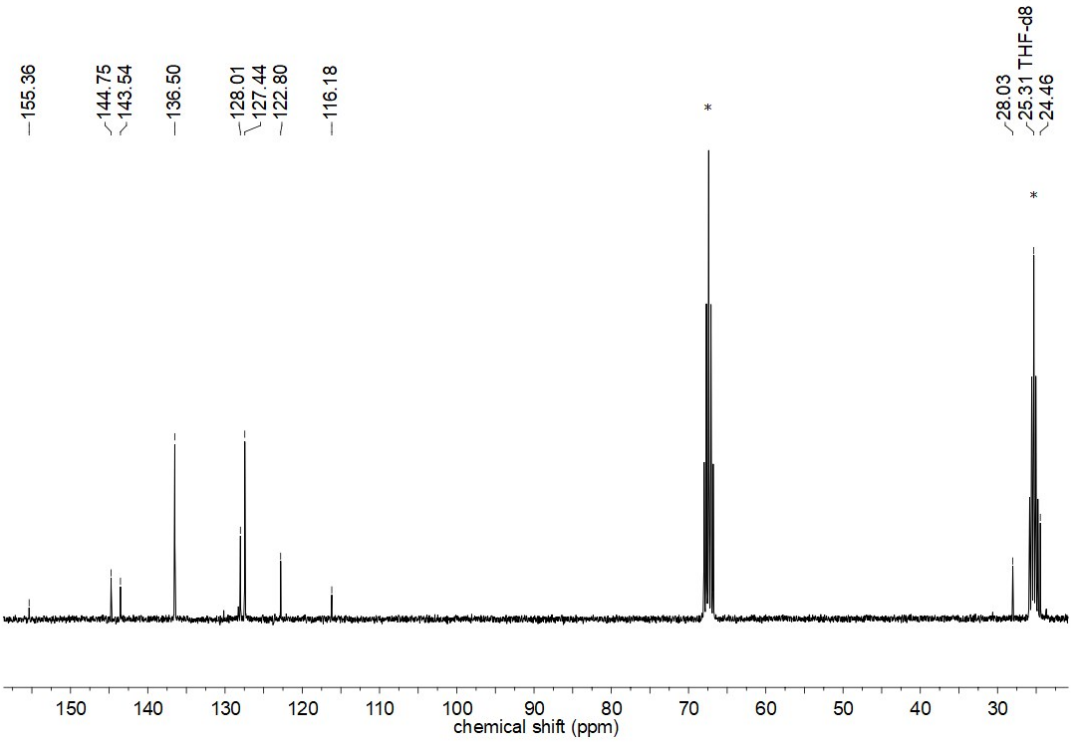

Figure S22. ^{13}C NMR spectrum (75.5 MHz, 300 K) of **LiL^{3}** in THF-d_8. (* solvent)

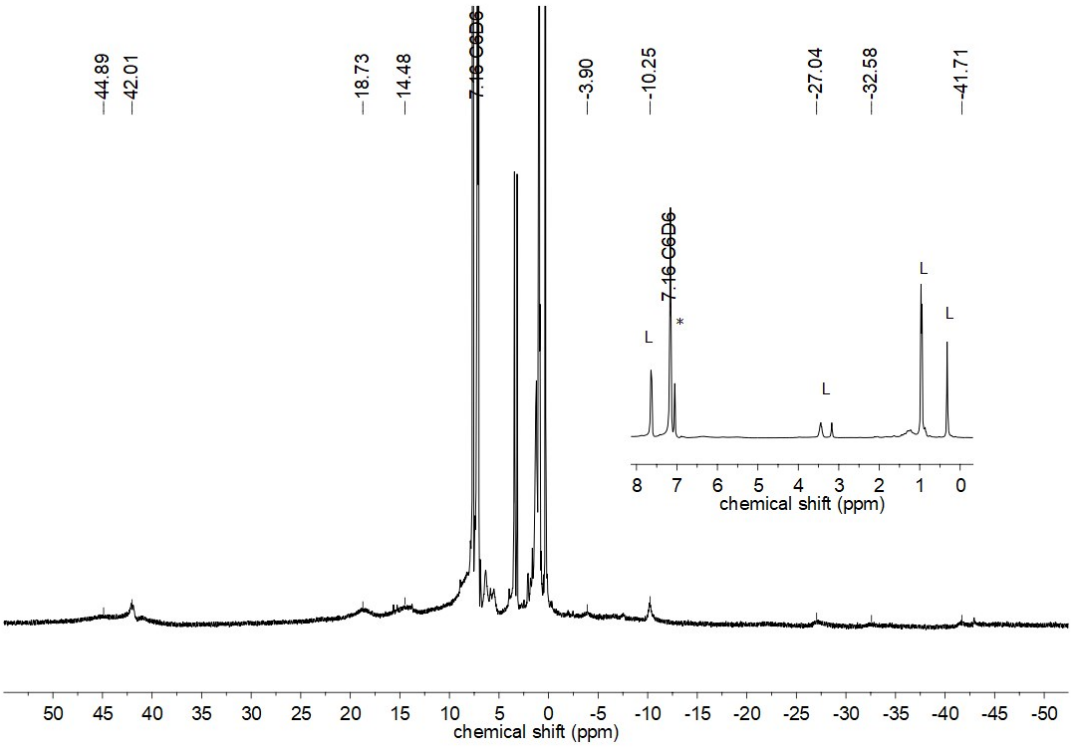

Figure S23. ^{1}H NMR spectrum (300.2 MHz, 300 K) of **[FeL$^{3}_{2}$]** in C_6D_6. (* solvent, ^{L} ligand impurities)

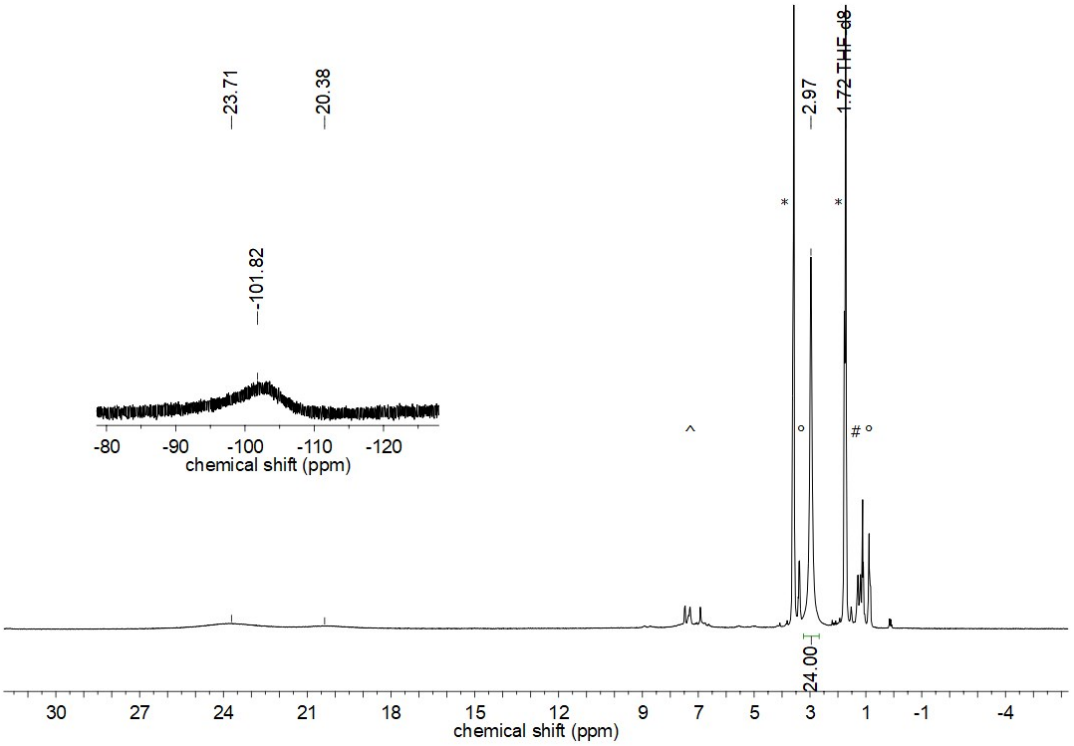

Figure S24. ^{1}H NMR spectrum (300.2 MHz, 300 K) of K{18c6}**[FeL$^{3}_{2}$]** in THF-d_8. (* solvent, ^ impurities, ° diethyl ether, # *n*-pentane)

−N(Dipp)SiMe$_2$(allyl) (L^4) containing compounds

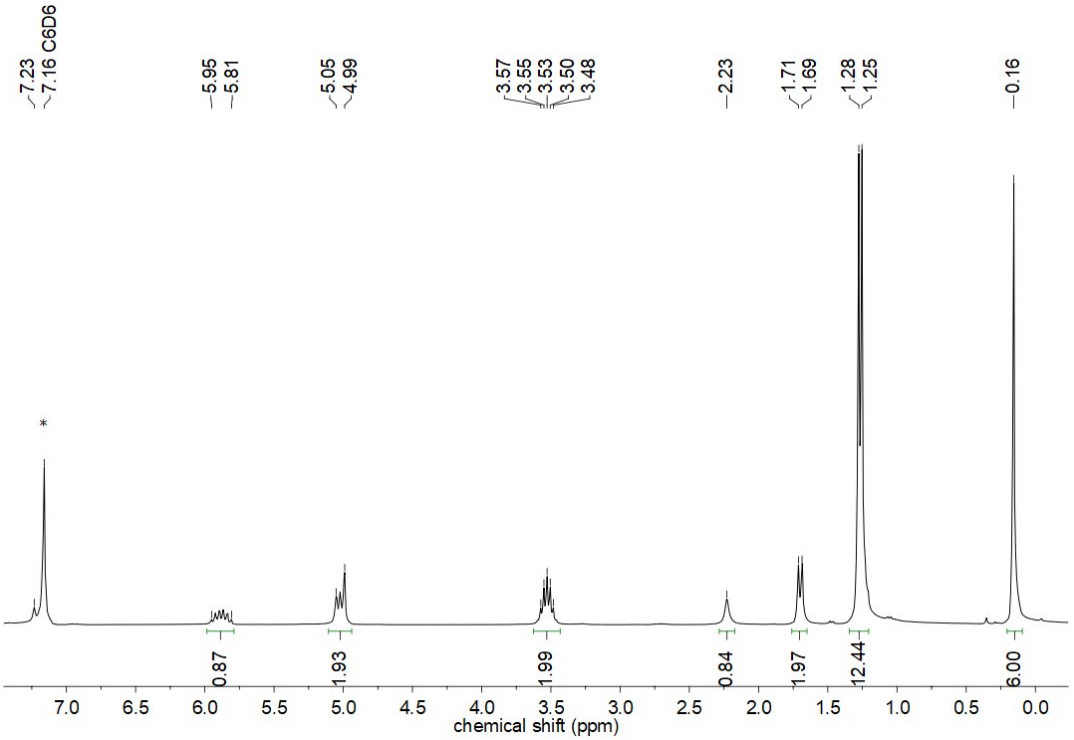

Figure S25. ^{1}H NMR spectrum (300.2 MHz, 300 K) of **HL^4** in C_6D_6. (* solvent)

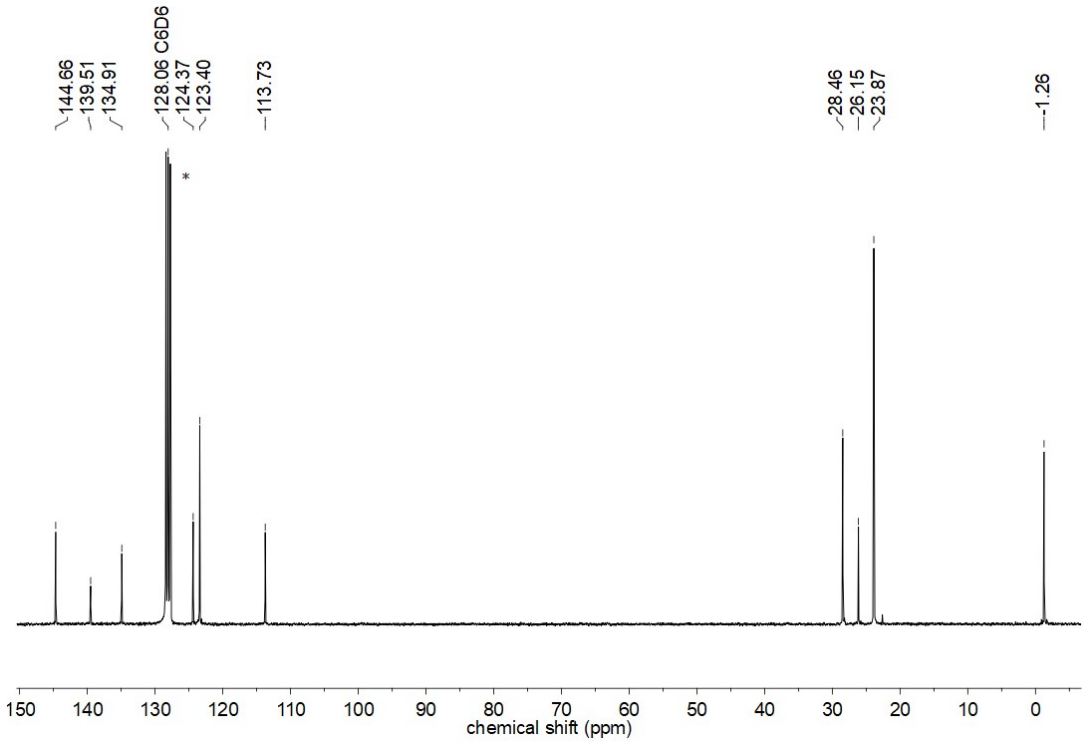

Figure S26. ^{13}C NMR spectrum (75.5 MHz, 300 K) of **HL^4** in C_6D_6. (* solvent)

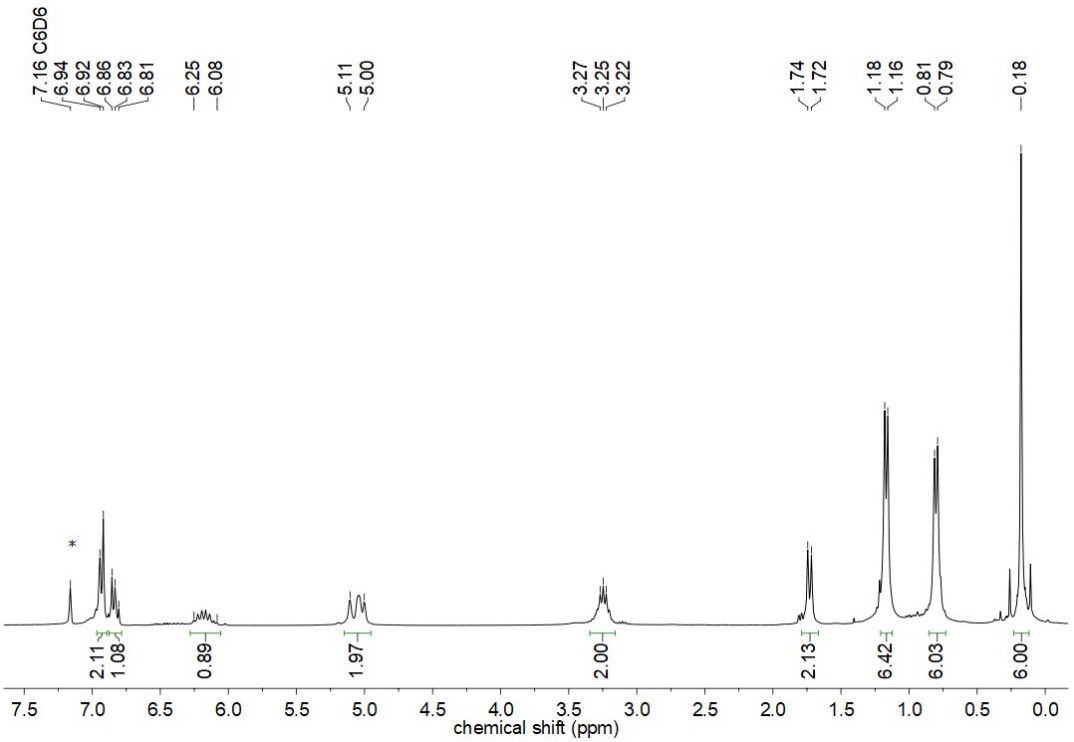

Figure S27. ^{1}H NMR spectrum (300.2 MHz, 300 K) of **LiL^{4}** in C_6D_6. (* solvent)

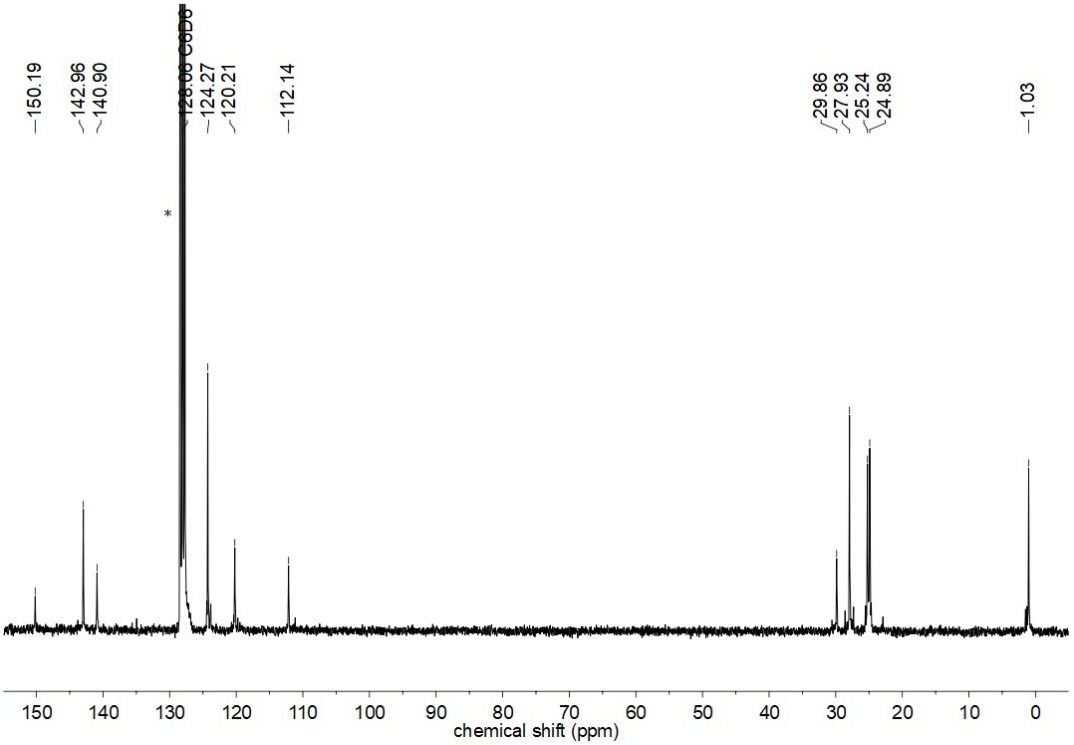

Figure S28. ^{13}C NMR spectrum (75.5 MHz, 300 K) of **LiL^{4}** in C_6D_6. (* solvent)

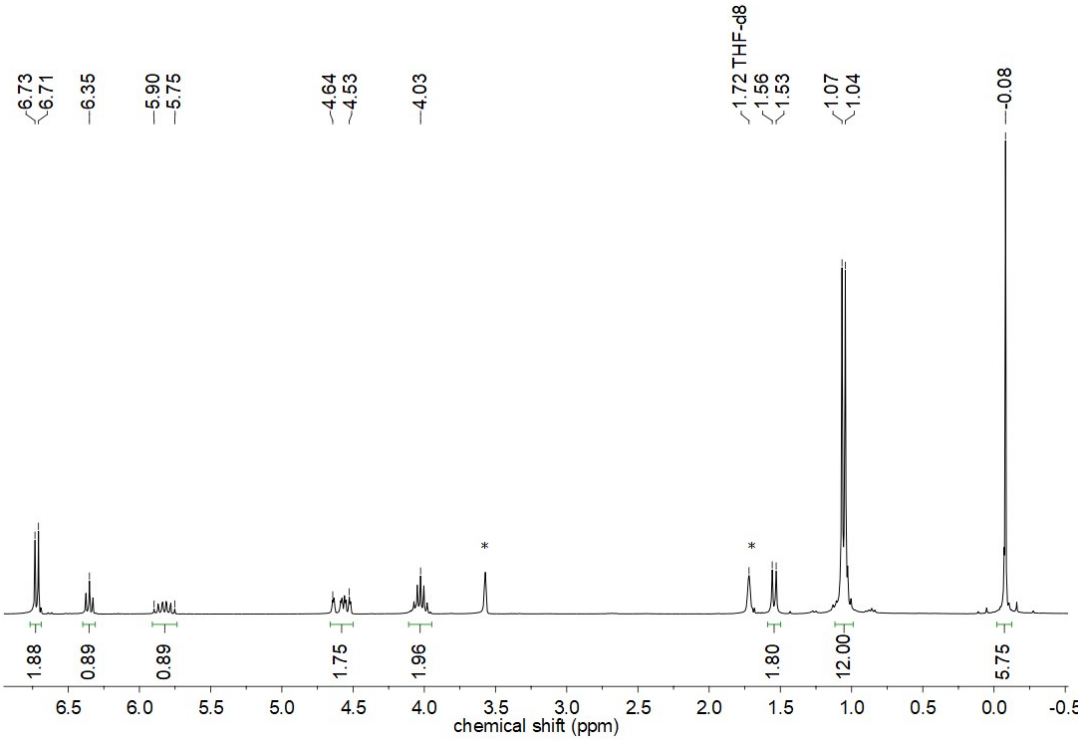

Figure S29. ^{1}H NMR spectrum (300.2 MHz, 300 K) of **LiL^{4}** in THF-d_8. (* solvent)

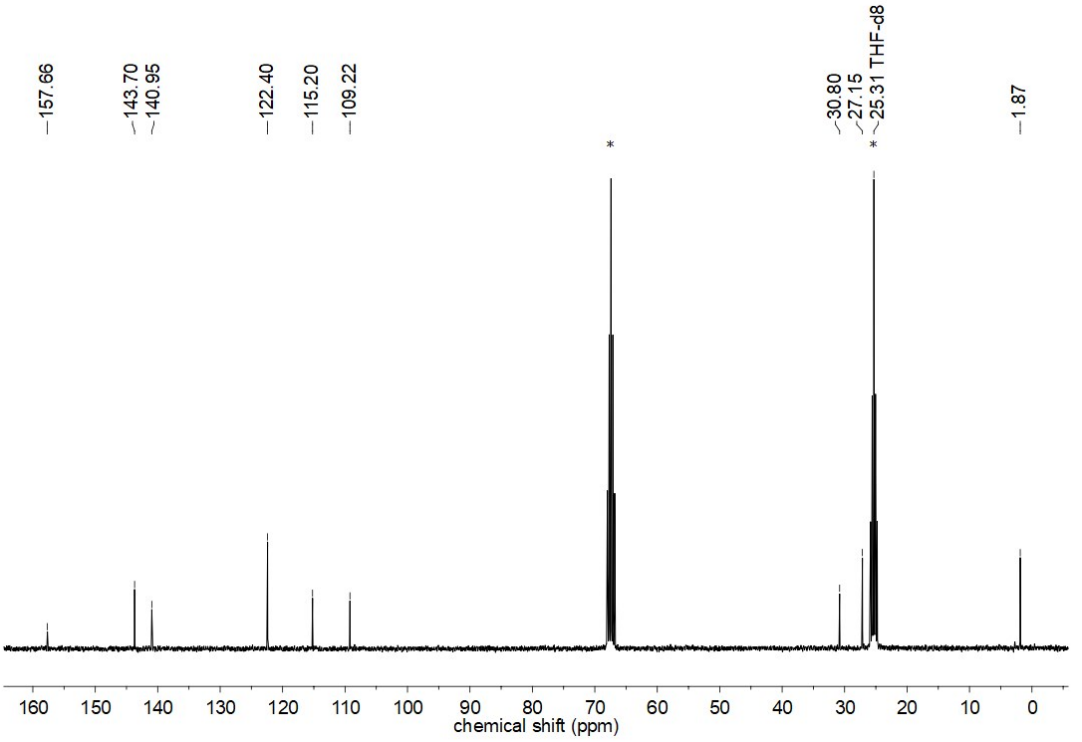

Figure S30. ^{13}C NMR spectrum (75.5 MHz, 300 K) of **LiL^{4}** in THF-d_8. (* solvent)

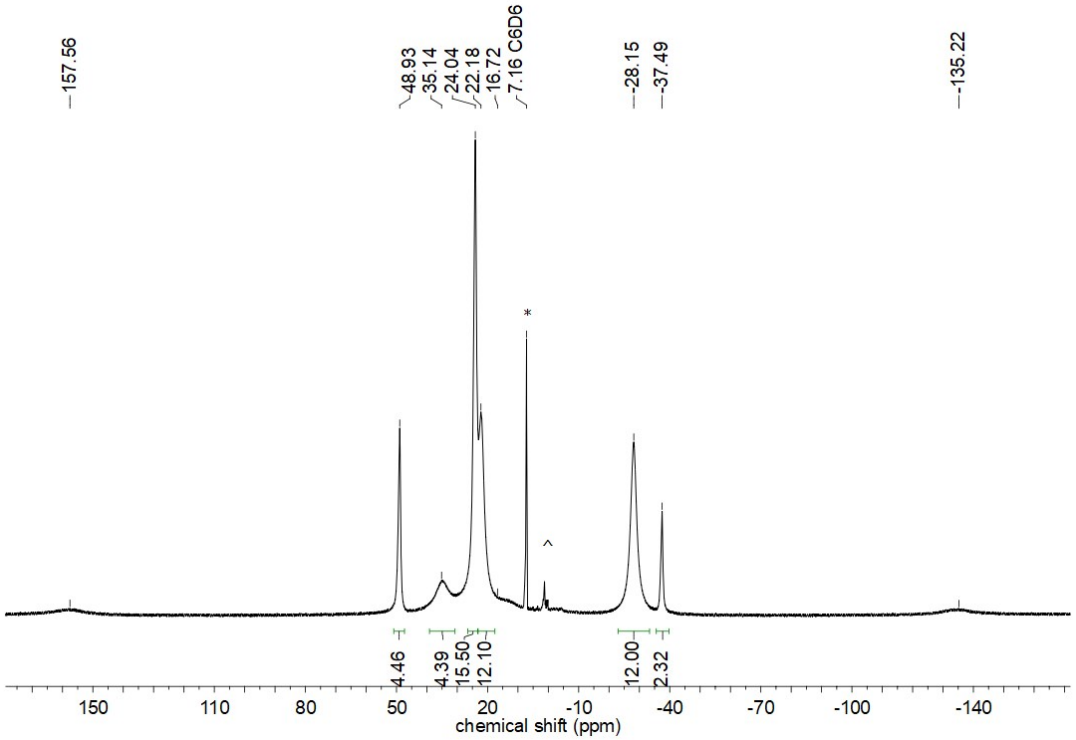

Figure S31. ^{1}H NMR spectrum (300.2 MHz, 300 K) of **[FeL$^4_2$]** in C_6D_6. (* solvent, ^ impurities)

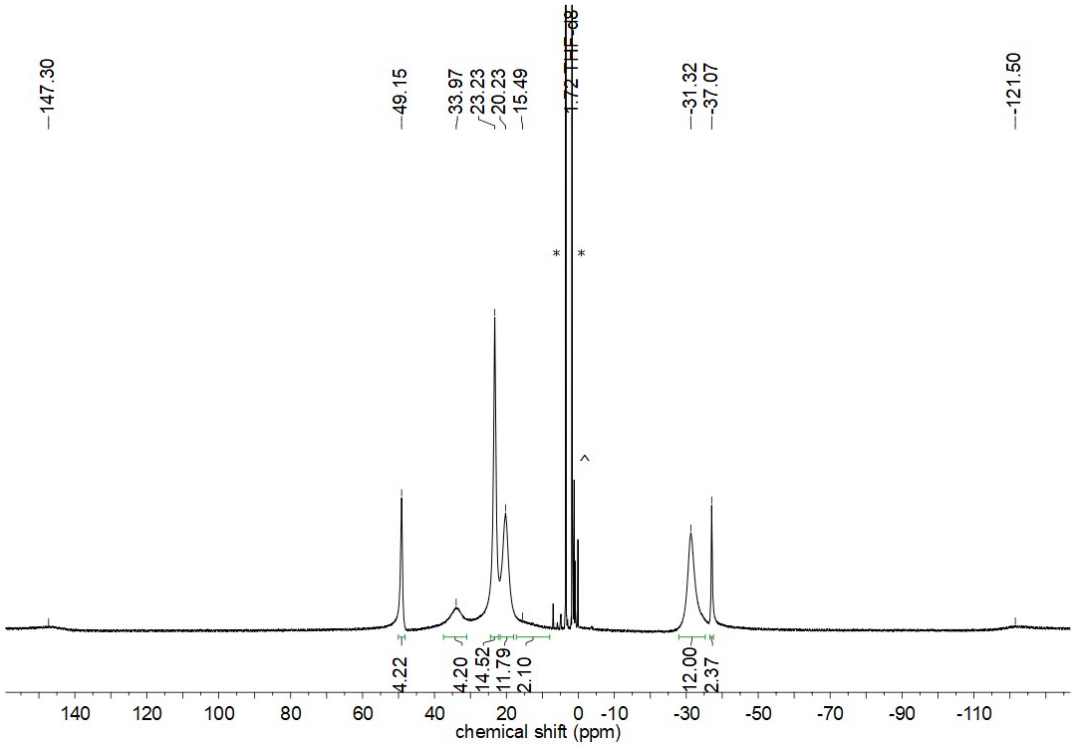

Figure S32. ^{1}H NMR spectrum (300.2 MHz, 300 K) of **[FeL$^4_2$]** in THF-d_8. (* solvent, ^ impurities)

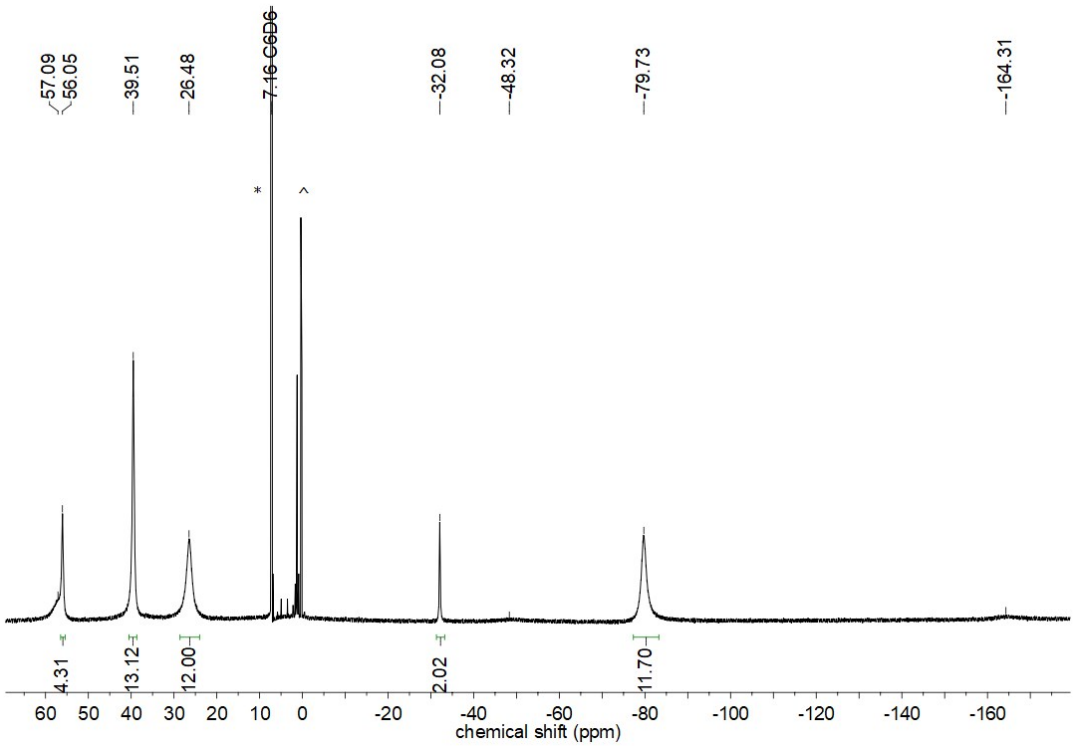

Figure S33. ^{1}H NMR spectrum (300.2 MHz, 300 K) of **[CoL$^4_2$]** in C_6D_6. (* solvent, ^ impurities)

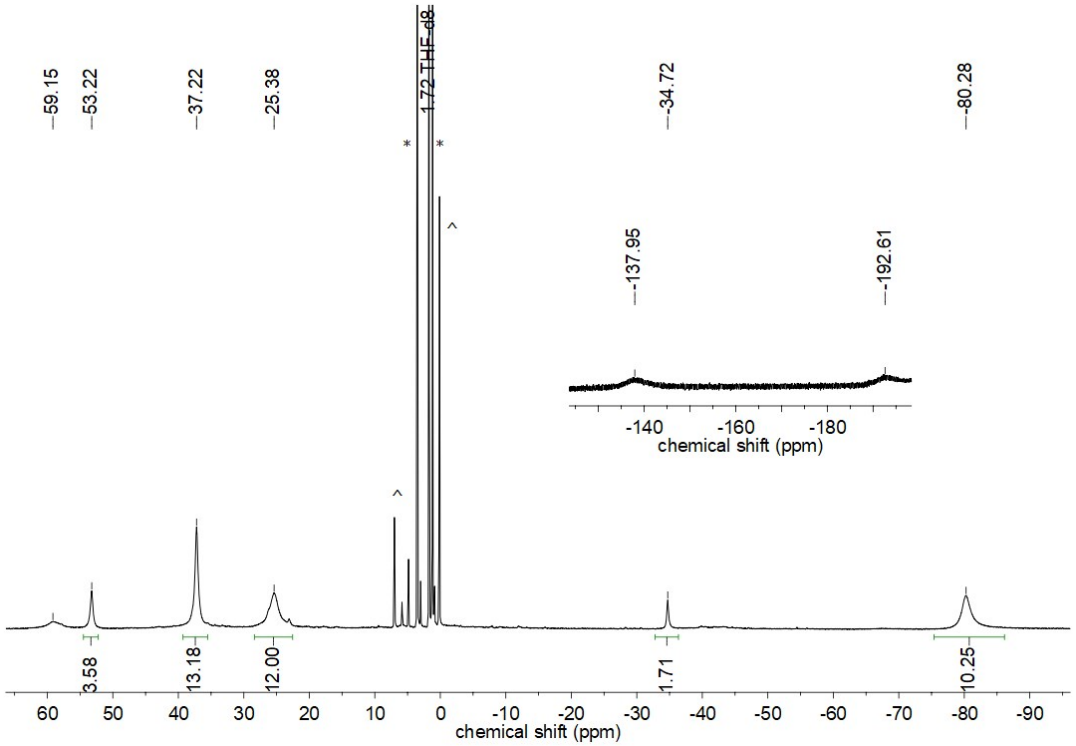

Figure S34. ^{1}H NMR spectrum (300.2 MHz, 300 K) of **[CoL$^4_2$]** in THF-d_8. (* solvent, ^ impurities)

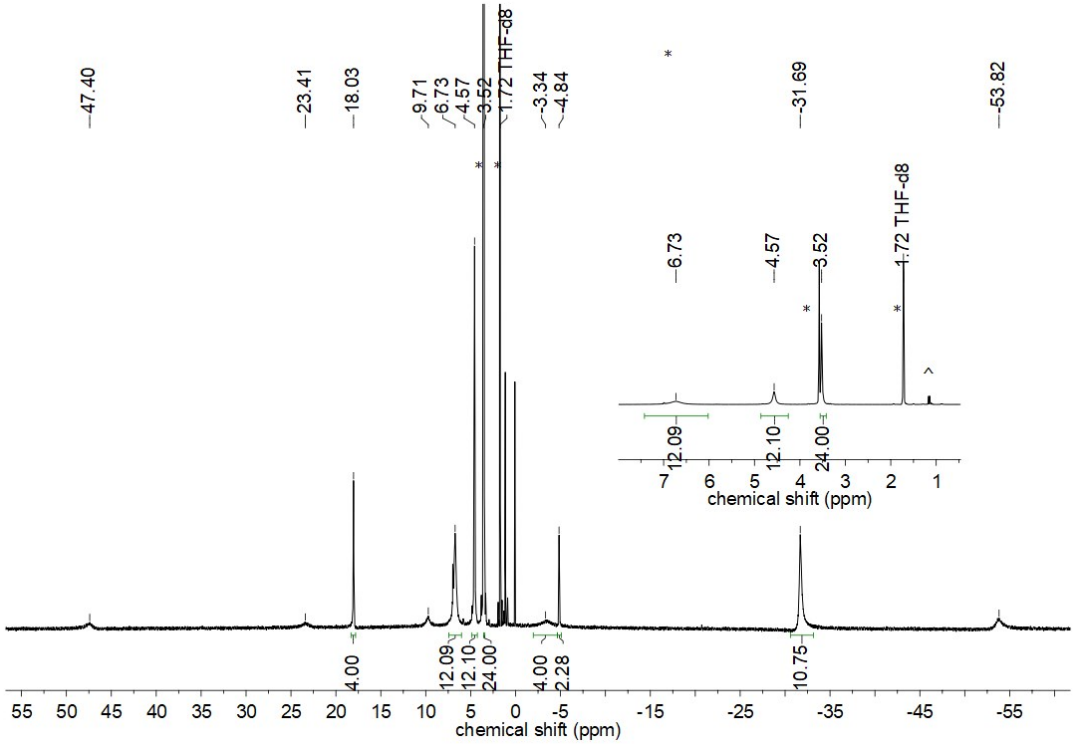

Figure S35. ^{1}H NMR spectrum (300.2 MHz, 300 K) of K{18c6}**[CoL$^{4}_{2}$]** in THF-d_8. (* solvent, ^ impurities)

Imido complexes

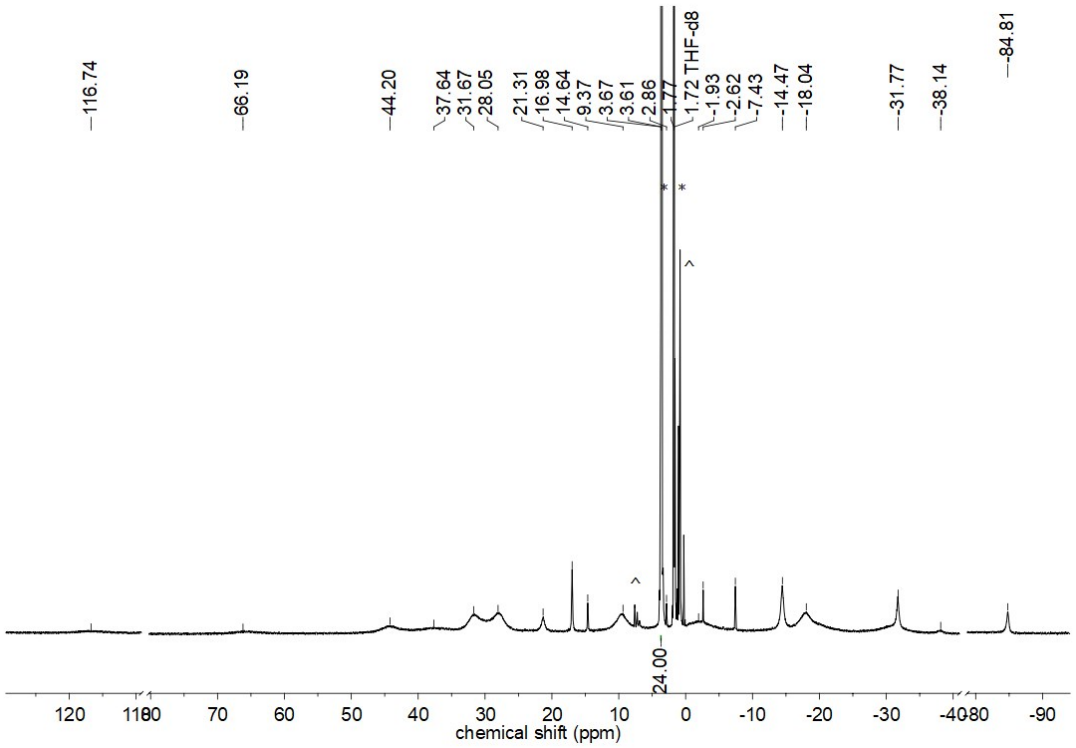

Figure S36. ^{1}H NMR spectrum (300.2 MHz, 300 K) of K{18c6}**[Co(NDipp)L$^{1}_{2}$]** in THF-d_8. (* solvent, ^ impurities)

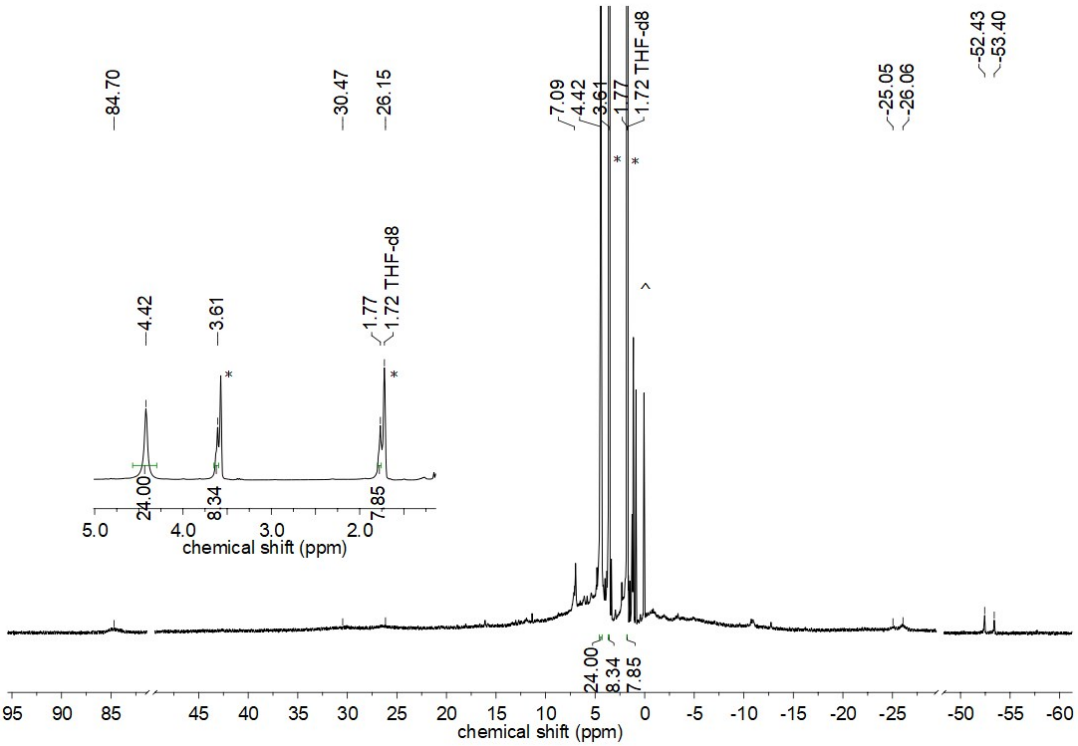

Figure S37. ^{1}H NMR spectrum (300.2 MHz, 300 K) of K{18c6}**[Co(NDipp)L$^{4}_{2}$]** in THF-d_8. (* solvent, ^ impurities)

2 UV/Vis spectra

−N(Dipp)SiMe$_2$Ph (L^1) containing compounds

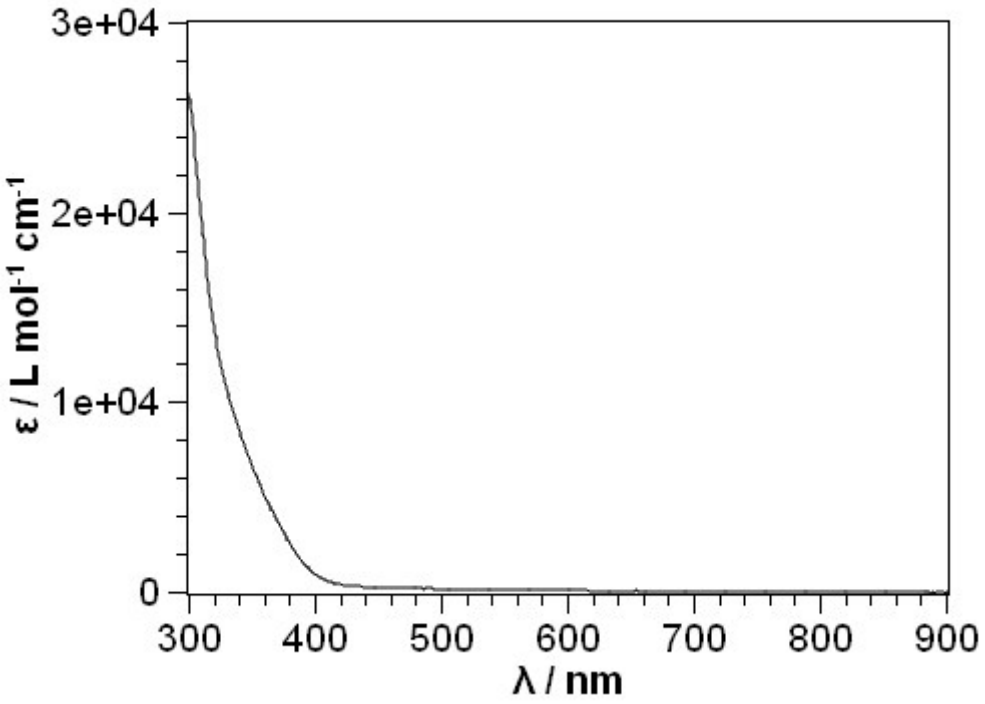

Figure S38. UV/Vis spectrum of **[MnL$^1_2$]** in Et$_2$O.

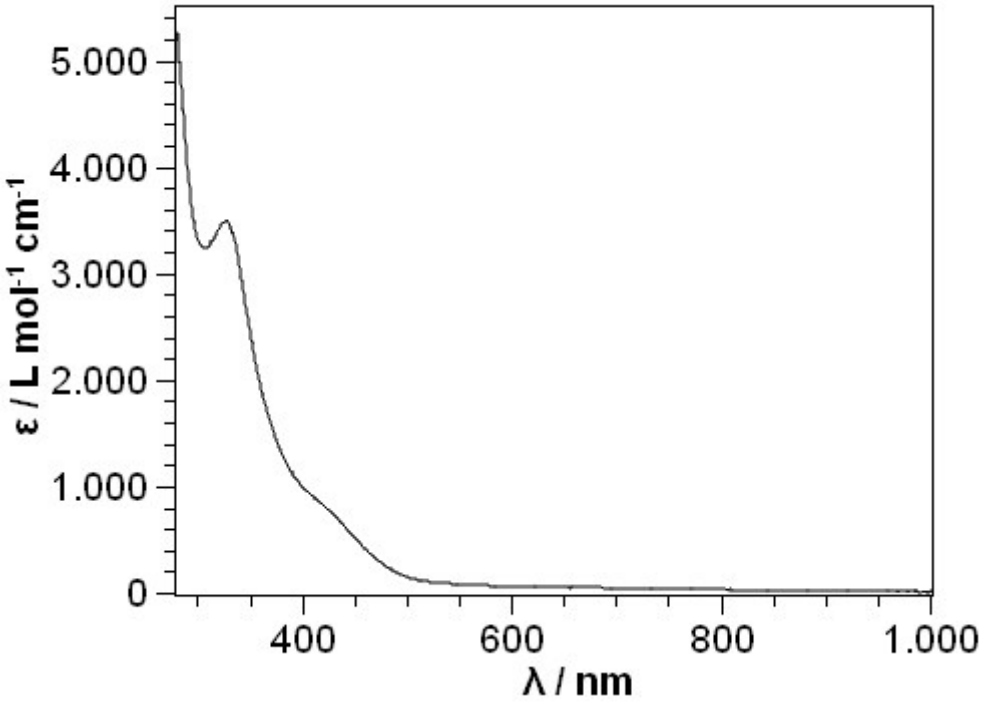

Figure S39. UV/Vis spectrum of **[FeL$^1_2$]** in Et$_2$O.

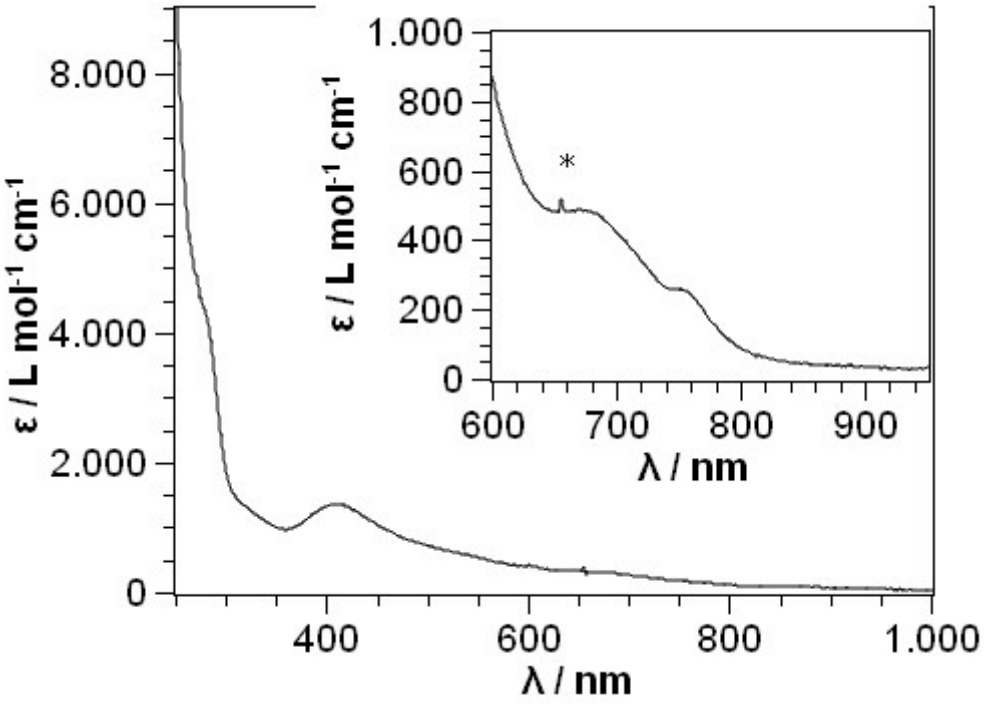

Figure S40. UV/Vis spectrum of **[CoL$^1_2$]** in Et_2O. The signal caused by detector exchange is indicated by *.

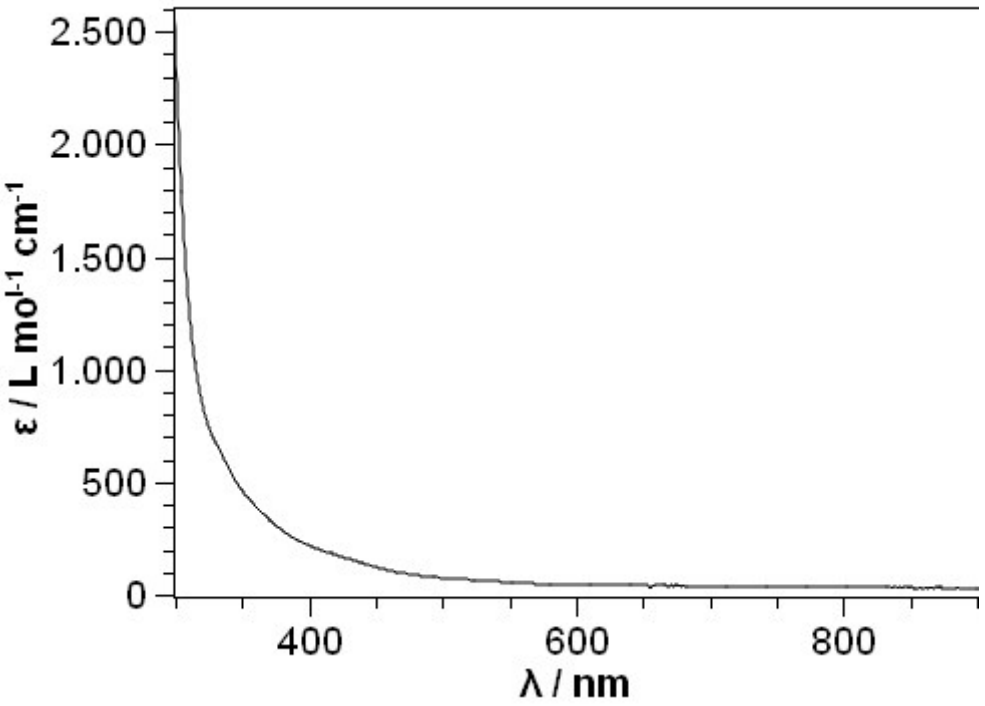

Figure S41. UV/Vis spectrum of K{18c6}**[MnL^{1}L^{1*}]** in THF.

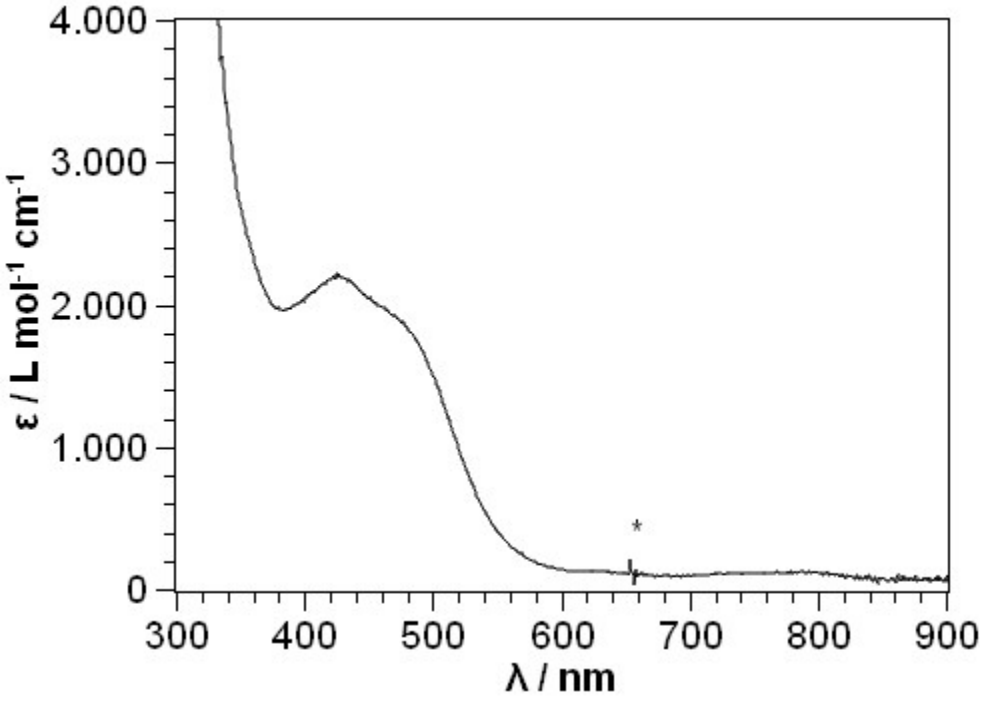

Figure S42. UV/Vis spectrum of K{18c6}**[FeL$^1_2$]** in Et_2O.

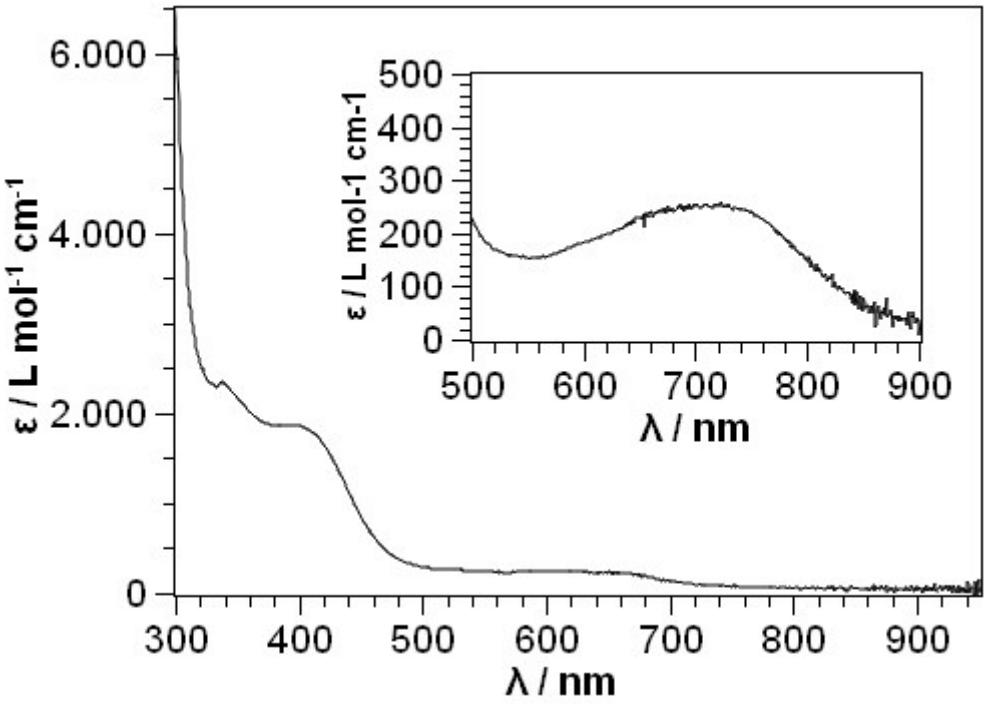

Figure S43. UV/Vis spectrum of K{18c6}**[CoL$^1_2$]** in Et_2O.

−N(Dipp)SiMePh$_2$ (L^2) containing compounds

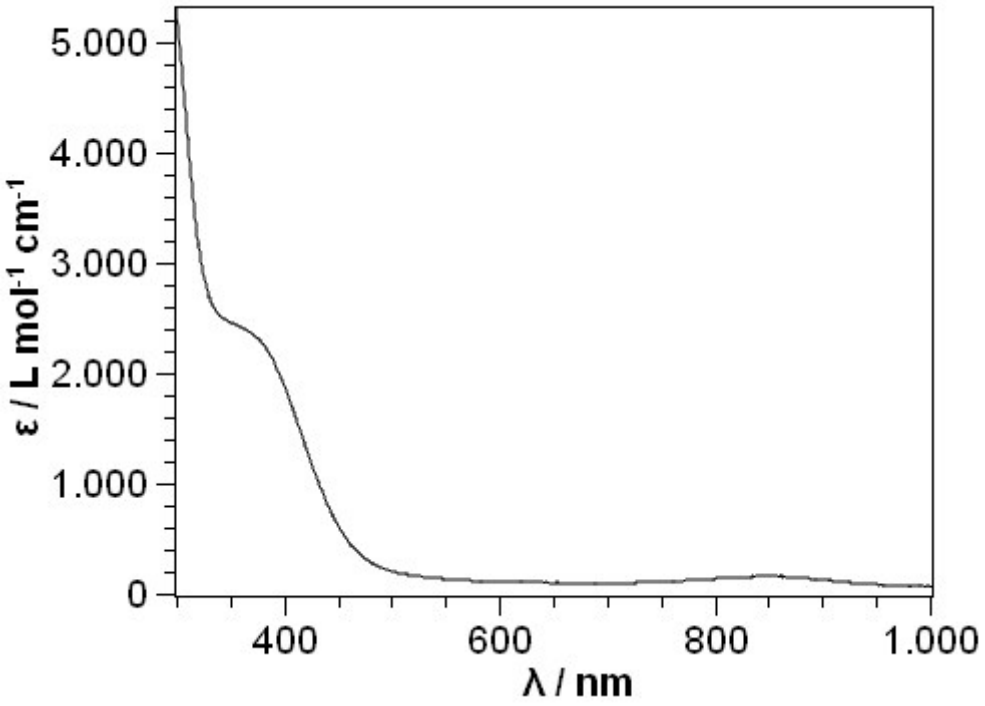

Figure S44. UV/Vis spectrum of **[CrL$^2_2$]** in Et_2O.

−N(Dipp)SiPh$_3$ (L^3) containing compounds

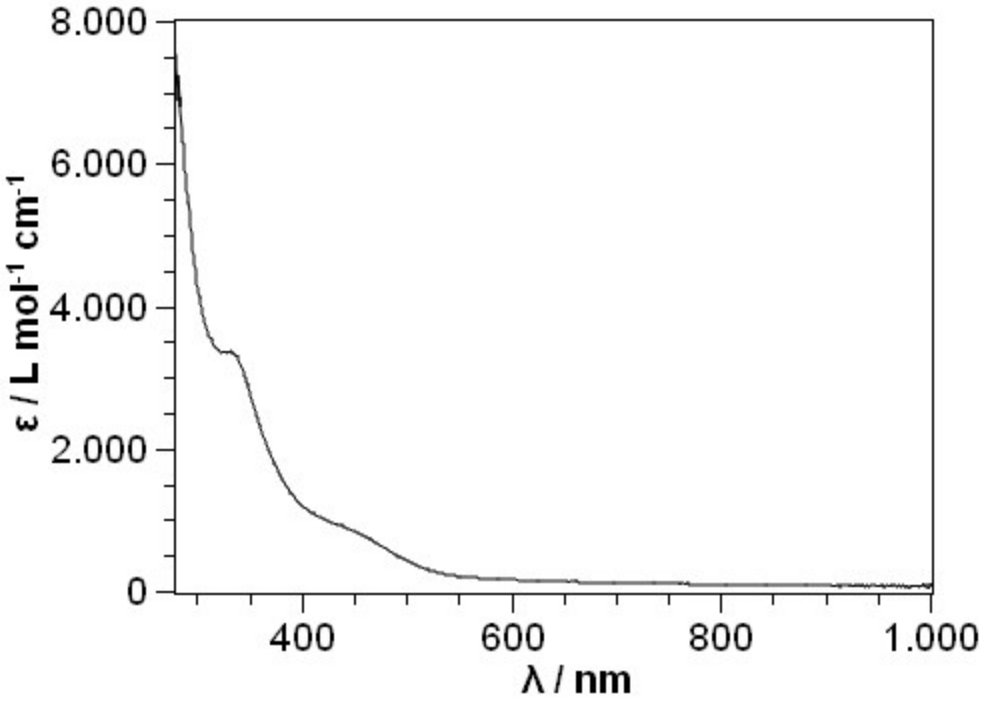

Figure S45. UV/Vis spectrum of **[FeL$^3_2$]** in Et_2O.

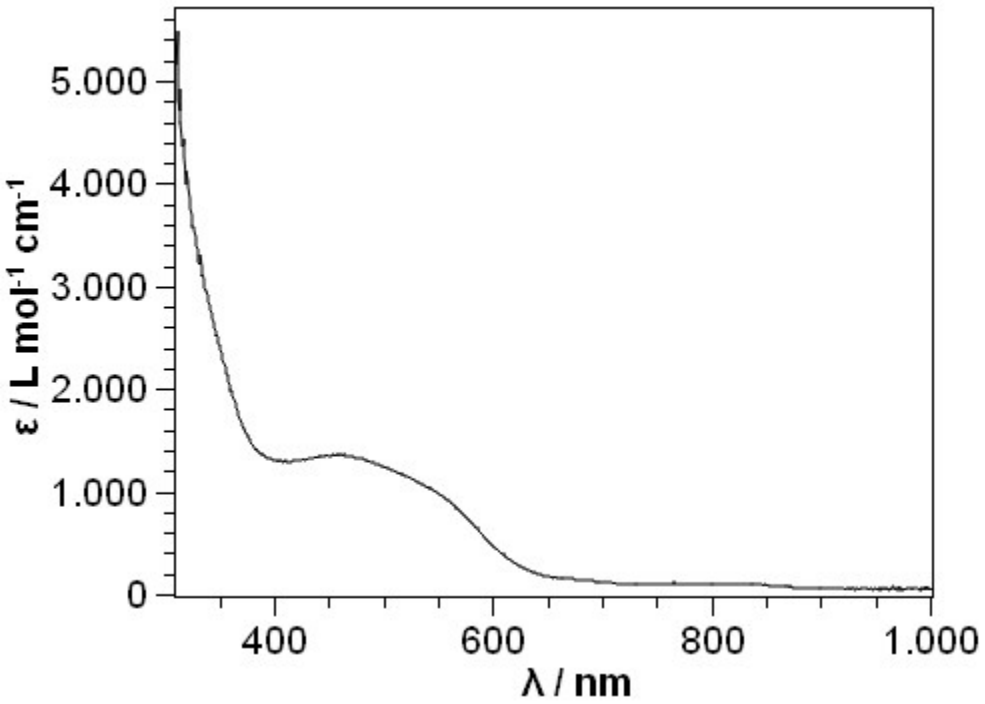

Figure S46. UV/Vis spectrum of K{18c6}**[FeL$^3_2$]** in THF.

−N(Dipp)SiMe$_2$(allyl) (L^4) containing compounds

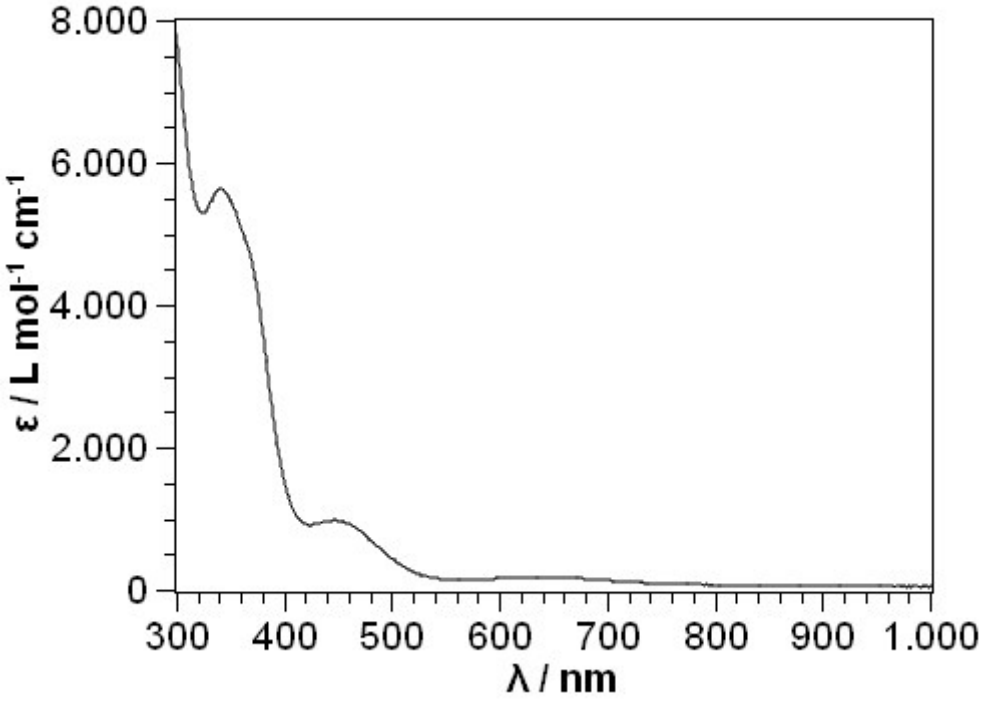

Figure S47. UV/Vis spectrum of **[CrL$^4_2$]** in Et_2O.

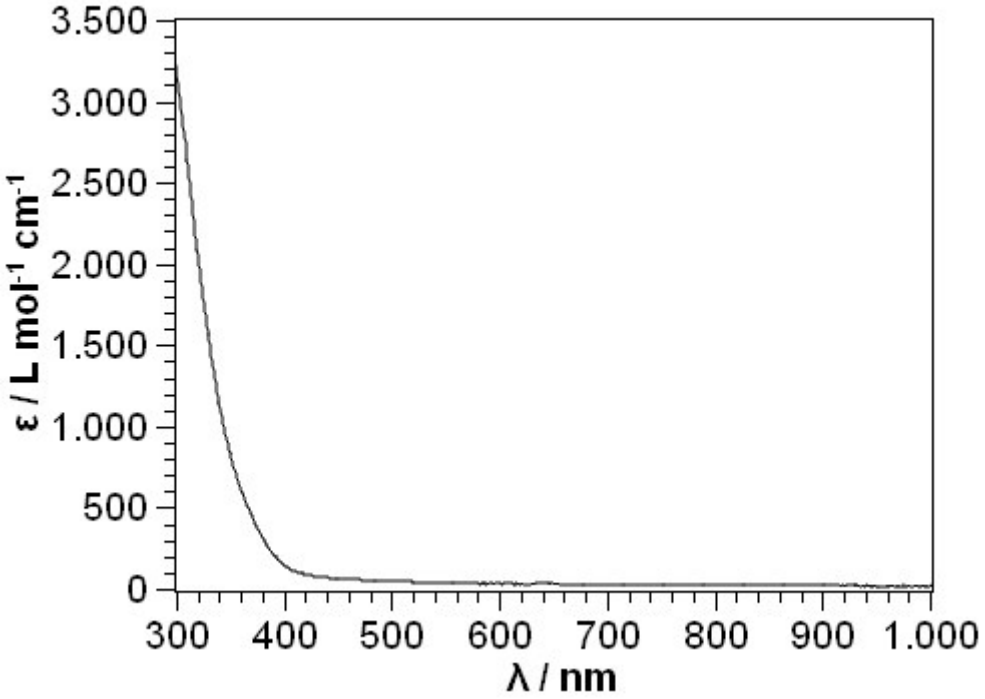

Figure S48. UV/Vis spectrum of **[MnL$^4_2$]** in Et_2O.

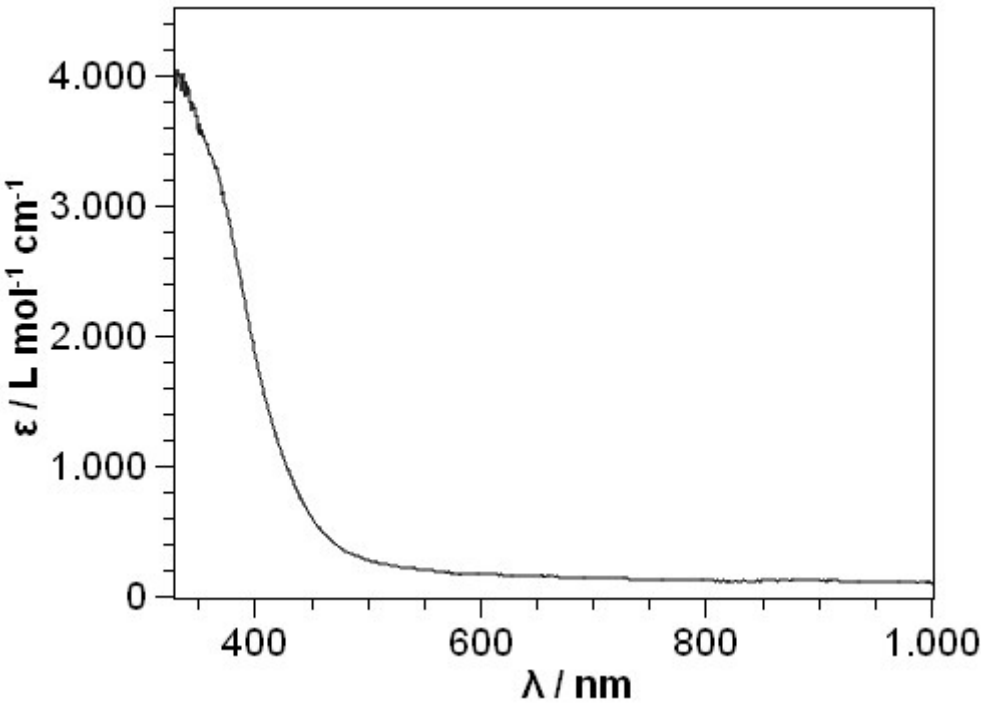

Figure S49. UV/Vis spectrum of **[FeL$^4_2$]** in Et_2O.

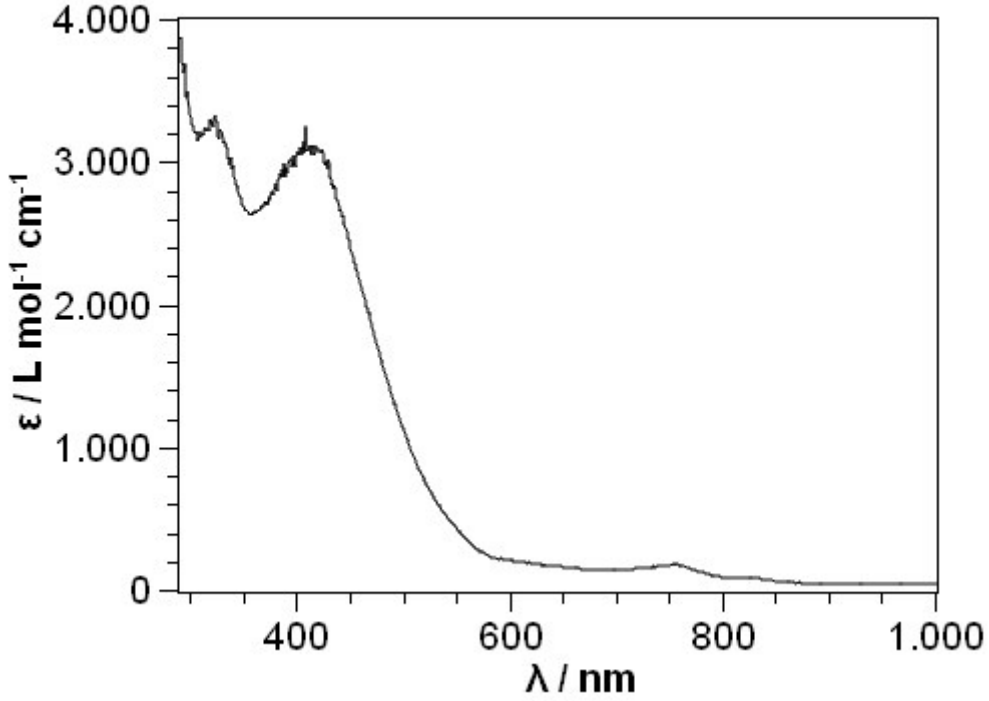

Figure S50. UV/Vis spectrum of **[CoL$^4_2$]** in Et_2O.

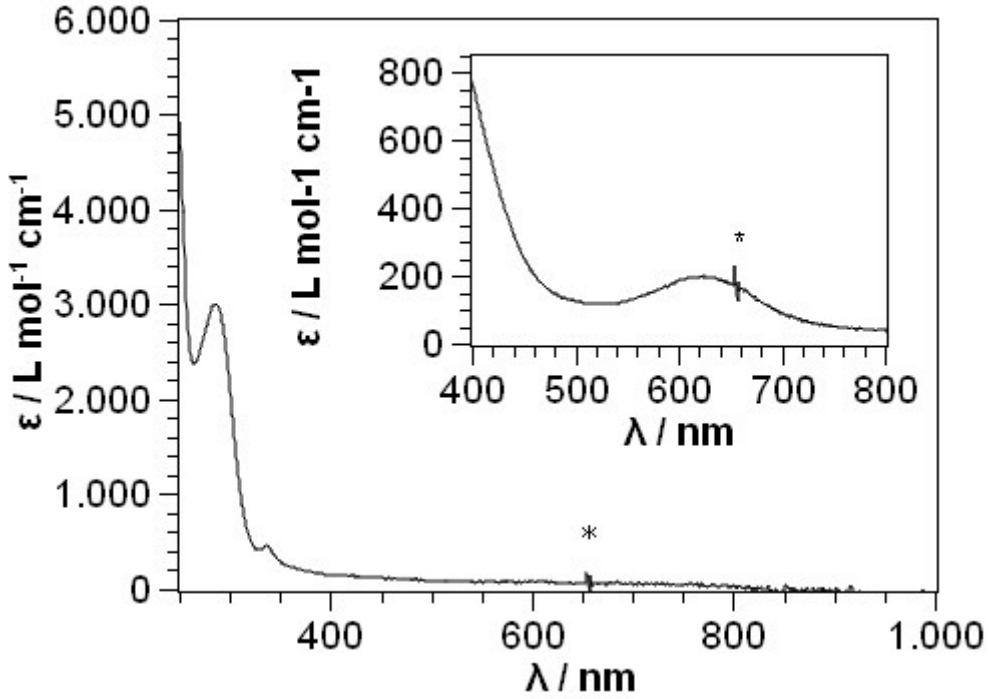

Figure S51. UV/Vis spectrum of $(K\{18c6\})_2$**[CrL$^4_2$]$_2$** in THF. The signal caused by detector exchange is indicated by *.

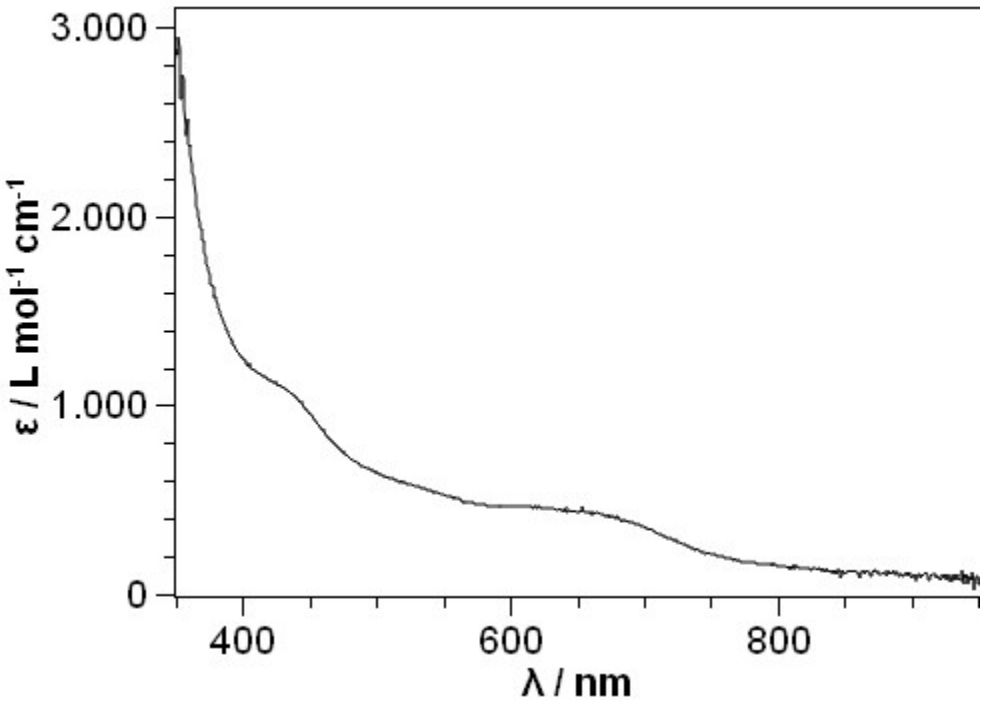

Figure S52. UV/Vis spectrum of K{18c6}**[CoL$^4_2$]** in THF.

Imido complexes

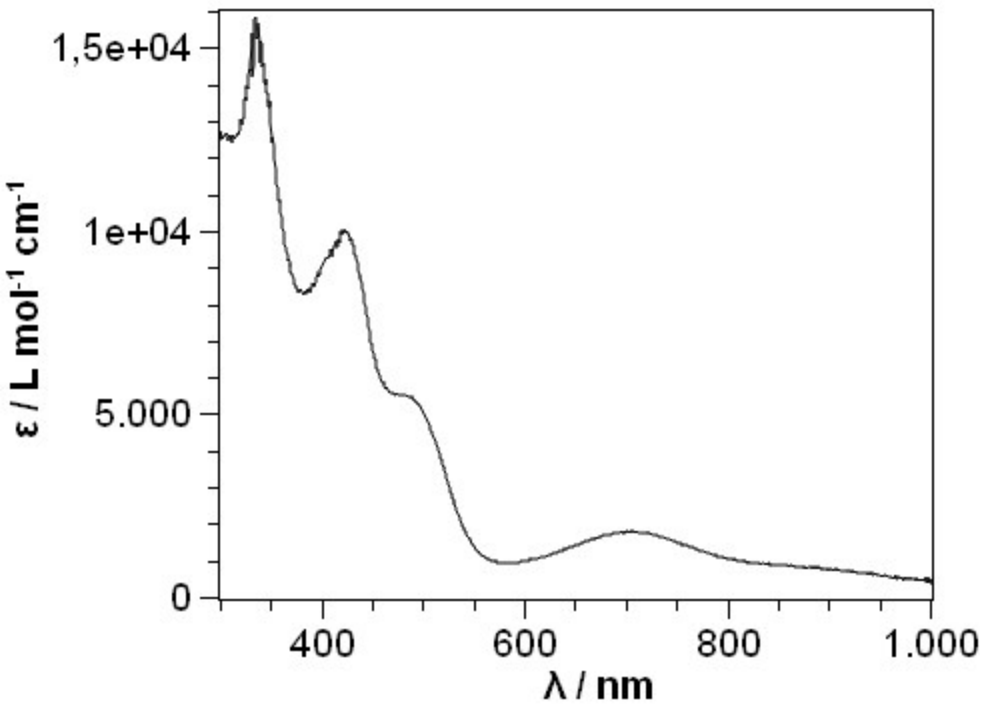

Figure S53. UV/Vis spectrum of K{18c6}**[Co(NDipp)L$^1_2$]** in THF.

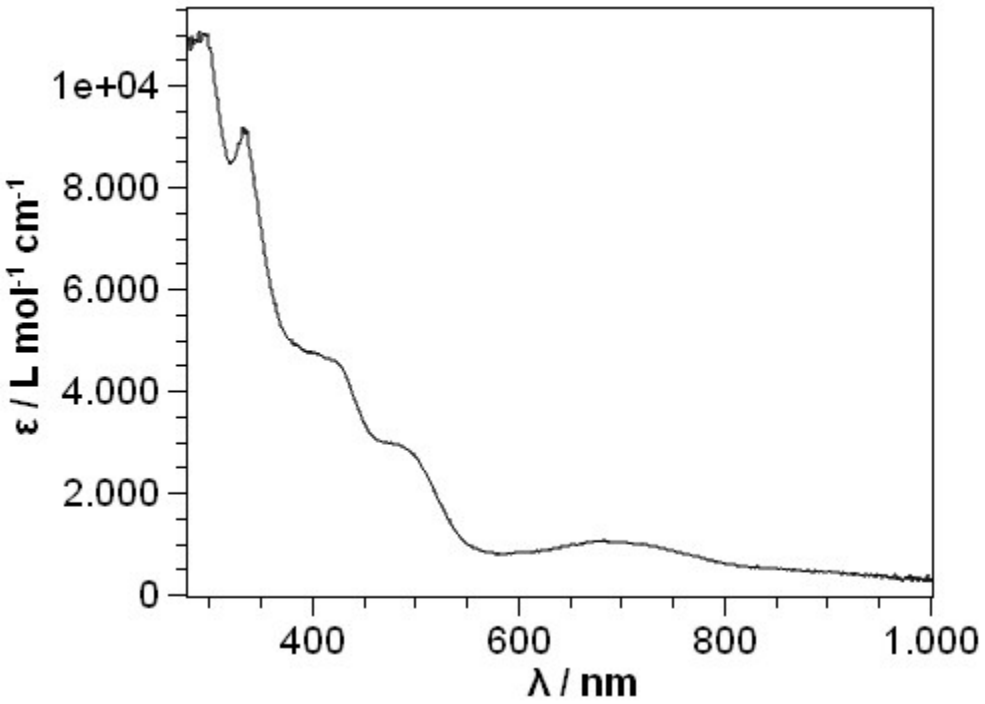

Figure S54. UV/Vis spectrum of K{18c6}**[Co(NDipp)L$^4_2$]** in THF.

3 IR spectra

−N(Dipp)Si(Me_2Ph) (L^1) containing compounds

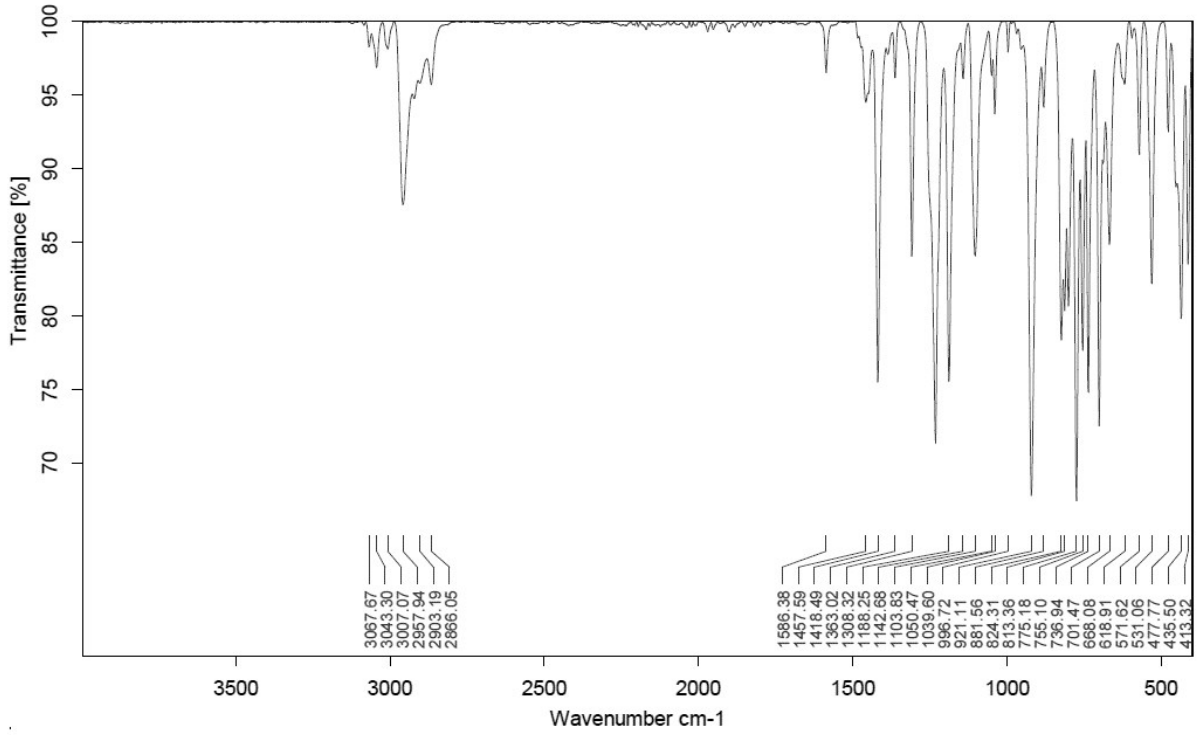

Figure S55. IR spectrum of **LiL^1**.

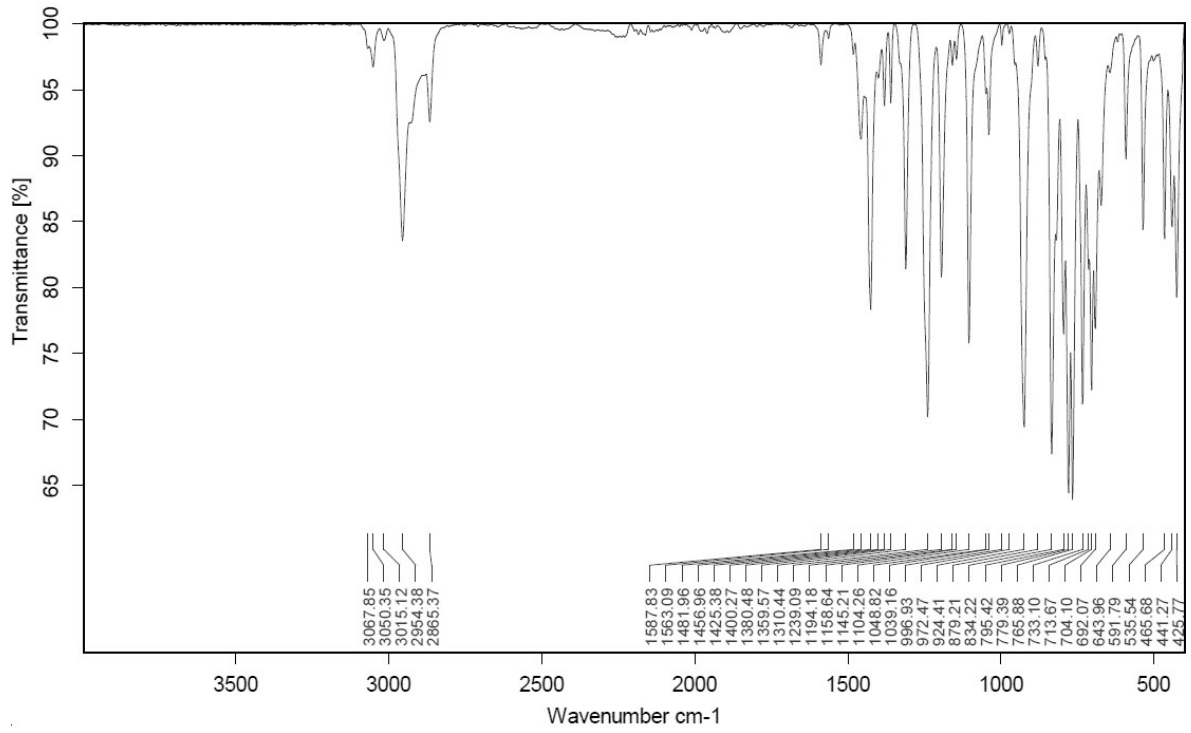

Figure S56. IR spectrum of **[MnL^1_2]**.

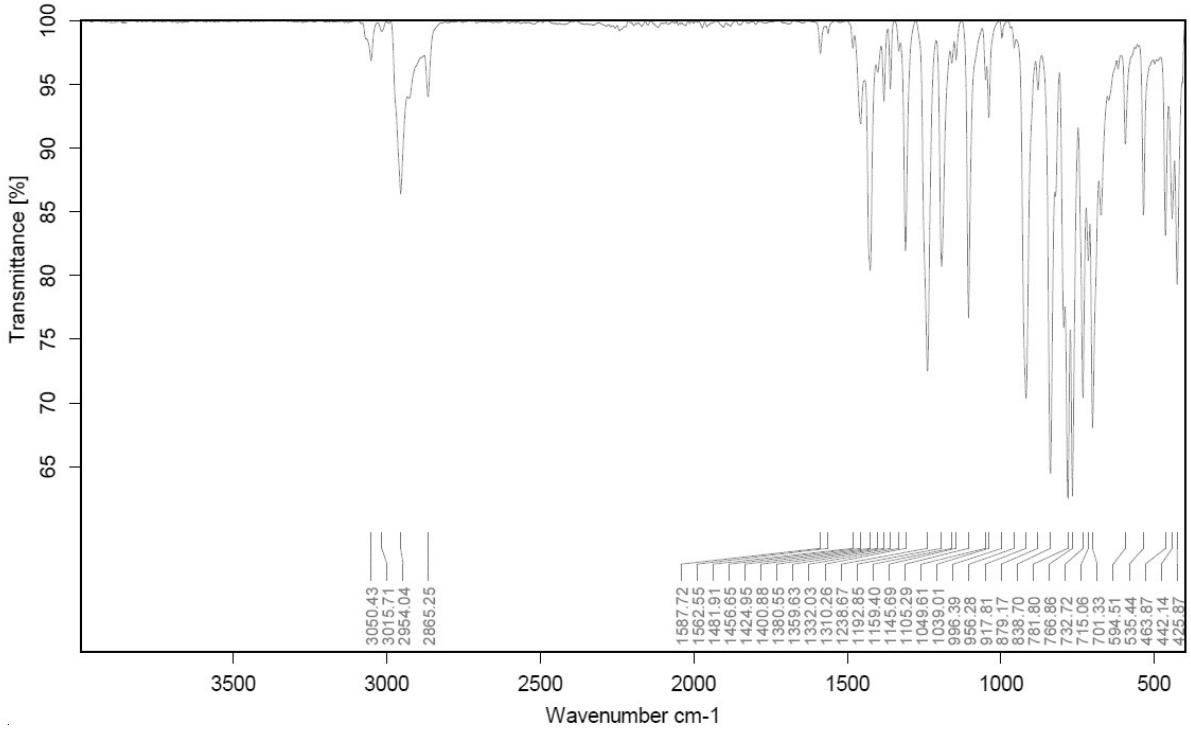

Figure S57. IR spectrum of **[FeL$^1_2$]**.

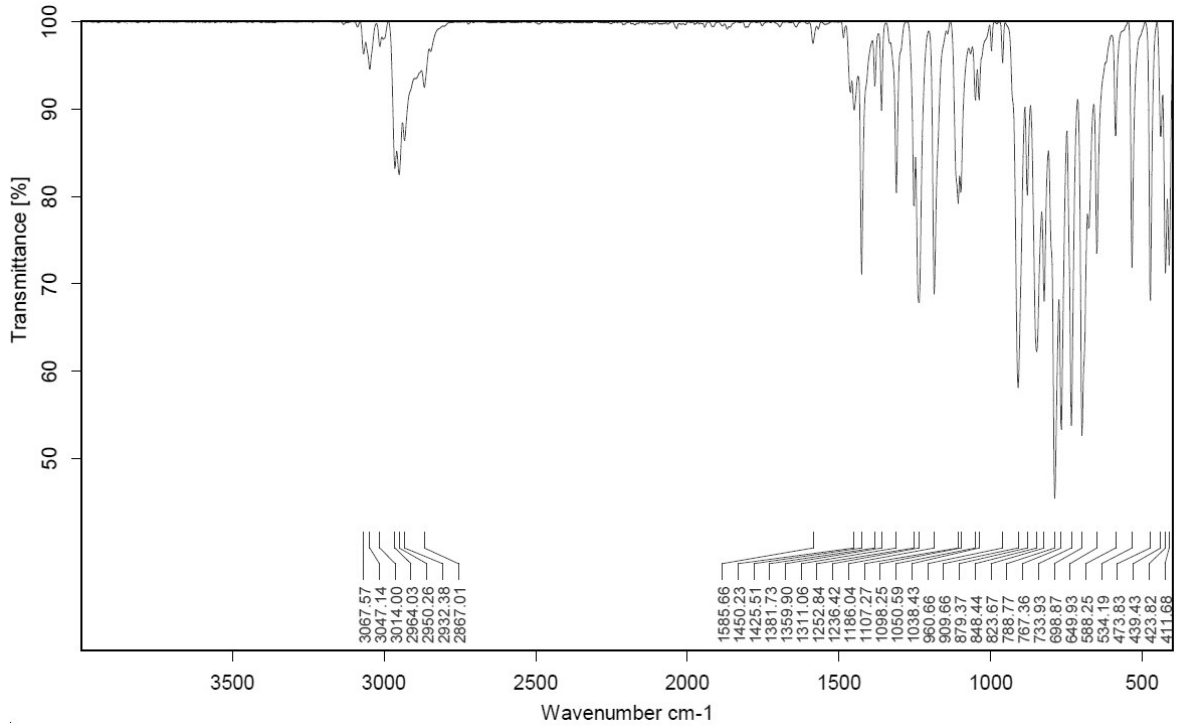

Figure S58. IR spectrum of **[CoL$^1_2$]**.

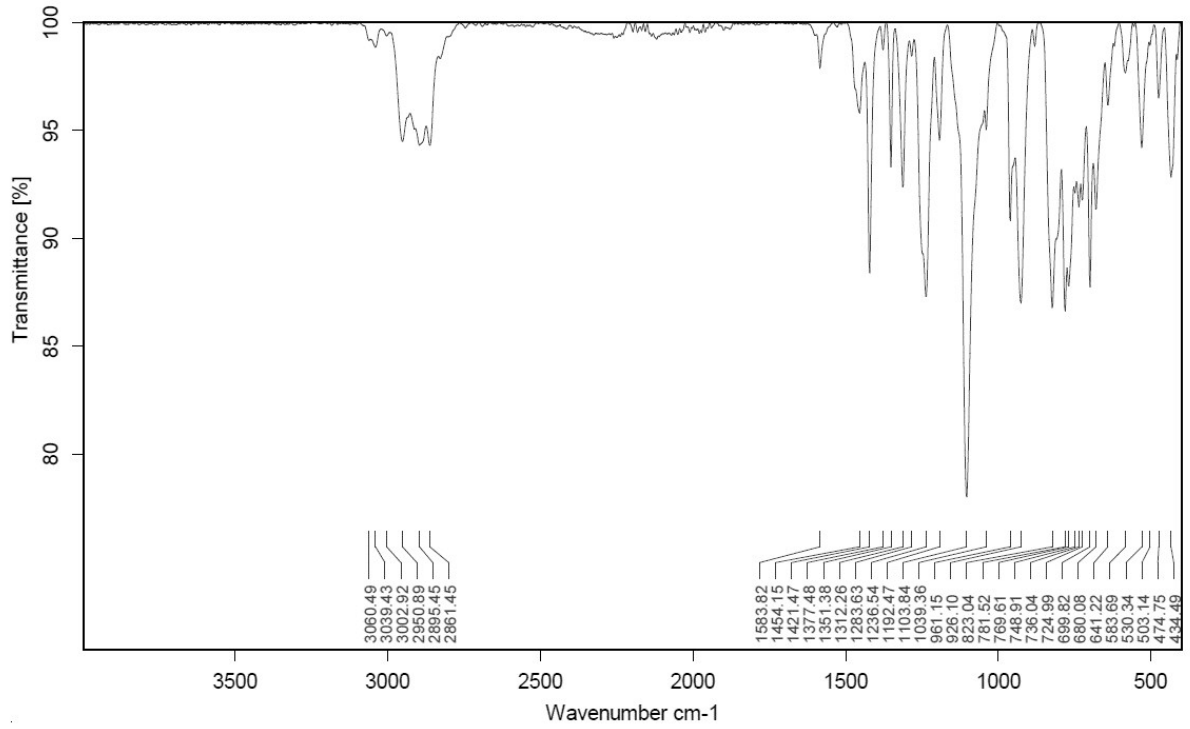

Figure S59. IR spectrum of K{18c6}**[MnL^{1}L^1*]**.

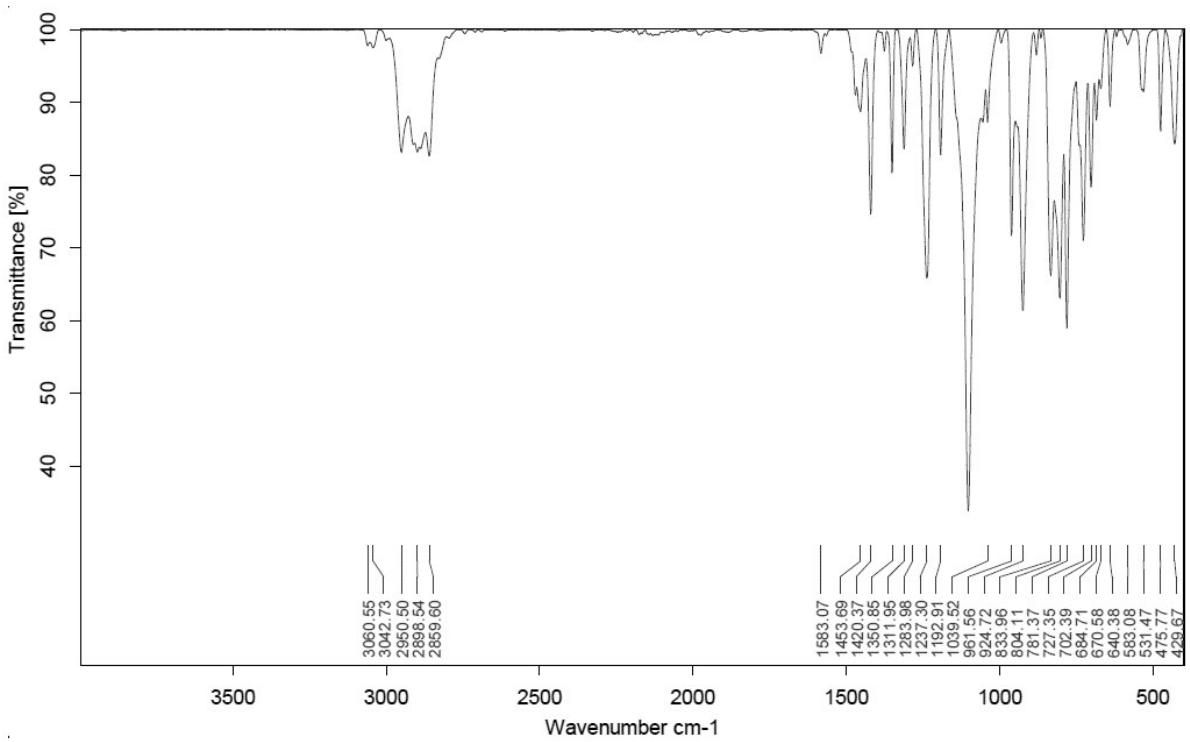

Figure S60. IR spectrum of K{18c6}**[FeL$^1_2$]**.

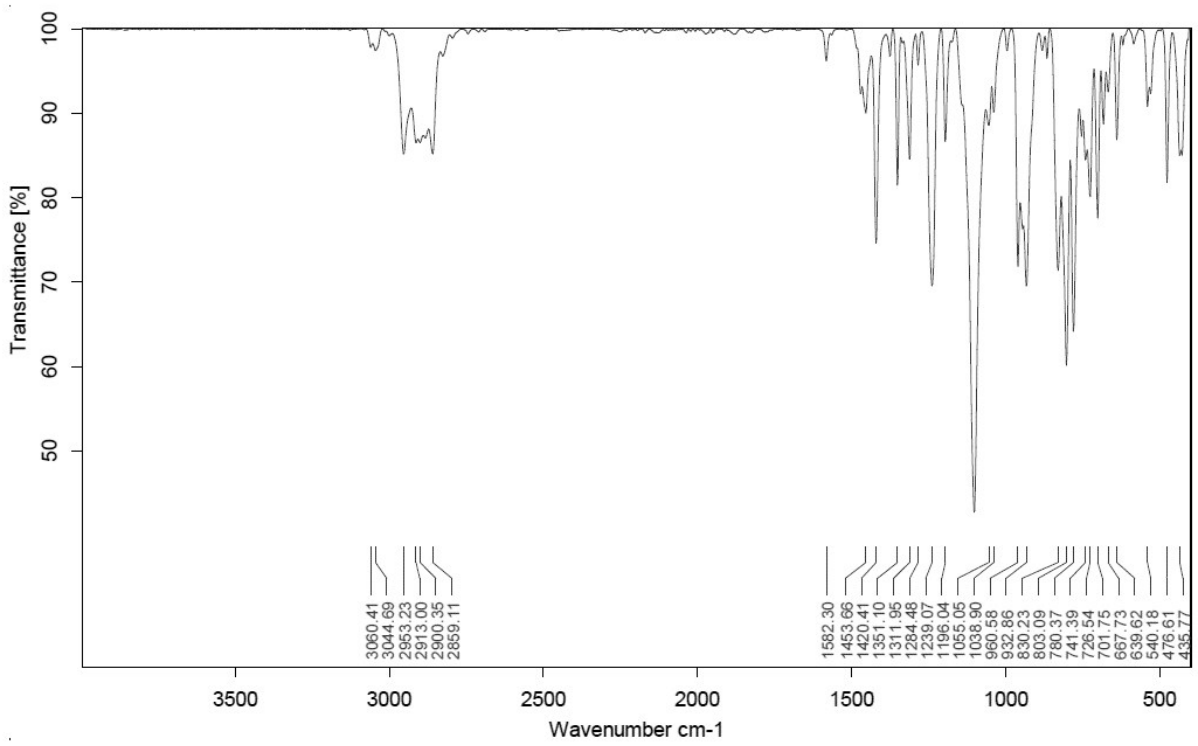

Figure S61. IR spectrum of K{18c6}**[CoL$^1_2$]**.

−N(Dipp)SiMePh$_2$ (L^2) containing compounds

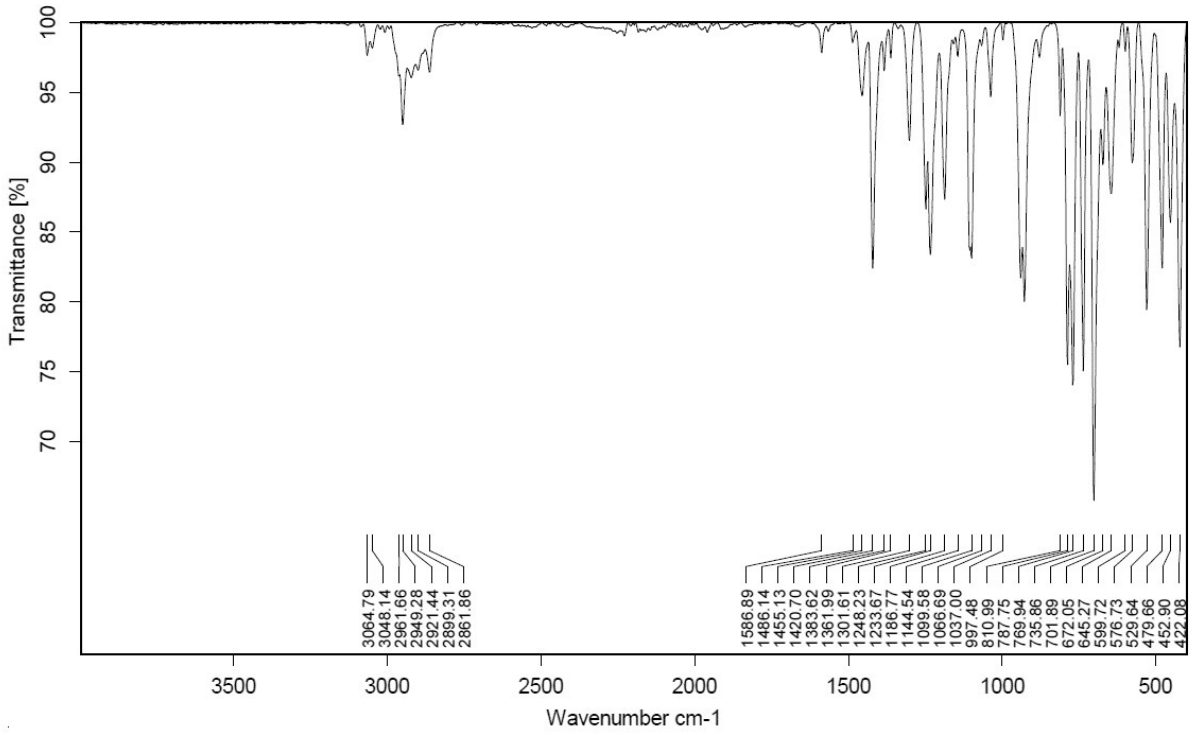

Figure S62. IR spectrum of **LiL^2**.

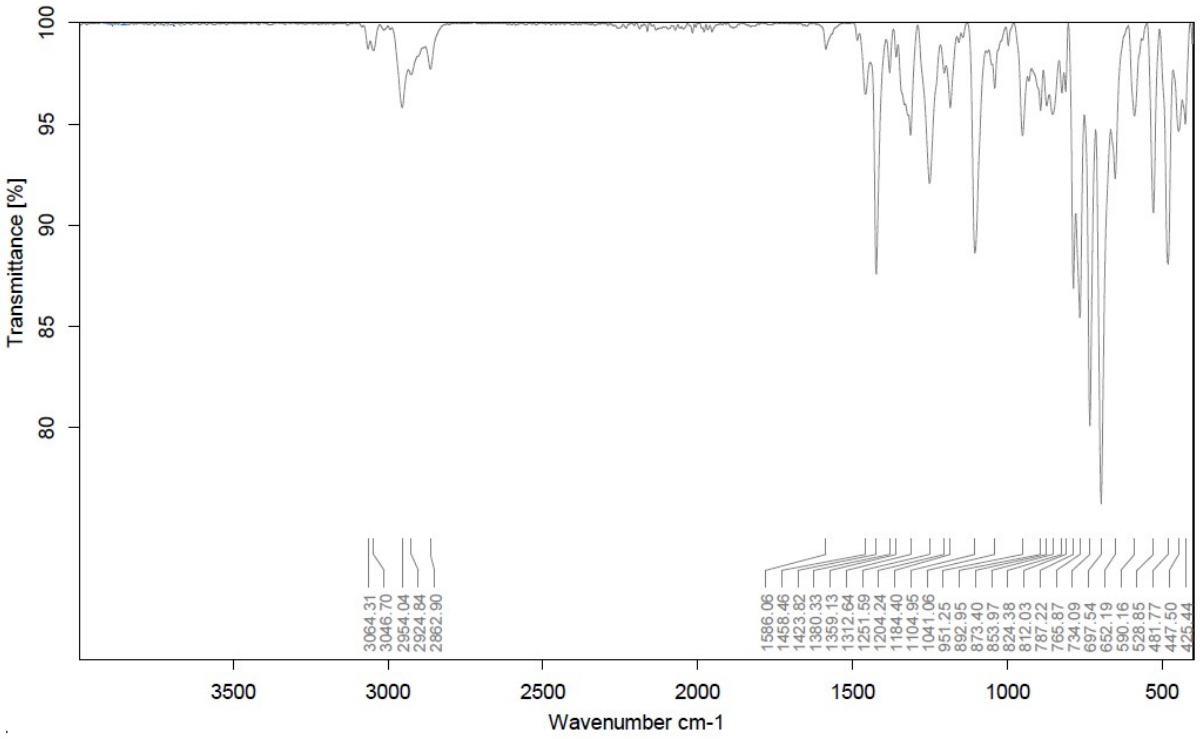

Figure S63. IR spectrum of **[CrL$^2_2$]**.

−N(Dipp)SiPh$_3$ (L^3) containing compounds

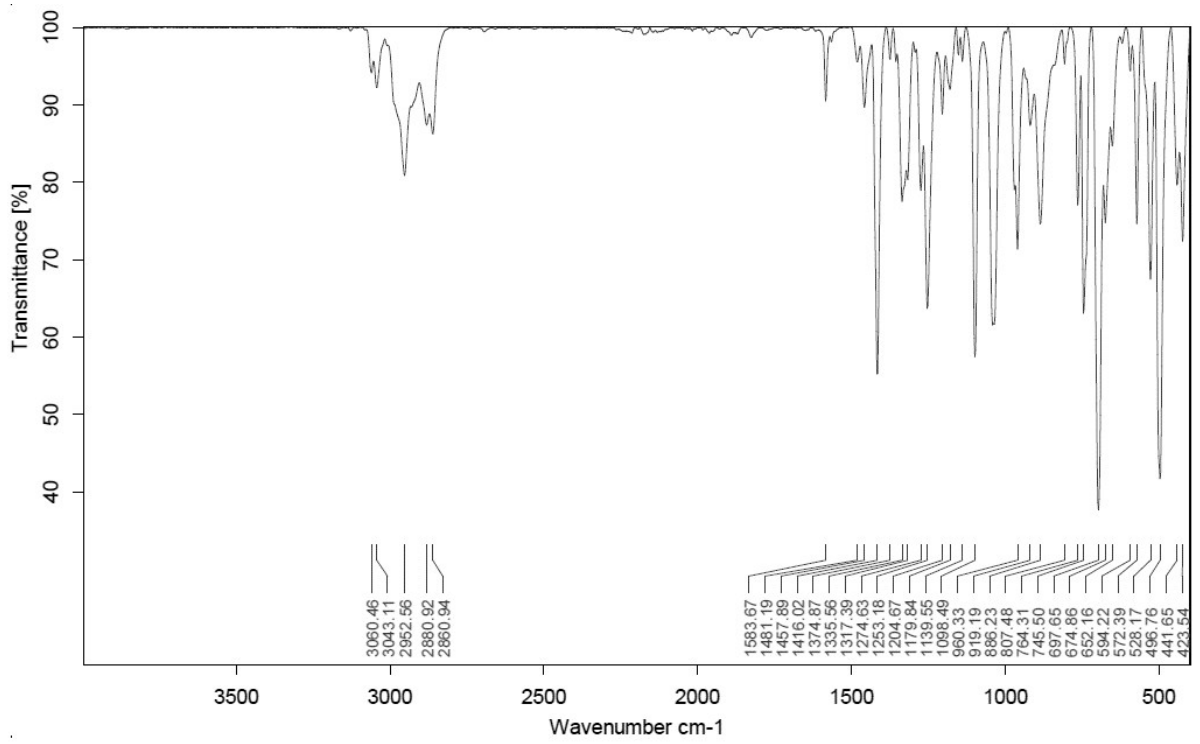

Figure S64. IR spectrum of **LiL^3**.

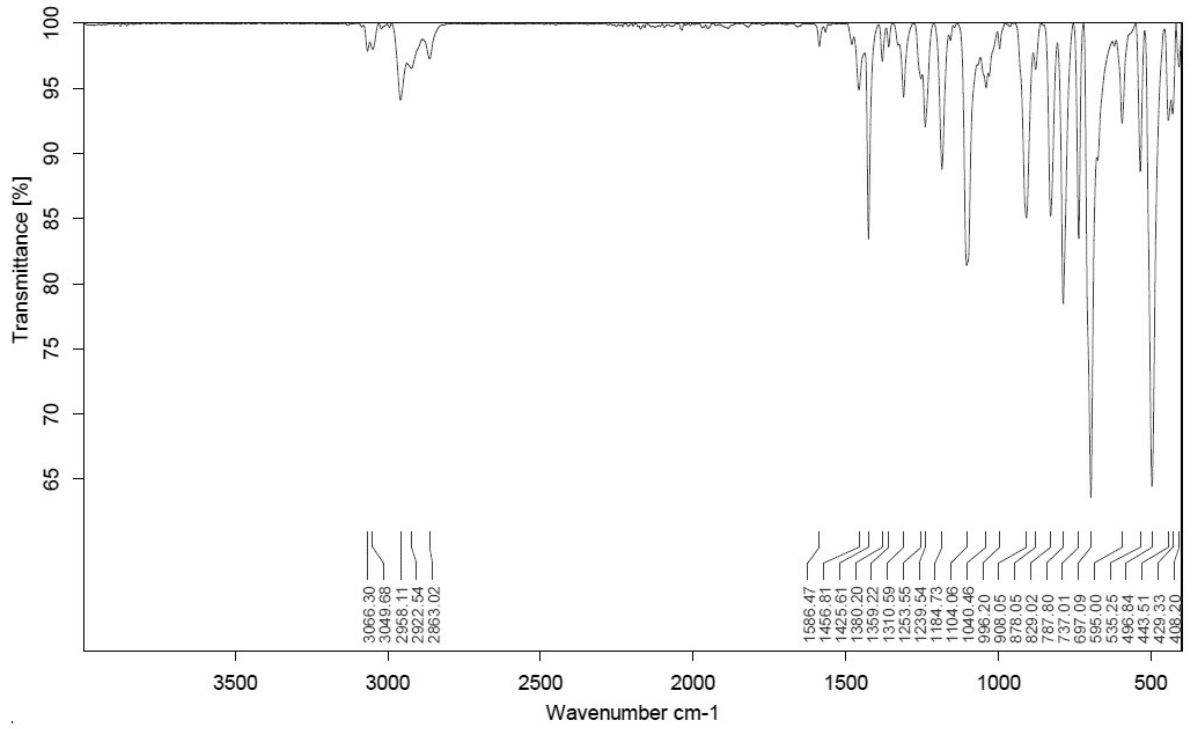

Figure S65. IR spectrum of **[FeL$^3_2$]**.

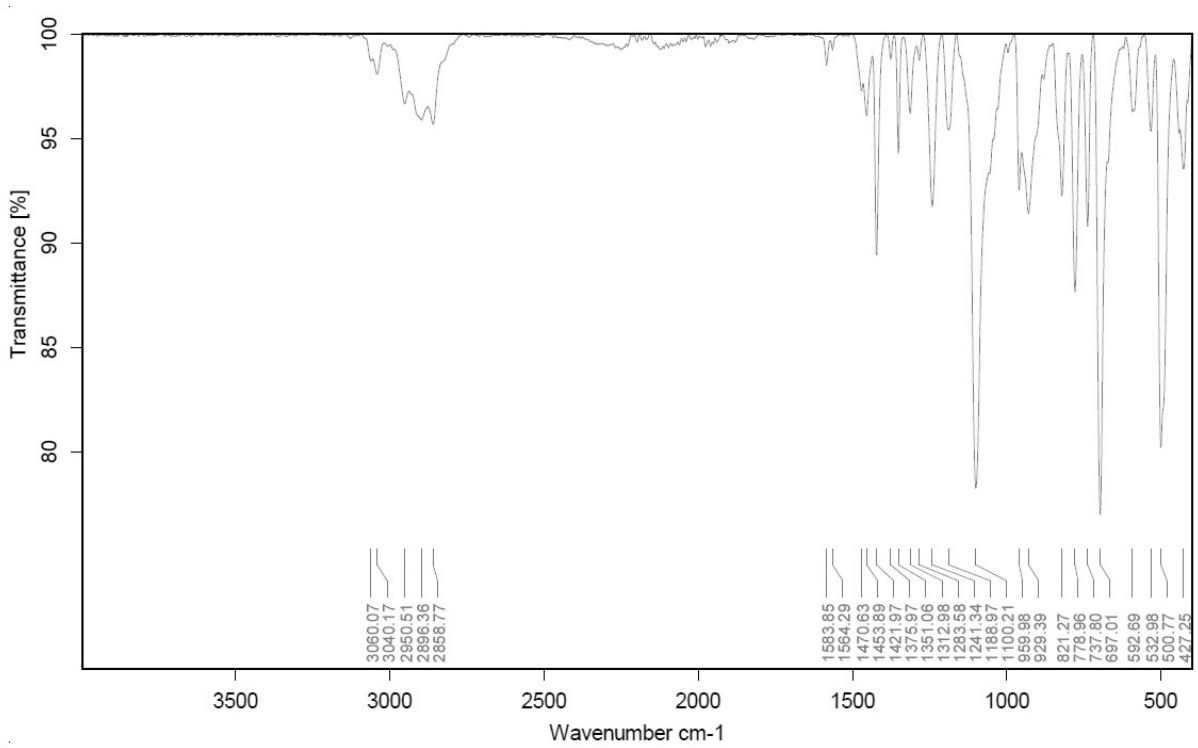

Figure S66. IR spectrum of K{18c6}**[FeL$^3_2$]**.

−N(Dipp)SiMe$_2$(allyl) (L^4) containing compounds

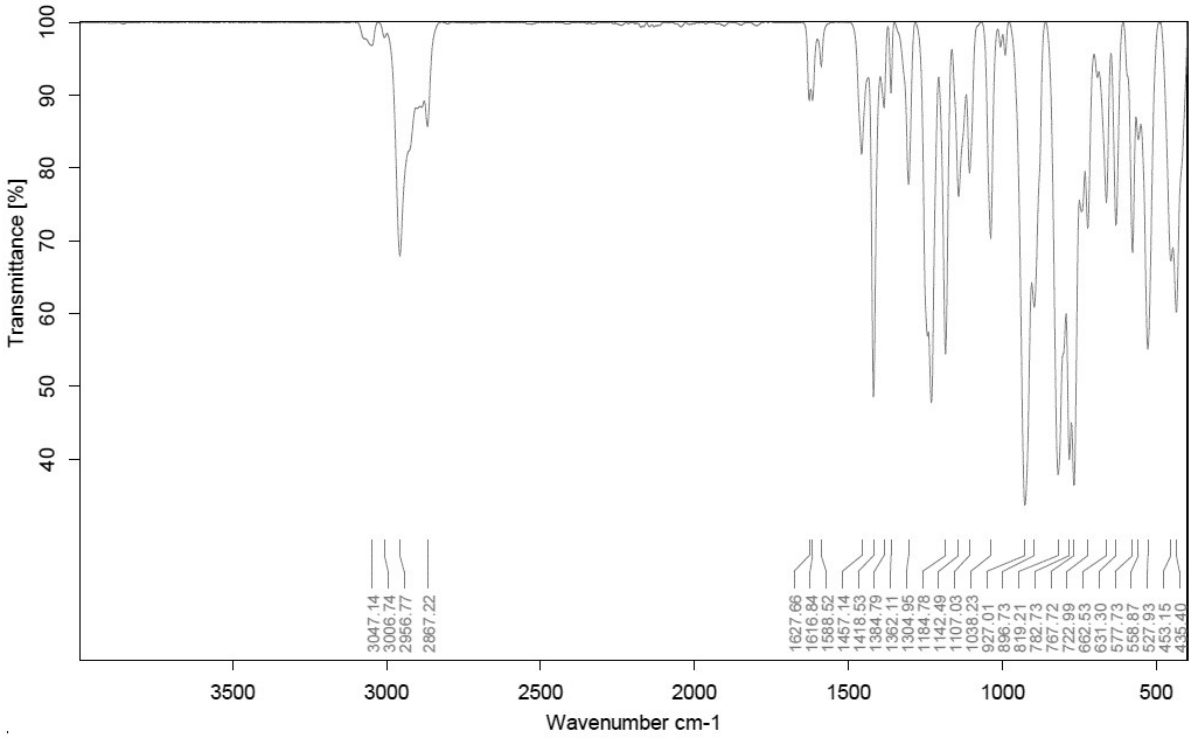

Figure S67. IR spectrum of **LiL^4**.

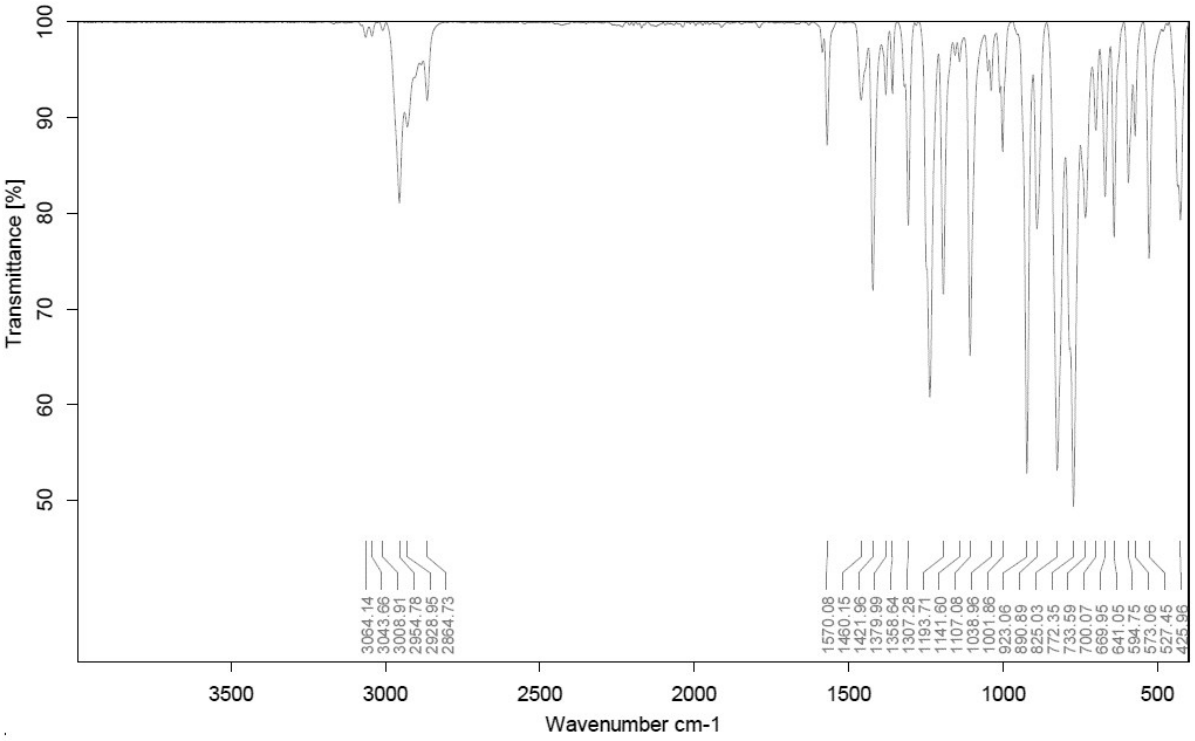

Figure S68. IR spectrum of **[CrL$^4_2$]**.

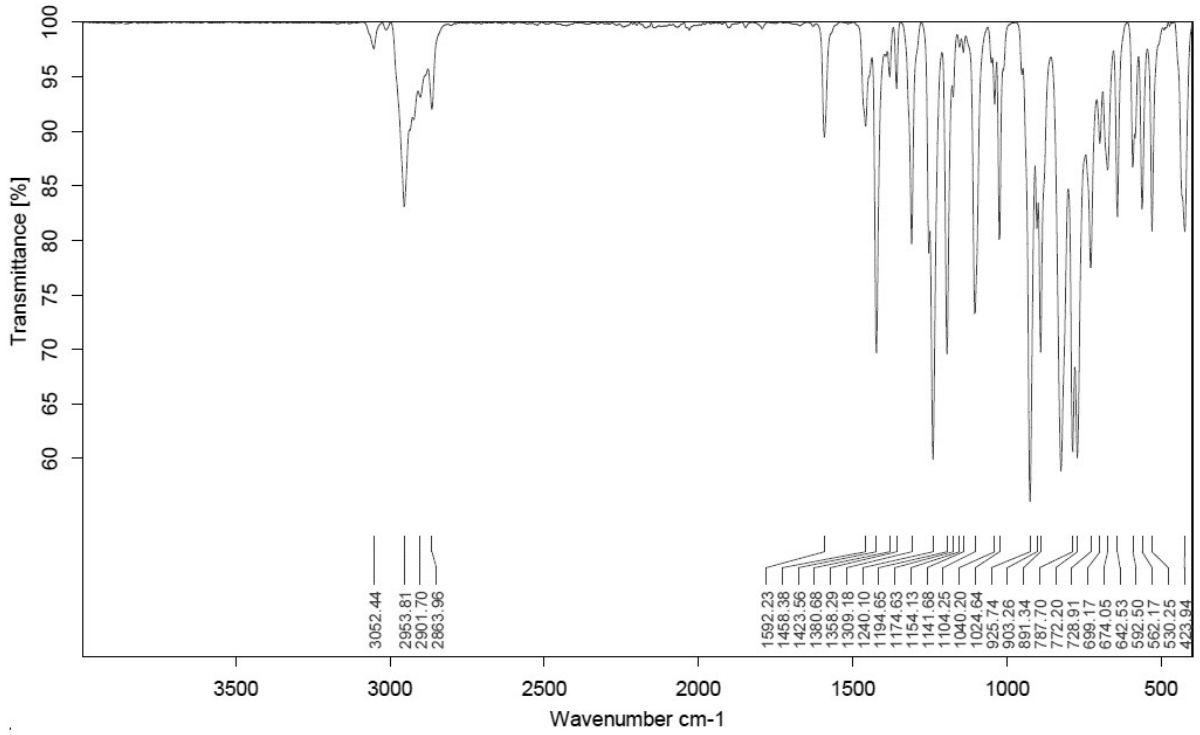

Figure S69. IR spectrum of **[MnL$^4_2$]**.

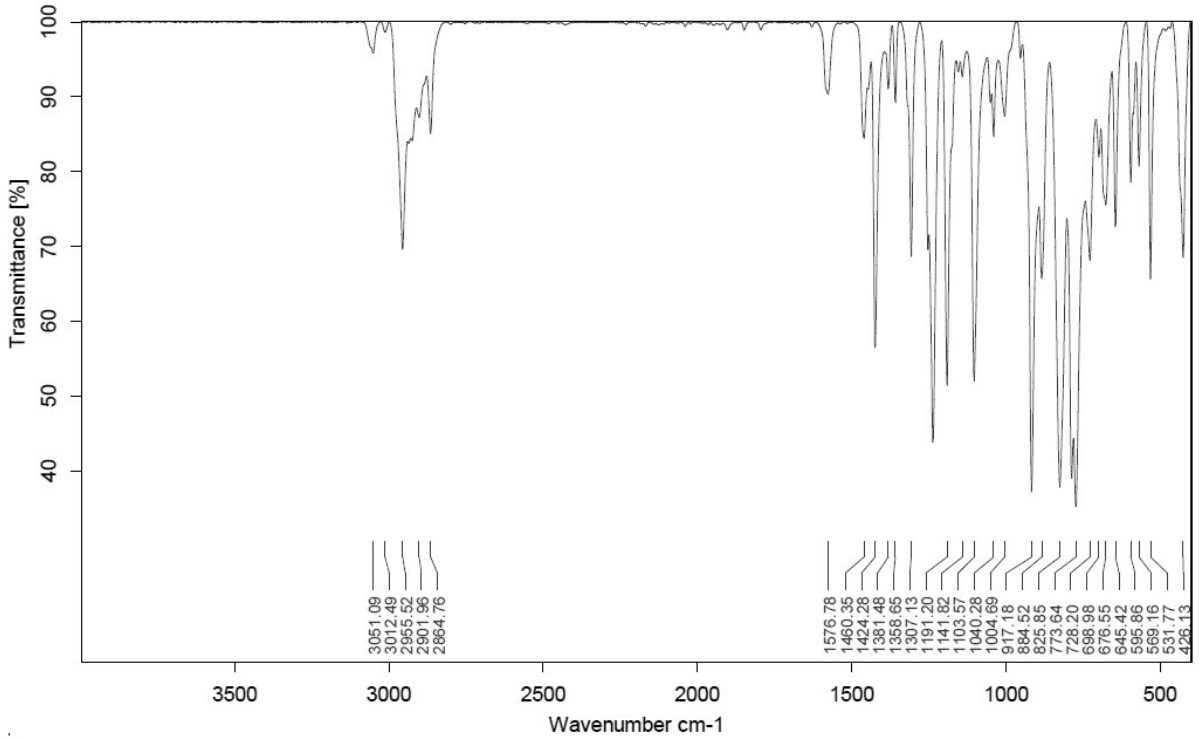

Figure S70. IR spectrum of **[FeL$^4_2$]**.

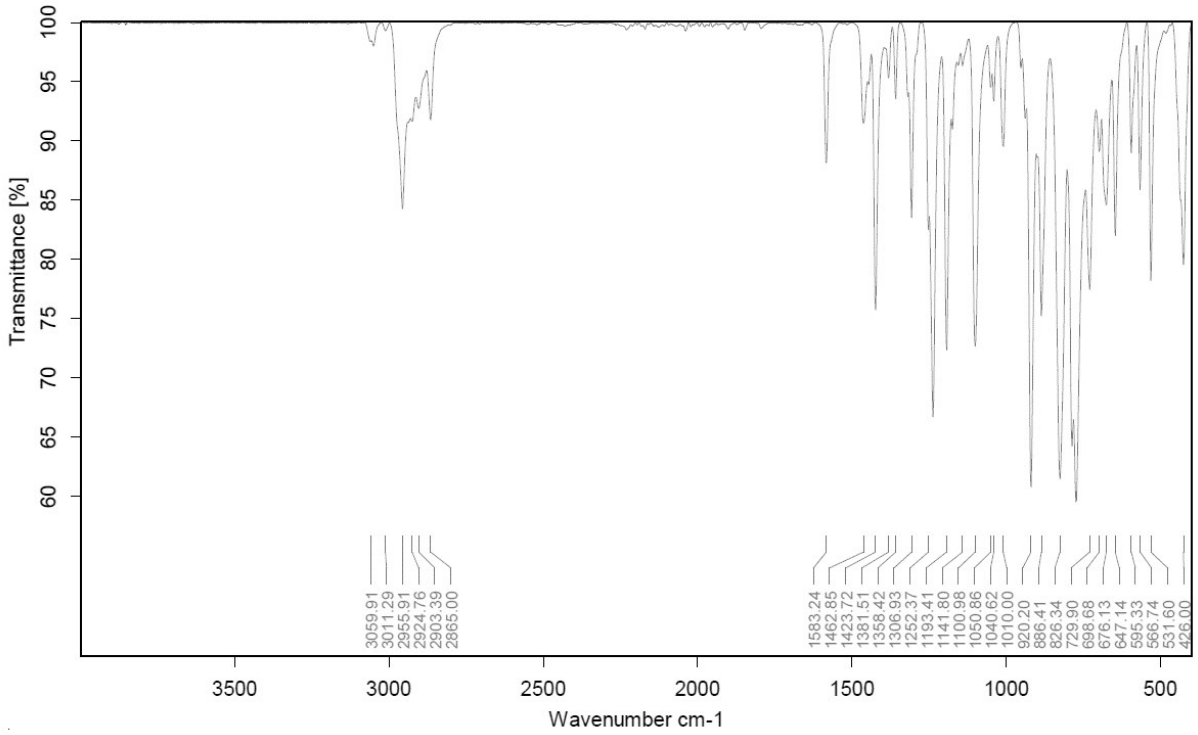

Figure S71. IR spectrum of **[CoL$^4_2$]**.

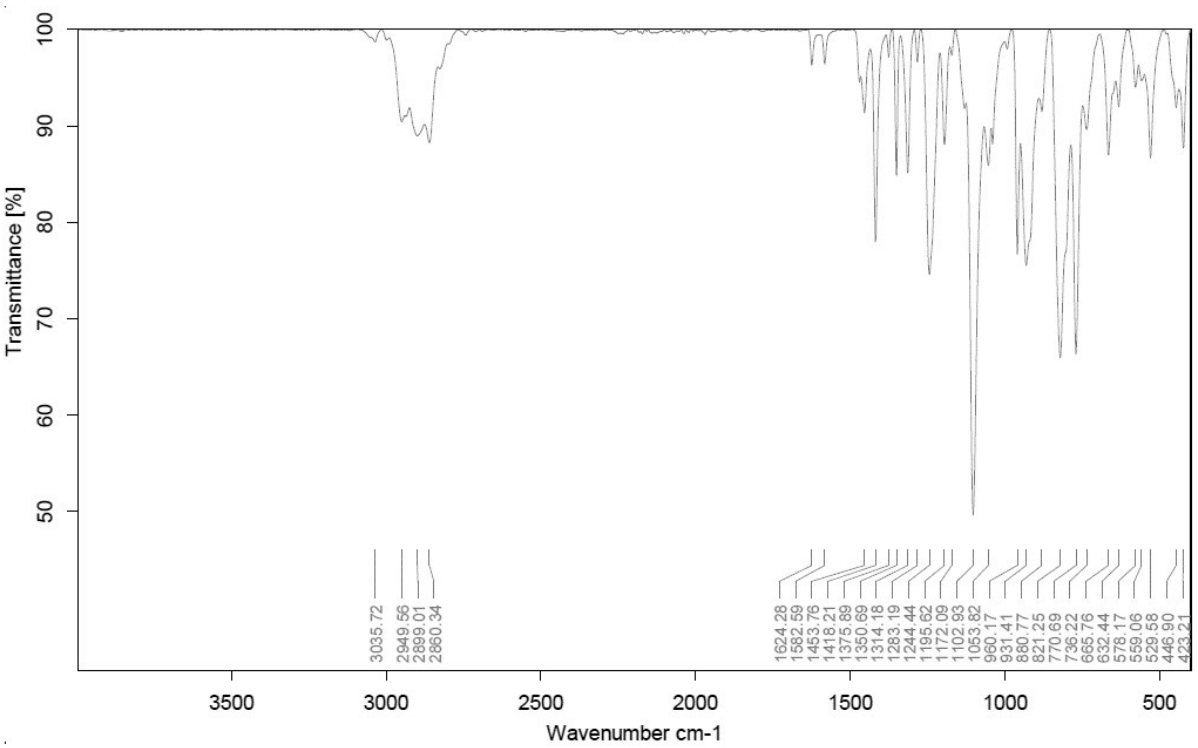

Figure S72. IR spectrum of (K{18c6})$_2$**[CrL$^4_2$]$_2$**.

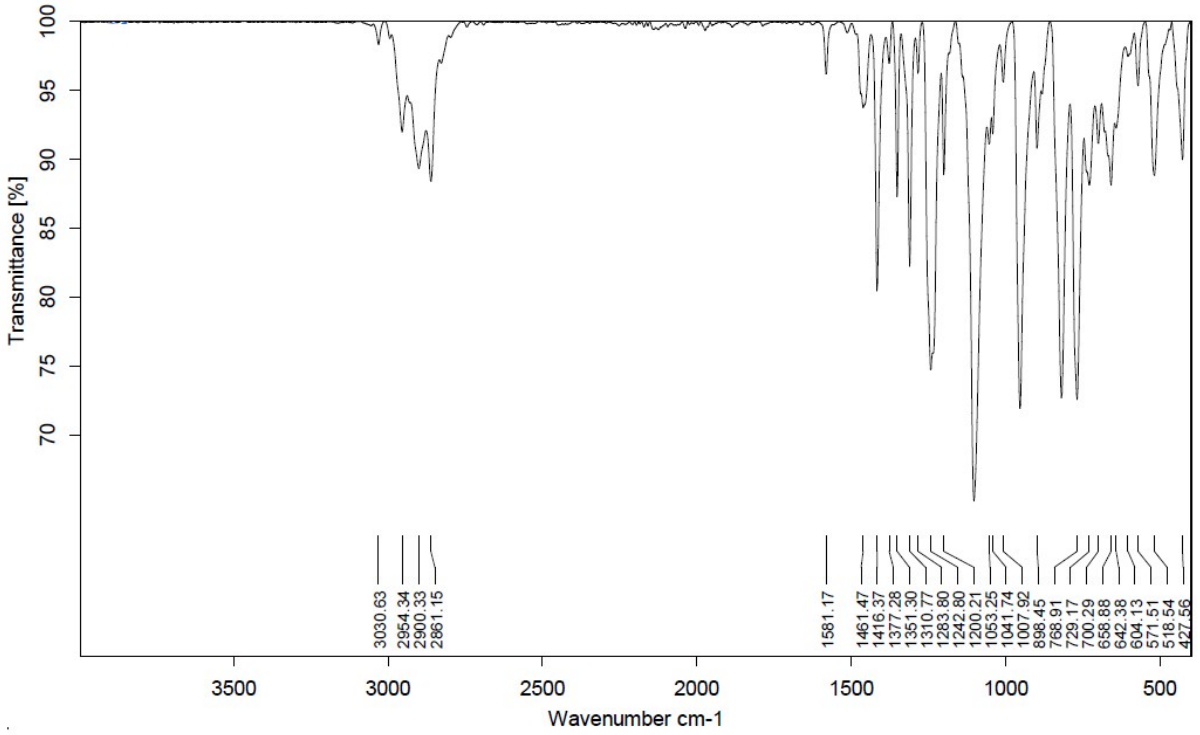

Figure S73. IR spectrum of K{18c6}**[CoL$^4_2$]**.

Imido complexes

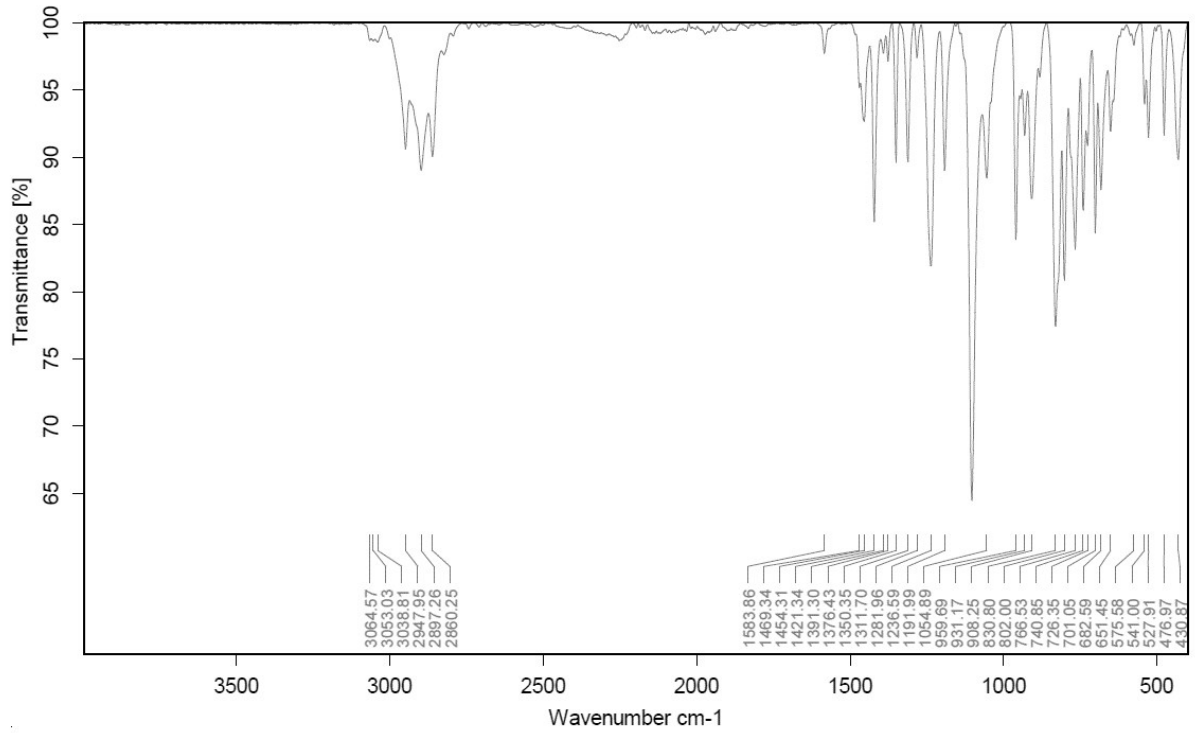

Figure S74. IR spectrum of K{18c6}**[Co(NDipp)L$^1_2$]**.

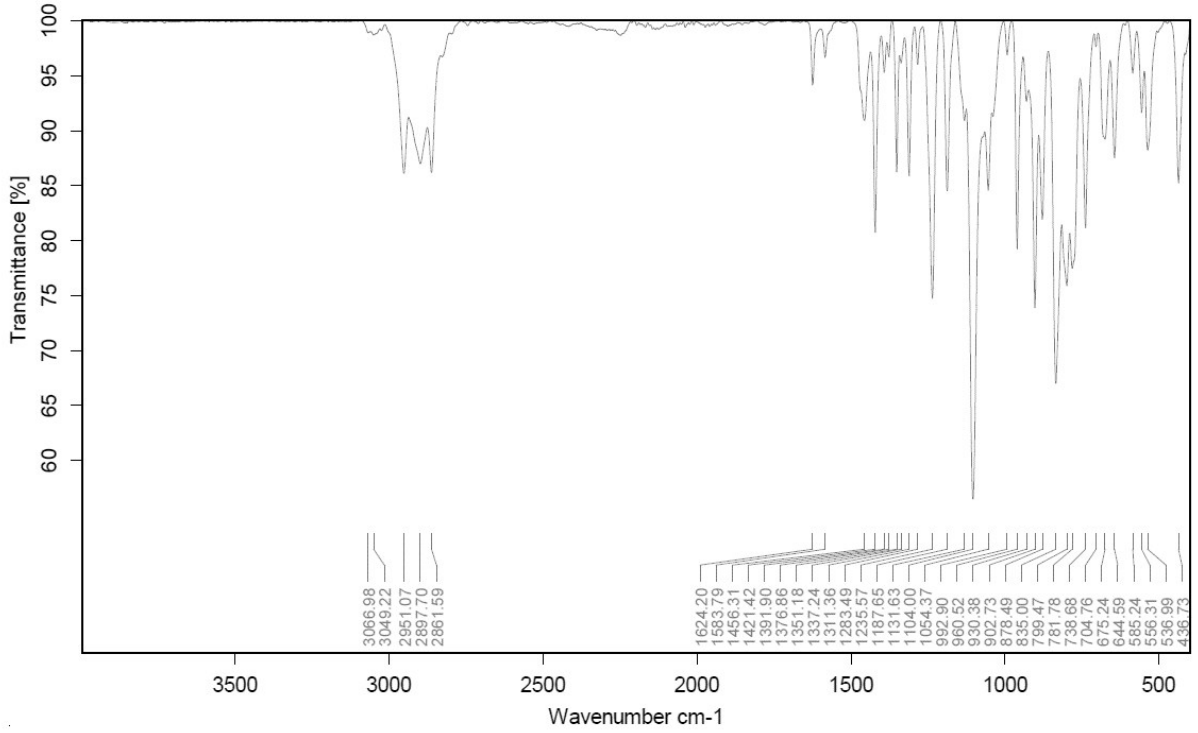

Figure S75. IR spectrum of K{18c6}**[Co(NDipp)L$^4_2$]**.

4 X-Ray Diffraction Analysis and Molecular Structures

−N(Dipp)SiMe$_2$Ph (L^1) containing compounds

Table S1. Crystal data and structure refinement of **LiL^1**

Empirical formula	$C_{40}H_{56}Li_2N_2Si_2$
Formula weight	634.92
Temperature /K	100.0
Crystal system	monoclinic
Space group	$P2_1/n$
a /Å	11.4917(10)
b /Å	12.5476(17)
c /Å	12.9022(11)
α /°	90
β /°	92.171(7)
γ /°	90
Volume /Å^3	1859.1(3)
Z	2
ρ_{calc} /g·cm^3	1.134
μ /mm^{-1}	0.125
F(000)	688.0
Crystal size /mm^3	0.931 × 0.293 × 0.188
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.808 to 53.434
Index ranges	−13 ≤ *h* ≤ 14, −15 ≤ *k* ≤ 15, −15 ≤ *l* ≤ 16
Reflections collected	16372
Independent reflections	3939 [R_{int} = 0.0744, R_{sigma} = 0.0671]
Data/restraints/parameters	3939/0/320
Goodness-of-fit on F^2	0.899
Final *R* indexes [*I*>=2σ (*I*)]	R_1 = 0.0377, wR_2 = 0.0812
Final *R* indexes [all data]	R_1 = 0.0700, wR_2 = 0.0886
Largest diff. peak/hole / e Å^{-3}	0.30/−0.22

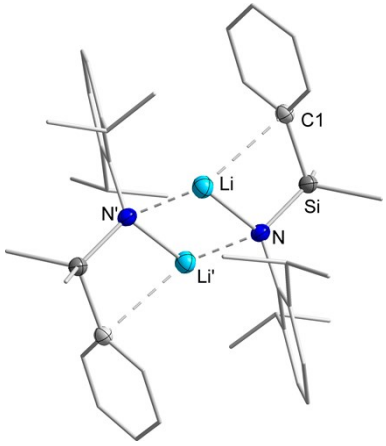

Figure S76. Molecular structure of (**LiL^1**)$_2$. All hydrogen atoms are omitted for clarity.

Table S2. Crystal data and structure refinement of **[MnL$^1_2$]**

Empirical formula	$C_{40}H_{56}MnN_2Si_2$
Formula weight	675.98
Temperature /K	100
Crystal system	triclinic
Space group	P−1
a /Å	11.5053(6)
b /Å	19.5096(13)
c /Å	19.5355(11)
α /°	117.392(4)
β /°	97.873(4)
γ /°	90.877(5)
Volume /Å^3	3841.3(4)
Z	4
ρ_{calc} /g·cm^3	1.169
μ /mm^{-1}	0.435
F(000)	1452.0
Crystal size /mm^3	0.413 × 0.199 × 0.144
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.008 to 54.178
Index ranges	−14 ≤ *h* ≤ 13, −24 ≤ *k* ≤ 24, −24 ≤ *l* ≤ 24
Reflections collected	38338
Independent reflections	38338 [R_{int} = 0.2443, R_{sigma} = 0.1343]
Data/restraints/parameters	38338/0/836
Goodness-of-fit on F^2	0.911
Final *R* indexes [*I*>=2σ (*I*)]	R_1 = 0.0633, wR_2 = 0.1460
Final *R* indexes [all data]	R_1 = 0.1521, wR_2 = 0.1750
Largest diff. peak/hole / e Å^{-3}	0.63/−0.86

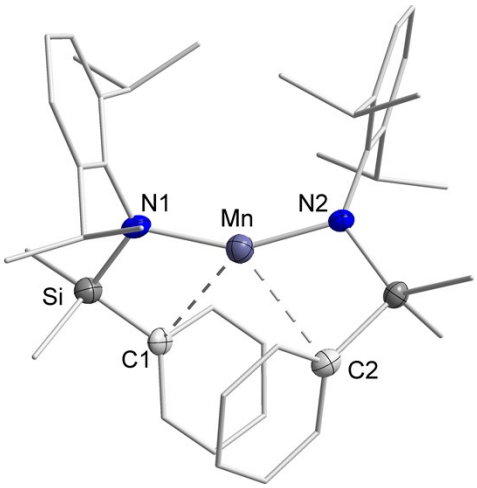

Figure S77. Molecular structure of **[MnL$^1_2$]**. All hydrogen atoms and a second, independent molecule are omitted for clarity. The structure was refined as a twin, twin ratio refined to 0.2465(8).

Table S3. Crystal data and structure refinement of **[FeL$^1_2$]**

Empirical formula	$C_{80}H_{112}Fe_2N_4Si_4$
Formula weight	1353.79
Temperature /K	100.01
Crystal system	triclinic
Space group	P−1
a /Å	11.4603(5)
b /Å	19.4567(9)
c /Å	19.5695(9)
α /°	117.2580(10)
β /°	90.819(2)
γ /°	97.965(2)
Volume /Å^3	3826.6(3)
Z	2
ρ_{calc} /g·cm^3	1.175
μ /mm^{-1}	0.485
F(000)	1456.0
Crystal size /mm^3	0.262 × 0.186 × 0.124
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.054 to 54.578
Index ranges	−14 ≤ *h* ≤ 14, −25 ≤ *k* ≤ 25, −24 ≤ *l* ≤ 25
Reflections collected	73224
Independent reflections	17162 [R_{int} = 0.0571, R_{sigma} = 0.0531]
Data/restraints/parameters	17162/0/835
Goodness-of-fit on F^2	1.038
Final *R* indexes [*I*>=2σ (*I*)]	R_1 = 0.0408, wR_2 = 0.0755
Final *R* indexes [all data]	R_1 = 0.0686, wR_2 = 0.0838
Largest diff. peak/hole / e Å^{-3}	0.35/−0.30

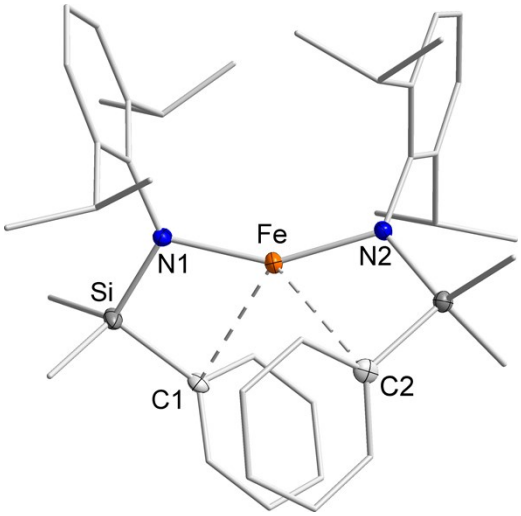

Figure S78. Molecular structure of **[FeL$^1_2$]**. All hydrogen atoms and a second, independent molecule are omitted for clarity.

Table S4. Crystal data and structure refinement of **[CoL$^1_2$]**

Empirical formula	$C_{40}H_{56}CoN_2Si_2$
Formula weight	680.008
Temperature/K	99.96
Crystal system	triclinic
Space group	P−1
a/Å	11.5124(5)
b/Å	19.4083(8)
c/Å	19.4427(8)
α/°	116.737(1)
β/°	98.024(1)
γ/°	91.028(2)
Volume/Å^3	3825.7(3)
Z	4
ρ_{calc}g/cm^3	1.181
μ/mm^{-1}	0.540
F(000)	1462.5
Crystal size/mm^3	0.486 × 0.213 × 0.192
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.24 to 58.5
Index ranges	−15 ≤ *h* ≤ 15, −26 ≤ *k* ≤ 26, −26 ≤ *l* ≤ 25
Reflections collected	75032
Independent reflections	19910 [R_{int} = 0.0525, R_{sigma} = 0.0618]
Data/restraints/parameters	19910/0/885
Goodness-of-fit on F^2	1.053
Final *R* indexes [*I*>=2σ (*I*)]	R_1 = 0.0456, wR_2 = 0.0801
Final *R* indexes [all data]	R_1 = 0.0844, wR_2 = 0.0924
Largest diff. peak/hole / e Å^{-3}	0.63/−0.66

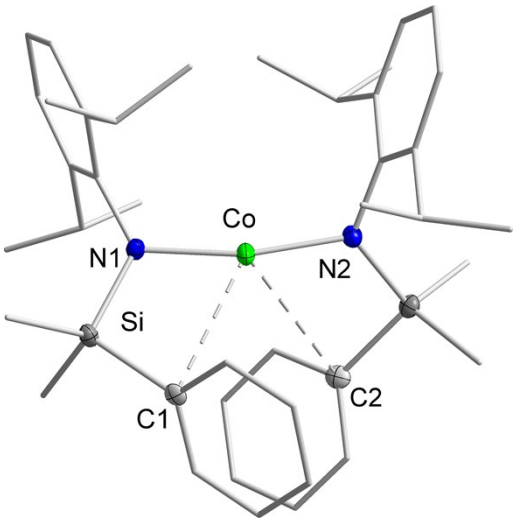

Figure S79. Molecular structure of **[CoL$^1_2$]**. All hydrogen atoms and a second, independent molecule are omitted for clarity.

Table S5. Crystal data and structure refinement of K{18c6}**[MnL^{1}L^{1*}]**

Empirical formula	$C_{52}H_{79}KMnN_2O_6Si_2$
Formula weight	978.39
Temperature/K	100
Crystal system	monoclinic
Space group	Pn
a/Å	13.0249(6)
b/Å	14.7896(6)
c/Å	14.3462(6)
α/°	90
β/°	101.315(2)
γ/°	90
Volume/Å^3	2709.8(2)
Z	2
ρ_{calc}g/cm^3	1.199
μ/mm^{-1}	3.457
F(000)	1050.0
Crystal size/mm^3	0.212 × 0.134 × 0.115
Radiation	Cu Kα (λ = 1.54186)
2Θ range for data collection/°	5.976 to 151.934
Index ranges	−14 ≤ *h* ≤ 16, −18 ≤ *k* ≤ 16, −18 ≤ *l* ≤ 14
Reflections collected	33826
Independent reflections	11326 [R_{int} = 0.0421, R_{sigma} = 0.0412]
Data/restraints/parameters	11326/3659/1058
Goodness-of-fit on F^2	0.945
Final *R* indexes [*I*>=2σ (*I*)]	R_1 = 0.0484, wR_2 = 0.1211
Final *R* indexes [all data]	R_1 = 0.0812, wR_2 = 0.1371
Largest diff. peak/hole / e Å^{-3}	0.24/−0.23
Flack parameter	0.529(12)

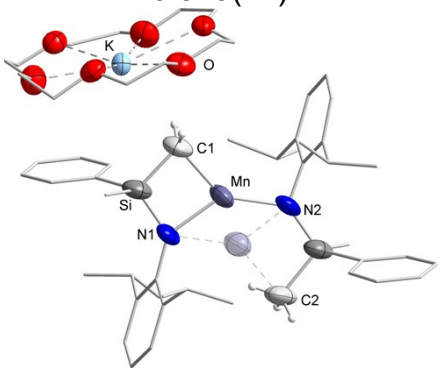

Figure S80. Molecular structure of K{18c6}**[MnL^{1}L^{1*}]**. Unnecessary hydrogen atoms are omitted for clarity. The structure was refined as a twin, twin ratio refined to 0.529(12). Disorders were found for all atoms with different occupancies (anion: part 1 (depicted): 69%; part 2 (indicated for Mn): 31%; K{18c6}: both part 3 (depicted) / 4: 50%)

Table S6. Crystal data and structure refinement of K{18c6}**[FeL$^1_2$]**

Empirical formula	$C_{56}H_{90}FeKN_2O_7Si_2$
Formula weight	1054.42
Temperature /K	100.0
Crystal system	triclinic
Space group	P−1
a /Å	18.141(2)
b /Å	19.9930(19)
c /Å	20.561(2)
α /°	60.863(7)
β /°	66.609(9)
γ /°	79.327(9)
Volume /Å^3	5977.9(13)
Z	4
ρ_{calc} /g·cm^3	1.172
μ /mm^{-1}	0.410
F(000)	2276.0
Crystal size /mm^3	0.702 × 0.604 × 0.161
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.894 to 50
Index ranges	−21 ≤ *h* ≤ 21, −23 ≤ *k* ≤ 23, −24 ≤ *l* ≤ 22
Reflections collected	41617
Independent reflections	20923 [R_{int} = 0.0650, R_{sigma} = 0.0742]
Data/restraints/parameters	20923/174/1394
Goodness-of-fit on F^2	1.042
Final *R* indexes [*I*>=2σ (*I*)]	R_1 = 0.0773, wR_2 = 0.2276
Final *R* indexes [all data]	R_1 = 0.1104, wR_2 = 0.2420
Largest diff. peak/hole / e Å^{-3}	0.98/−0.53

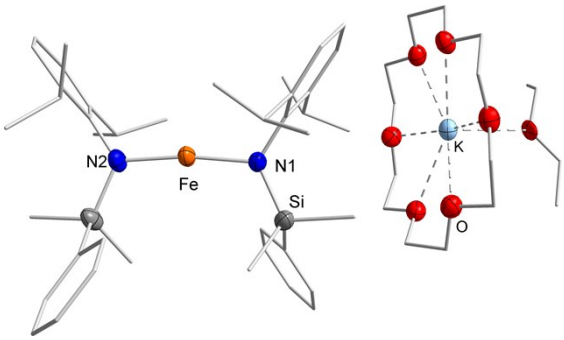

Figure S81. Molecular structure of K{18c6}**[FeL$^1_2$]**. All hydrogen atoms and a second, independent molecule with disorders in two phenyl rings and two *iso*-propyl groups (all parts: 50%) are omitted for clarity. A disorder in the Et_2O molecule (part 1 (depicted): 70%; part 2: 30%) is found. The dataset is based on a measurement comprising approximately 75% data for the crystal presented here + 25% data from other individuums, which could not be indexed. Partial reflection overlap of the parasitic scattering leads to a high wR_2 value.

Table S7. Crystal data and structure refinement of K{18c6}**[CoL$^1_2$]**

Empirical formula	$C_{52}H_{80}CoKN_2O_6Si_2$
Formula weight	983.39
Temperature /K	100.0
Crystal system	triclinic
Space group	P−1
a /Å	10.688(2)
b /Å	15.427(3)
c /Å	17.610(4)
α /°	85.095(6)
β /°	75.862(6)
γ /°	77.123(6)
Volume /Å^3	2743.5(10)
Z	2
ρ_{calc} /g·cm^3	1.190
μ /mm^{-1}	0.478
F(000)	1056.0
Crystal size /mm^3	0.62 × 0.274 × 0.124
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.172 to 49.998
Index ranges	−12 ≤ *h* ≤ 12, −18 ≤ *k* ≤ 16, −20 ≤ *l* ≤ 20
Reflections collected	29137
Independent reflections	9518 [R_{int} = 0.1123, R_{sigma} = 0.1104]
Data/restraints/parameters	9518/6/599
Goodness-of-fit on F^2	1.050
Final *R* indexes [*I*>=2σ (*I*)]	R_1 = 0.0683, wR_2 = 0.1386
Final *R* indexes [all data]	R_1 = 0.1335, wR_2 = 0.1551
Largest diff. peak/hole / e Å^{-3}	0.65/−0.43

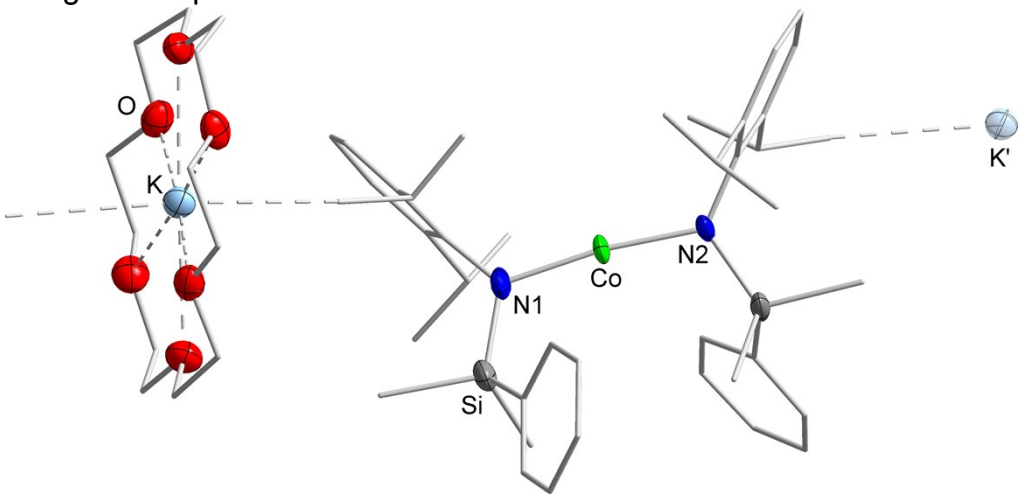

Figure S82. Molecular structure of K{18c6}**[CoL$^1_2$]**. All hydrogen atoms are omitted for clarity. A disorder in one methyl group (part 1 (depicted): 30%; part 2: 70%) is found.

−N(Dipp)SiMePh$_2$ (L^2) containing compounds

Table S8. Crystal data and structure refinement of **LiL^2**

Empirical formula	$C_{37}H_{54}LiNO_3Si$
Formula weight	595.84
Temperature /K	100.0
Crystal system	triclinic
Space group	P1
a /Å	10.0915(5)
b /Å	10.2440(5)
c /Å	17.2833(9)
α /°	87.900(2)
β /°	86.203(2)
γ /°	76.965(2)
Volume /Å^3	1736.41(15)
Z	2
ρ_{calc} /g·cm^3	1.140
μ /mm^{-1}	0.102
F(000)	648.0
Crystal size /mm^3	0.412 × 0.36 × 0.176
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.082 to 58.948
Index ranges	−13 ≤ *h* ≤ 13, −14 ≤ *k* ≤ 14, −23 ≤ *l* ≤ 23
Reflections collected	101241
Independent reflections	18604 [R_{int} = 0.0344, R_{sigma} = 0.0281]
Data/restraints/parameters	18604/3/803
Goodness-of-fit on F^2	1.047
Final *R* indexes [*I*>=2σ (*I*)]	R_1 = 0.0373, wR_2 = 0.0926
Final *R* indexes [all data]	R_1 = 0.0423, wR_2 = 0.0952
Largest diff. peak/hole / e Å^{-3}	0.76/−0.41
Flack parameter	0.001(15)

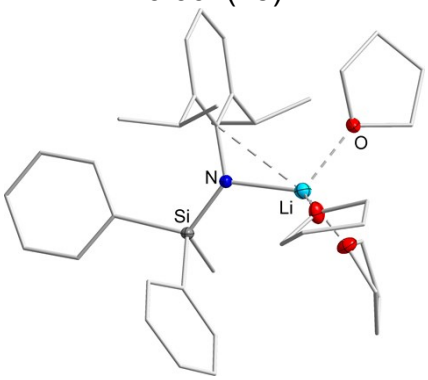

Figure S83. Molecular structure of **LiL^2**. All hydrogen atoms and a second, independent molecule with a disorder in one THF molecule (part 1: 70%; part 2: 30%) are omitted for clarity.

Table S9. Crystal data and structure refinement of **[CrL$^2_2$]**

Empirical formula	$C_{50}H_{60}Cr_{0.82}Li_{0.35}N_2Si_2$
Formula weight	790.51
Temperature /K	100.0
Crystal system	triclinic
Space group	P−1
a /Å	11.8650(11)
b /Å	12.9730(13)
c /Å	16.4026(16)
α /°	84.911(8)
β /°	88.653(8)
γ /°	68.582(7)
Volume /Å^3	2341.0(4)
Z	2
ρ_{calc} /g·cm^3	1.121
μ /mm^{-1}	0.291
F(000)	846.0
Crystal size /mm^3	0.233 × 0.203 × 0.121
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.986 to 53.542
Index ranges	−14 ≤ *h* ≤ 14, −14 ≤ *k* ≤ 16, −20 ≤ *l* ≤ 20
Reflections collected	20595
Independent reflections	9847 [R_{int} = 0.0399, R_{sigma} = 0.0426]
Data/restraints/parameters	9847/53/612
Goodness-of-fit on F^2	1.068
Final *R* indexes [*I*>=2σ (*I*)]	R_1 = 0.0337, wR_2 = 0.0822
Final *R* indexes [all data]	R_1 = 0.0506, wR_2 = 0.0863
Largest diff. peak/hole / e Å^{-3}	0.37/−0.30

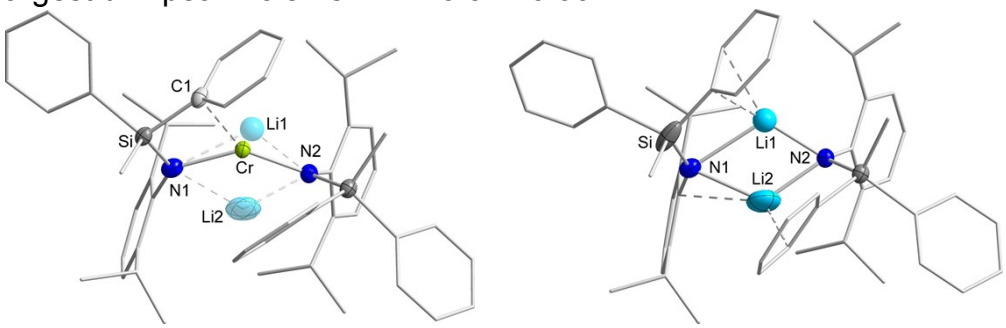

Figure S84. Molecular structure of **[CrL$^2_2$]** (left). All hydrogen atoms are omitted for clarity. One free *n*-pentane molecule is disordered over multiple positions on a symmetry element and has thus been squeezed. A disorder in one $SiMePh_2$ fragment and one phenyl group (part 1 (depicted): 83%; part 2: 17%) is found. Additionally, the chromium atom is only present in part 1 (83%), while co-crystallized dimeric $(LiL^2)_2$ is present in part 2 (17%, left: indicated; right: isolated). Due to its proximity to the chromium atom, Li1 could not be modelled anisotropically.

−N(Dipp)SiPh$_3$ (L^3) containing compounds

Table S10. Crystal data and structure refinement of **HL^3**

Empirical formula	$C_{60}H_{66}N_2Si_2$
Formula weight	871.32
Temperature /K	100.0
Crystal system	monoclinic
Space group	$P2_1$
a /Å	10.9870(13)
b /Å	8.9441(7)
c /Å	12.9460(13)
α /°	90
β /°	93.863(9)
γ /°	90
Volume /Å^3	1269.3(2)
Z	1
ρ_{calc} /g·cm^3	1.140
μ /mm^{-1}	0.110
F(000)	468.0
Crystal size /mm^3	0.543 × 0.46 × 0.157
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.034 to 53.616
Index ranges	−13 ≤ *h* ≤ 13, −10 ≤ *k* ≤ 11, −16 ≤ *l* ≤ 16
Reflections collected	11229
Independent reflections	5138 [R_{int} = 0.0319, R_{sigma} = 0.0294]
Data/restraints/parameters	5138/1/297
Goodness-of-fit on F^2	1.023
Final *R* indexes [*I*>=2σ (*I*)]	R_1 = 0.0319, wR_2 = 0.0811
Final *R* indexes [all data]	R_1 = 0.0365, wR_2 = 0.0826
Largest diff. peak/hole / e Å^{-3}	0.28/−0.15
Flack parameter	0.00(4)

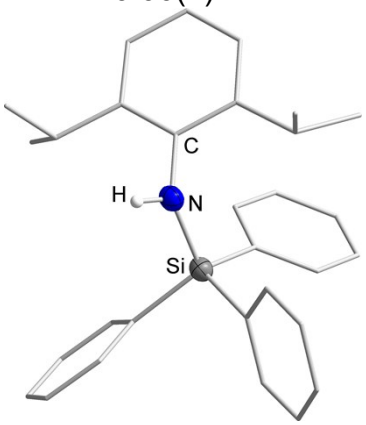

Figure S85. Molecular structure of **HL^3**. Unnecessary hydrogen atoms are omitted for clarity.

Table S11. Crystal data and structure refinement of **LiL^3**

Empirical formula	$C_{38}H_{48}LiNO_2Si$
Formula weight	585.80
Temperature /K	100.0
Crystal system	orthorhombic
Space group	Pbca
a /Å	10.6101(7)
b /Å	16.8895(10)
c /Å	38.289(3)
α /°	90
β /°	90
γ /°	90
Volume /Å^3	6861.3(8)
Z	8
ρ_{calc} /g·cm^3	1.134
μ /mm^{-1}	0.101
F(000)	2528.0
Crystal size /mm^3	0.288 × 0.192 × 0.181
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.656 to 53.492
Index ranges	−13 ≤ *h* ≤ 13, −21 ≤ *k* ≤ 20, −48 ≤ *l* ≤ 48
Reflections collected	55029
Independent reflections	7263 [R_{int} = 0.1141, R_{sigma} = 0.1028]
Data/restraints/parameters	7263/0/404
Goodness-of-fit on F^2	0.797
Final *R* indexes [*I*>=2σ (*I*)]	R_1 = 0.0379, wR_2 = 0.0819
Final *R* indexes [all data]	R_1 = 0.0958, wR_2 = 0.0892
Largest diff. peak/hole / e Å^{-3}	0.25/−0.24

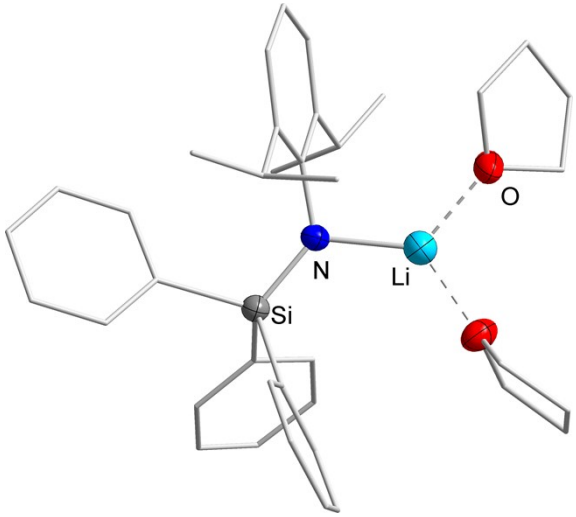

Figure S86. Molecular structure of **LiL^3**. All hydrogen atoms are omitted for clarity. A disorder in one THF molecule (both part 1 (depicted) / 2: 50%) is found.

Table S12. Crystal data and structure refinement of **LiL³**

Empirical formula	$C_{38}H_{48}LiNO_2Si$
Formula weight	585.80
Temperature /K	100.0
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a /Å	9.750(3)
b /Å	15.312(5)
c /Å	45.002(11)
α /°	90
β /°	90
γ /°	90
Volume /Å³	6719(3)
Z	8
ρ_{calc} /g·cm³	1.158
μ /mm⁻¹	0.103
F(000)	2528.0
Crystal size /mm³	0.287 × 0.155 × 0.11
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.552 to 52.13
Index ranges	−12 ≤ *h* ≤ 12, −18 ≤ *k* ≤ 18, −55 ≤ *l* ≤ 55
Reflections collected	97307
Independent reflections	13263 [R_{int} = 0.0433, R_{sigma} = 0.0272]
Data/restraints/parameters	13263/0/810
Goodness-of-fit on F^2	1.073
Final *R* indexes [*I*>=2σ (*I*)]	R_1 = 0.0405, wR_2 = 0.0950
Final *R* indexes [all data]	R_1 = 0.0459, wR_2 = 0.0975
Largest diff. peak/hole / e Å⁻³	0.53/−0.25
Flack parameter	0.00(2)

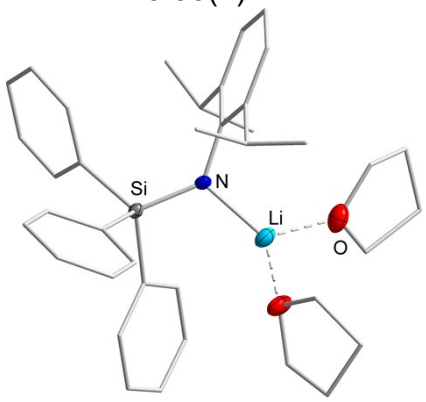

Figure S87. Molecular structure of **LiL³**. All hydrogen atoms and a second, independent molecule with a disorder in one THF molecule (part 1: 70%; part 2: 30%) are omitted for clarity. A disorder in one THF molecule (both part 1 (depicted) / 2: 50%) is found.

Table S13. Crystal data and structure refinement of **[FeL$^3_2$]**

Empirical formula	$C_{60}H_{64}FeN_2Si_2$
Formula weight	925.16
Temperature /K	99.99
Crystal system	triclinic
Space group	P−1
a /Å	12.2746(11)
b /Å	13.7722(10)
c /Å	17.6349(11)
α /°	72.165(2)
β /°	88.812(2)
γ /°	86.503(2)
Volume /Å^3	2832.6(4)
Z	2
ρ_{calc} /g·cm^3	1.085
μ /mm^{-1}	0.344
F(000)	984.0
Crystal size /mm^3	0.167 × 0.104 × 0.068
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.422 to 49.998
Index ranges	−14 ≤ *h* ≤ 14, −16 ≤ *k* ≤ 16, −20 ≤ *l* ≤ 20
Reflections collected	66757
Independent reflections	9966 [R_{int} = 0.1147, R_{sigma} = 0.0766]
Data/restraints/parameters	9966/18/588
Goodness-of-fit on F^2	1.081
Final *R* indexes [*I*>=2σ (*I*)]	R_1 = 0.0584, wR_2 = 0.1302
Final *R* indexes [all data]	R_1 = 0.0930, wR_2 = 0.1391
Largest diff. peak/hole / e Å^{-3}	0.77/−0.82

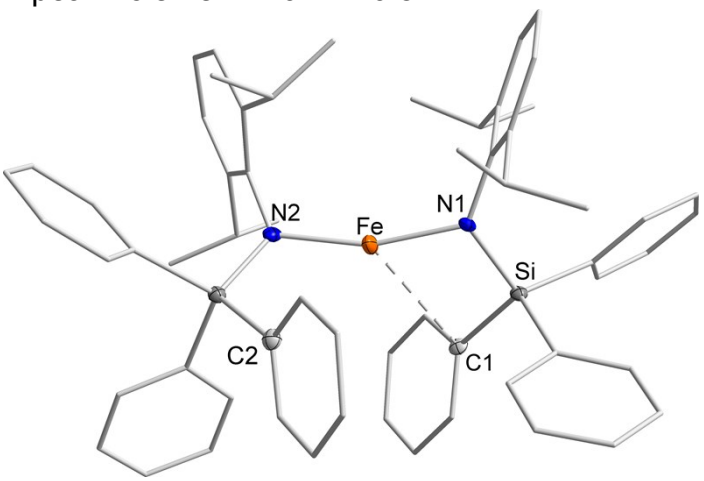

Figure S88. Molecular structure of **[FeL$^3_2$]**. All hydrogen atoms are omitted for clarity. One free *n*-pentane molecule is disordered over multiple positions and has thus been squeezed.

Table S14. Crystal data and structure refinement of K{18c6}**[FeL$^3_2$]**

Empirical formula	$C_{80}H_{104}FeKN_2O_8Si_2$
Formula weight	1372.78
Temperature /K	100.0
Crystal system	triclinic
Space group	P−1
a /Å	12.5267(8)
b /Å	13.5299(9)
c /Å	24.9620(15)
α /°	79.978(2)
β /°	88.219(2)
γ /°	73.252(2)
Volume /Å^3	3988.6(4)
Z	2
ρ_{calc} /g·cm^3	1.143
μ /mm^{-1}	0.323
F(000)	1470.0
Crystal size /mm^3	0.263 × 0.243 × 0.144
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.808 to 50
Index ranges	−14 ≤ *h* ≤ 14, −16 ≤ *k* ≤ 16, −29 ≤ *l* ≤ 29
Reflections collected	54903
Independent reflections	14023 [R_{int} = 0.0870, R_{sigma} = 0.1105]
Data/restraints/parameters	14023/186/903
Goodness-of-fit on F^2	1.037
Final *R* indexes [*I*>=2σ (*I*)]	R_1 = 0.0713, wR_2 = 0.1399
Final *R* indexes [all data]	R_1 = 0.1203, wR_2 = 0.1515
Largest diff. peak/hole / e Å^{-3}	0.44/−0.49

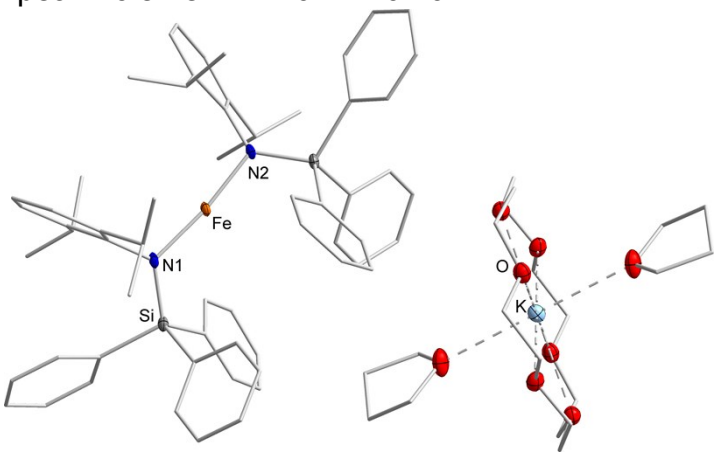

Figure S89. Molecular structure of K{18c6}**[FeL$^3_2$]**. All hydrogen atoms are omitted for clarity. One free *n*-pentane molecule is disordered over multiple positions and has thus been squeezed. A disorder in the THF molecule (both part 1 (depicted) / part 2: 50%) is found.

−N(Dipp)SiMe$_2$(allyl) (L^4) containing compounds

Table S15. Crystal data and structure refinement of **[CrL$^4_2$]**

Empirical formula	$C_{34}H_{56}CrN_2Si_2$
Formula weight	600.98
Temperature /K	100.0
Crystal system	triclinic
Space group	P−1
a /Å	9.5587(5)
b /Å	12.8751(7)
c /Å	16.1547(8)
α /°	67.981(2)
β /°	86.382(2)
γ /°	70.002(2)
Volume /Å^3	1727.15(16)
Z	2
ρ_{calc} /g·cm^3	1.156
μ /mm^{-1}	0.424
F(000)	652.0
Crystal size /mm^3	0.445 × 0.226 × 0.206
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.548 to 56.518
Index ranges	−12 ≤ *h* ≤ 12, −16 ≤ *k* ≤ 17, −21 ≤ *l* ≤ 21
Reflections collected	26070
Independent reflections	8502 [R_{int} = 0.0302, R_{sigma} = 0.0360]
Data/restraints/parameters	8502/0/380
Goodness-of-fit on F^2	1.027
Final *R* indexes [*I*>=2σ (*I*)]	R_1 = 0.0364, wR_2 = 0.0893
Final *R* indexes [all data]	R_1 = 0.0485, wR_2 = 0.0957
Largest diff. peak/hole / e Å^{-3}	0.53/−0.51

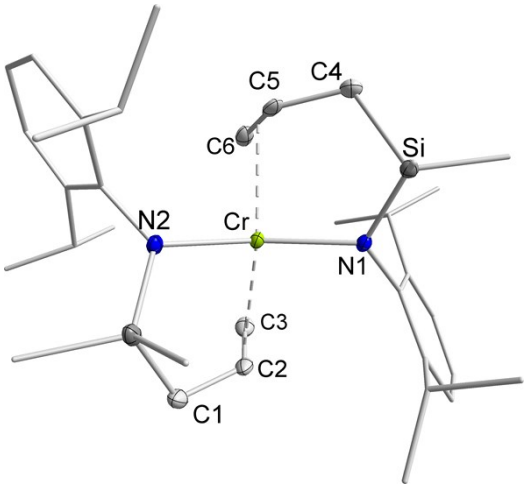

Figure S90. Molecular structure of **[CrL$^4_2$]**. All hydrogen atoms are omitted for clarity.

Table S16. Crystal data and structure refinement of **[MnL$^4_2$]**

Empirical formula	$C_{34}H_{56}MnN_2Si_2$
Formula weight	603.92
Temperature /K	100.0
Crystal system	monoclinic
Space group	$P2_1/n$
a /Å	15.9153(12)
b /Å	13.0196(8)
c /Å	17.0810(16)
α /°	90
β /°	97.079(7)
γ /°	90
Volume /Å^3	3512.4(5)
Z	4
ρ_{calc} /g·cm^3	1.142
μ /mm^{-1}	0.468
F(000)	1308.0
Crystal size /mm^3	0.491 × 0.029 × 0.016
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.736 to 53.5
Index ranges	−20 ≤ *h* ≤ 20, −16 ≤ *k* ≤ 16, −21 ≤ *l* ≤ 21
Reflections collected	31624
Independent reflections	7421 [R_{int} = 0.0466, R_{sigma} = 0.0466]
Data/restraints/parameters	7421/0/372
Goodness-of-fit on F^2	0.941
Final *R* indexes [*I*>=2σ (*I*)]	R_1 = 0.0357, wR_2 = 0.0830
Final *R* indexes [all data]	R_1 = 0.0603, wR_2 = 0.0892
Largest diff. peak/hole / e Å^{-3}	0.36/−0.27

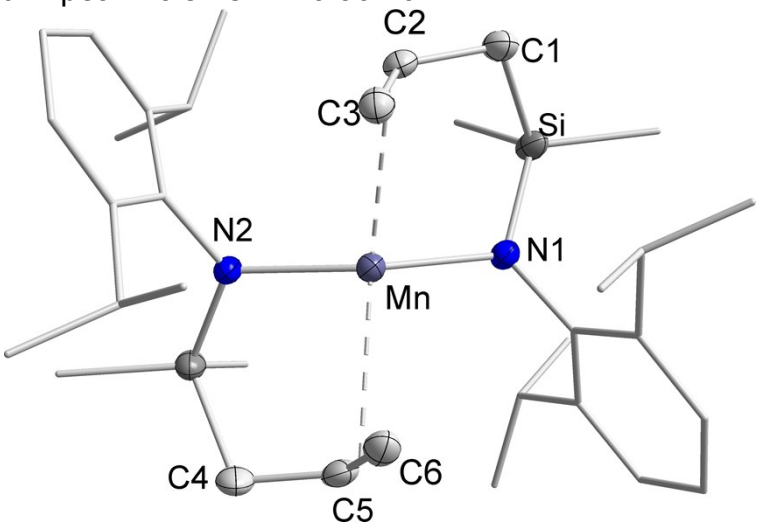

Figure S91. Molecular structure of **[MnL$^4_2$]**. All hydrogen atoms are omitted for clarity.

Table S17. Crystal data and structure refinement of **[FeL$^4_2$]**

Empirical formula	$C_{34}H_{56}FeN_2Si_2$
Formula weight	604.83
Temperature /K	99.99
Crystal system	monoclinic
Space group	$P2_1/n$
a /Å	15.7788(7)
b /Å	13.0161(6)
c /Å	17.0238(8)
α /°	90
β /°	97.370(2)
γ /°	90
Volume /Å^3	3467.4(3)
Z	4
ρ_{calc} /g·cm^3	1.159
μ /mm^{-1}	0.528
F(000)	1312.0
Crystal size /mm^3	0.34 × 0.339 × 0.24
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.826 to 59.104
Index ranges	−21 ≤ *h* ≤ 21, −18 ≤ *k* ≤ 17, −23 ≤ *l* ≤ 23
Reflections collected	45644
Independent reflections	9681 [R_{int} = 0.0314, R_{sigma} = 0.0264]
Data/restraints/parameters	9681/0/388
Goodness-of-fit on F^2	1.020
Final *R* indexes [*I*>=2σ (*I*)]	R_1 = 0.0305, wR_2 = 0.0733
Final *R* indexes [all data]	R_1 = 0.0399, wR_2 = 0.0776
Largest diff. peak/hole / e Å^{-3}	0.41/−0.29

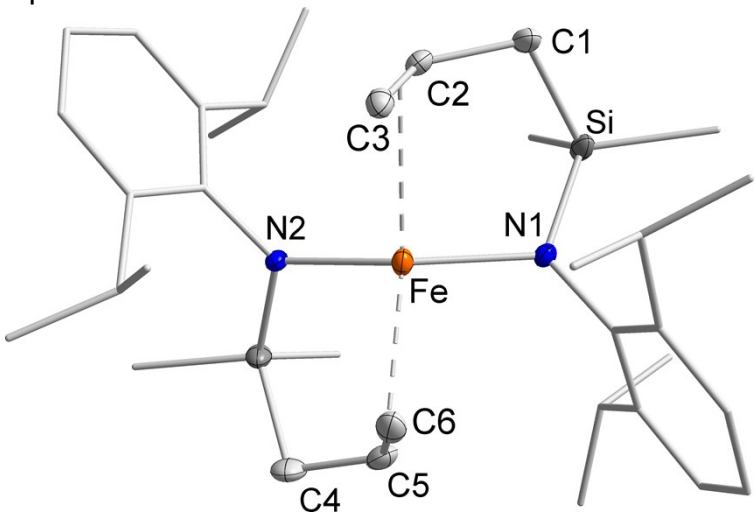

Figure S92. Molecular structure of **[FeL$^4_2$]**. All hydrogen atoms (partially disordered with both part 1 / 2: 50% due to free rotation of CH_3 fragments) are omitted for clarity.

Table S18. Crystal data and structure refinement of **[CoL$^4_2$]**

Empirical formula	$C_{34}H_{56}CoN_2Si_2$
Formula weight	607.91
Temperature /K	100.0
Crystal system	monoclinic
Space group	$P2_1/n$
a /Å	15.7778(8)
b /Å	13.0041(7)
c /Å	17.0121(9)
α /°	90
β /°	97.284(2)
γ /°	90
Volume /Å^3	3462.3(3)
Z	4
ρ_{calc} /g·cm^3	1.166
μ /mm^{-1}	0.589
F(000)	1316.0
Crystal size /mm^3	0.64 × 0.344 × 0.298
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.562 to 68.872
Index ranges	−25 ≤ *h* ≤ 25, −20 ≤ *k* ≤ 20, −27 ≤ *l* ≤ 27
Reflections collected	117460
Independent reflections	14585 [R_{int} = 0.0360, R_{sigma} = 0.0224]
Data/restraints/parameters	14585/0/404
Goodness-of-fit on F^2	1.050
Final *R* indexes [*I*>=2σ (*I*)]	R_1 = 0.0305, wR_2 = 0.0744
Final *R* indexes [all data]	R_1 = 0.0413, wR_2 = 0.0789
Largest diff. peak/hole / e Å^{-3}	0.43/−0.38

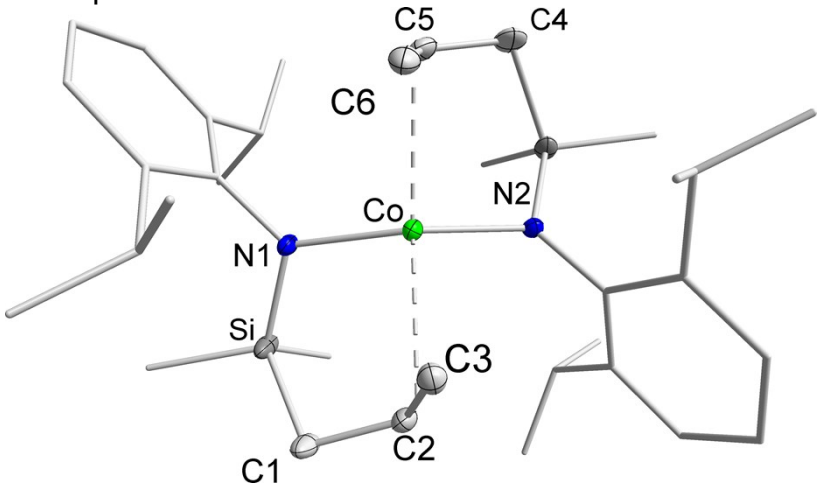

Figure S93. Molecular structure of **[CoL$^4_2$]**. All hydrogen atoms (partially disordered with both part 1 / 2: 50% due to free rotation of CH_3 fragments) are omitted for clarity.

Table S19. Crystal data and structure refinement of (K{18c6})$_2$**[CrL$^4_2$]$_2$**

Empirical formula	$C_{54}H_{94}CrKN_2O_8Si_2$
Formula weight	1046.59
Temperature /K	99.88
Crystal system	monoclinic
Space group	C2/c
a /Å	31.9234(17)
b /Å	12.8832(6)
c /Å	33.0790(16)
α /°	90
β /°	101.405(2)
γ /°	90
Volume /Å^3	13335.9(11)
Z	8
ρ_{calc} /g·cm^3	1.043
μ /mm^{-1}	0.314
F(000)	4528.0
Crystal size /mm^3	0.321 × 0.269 × 0.224
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.96 to 51.478
Index ranges	−33 ≤ *h* ≤ 38, −15 ≤ *k* ≤ 15, −40 ≤ *l* ≤ 39
Reflections collected	47610
Independent reflections	12301 [R_{int} = 0.0548, R_{sigma} = 0.0750]
Data/restraints/parameters	12301/1260/986
Goodness-of-fit on F^2	1.030
Final *R* indexes [*I*>=2σ (*I*)]	R_1 = 0.1095, wR_2 = 0.2809
Final *R* indexes [all data]	R_1 = 0.1809, wR_2 = 0.3278
Largest diff. peak/hole / e Å^{-3}	0.42/−0.45

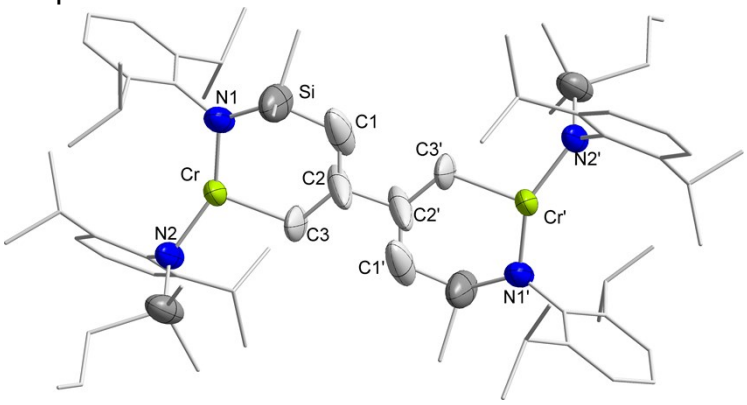

Figure S94. Anionic section of (K{18c6})$_2$**[CrL$^4_2$]$_2$**. All hydrogen atoms are omitted for clarity. The structure suffered from intrinsic crystallographic flaws, due to weakly diffracting crystals, which could not be overcome despite multiple attempts. Disorders were found for the crown ether, THF molecules, *iso*-propyl groups and the allyl moiety in different occupancies of 50% (part 1/2), 75% (part 3) or 25% (part 4/5).

Table S20. Crystal data and structure refinement of K{18c6}**[CoL$^4_2$]**

Empirical formula	$C_{46}H_{80}CoKN_2O_6Si_2$
Formula weight	911.33
Temperature /K	100.0
Crystal system	monoclinic
Space group	$P2_1/n$
a /Å	13.0369(5)
b /Å	22.1041(11)
c /Å	18.2404(7)
α /°	90
β /°	110.376(3)
γ /°	90
Volume /Å^3	4927.4(4)
Z	4
ρ_{calc} /g·cm^3	1.228
μ /mm^{-1}	0.527
F(000)	1968.0
Crystal size /mm^3	0.415 × 0.395 × 0.101
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.97 to 53.496
Index ranges	−16 ≤ *h* ≤ 16, −27 ≤ *k* ≤ 27, −23 ≤ *l* ≤ 22
Reflections collected	39565
Independent reflections	10419 [R_{int} = 0.0402, R_{sigma} = 0.0362]
Data/restraints/parameters	10419/0/574
Goodness-of-fit on F^2	1.025
Final *R* indexes [*I*>=2σ (*I*)]	R_1 = 0.0316, wR_2 = 0.0703
Final *R* indexes [all data]	R_1 = 0.0527, wR_2 = 0.0764
Largest diff. peak/hole / e Å^{-3}	0.30/−0.33

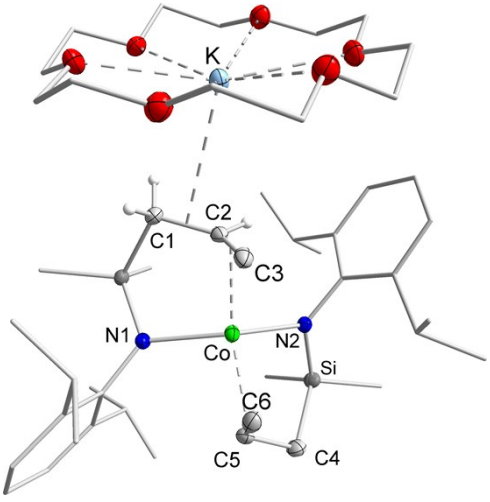

Figure S95. Molecular structure of K{18c6}**[CoL$^4_2$]**. Unnecessary hydrogen atoms are omitted for clarity.

Imido cobalt complexes

Table S21. Crystal data and structure refinement of K{18c6}**[Co(NDipp)L$^1_2$]**

Empirical formula	$C_{72}H_{113}CoKN_3O_8Si_2$
Formula weight	1302.86
Temperature /K	100.0
Crystal system	monoclinic
Space group	C2/c
a /Å	10.1708(6)
b /Å	25.7371(18)
c /Å	28.1136(15)
α /°	90
β /°	90.265(5)
γ /°	90
Volume /Å^3	7359.1(8)
Z	4
ρ_{calc} /g·cm^3	1.176
μ /mm^{-1}	0.375
F(000)	2816.0
Crystal size /mm^3	0.501 × 0.218 × 0.152
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.18 to 53.508
Index ranges	−12 ≤ *h* ≤ 12, −32 ≤ *k* ≤ 32, −35 ≤ *l* ≤ 35
Reflections collected	31700
Independent reflections	7779 [R_{int} = 0.0427, R_{sigma} = 0.0293]
Data/restraints/parameters	7779/0/422
Goodness-of-fit on F^2	1.053
Final *R* indexes [*I*>=2σ (*I*)]	R_1 = 0.0341, wR_2 = 0.0871
Final *R* indexes [all data]	R_1 = 0.0469, wR_2 = 0.0913
Largest diff. peak/hole / e Å^{-3}	0.66/−0.46

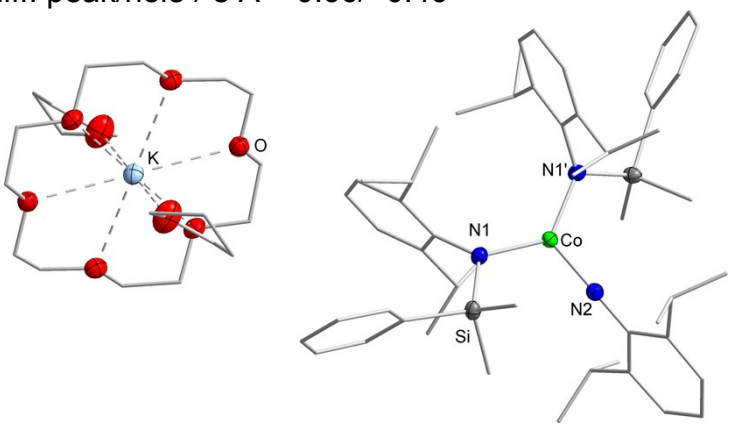

Figure S96. Molecular structure of K{18c6}**[Co(NDipp)L$^1_2$]**. All hydrogen atoms are omitted for clarity. A disorder in the THF molecule (part 1 (depicted): 75%; part 2: 25%) is omitted for clarity.

Table S22. Crystal data and structure refinement of K{18c6}**[Co(NDipp)L$^4_2$]**

Empirical formula	$C_{70}H_{121}CoKN_3O_9Si_2$
Formula weight	1302.90
Temperature /K	100.03
Crystal system	triclinic
Space group	P−1
a /Å	13.0565(5)
b /Å	15.5862(7)
c /Å	19.4665(8)
α /°	102.682(2)
β /°	100.886(2)
γ /°	94.621(2)
Volume /Å^3	3764.4(3)
Z	2
ρ_{calc} /g·cm^3	1.148
μ /mm^{-1}	0.367
F(000)	1412.0
Crystal size /mm^3	0.358 × 0.238 × 0.203
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.866 to 61.622
Index ranges	−17 ≤ *h* ≤ 18, −19 ≤ *k* ≤ 22, −27 ≤ *l* ≤ 27
Reflections collected	77935
Independent reflections	19892 [R_{int} = 0.0429, R_{sigma} = 0.0479]
Data/restraints/parameters	19892/26/876
Goodness-of-fit on F^2	1.037
Final *R* indexes [*I*>=2σ (*I*)]	R_1 = 0.0595, wR_2 = 0.1282
Final *R* indexes [all data]	R_1 = 0.0922, wR_2 = 0.1432
Largest diff. peak/hole / e Å^{-3}	0.81/−0.71

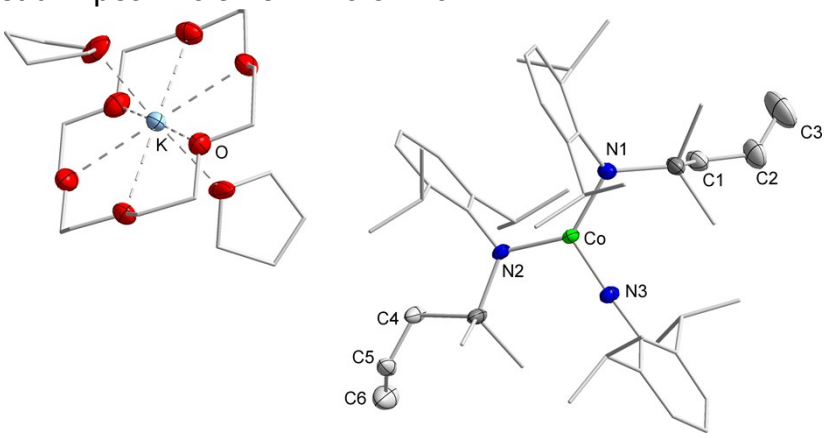

Figure S97. Molecular structure of K{18c6}**[Co(NDipp)L$^4_2$]**. All hydrogen atoms and one free, disordered THF molecule (part 1: 70%; part 2: 30%) are omitted for clarity. Disorders in both coordinated THF molecules (part 1 (depicted) / part 2: 50%) and both allyl moieties (part 1 (depicted): 70%; part 2: 30%) are omitted for clarity.