Supporting Information

Benzoquinonoid-bridged dinuclear actinide complexes

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Contents

General experimental details

If not otherwise mentioned, all manipulations were carried out in a dry, nitrogen-filled glovebox. Solvents were dried by an MBraun solvent purification system. 2,5-dihydroxy-benzoquinone, 2-fluoropyridine, tris(2-aminoethyl)amine and K_2CO_3 were used as commercially available. H_2Q^{OMe},[1] $ThCl_4(DME)_2$[2] and $UI_4(1,4\text{-dioxane})_2$[3] were synthesised according to literature procedures.

NMR spectra were collected at 300 K on Bruker AV-300, AVB-400, AV-500 or AV-600 spectrometers at 300 K. ^1H and $^{13}C\{^1H\}$ NMR spectra are reported in chemical shift (δ / ppm) and were calibrated against an external standard ($SiMe_4$: $\delta_H = 0$ ppm; $\delta_C = 0$ ppm) and referenced against the residual solvent resonances. NMR spectra are presented using MestReNova 10.0.2. Elemental analyses were carried out the University of California, Berkeley. UV-visible spectra were collected on a Varian Cary 50 UV-visible spectrophotometer using a Schlenk-adapted 1 cm quartz cell at ambient temperature. FT-IR spectra were recorded at ambient temperature on a Thermo Scientific Nicolet iS10 FT-IR spectrophotometer using Nujol mulls of the compound pressed between KBr plates.

Single-crystal X-ray diffraction data were collected using a Bruker Quazar instrument at 100 K using Mo-Kα radiation (λ = 0.71073 Å). Structural solution was carried out using either intrinsic phasing methods (for **1**, **2**, **2-dimer**, **5** and **6**) in the ShelXT program, or direct methods (for **3**) and Patterson methods (for **6**$^-$) in the ShelXS program. Structures were refined using a full-matrix least-square refinement on $|F|^2$ using ShelXL.[4] All programs were used within the WinGX suite. All non-hydrogen atoms were refined with anisotropic displacement parameters, and hydrogen atoms were placed at calculated positions and included in the refinement using a constrained model. Tables S1 and S2 contain the CCDC numbers to the obtained structures.

Cyclic voltammograms were recorded using a Gamry Instruments Reference 600 potentiostat and Gamry Framework software. Experiments were carried out in a N_2 glovebox in a 7 mL vial as the electrochemical cell. A Pt-disc working electrode was used, along with a Pt-gauze counter electrode and a Pt-wire quasi-reference electrode. The solution employed was approximately 1 mM of the analyte with 0.1 M [^{n}Bu_4N][PF_6] as the supporting electrolyte, in 3 mL of dry and deoxygenated THF. All potentials were referenced against ferrocene ($E_{1/2}$, $[FeCp_2]^{+/0}$ = 0.0 V).

Magnetic susceptibility measurements were performed using a Quantum Design MPMS2 SQUID magnetometer. DC magnetic susceptibility measurements were performed at temperatures ranging from 2-300 K under applied DC fields of 1000 Oe (0.1 T), 5000 Oe (0.5 T), 20000 Oe (2.0 T), and 70000 Oe (7.0 T). All data were corrected for diamagnetic contributions from the core diamagnetism estimated using Pascal's constants[5] to give $\chi_{dia} = -0.00077996$ emu/mol. Magnetic samples were prepared by adding crystalline powder of the compound (14.0 mg) to a 7 mm quartz tube, which was subsequently packed with glass wool to preventing crystallite torqueing. The tubes were fitted with Teflon selable adapters, evacuated on a Schlenk line or using a glove box vacuum pump, and flame-sealed under static vacuum using a H_2/O_2 torch.

All DFT calculations were carried out using Gaussian09[6] on the University of Edinburgh's Eddie3 server system. The unrestricted B3PW91 functional was employed, using Becke's

3-parameter hybrid functional[7] along with Perdew/Wang's non-local correlation functional.[8] The uranium atoms were described using the ECP78MWB pseudopotential from the Stuttgart-Köln ECP library, along with its adapted segmented basis set.[9] All other light atoms were described by the 6-31G(d,p) Pople basis set.[10] Stationary points were confirmed as minimum-energy structures and contained no imaginary frequencies. The minimum-energy structure for **6** was only obtained using the "opt=verytight", "int=(grid=ultrafine)", "cphf=(grid=fine)" and "scf=tight" keywords in Gaussian09. The amount of spin-contamination in the open-shell calculations is less than 6 % in all cases. The "noraman" Gaussian09 option was used for both optimisation and frequency calculations for efficiency. Initial-guess geometries were generated from X-ray crystal structures using Mercury 3.8, and the full molecule was used as input; for **6**$^{–}$, the $[K(18\text{-}c\text{-}6)(thf)_2]^+$ moiety was omitted for efficiency. Molecular orbitals were inspected using Jmol 14.4.0. Molecular-orbital and spin-density surfaces were rendered using UCSF Chimera 1.11,[11] from cube files generated using Gaussian09 "formchk" and "cubegen" utilities, and are displayed at an iso-value of 0.02. The spin-density difference-plot cube file was generated using the Gaussian09 "cubman" subtraction utility.

All spectra were plotted using MagicPlot Student 2.7.2.

NMR spectra

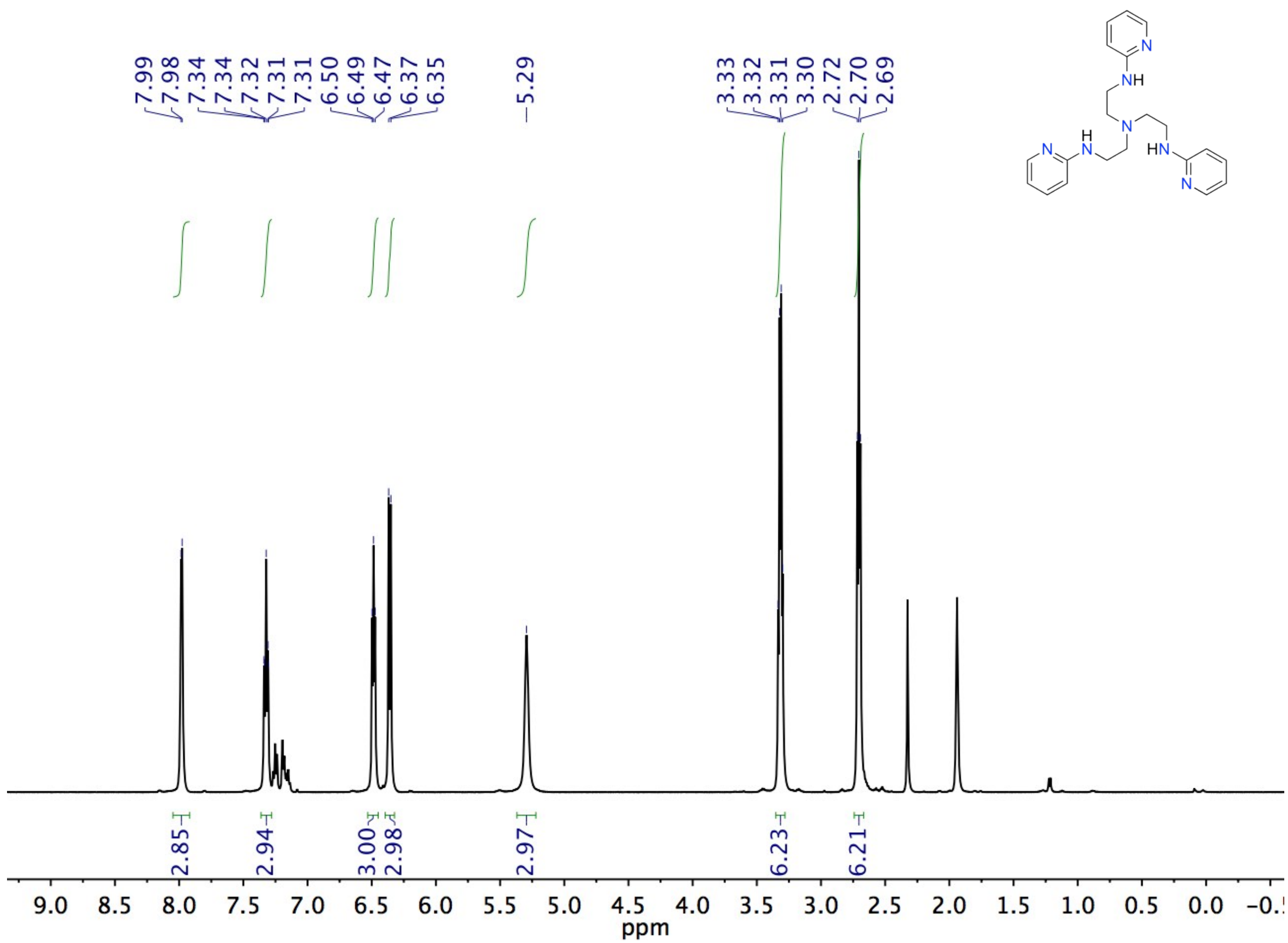


Figure S1. ^{1}H NMR of $\mathbf{H_3L}$ in CD_3CN. Toluene is present in the spectrum.

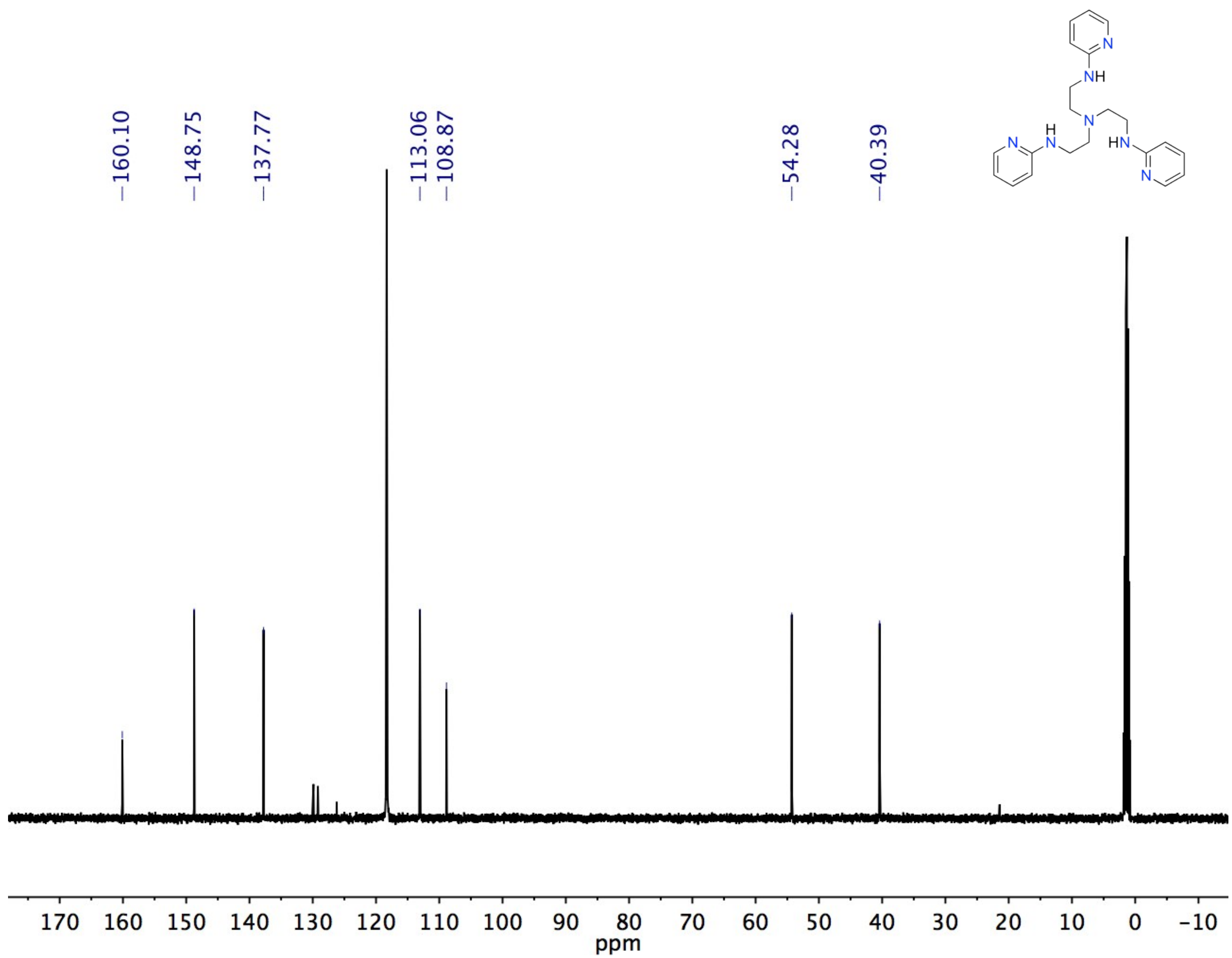


Figure S2. $^{13}C\{^1H\}$ NMR spectrum of $\mathbf{H_3L}$ in CD_3CN. Toluene is present in the spectrum.

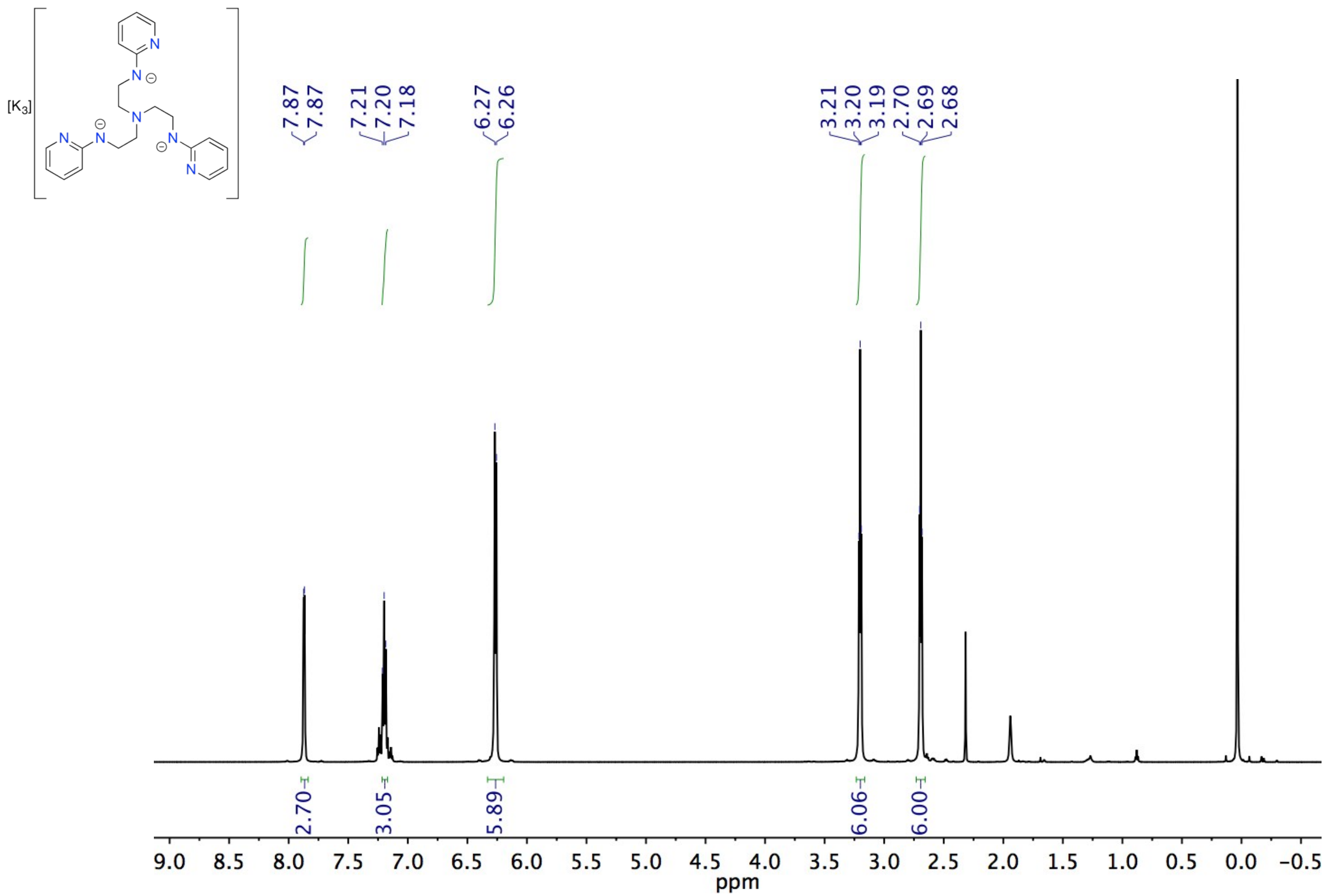


Figure S3. ^{1}H NMR spectrum of **K_3L** in CD_3CN.

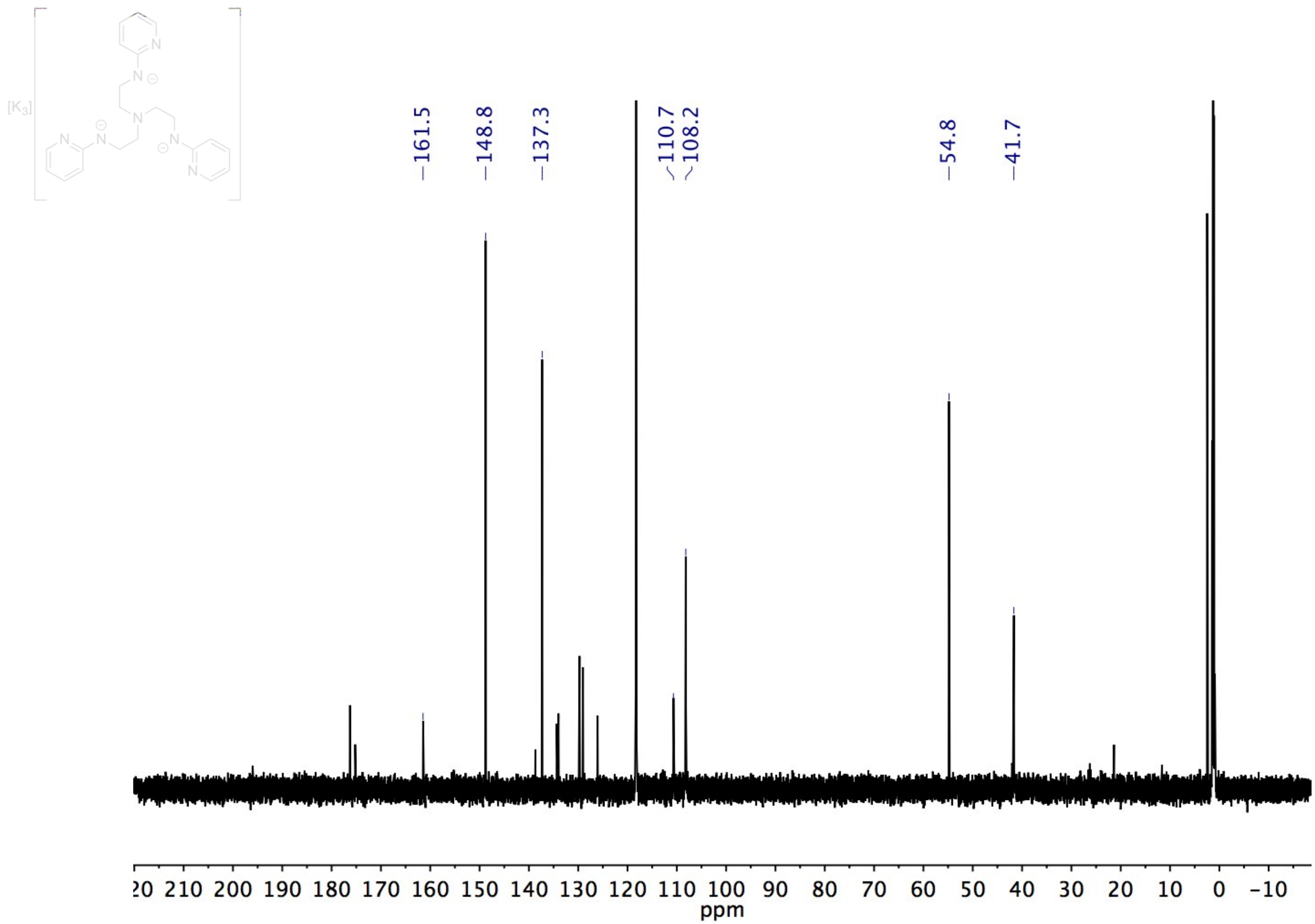


Figure S4. $^{13}C\{^1H\}$ NMR spectrum of **K_3L** in CD_3CN. Resonances between 127 and 138 ppm as well as at 21 ppm belong to toluene. Signals at 175 ppm are an impurity from the solvent.

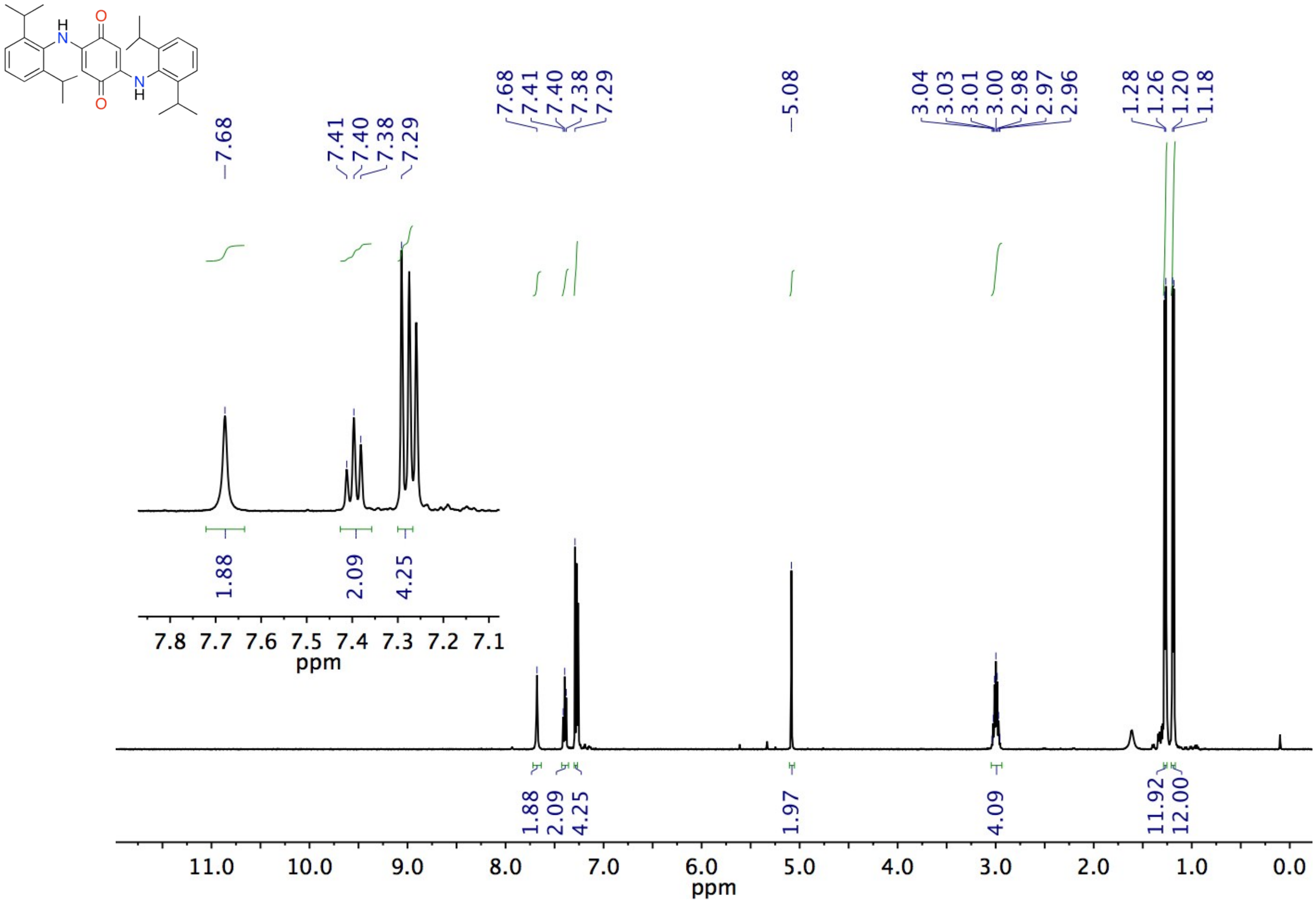


Figure S5. ^{1}H NMR spectrum of **H_2Q^{Dipp}** in $CDCl_3$.

H
N
O
O
N
H

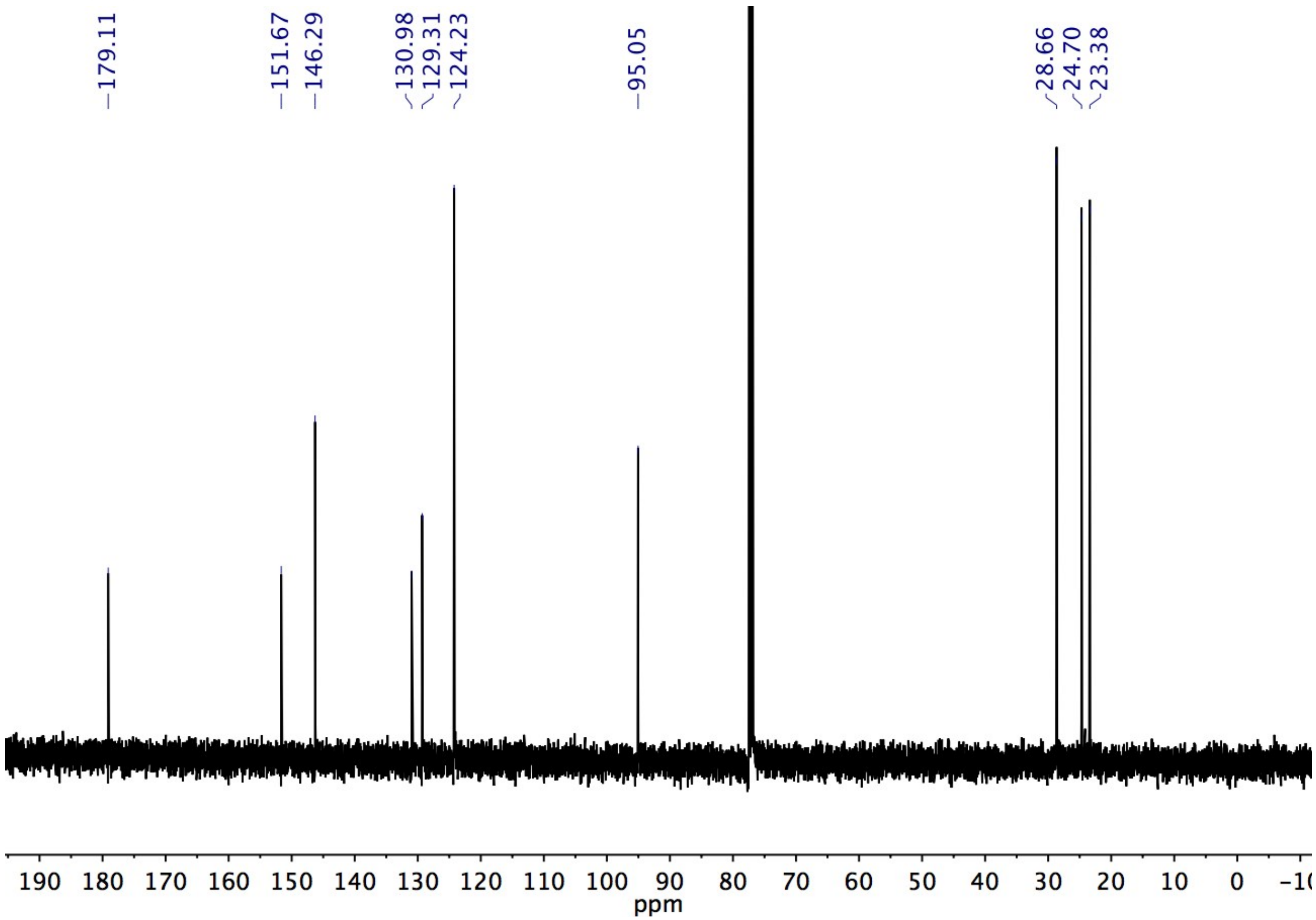
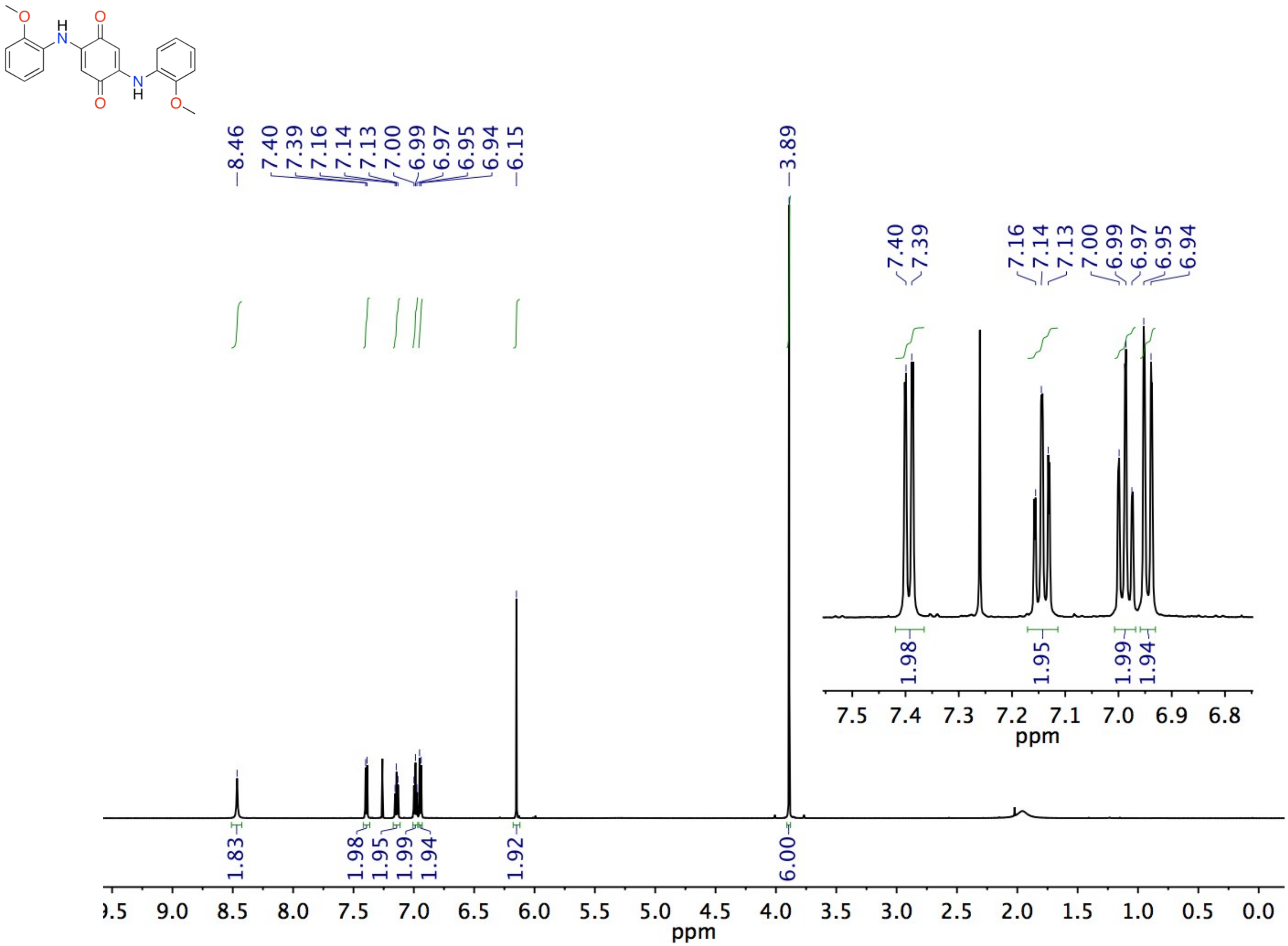

179.11
151.67
146.29
130.98
129.31
124.23
95.05
28.66
24.70
23.38
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
ppm

Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of $\mathbf{H_2Q^{Dipp}}$ in $CDCl_3$.



8.46
7.40
7.39
7.16
7.14
7.13
7.00
6.99
6.97
6.95
6.94
6.15
3.89
1.83
1.98
1.95
1.99
1.94
1.92
6.00
ppm

Figure S7. [1]H NMR spectrum of $\mathbf{H_2Q^{OMe}}$ in $CDCl_3$.

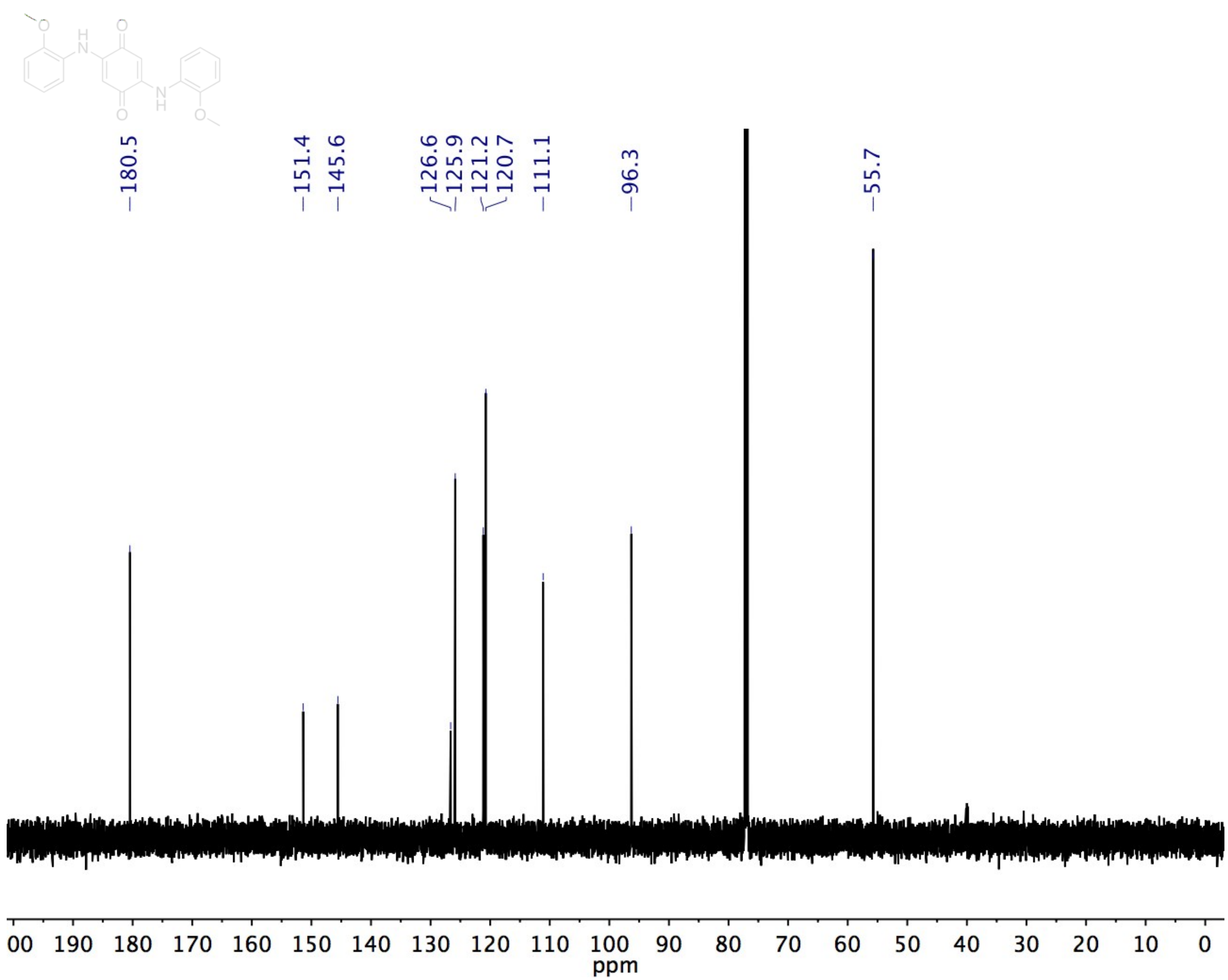

180.5
151.4
145.6
126.6
125.9
121.2
120.7
111.1
96.3
55.7
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum of $\mathbf{H_2Q^{OMe}}$ in $CDCl_3$.

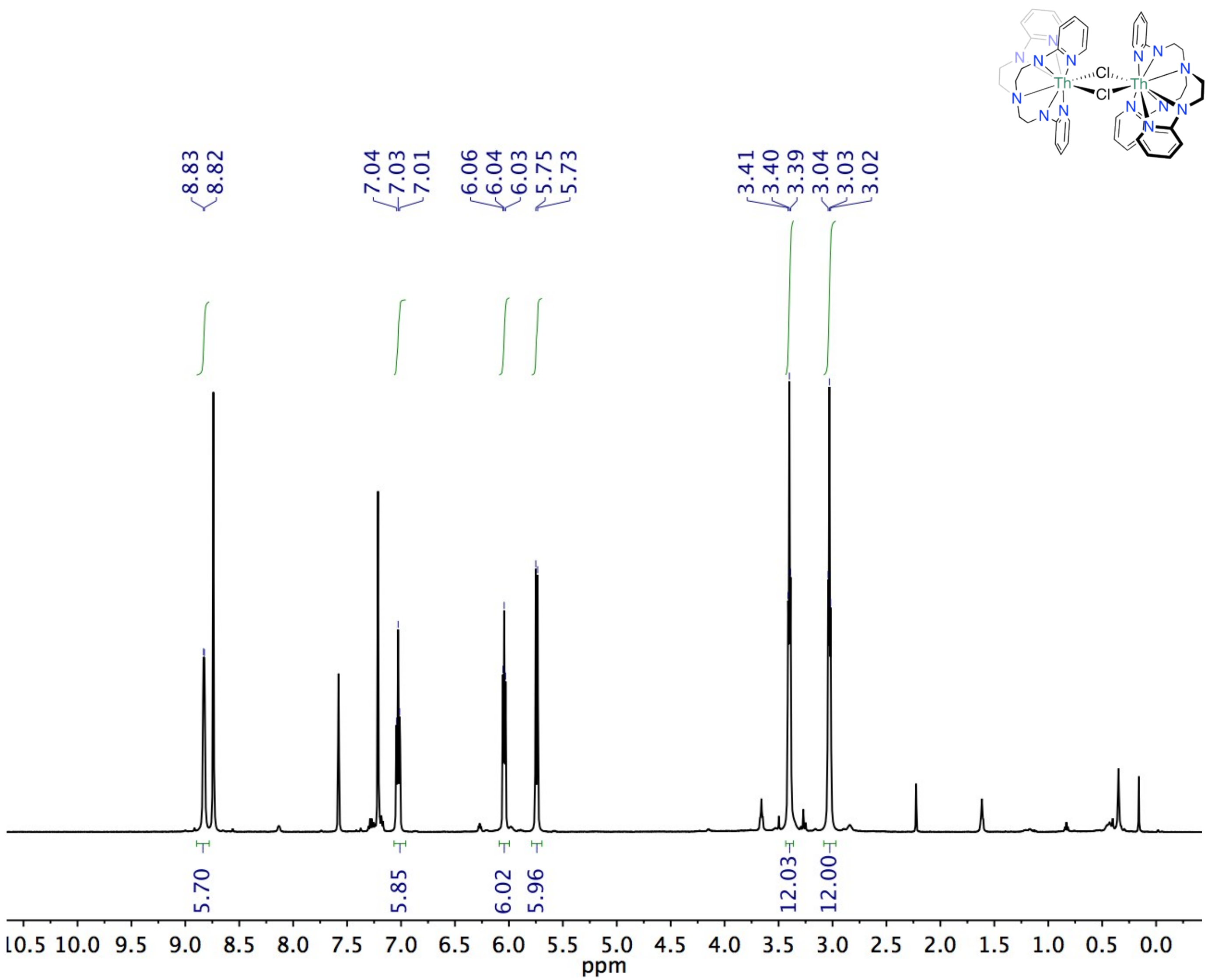


Figure S9. ^{1}H NMR spectrum of **1** in d_5-pyridine.

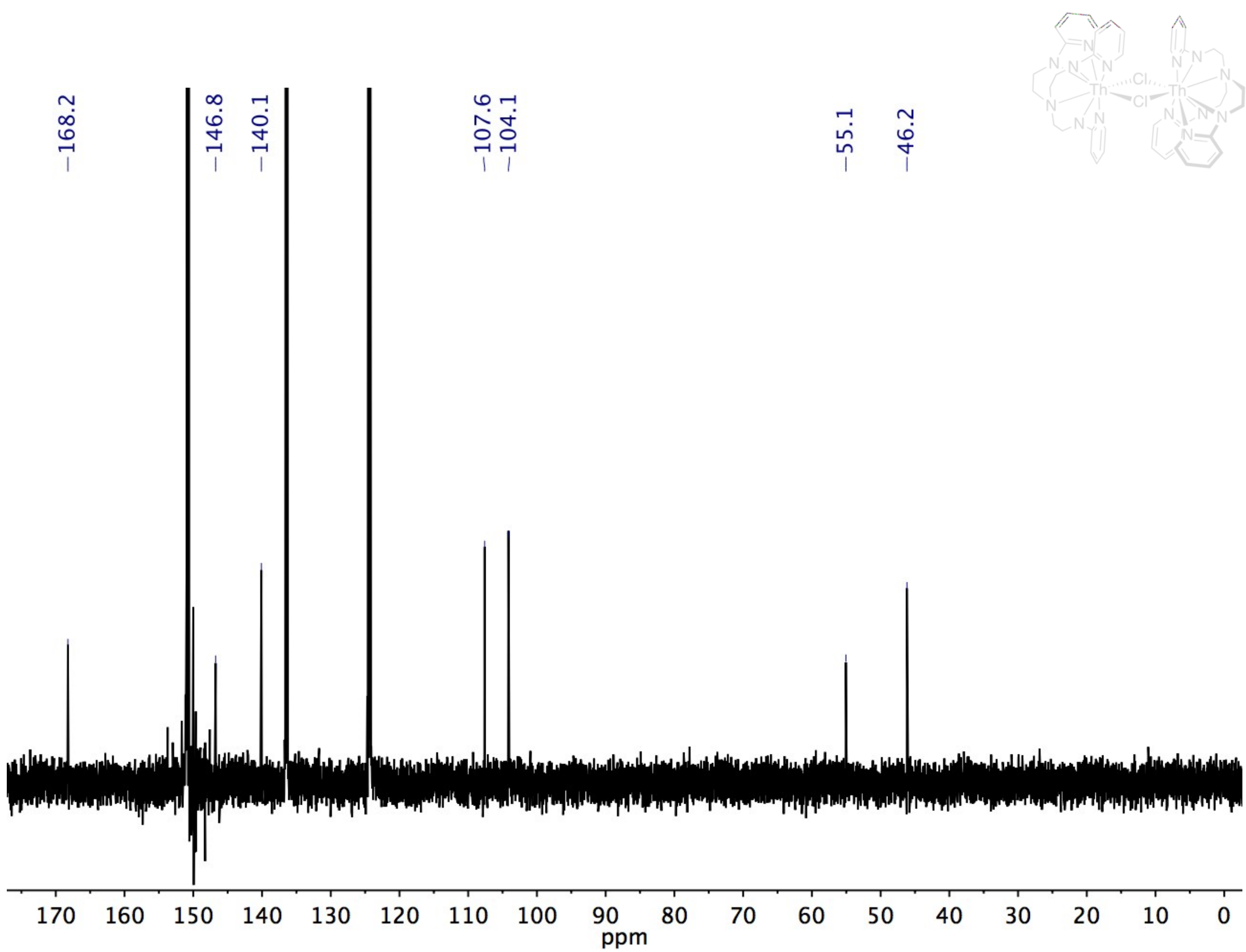


Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum of **1** in d_5-pyridine.

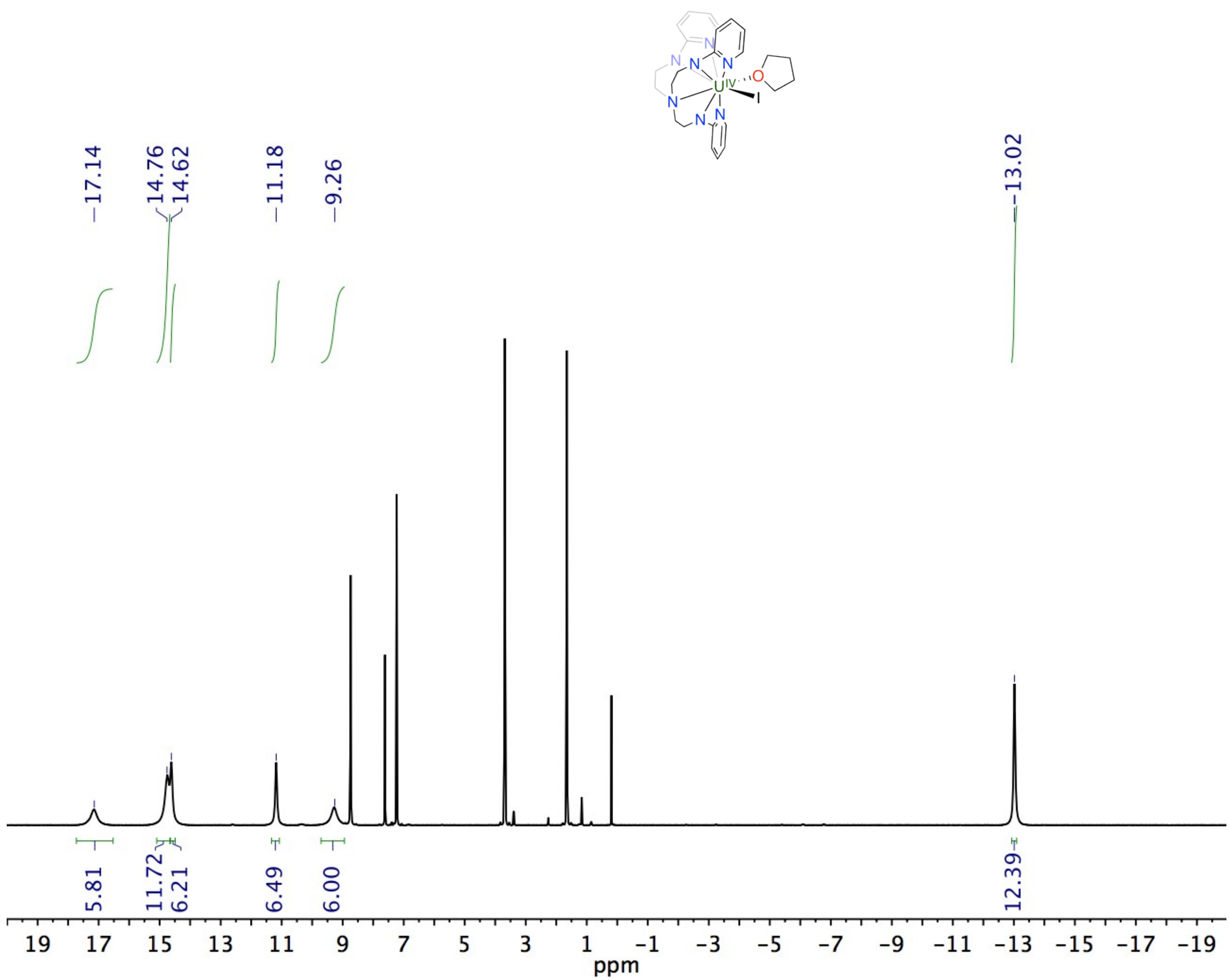


Figure S11. ^{1}H NMR spectrum of **2** in d_5-pyridine (3 eq of THF are present from the crystals; previously bound THF are most likely displaced by d_5-pyridine).

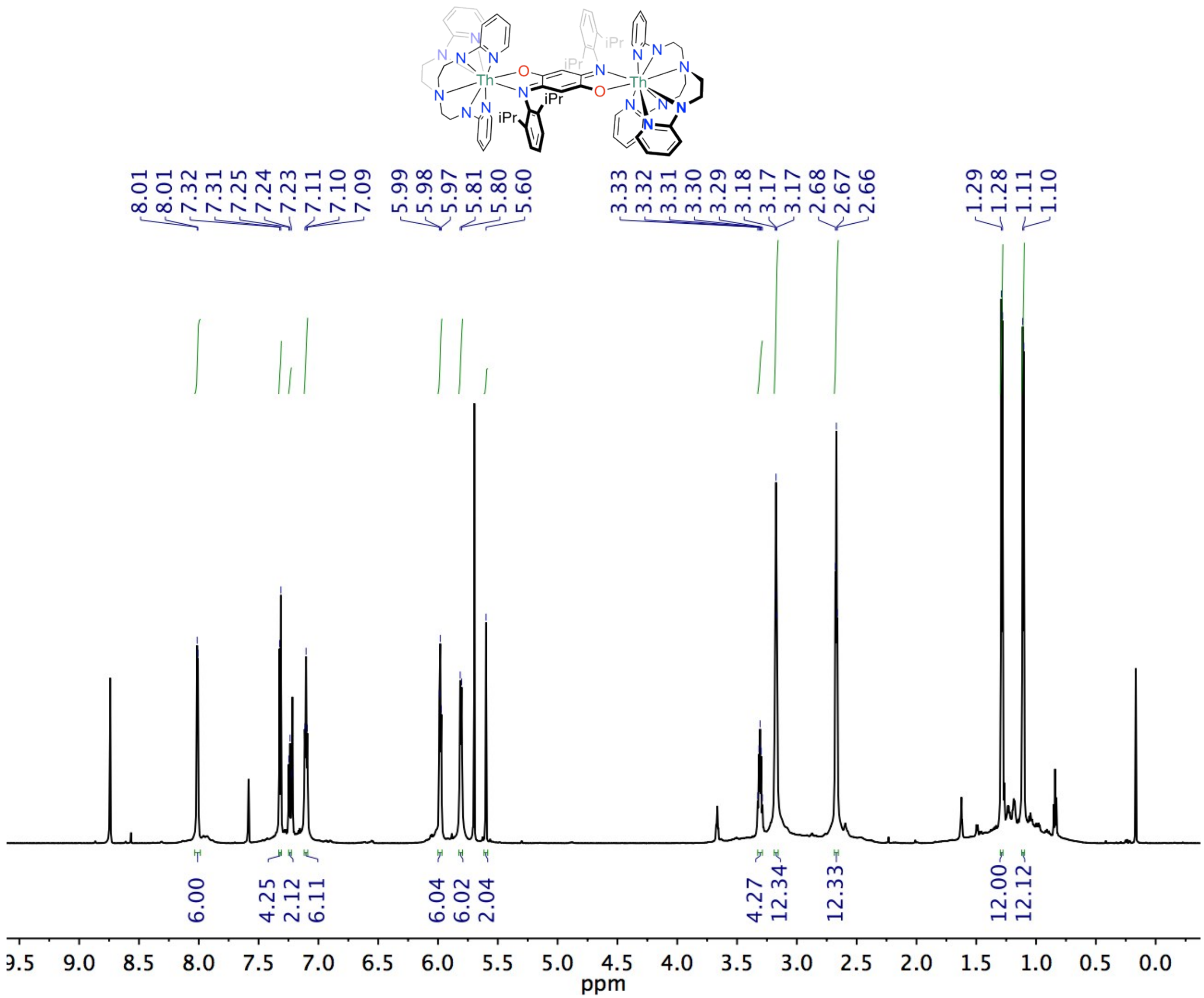


Figure S12. ¹H NMR spectrum of **3** in d_5-pyridine.

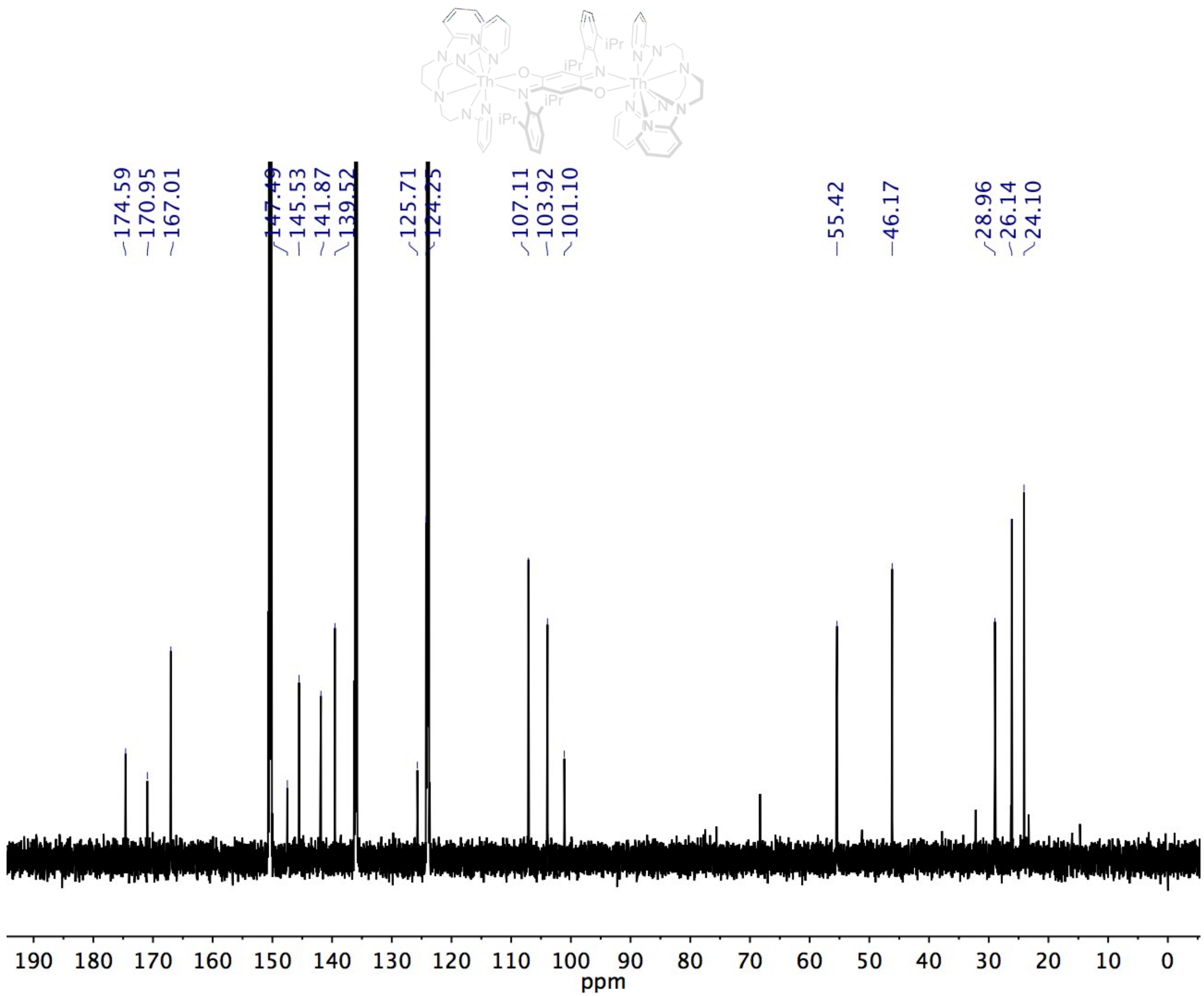


Figure S13. $^{13}C\{^1H\}$ NMR spectrum of **3** in d_5-pyridine.

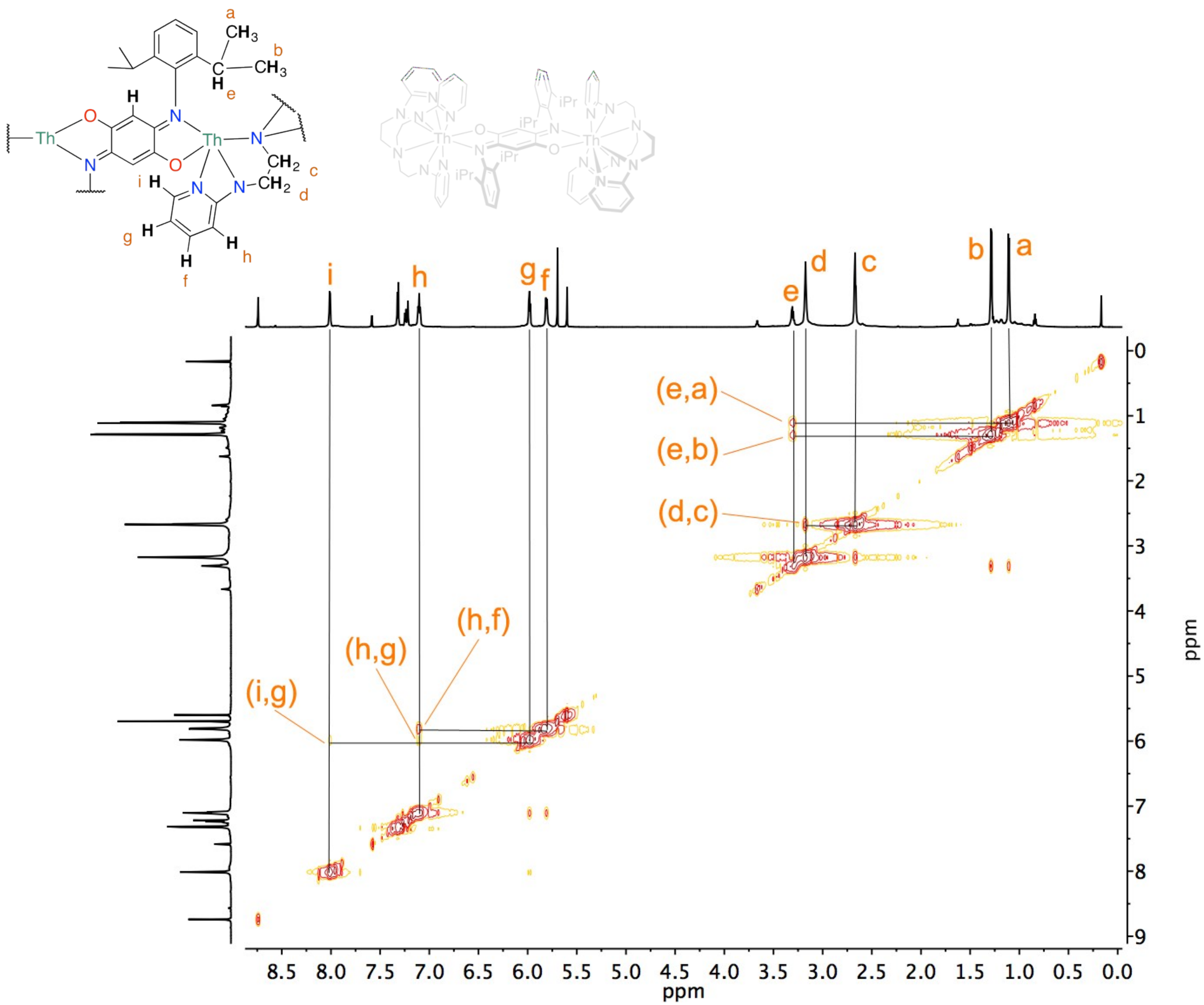


Figure S14. ^{1}H COSY NMR spectrum of **3** in d_5-pyridine.

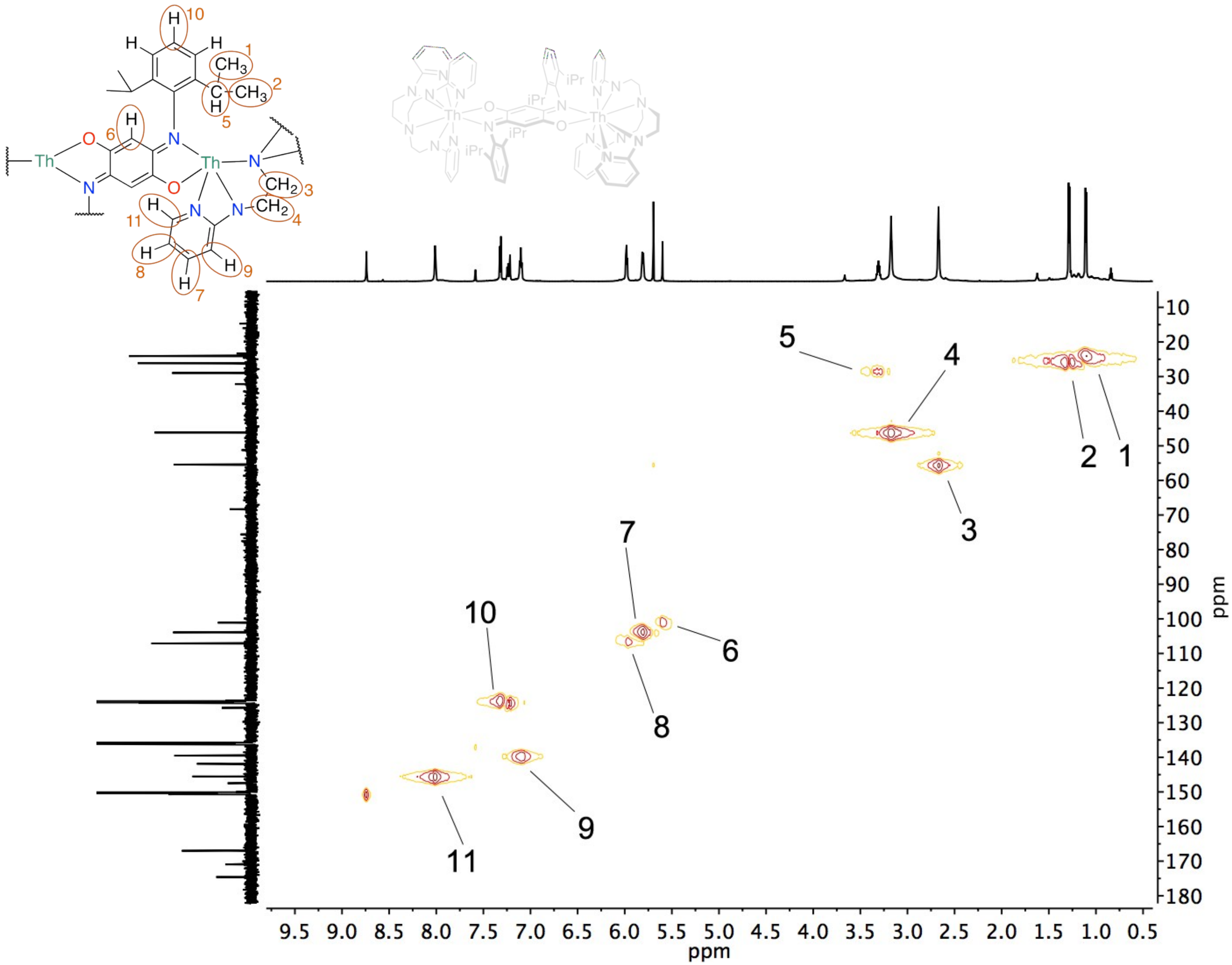
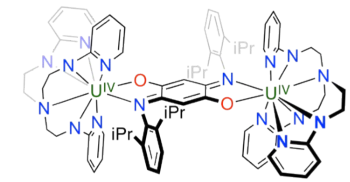


Figure S15. ^{1}H-^{13}C HSQC NMR spectrum of **3** in d_5-pyridine.



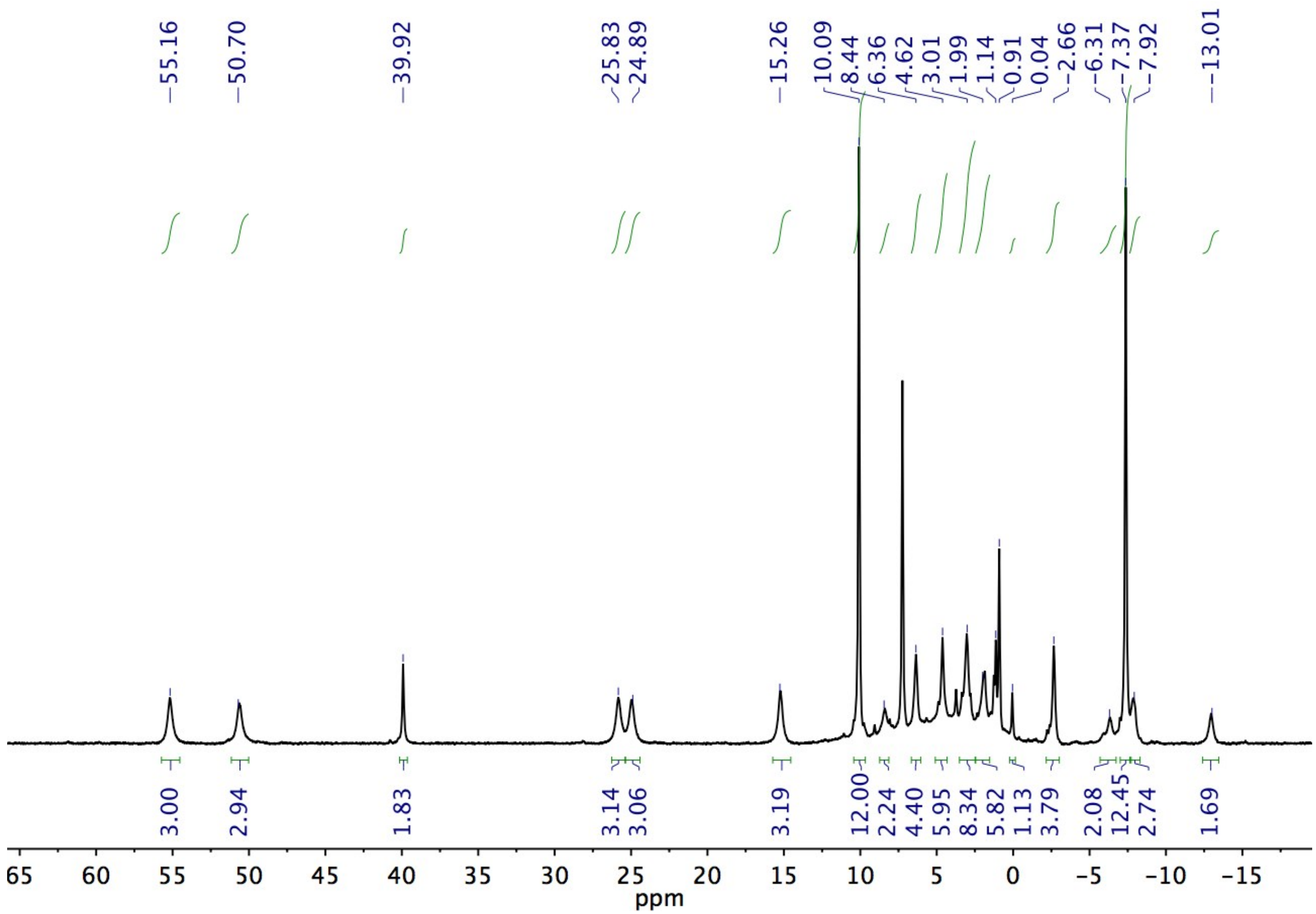
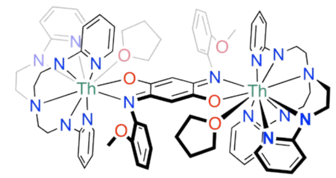


Figure S16. Uninformative ^{1}H NMR spectrum from the attempted synthesis of **4** in $CDCl_3$. Two pyridyl resonances have not been located.



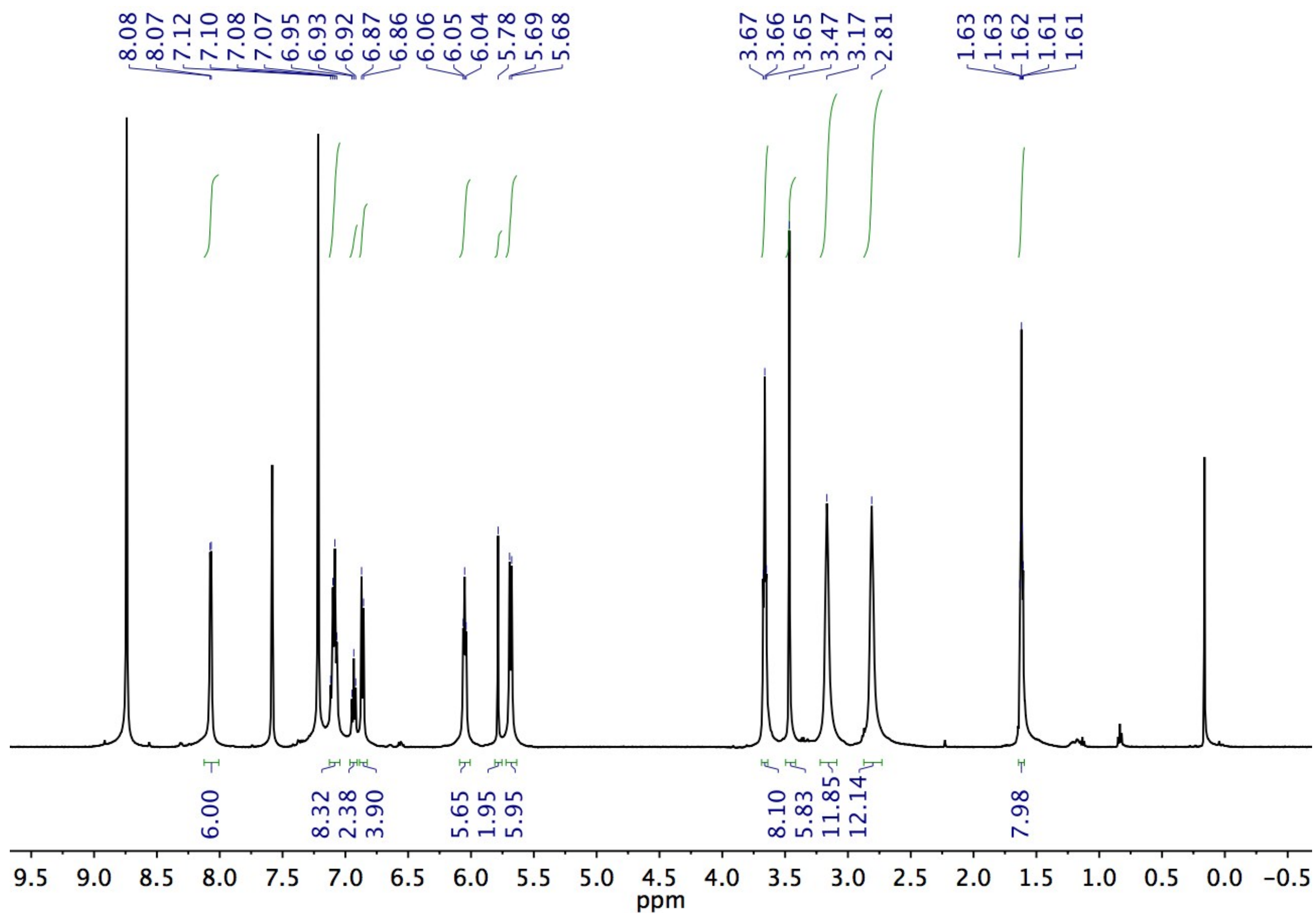


Figure S17. ^{1}H NMR spectrum of **5** in d_5-pyridine.

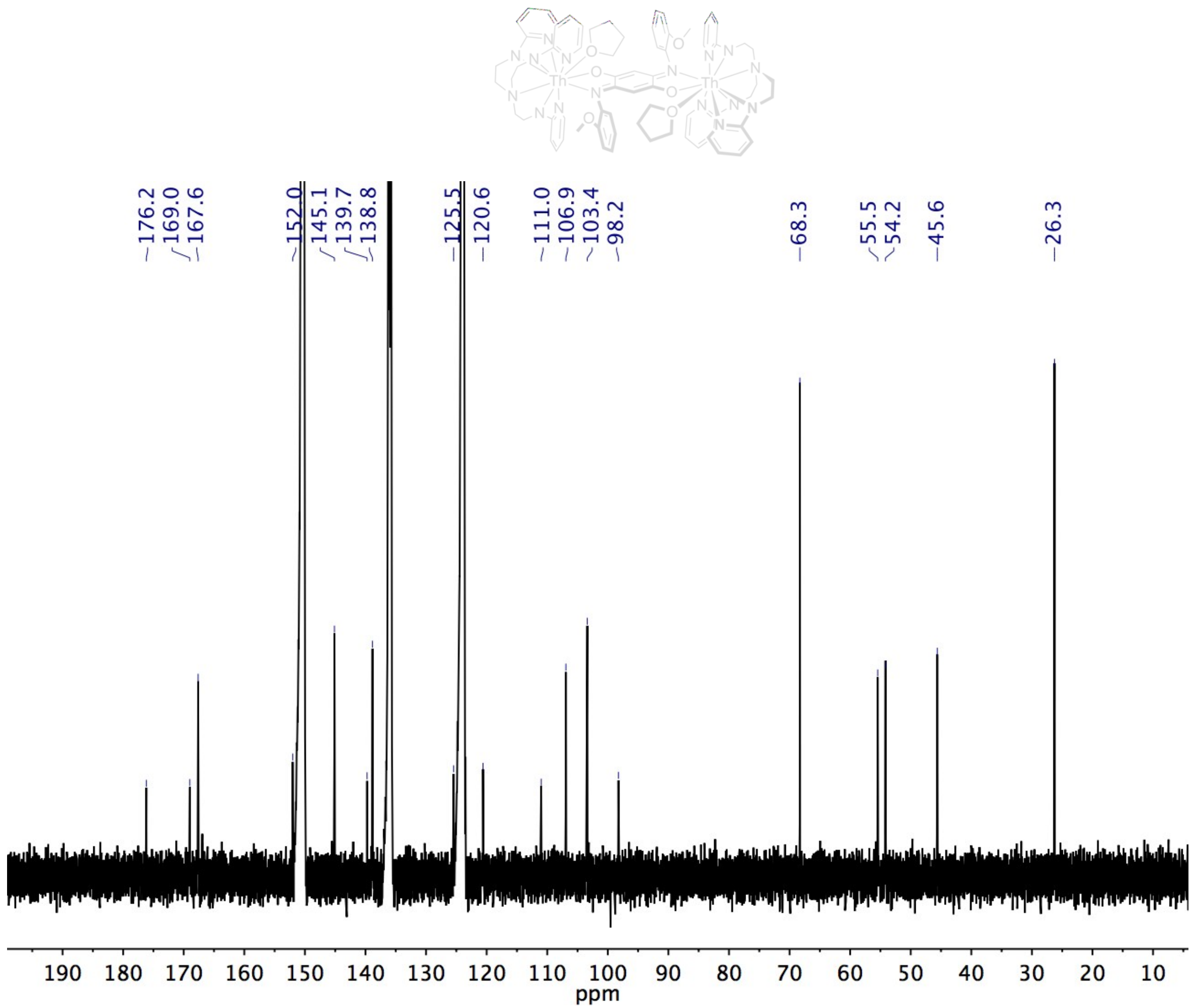


Figure S18. $^{13}C\{^{1}H\}$ NMR spectrum of **5** in d_5-pyridine.

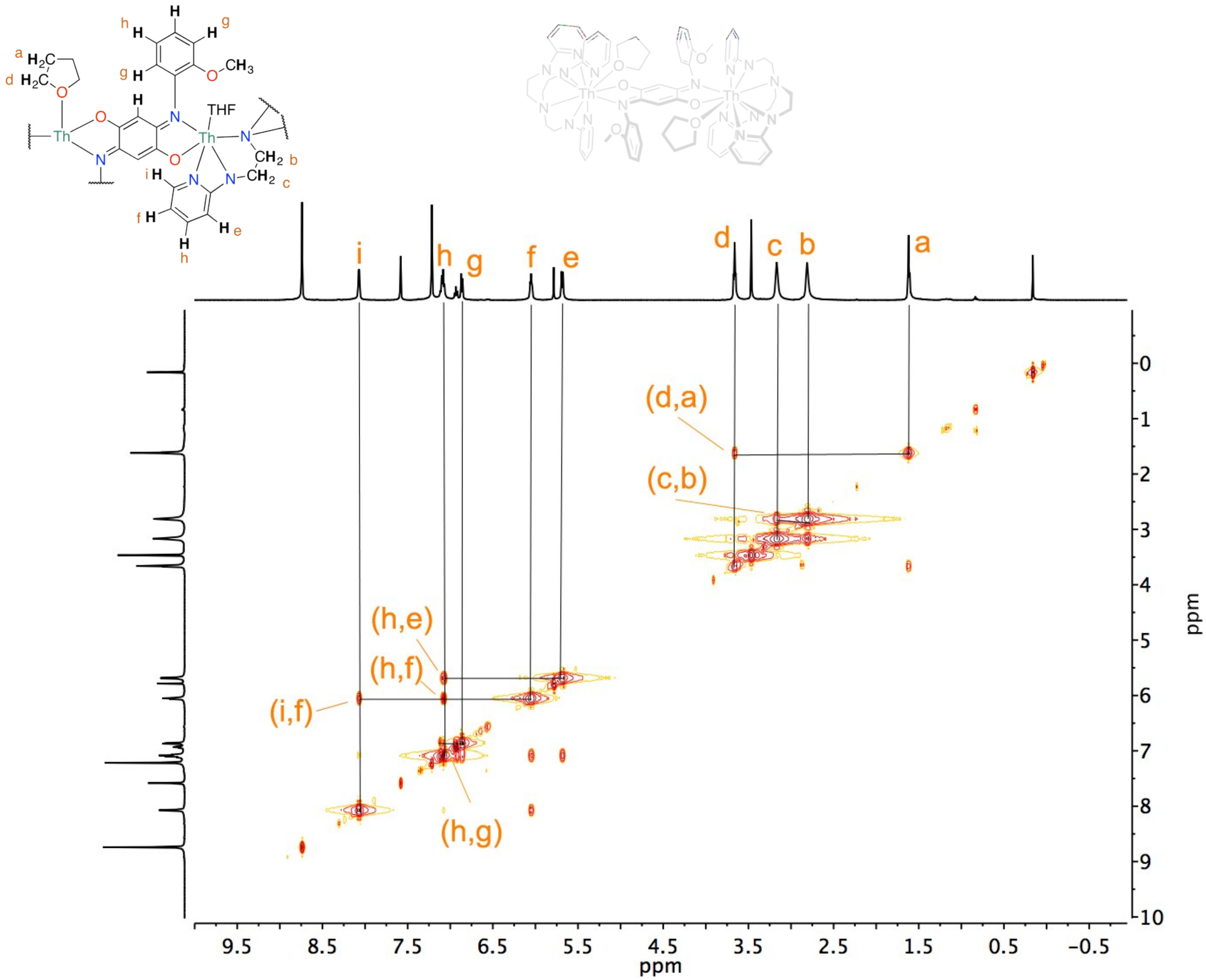


Figure S19. ^{1}H COSY NMR spectrum of **5** in d_5-pyridine.

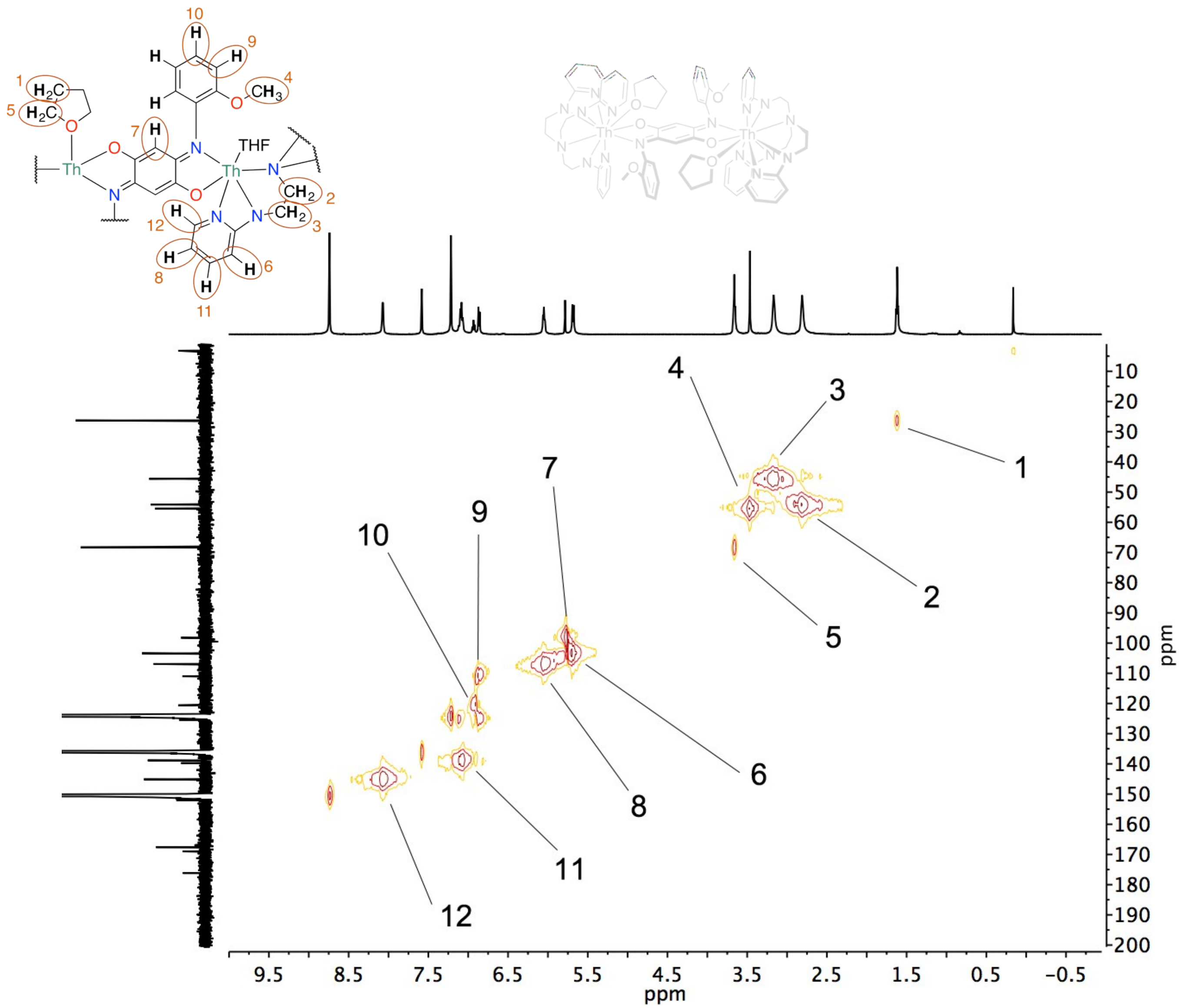
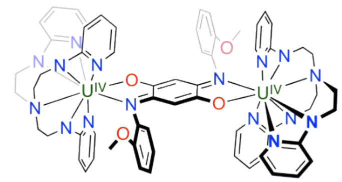


Figure S20. ^{1}H-^{13}C HSQC NMR spectrum of **5** in d_5-pyridine.



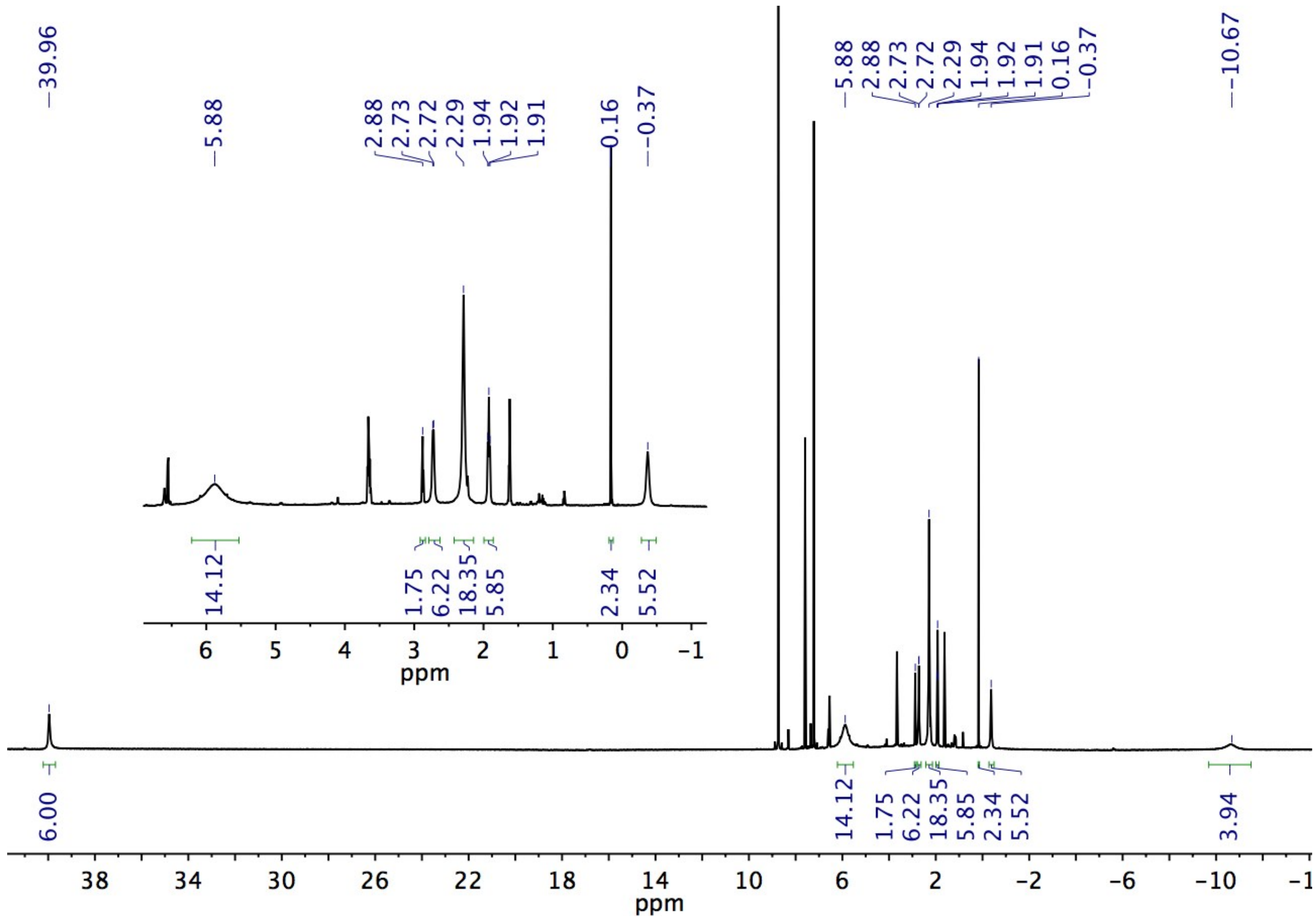


Figure S21. ^{1}H NMR spectrum of **6** in d_5-pyridine.

UV/Vis-spectra

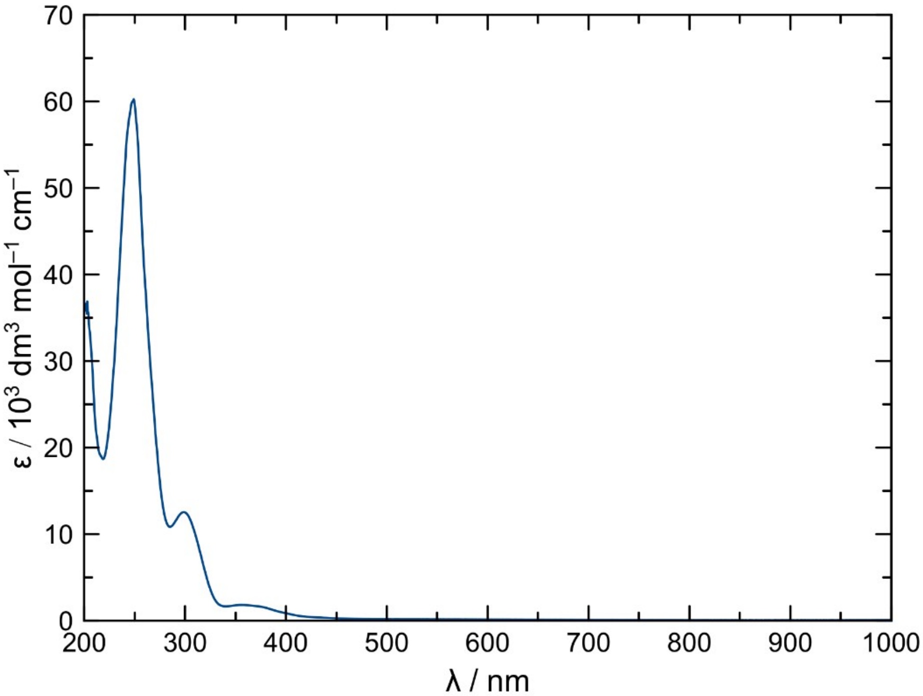


Figure S22. UV/visible absorption spectrum of $\mathbf{K_3L}$ in CH_3CN.

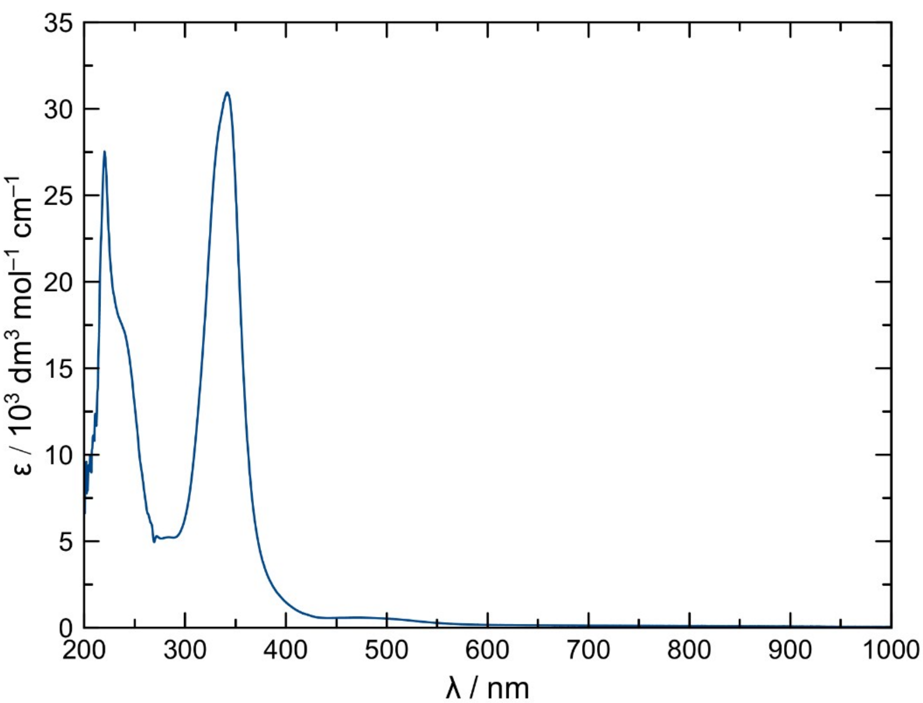


Figure S23. UV/visible absorption spectrum of $\mathbf{H_2Q^{Dipp}}$ in THF.

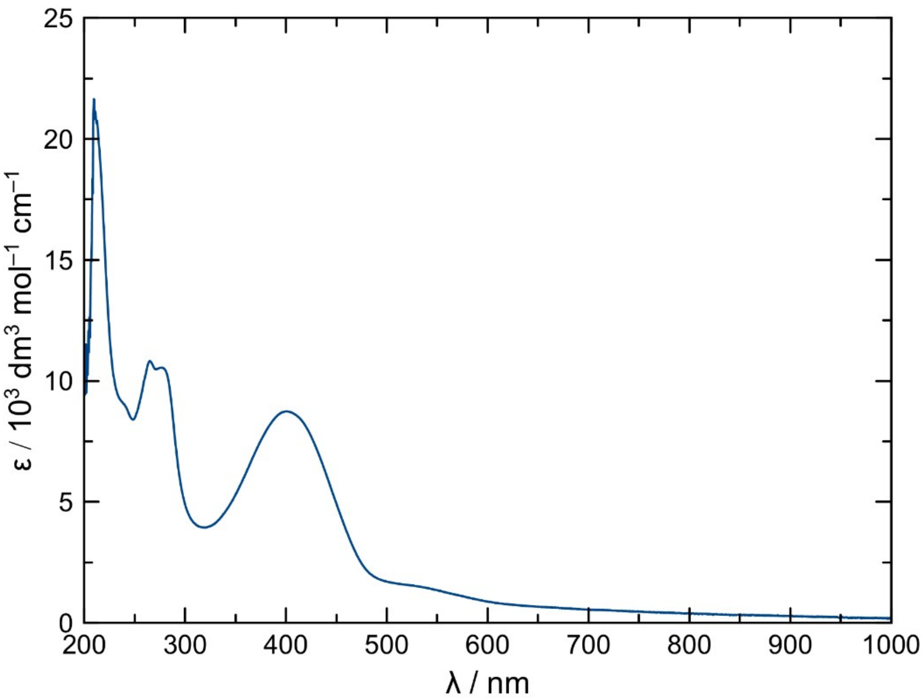


Figure S24. UV/visible absorption spectrum of $\mathbf{H_2Q^{OMe}}$ in THF.

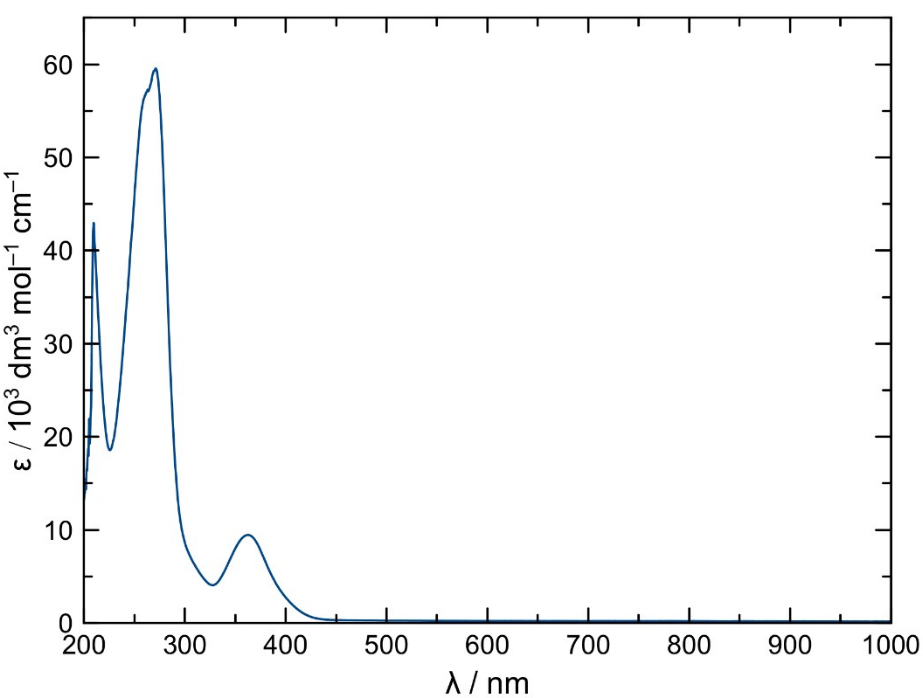


Figure S25. UV/visible absorption spectrum of **1** in THF.

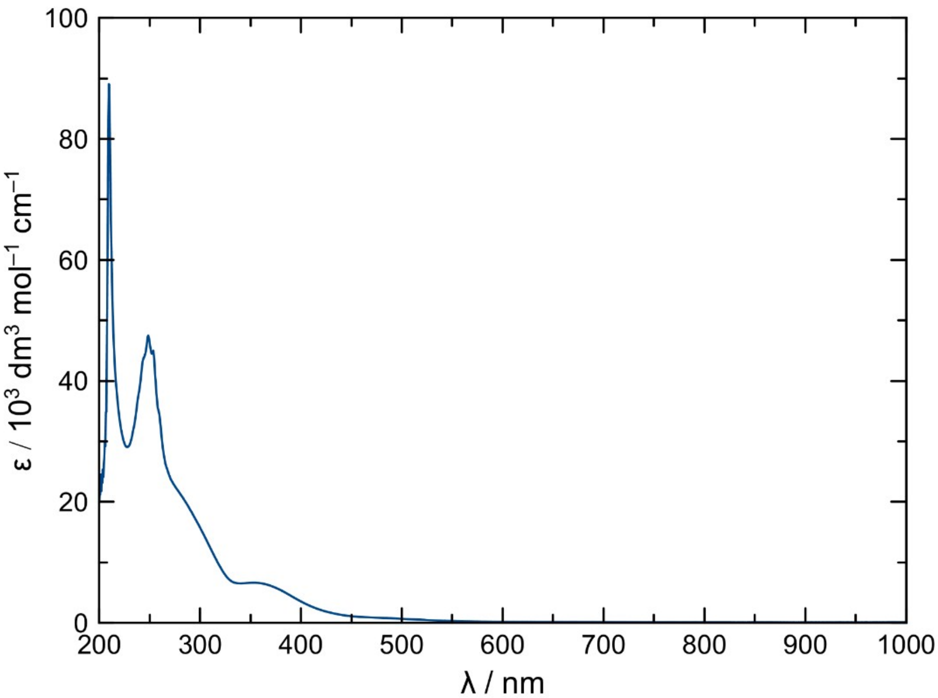


Figure S26. UV/visible absorption spectrum of **2** in THF.

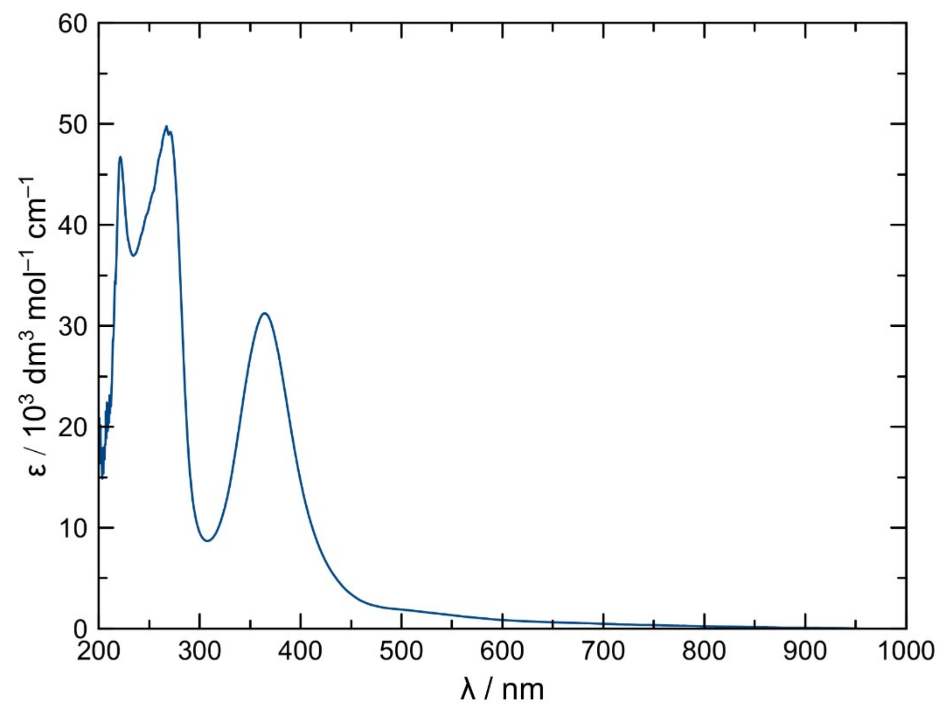


Figure S27. UV/visible absorption spectrum of **3** in THF.

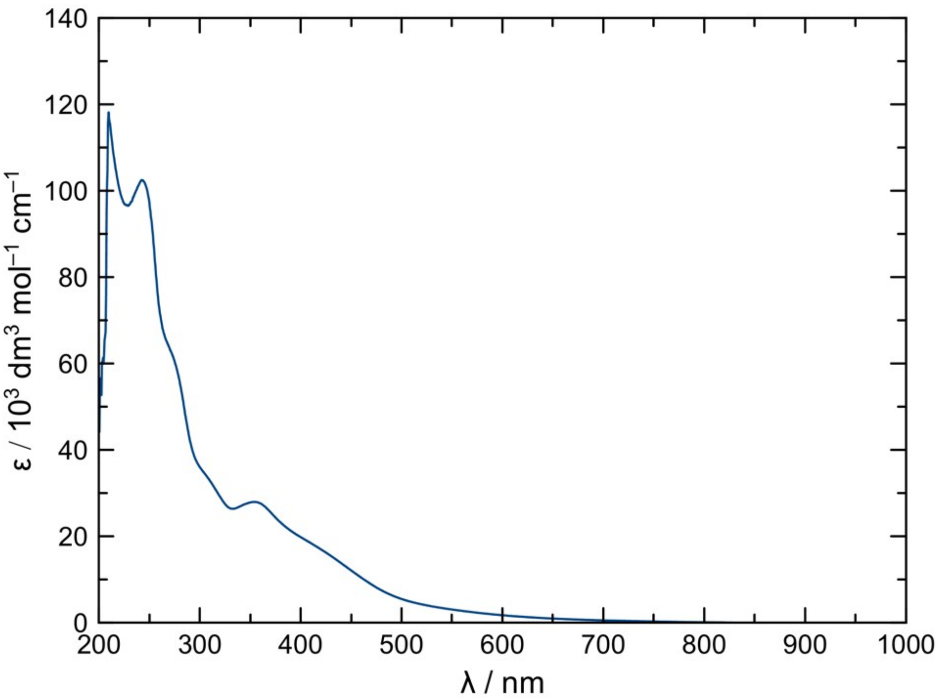


Figure S28. UV/visible absorption spectrum of **5** in THF.

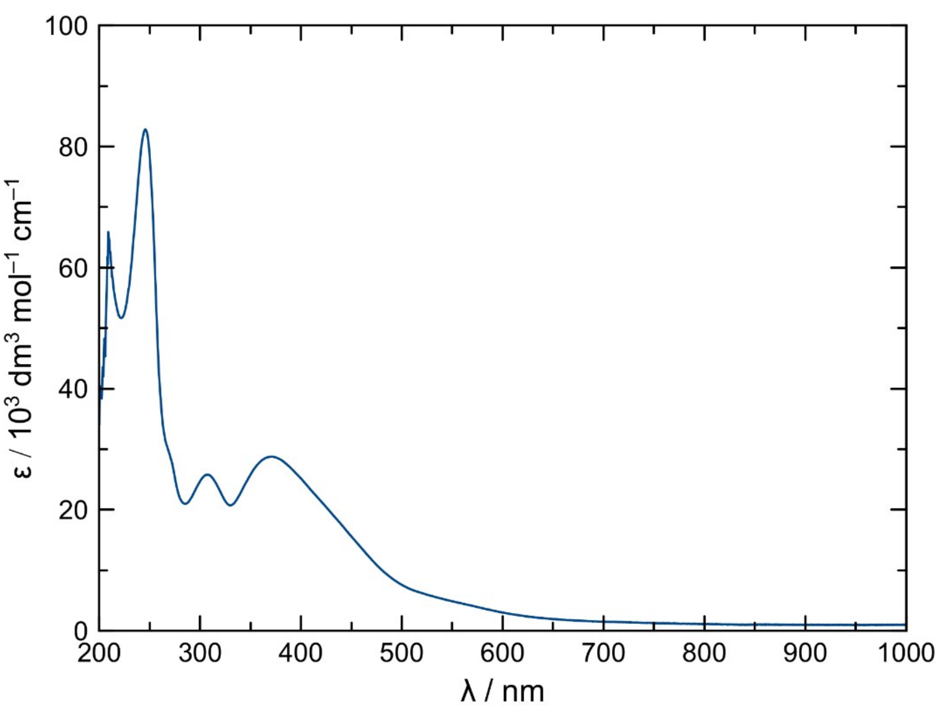


Figure S29. UV/visible absorption spectrum of **6** in THF.

IR-spectra

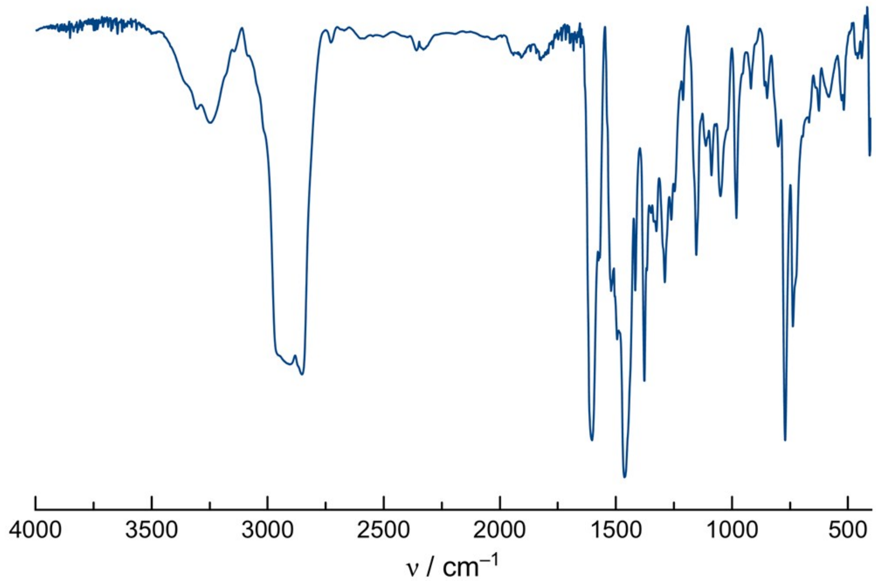


Figure S30. FT-IR spectrum of **H_3L**. ν / cm^{-1}: 3307 (w), 3251 (w), 1604 (s), 1521 (s, sh), 1495 (s, sh), 1464 (s), 1416 (m), 1378 (s), 1349 (w), 1337 (w), 1288 (m), 1261 (w), 1246 (w), 1209 (w), 1153 (m), 1113 (w), 1088 (w), 1050 (m), 981 (m), 920 (w), 861 (w), 849 (w), 801 (w), 770 (s), 737 (s), 667 (w), 626 (w), 581 (w), 528 (w), 518 (w), 458 (w), 441 (w).

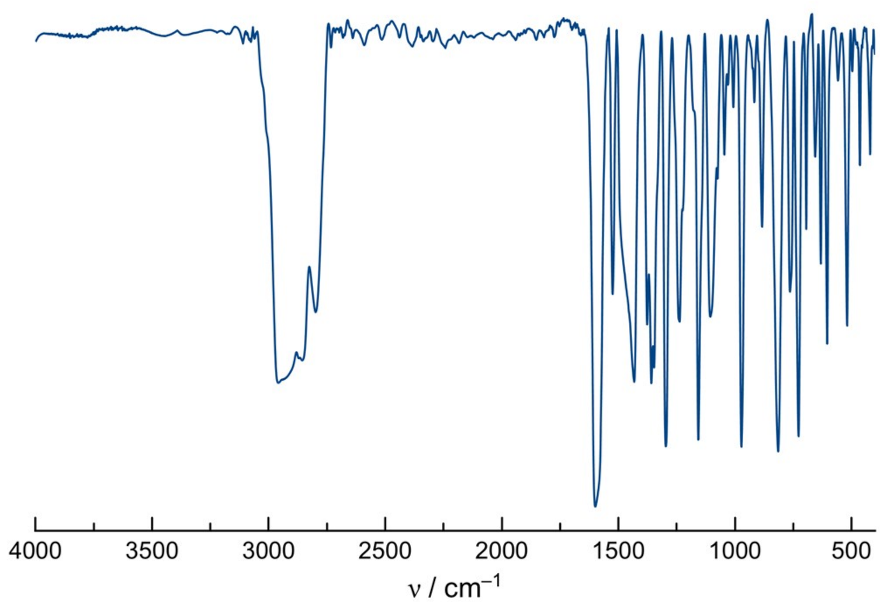


Figure S31. FT-IR spectrum of **K_3L**. ν / cm^{-1}: 1600 (s), 1525 (s), 1432 (s), 1378 (s), 1359 (s), 1347 (s), 1296 (s), 1237 (s), 1224 (s), 1156 (s), 1106 (s), 1046 (w), 1030 (w), 1007 (w), 972 (s), 917 (s), 883 (m), 815 (s), 764 (s), 727 (s), 694 (m), 657 (m), 633 (m), 604 (s), 558 (w), 520 (s), 497 (w), 464 (m), 420 (m).

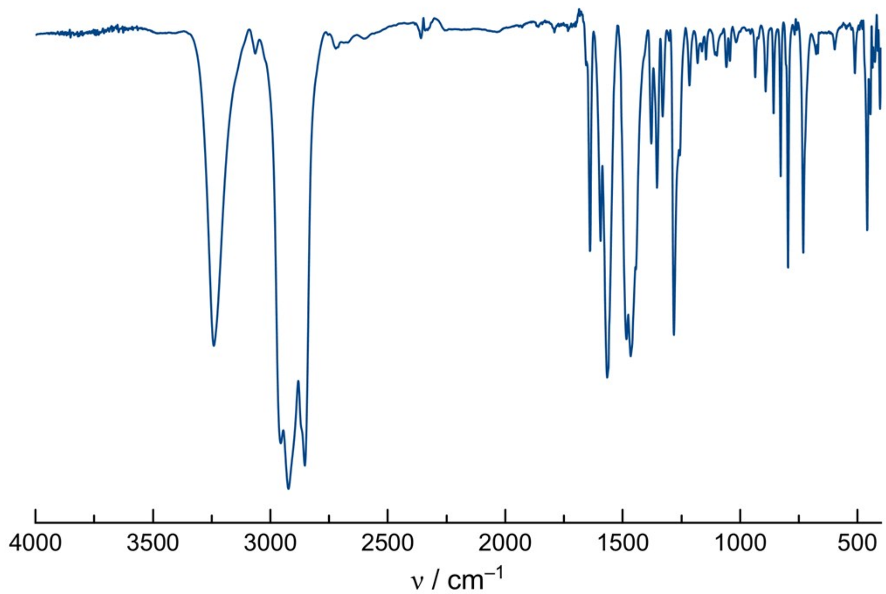


Figure S32. FT-IR spectrum of $\mathbf{H_2Q^{Dipp}}$. ν / cm^{-1}: 3241 (s), 1639 (s), 1594 (s), 1565 (s), 1486 (s), 1466 (s), 1379 (w), 1354 (m), 1330 (w), 1282 (s), 1256 (m, sh), 1215 (w), 1181 (w), 1162 (w), 1145 (w), 1099 (w), 1058 (w), 1043 (w), 1016 (w), 935 (w), 891 (w), 857 (w), 827 (m), 796 (s), 731 (s), 668 (w), 597 (w), 511 (w), 459 (s), 446 (m), 426 (w), 404 (w).

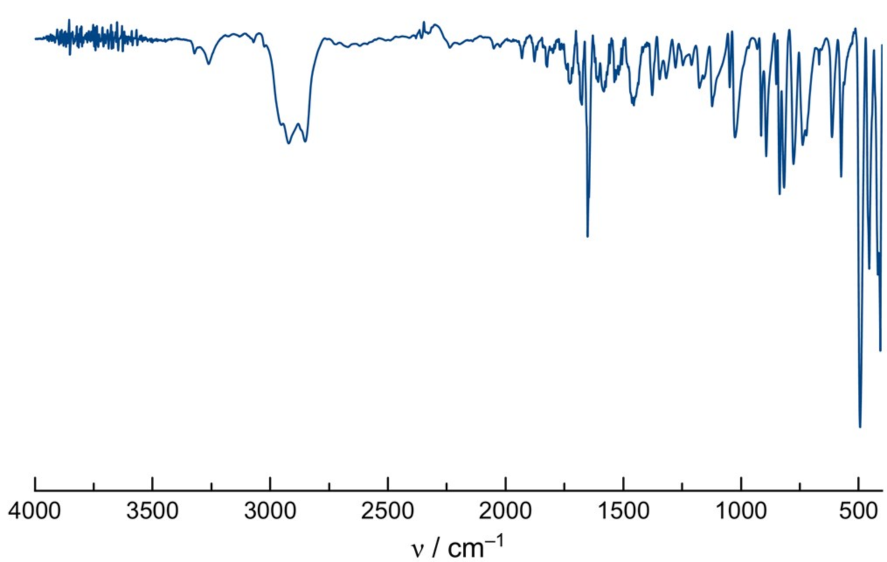


Figure S33. FT-IR spectrum of $\mathbf{H_2Q^{OMe}}$. ν / cm^{-1}: 3322 (w), 3264 (w), 1930 (w), 1877 (w), 1824 (w), 1728 (w), 1679 (w), 1652 (s), 1606 (w), 1583 (w), 1523 (w), 1454 (w), 1378 (w), 1345 (w), 1317 (w), 1276 (w), 1247 (w), 1209 (w), 1177 (w), 1155 (w), 1121 (w), 1047 (w), 1025 (m), 915 (m), 893 (m), 835 (m), 816 (m), 776 (m), 738 (m), 722 (m), 613 (m), 575 (m), 494 (s), 455 (s), 418 (s), 408 (s).

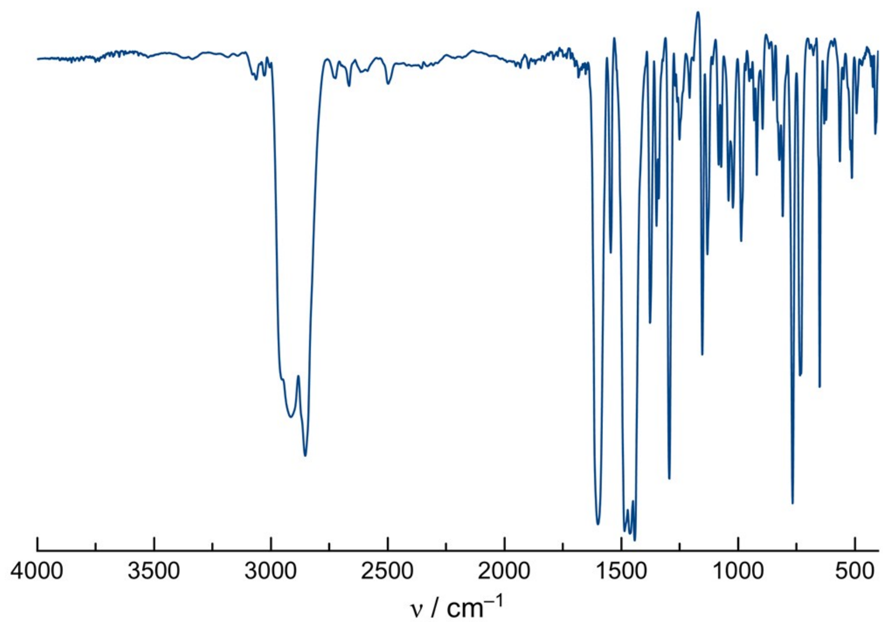


Figure S34. FT-IR spectrum of **1**. ν / cm^{-1}: 1599 (s), 1545 (m), 1487 (s), 1463 (s), 1442 (s), 1377 (m), 1349 (m), 1338 (m), 1293 (s), 1252 (w), 1209 (w), 1153 (s), 1130 (m), 1083 (w), 1071 (w), 1040 (w), 1022 (w), 986 (m), 931 (w), 920 (w), 896 (w), 850 (w), 824 (w), 808 (w), 767 (s), 730 (s), 650 (s), 631 (w), 622 (w), 564 (w), 512 (w), 493 (w), 411 (w).

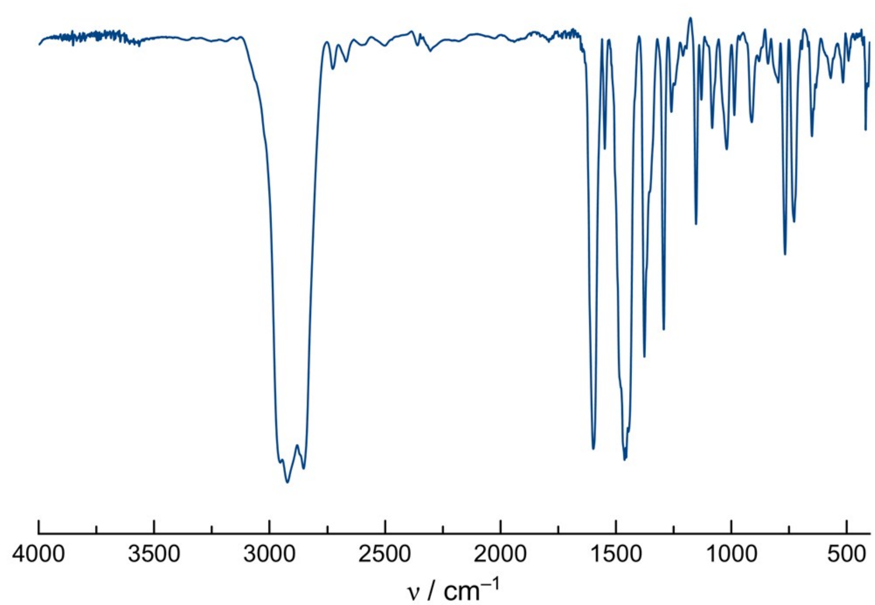


Figure S35. FT-IR spectrum of **2**. ν / cm^{-1}: 1598 (s), 1549 (w), 1461 (s), 1376 (s), 1292 (s), 1260 (w), 1244 (w), 1210 (w), 1194 (w), 1153 (m), 1130 (w), 1085 (w), 1022 (m), 989 (w), 912 (m), 880 (w), 842 (w), 796 (w), 767 (m), 728 (m), 650 (w), 569 (w), 516 (w), 494 (w), 418 (w).

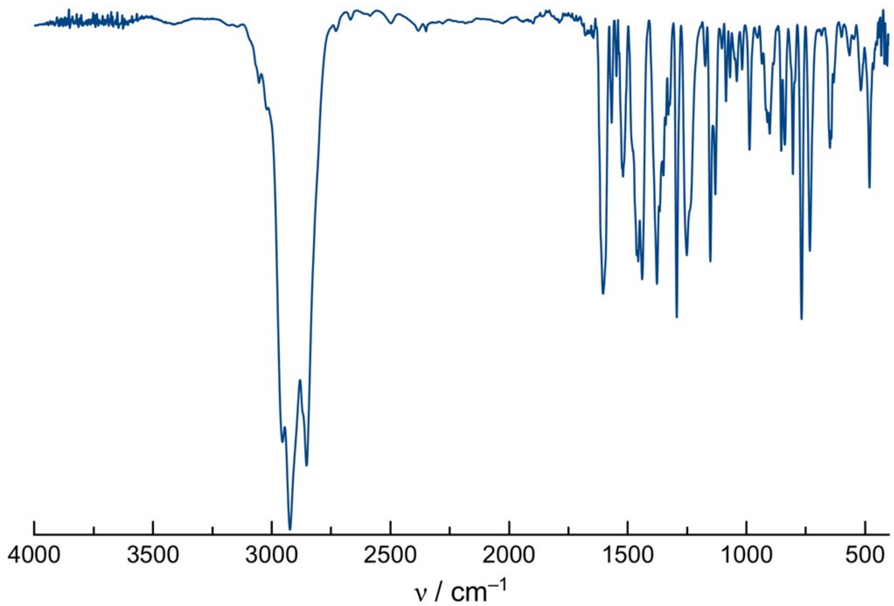


Figure S36. FT-IR spectrum of **3**. ν / cm^{-1}: 1604 (s), 1568 (m), 1549 (w), 1519 (m), 1463 (s), 1441 (s), 1377 (s), 1350 (m), 1328 (w), 1293 (s), 1250 (s), 1175 (w), 1152 (s), 1130 (m), 1106 (w), 1088 (w), 1068 (w), 1041 (w), 1017 (w), 987 (m), 934 (w), 902 (m), 853 (m), 838 (m), 805 (m), 796 (s), 732 (s), 647 (mO, 599 (w), 566 (w), 519 (w), 482 (s).

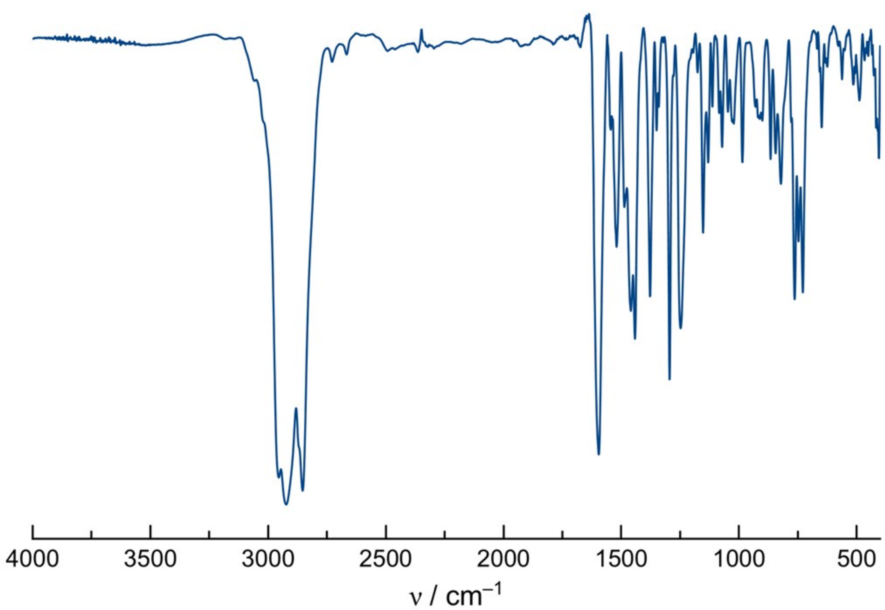


Figure S37. FT-IR spectrum of **5**. ν / cm^{-1}: 1594 (s), 1545 (m, sh), 1518 (s), 1486 (s, sh), 1462 (s), 1442 (s), 1378 (s), 1350 (w), 1339 (w), 1295 (s), 1248 (s), 1153 (s), 1131 (m), 1112 (w), 1084 (w), 1071 (w), 1047 (w), 1020 (w), 985 (m), 912 (m), 866 (m), 845 (m), 823 (m), 763 (s), 746 (m), 729 (s), 649 (w), 625 (w), 563 (w), 515 (w), 489 (w).

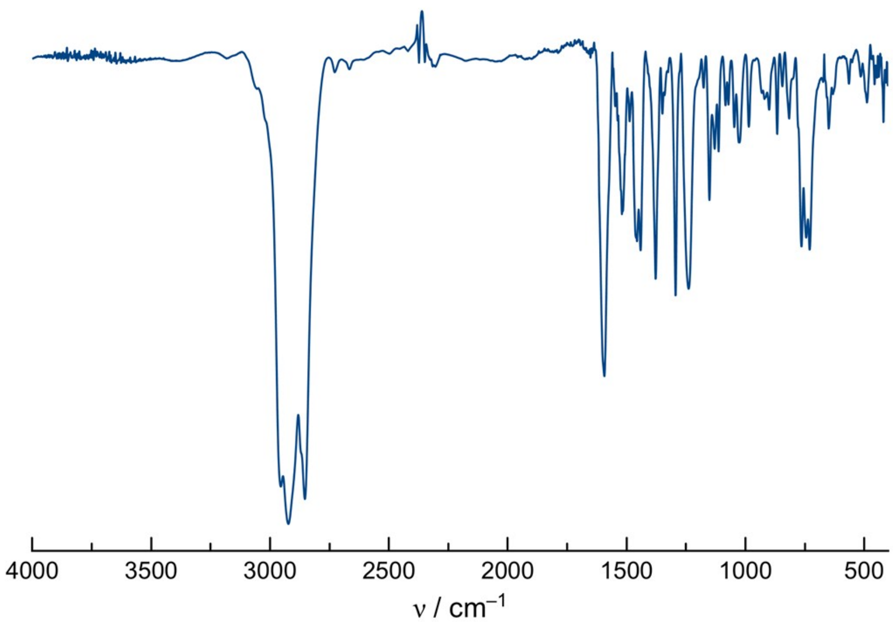


Figure S38. FT-IR spectrum of **6**. ν / cm^{-1}: 1594 (s), 1520 (m), 1489 (w), 1456 (m), 1443 (m), 1378 (s), 1351 (w), 1294 (s), 1240 (s), 1176 (w), 1150 (m), 1128 (w), 1112 (w), 1084 (w), 1071 (w), 1049 (w), 1025 (w), 985 (w), 921 (w), 900 (w), 868 (w), 844 (w), 817 (w), 764 (s), 743 (s), 729 (s), 649 (w), 625 (w), 565 (w), 517 (w), 489 (w), 457 (w), 418 (w).

X-ray crystallographic details

Table S1. X-ray crystallographic details for **1**, **2**, **2-dimer** and **3**.

	1	**2**	**2-dimer**	**3**
Chemical formula	$C_{42}H_{48}N_{14}Cl_2Th_2$	$2(C_{25}H_{32}N_7O_1U_1)\ 3(C_4H_8O_1)$	$C_{42}H_{48}N_{14}I_2U_2$	$C_{72}H_{84}N_{16}O_2Th_2$
M_r / g mol^{-1}	1283.92	1839.32	1478.80	1669.63
Crystal system	Monoclinic	Triclinic	Monoclinic	Monoclinic
Space group	P2(1)/n	P-1	P2(1)/n	C2/c
a / Å	13.3667(4)	12.6307(6)	13.6661(9)	27.6164(6)
b / Å	9.8584(3)	14.3188(6)	9.5267(6)	16.1837(3)
c / Å	16.0849(5)	18.4904(8)	16.578(1)	22,0451(5)
α / deg	90	90.085(2)	90	90
β / deg	95.518(1)	104.405(2)	94.929(3)	127.690(1)
γ / deg	90	90.085(2)	90	90
V / Å^3	2107.6(1)	3238.8(3)	2150.4(2)	7796.8(3)
Z	2	2	2	4
ρ / g cm^{-3}	2.021	1.886	2.284	1.422
F(000)	1224	1776	1376	13296
Radiation Type	MoK(α)	MoK(α)	MoK(α)	MoK(α)
μ / mm^{-1}	7.218	6.006	9.007	3.861
Crystal size / cm^3	0.2 × 0.1 × 0.05	0.15 × 0.13 × 0.11	0.1 × 0.08 × 0.07	0.09 × 0.07 × 0.05
Meas. Refl.	16056	75321	29570	34355
Indep. Refl.	4272	17397	3953	8062
Obsvd. [$I > 2\sigma(I)$] refl.	3920	11675	3585	5832
R_{int}	0.0437	0.0807	0.0957	0.0736
R [$F^2 > 2\sigma(F^2)$], wR(F^2)	0.0222	0.0513	0.0330	0.0423
S	0.0547	0.1109	0.0897	0.0934
G.O.F.	1.078	0.998	1.099	1.005
$\Delta\rho_{max}$ (e Å^{-3})	1.669	3.519	2.912	1.888
$\Delta\rho_{min}$ (e Å^{-3})	-0.852	-1.299	-1.239	-0.905
CCDC	1510088	1516433	1510089	1510091

Table S2. X-ray crystallographic details for **5**, **6** and **6⁻**.

	5	**6**	**6⁻**
Chemical formula	$C_{70}H_{78}N_{16}O_6Th_2$ $2(C_4H_6O)$	$C_{62}H_{64}N_{16}O_4U_2$	$[K(C_{18}H_{36}O_6)(C_4H_8O)_2][C_{62}H_{64}N_{16}O_4U_2]$ $2(C_4H_8O)$
M_r / g mol^{-1}	1843.73	1573.35	216517
Crystal system	Monoclinic	Orthorhombic	Triclinic
Space group	P2(1)/n	Pbca	P-1
a / Å	15.278(1)	9.590(1)	10.1836(3)
b / Å	13.533(2)	20.906(1)	13.3551(4)
c / Å	18.313(1)	28.940(2)	17.9008(5)
α / deg	90	90	110.811(1)
β / deg	90.453(5)	90	91.963(1)
γ / deg	90	90	100.295(1)
V / Å^3	3786.1(6)	5802.3(6)	2226.4(1)
Z	2	4	1
ρ / g cm^{-3}	1.617	1.801	1.615
F(000)	1828	3056	1087
Radiation Type	MoK(α)	MoK(α)	MoK(α)
μ / mm^{-1}	3.990	5.369	3.752
Crystal size / cm^3	0.09 × 0.09 × 0.07	0.05 × 0.04 × 0.01	0.12 × 0.08 × 0.04
Meas. Refl.	125549	55064	96441
Indep. Refl.	6960	5360	8165
Obsvd. [$I > 2\sigma(I)$] refl.	5909	3859	7510
R_{int}	0.0558	0.0898	0.0413
R [$F^2 > 2\sigma(F^2)$], wR(F^2)	0.0379	0.0454	0.0374
S	0.0918	0.1080	0.0958
G.O.F.	1.073	1.044	1.074
$\Delta\rho_{max}$ (e Å^{-3})	2.381	2.660	2.559
$\Delta\rho_{min}$ (e Å^{-3})	-1.050	-0.628	-1.406
CCDC	1526526	1526524	1526525

Table S3. Selected bonds lengths (in Å) and angles (in degrees) for all complexes characterised crystallographically.

Atoms	1	2	2-dimer	3	5	6	6⁻
M1 – Cl1/I1	2.912(8)	3.215(1)	3.311(1)	-	-	-	-
M1 – Cl1/I1		-		-	-	-	-
M1 – O100	-	2.562(5)	-	-	2.678(5)	-	-
M1 – N1	2.783(3)	2.789(5)	2.725(5)	2.904(4)	2.920(5)	2.831(5)	2.901(5)
M1 – N10	2.394(3)	2.343(5)	2.327(5)	2.434(5)	2.462(5)	2.355(6)	2.425(5)
M1 – N11	2.665(3)	2.613(5)	2.637(5)	2.593(4)	2.731(4)	2.604(6)	2.672(5)
M1 – N20	2.408(3)	2.357(5)	2.328(5)	2.433(4)	2.415(5)	2.344(6)	2.425(4)
M1 – N21	2.670(3)	2.597(5)	2.609(4)	2.582(4)	2.661(4)	2.605(6)	2.640(4)
M1 – N30	2.373(3)	2.327(5)	2.304(5)	2.442(4)	2.453(4)	2.360(6)	2.372(4)
M1 – N31	2.621(3)	2.563(5)	2.584(4)	2.604(4)	2.623(5)	2.578(6)	2.617(5)
M1 – O1	-	-		2.398(3)	2.376(4)	2.400(5)	2.263(3)
M1 – N2	-	-		2.687(4)	2.671(4)	2.497(5)	2.505(4)
C1 – C2	-	-		1.499(7)	1.504(7)	1.491(9)	1.449(7)
C2 – C3	-	-		1.423(7)	1.420(7)	1.413(9)	1.409(6)
C3 – C1	-	-		1.378(6)	1.370(7)	1.363(9)	1.388(6)
C1 – O1	-	-		1.277(6)	1.296(6)	1.288(7)	1.321(6)
C2 – N2	-	-		1.315(6)	1.299(7)	1.312(8)	1.360(6)
N2 – C40	-	-		1.456(6)	1.432(7)	1.442(8)	1.425(6)
M1 – M1	4.612(1)	-	5.125(1)	9.070(1)	9.053(1)	8.904(1)	8.850(1)
O1 - M1 – N1	-	-	-	179(9(1)	178.8(1)	173.6(2)	164.0(2)
O1 – M1 – N2	-	-	-	62.8(1)	62.8(1)	64.0(2)	65.7(1)

Cyclic voltamogramms

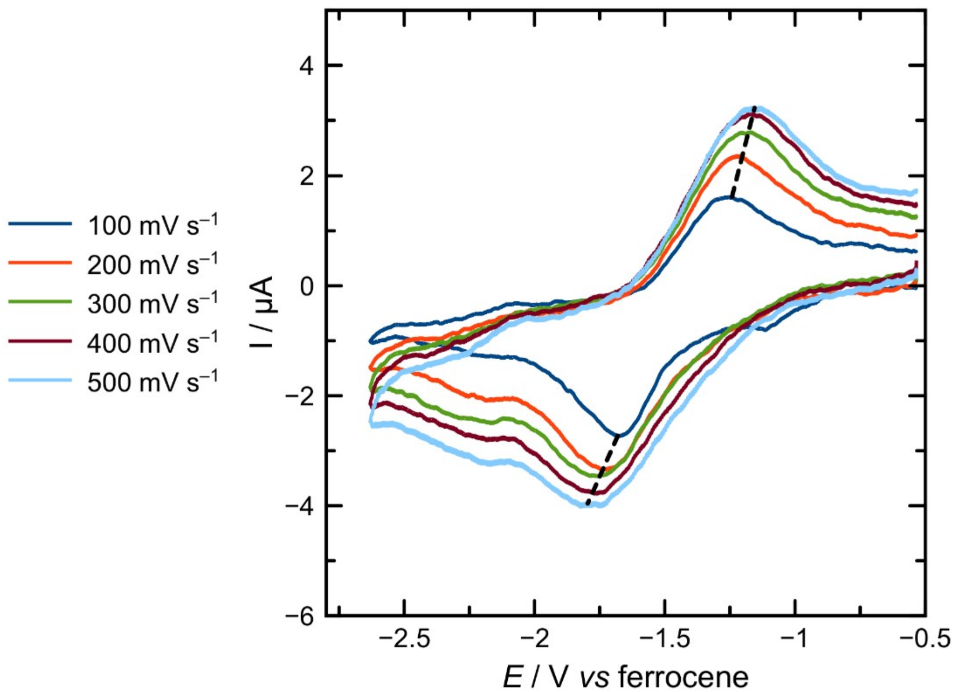


Figure S39. CVs of **5**, showing the reduction process at variable scan rates.

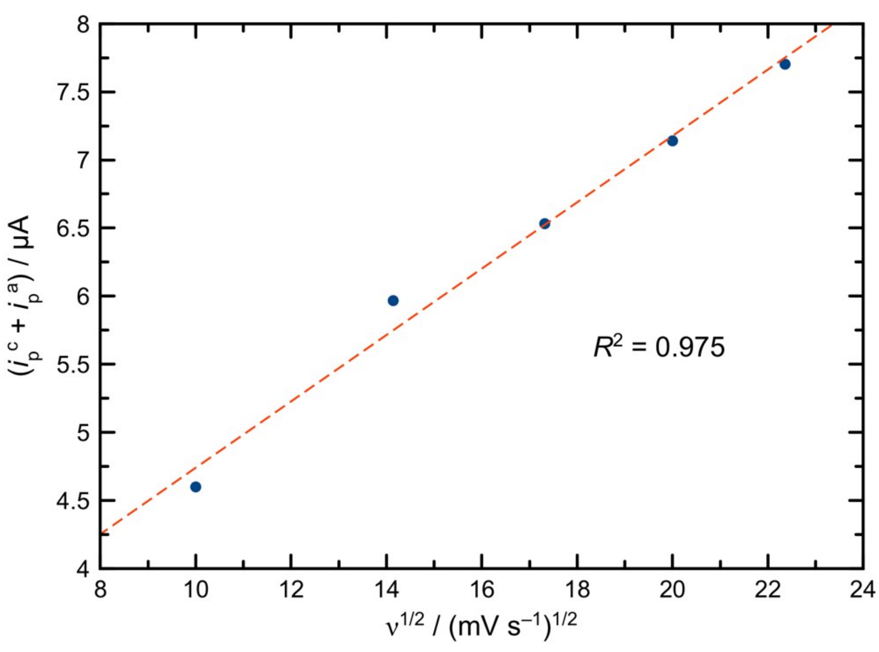


Figure S40. Plot of peak current against $\nu^{1/2}$ for the reduction of **5**. The linear response shows that the process is diffusion-controlled and suggests reversibility.

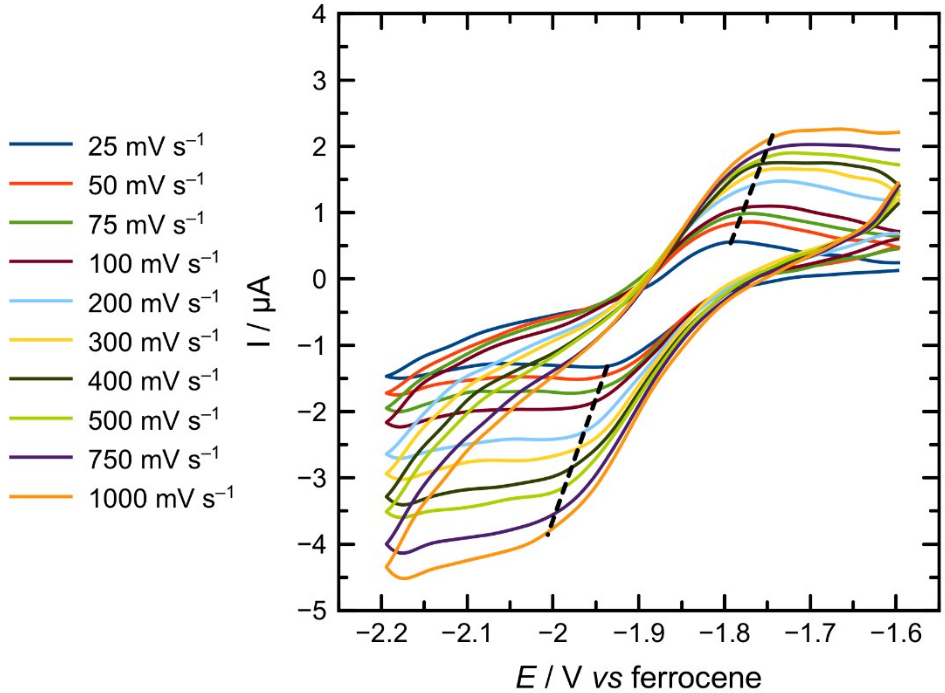


Figure S41. CVs of **6**, showing the reduction process at variable scan rates.

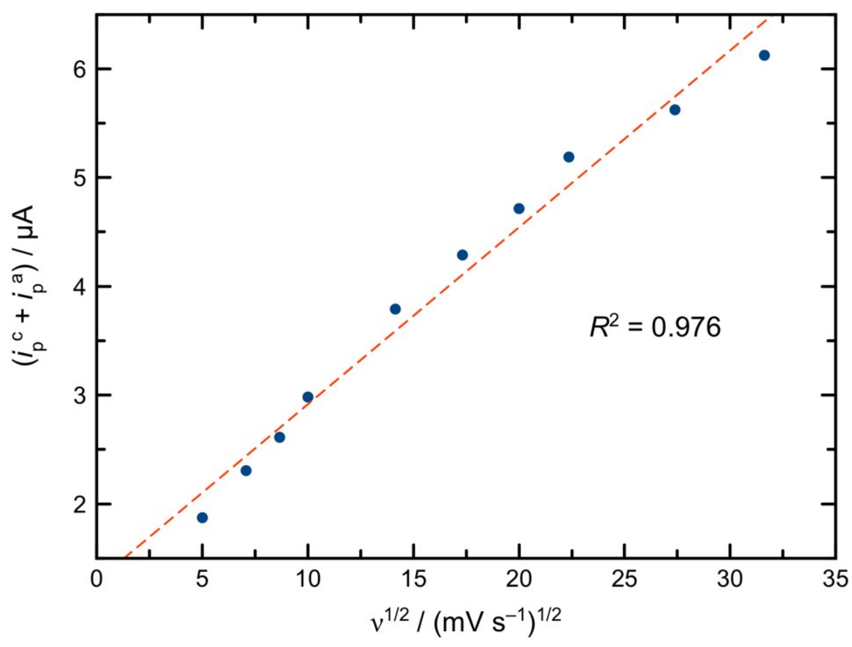


Figure S42. Plot of peak current against $\nu^{1/2}$ for the reduction of **6**. The linear response shows that the process is diffusion-controlled and suggests reversibility.

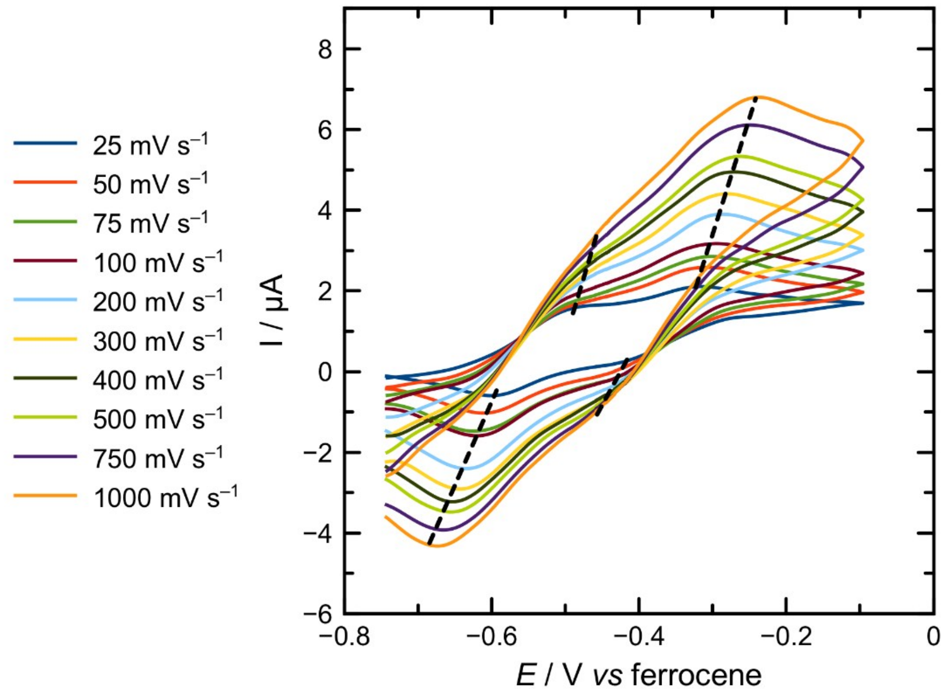


Figure S43. CVs of **6**, showing the two oxidation processes at variable scan rates.

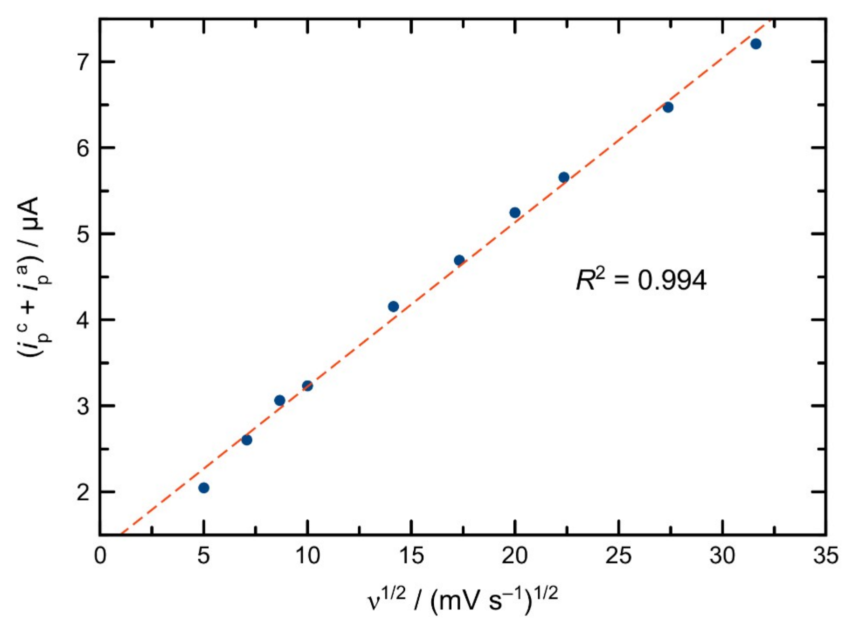


Figure S44. Plot of peak current against $\nu^{1/2}$ for the first oxidation of **6**. The linear response shows that the process is diffusion-controlled and suggests reversibility.

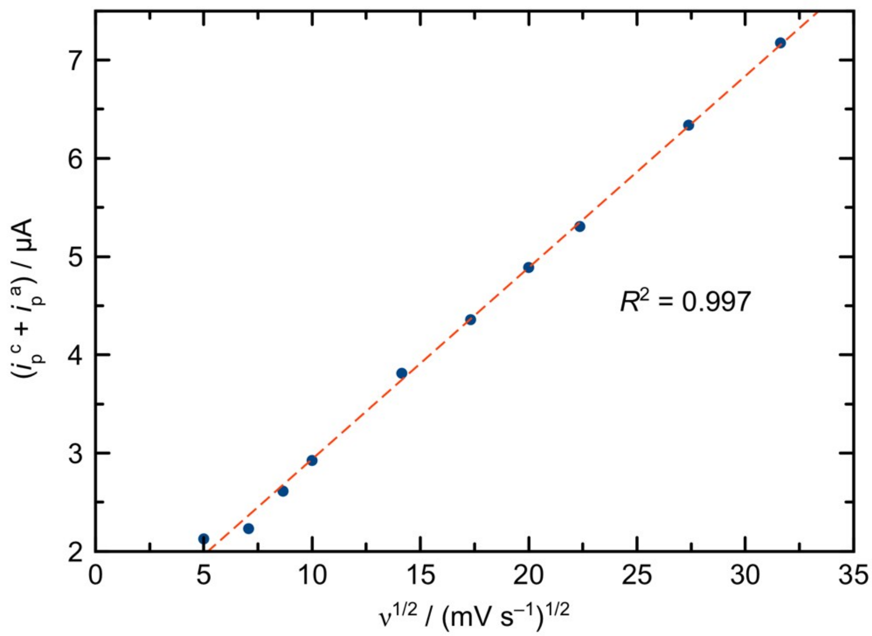


Figure S45. Plot of peak current against $\nu^{1/2}$ for the second oxidation of **6**. The linear response shows that the process is diffusion-controlled and suggests reversibility.

Magnetism

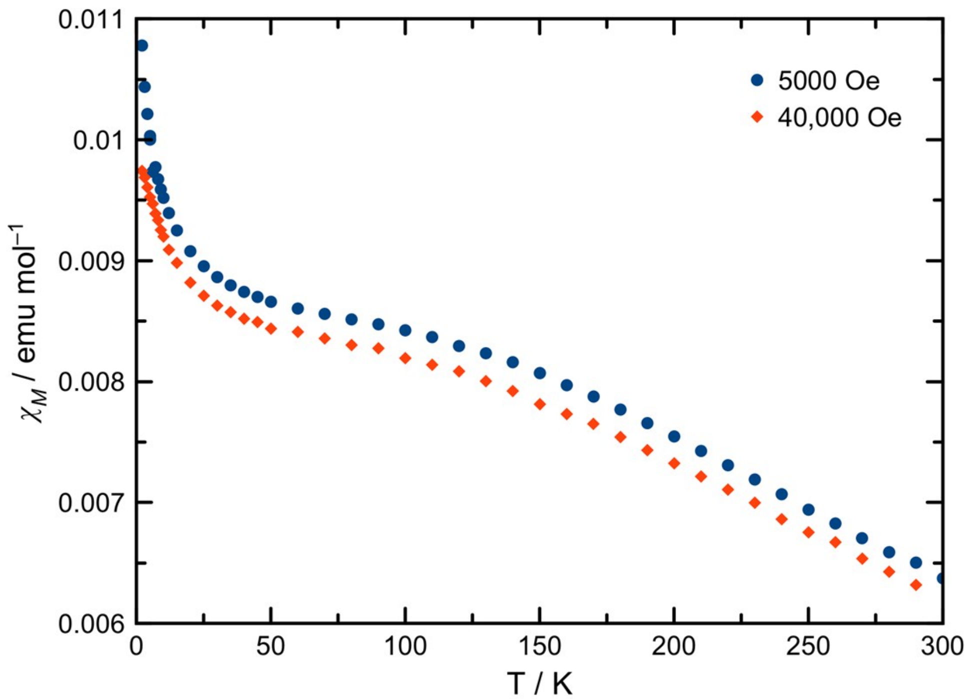


Figure S46. Variable-temperature DC magnetic susceptibility plot for **2-dimer**.

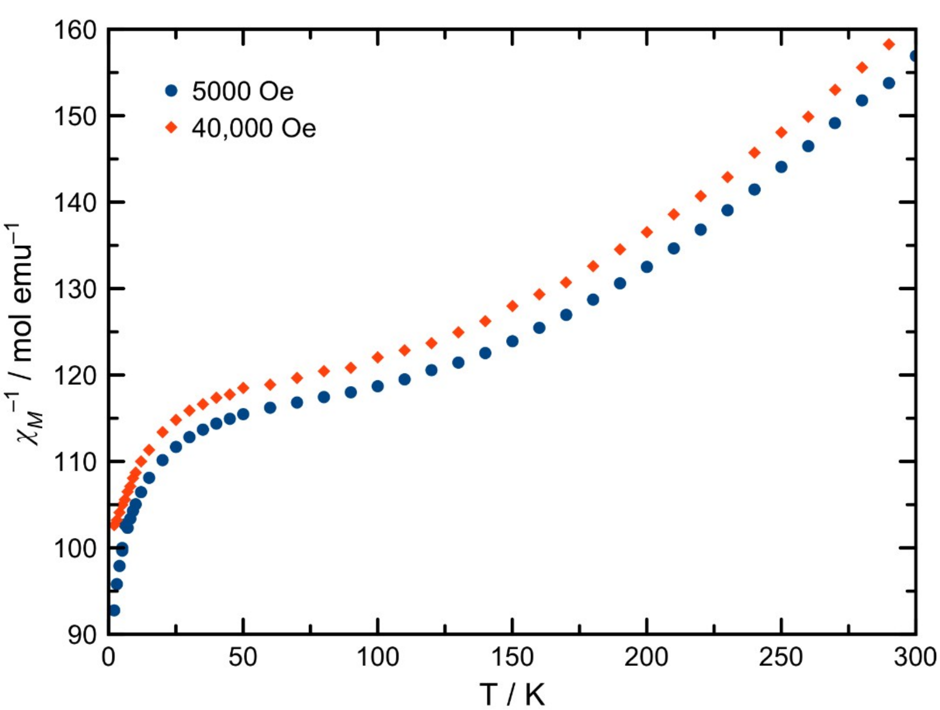


Figure S47. Variable-temperature DC magnetic inverse susceptibility plot for **2-dimer**.

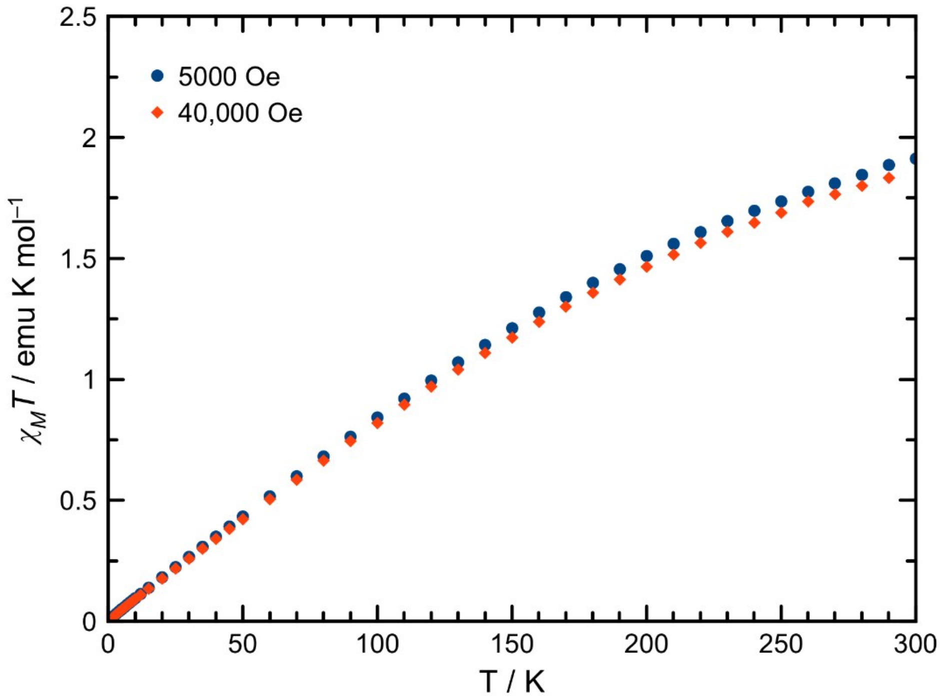


Figure S48. Variable-temperature DC magnetic susceptibility plot for **2-dimer**.

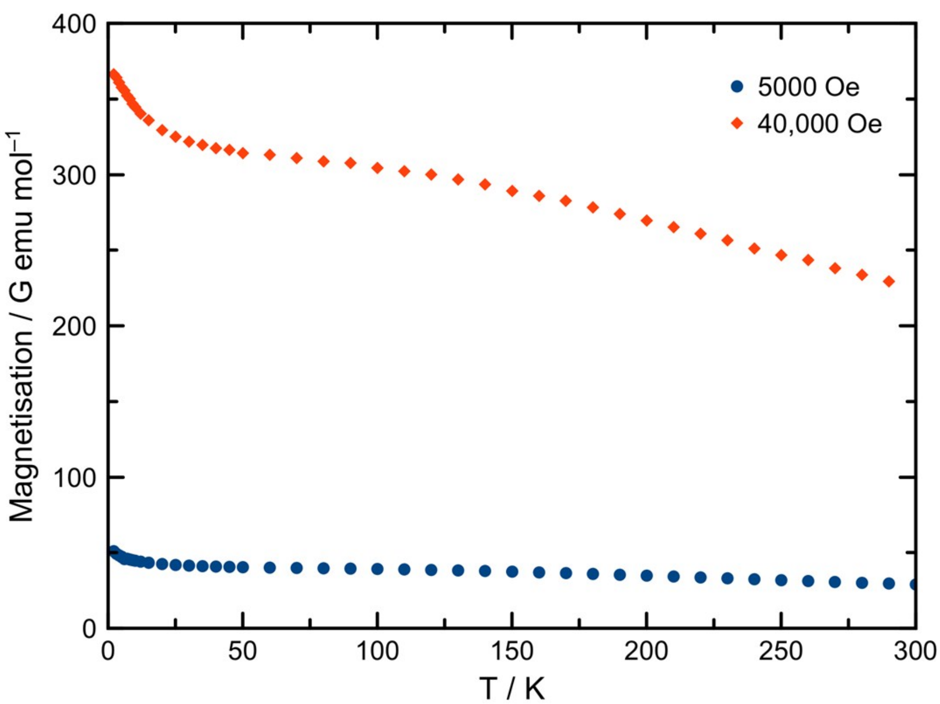


Figure S49. Variable-temperature magnetisation plot for **2-dimer**.

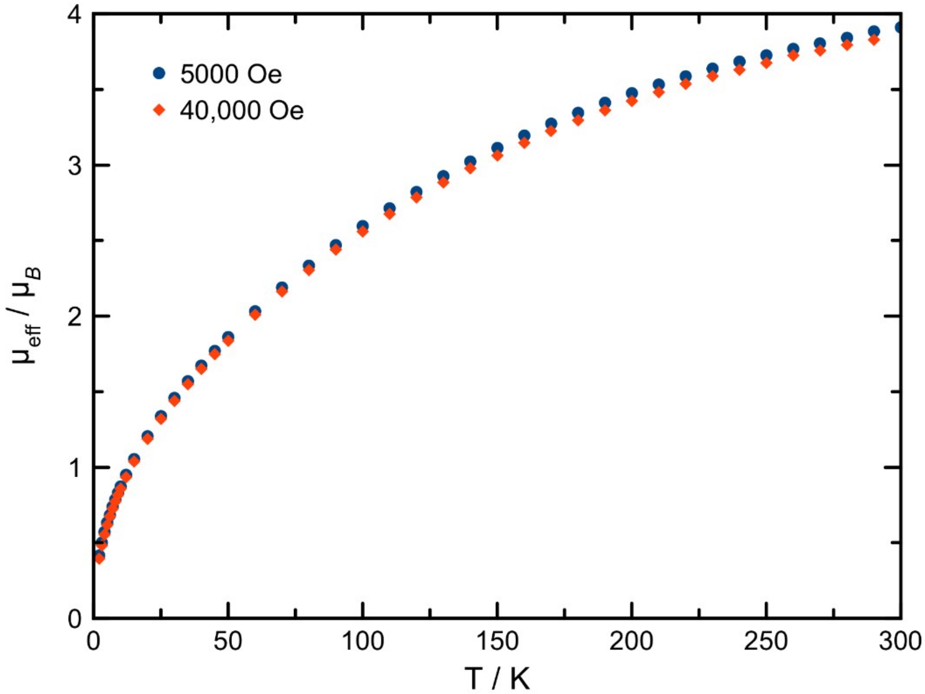


Figure S50. Temperature dependence of the magnetic moment for **2-dimer**.

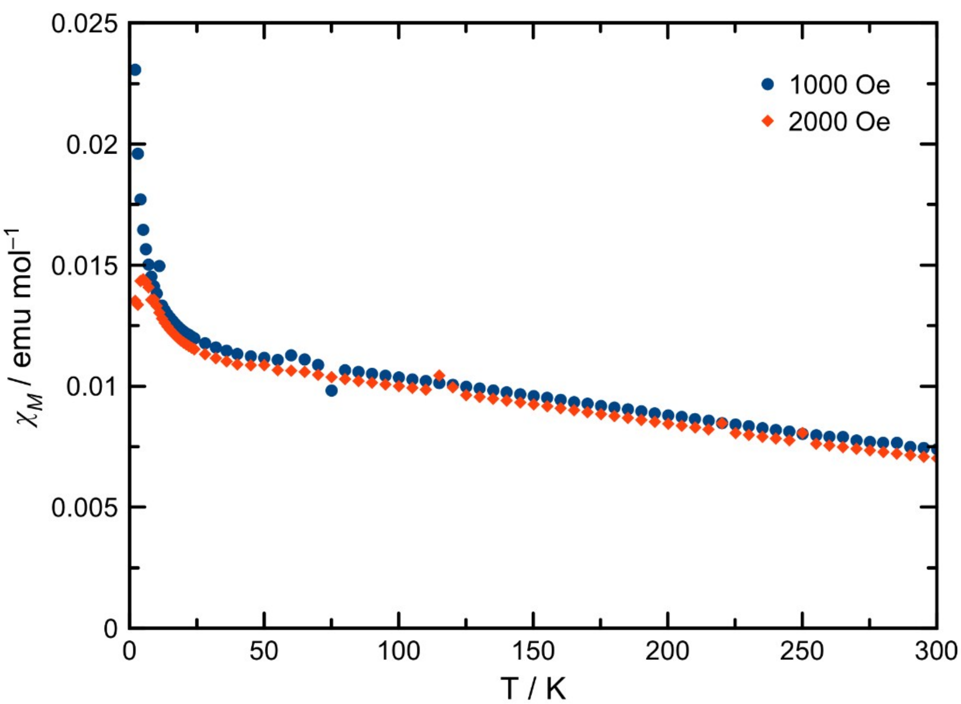


Figure S51. Variable-temperature DC magnetic susceptibility plot for **6**.

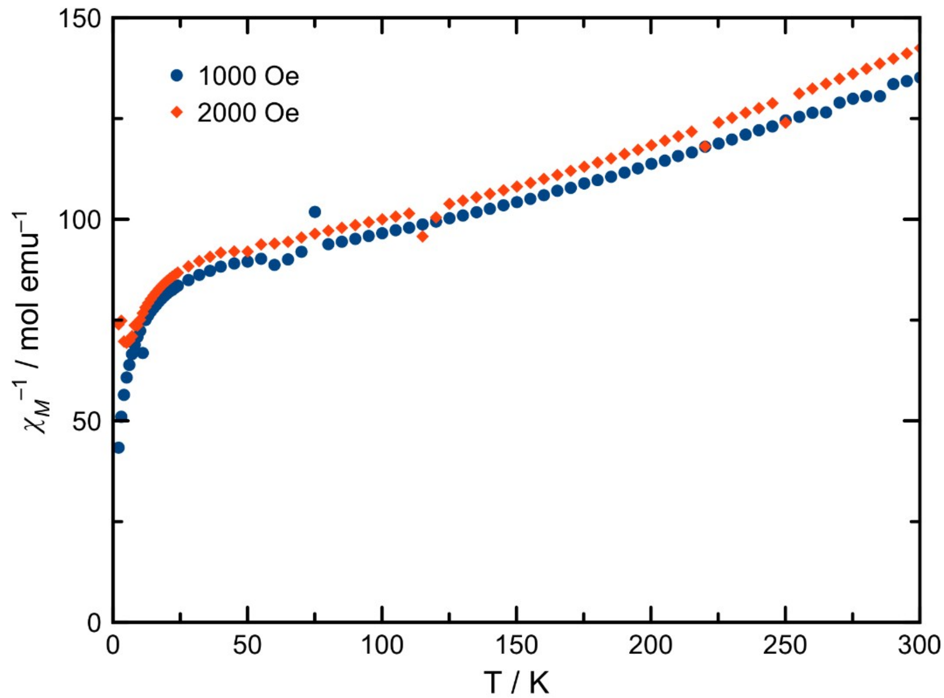


Figure S52. Variable-temperature inverse DC magnetic susceptibility plot for **6**.

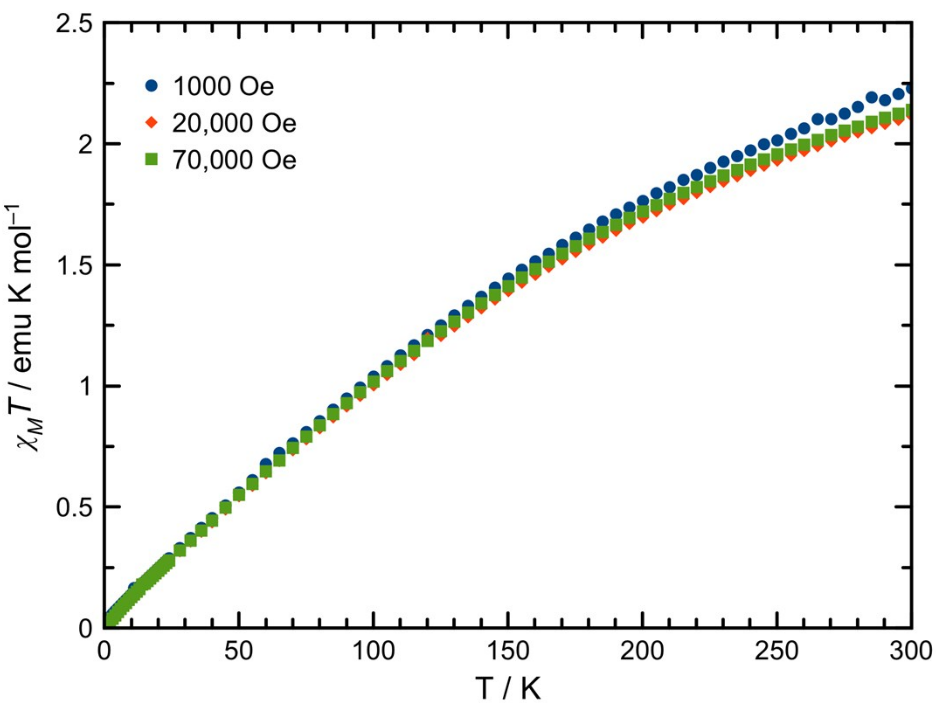


Figure S53. Variable-temperature DC magnetic susceptibility plot for **6**.

Figure S54. Variable-temperature magnetisation plot for **6**.

Figure S55. Temperature dependence of the magnetic moment for **6**.

Computational results

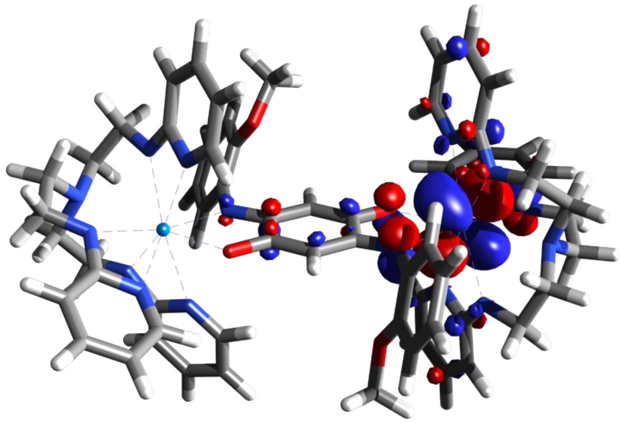


Figure S56. SOMO of **6**. *E* = –0.091173 Ha.

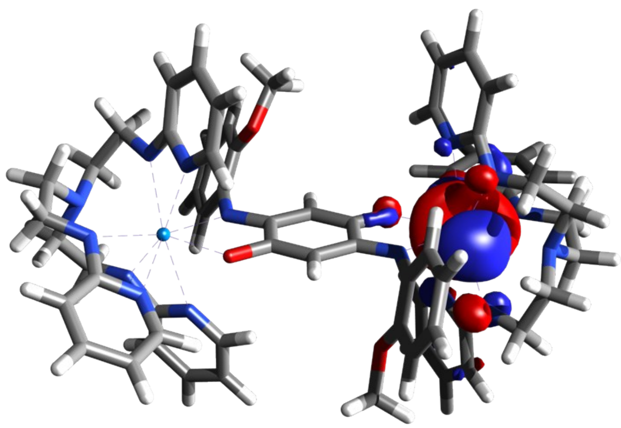


Figure S57. SOMO-1 of **6**. *E* = –0.118482 Ha.

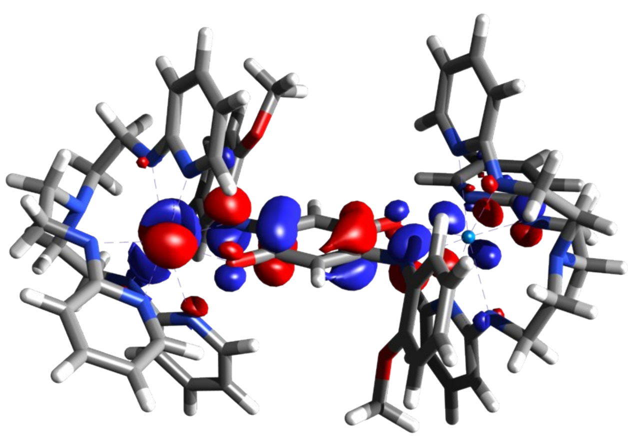


Figure S58. SOMO-2 of **6**. *E* = –0.128469 Ha.

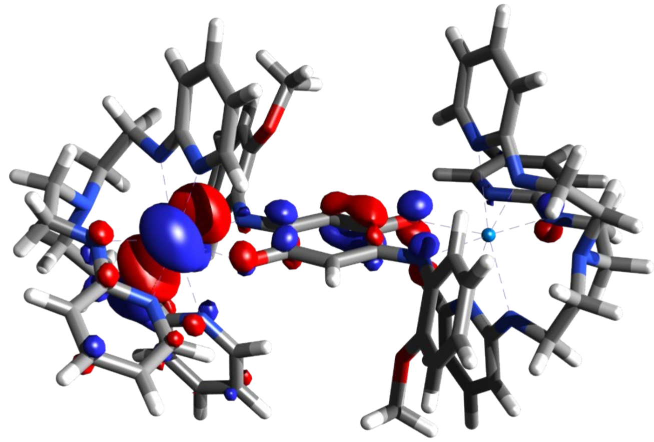


Figure S59. SOMO-3 of **6**. E = –0.150487 Ha.

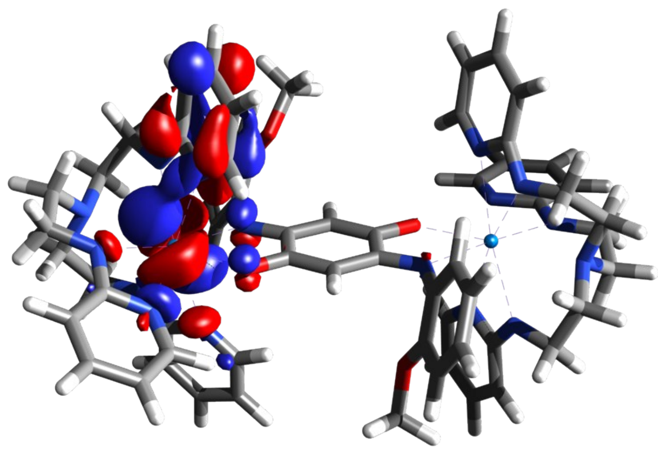


Figure S60. LUMO for **6**. E = –0.046756 Ha.

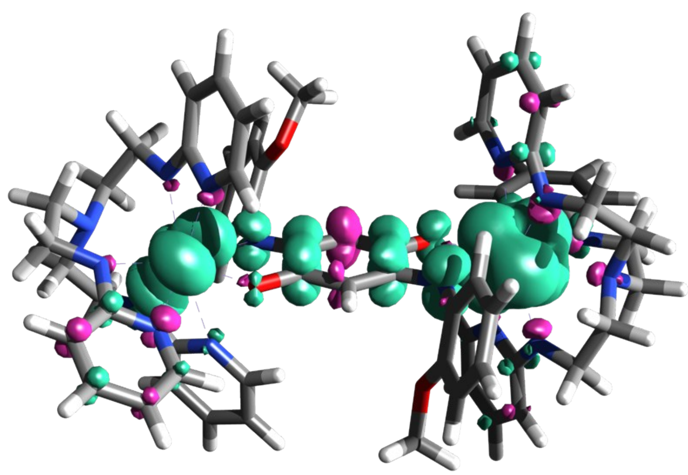


Figure S61. Spin-density plot for **6**, ρ(α)-ρ(β).

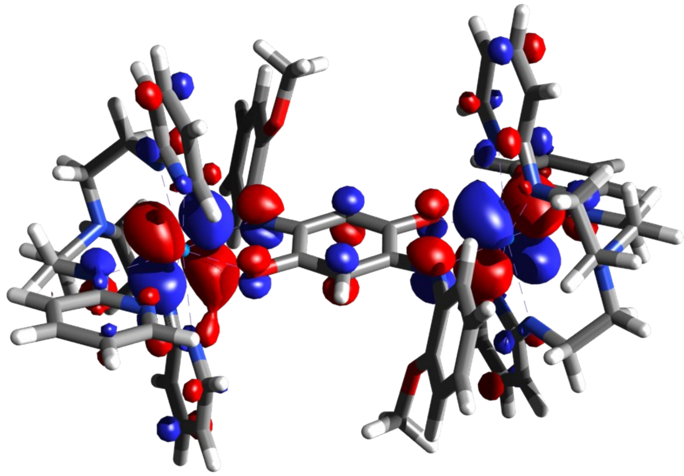


Figure S62. SOMO of **6**⁻ (quartet). E = –0.013037956 Ha.

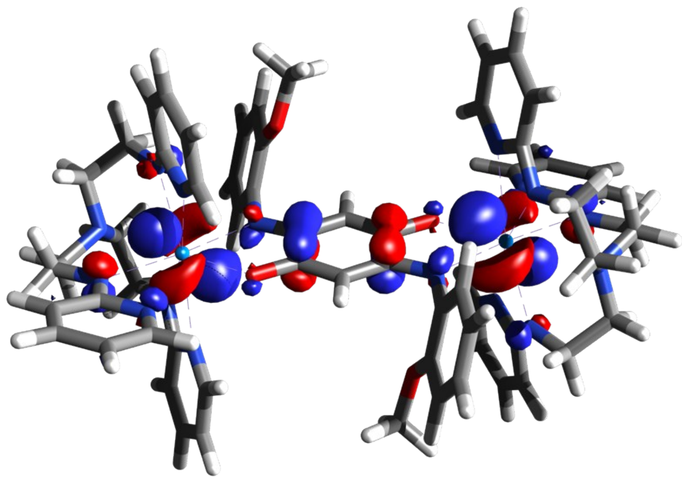


Figure S63. SOMO-1 of **6**⁻ (quartet). E = –0.045652464 Ha.

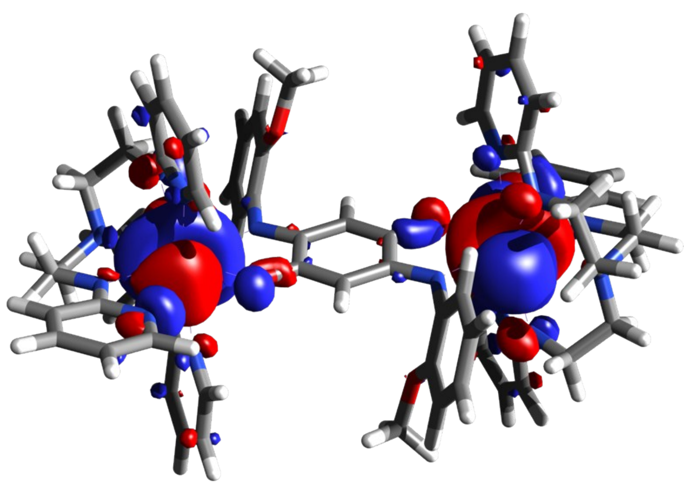


Figure S64. SOMO-2 of **6**⁻ (quartet). E = –0.04861292 Ha.

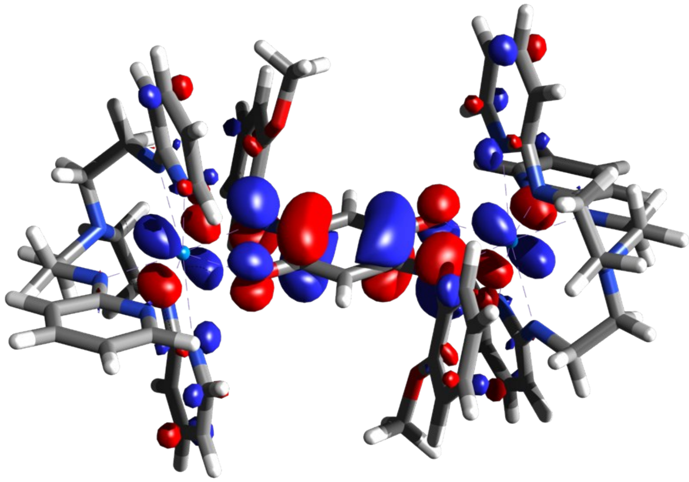


Figure S65. LUMO of **6**⁻ (quartet). E = 0.03518556 Ha.

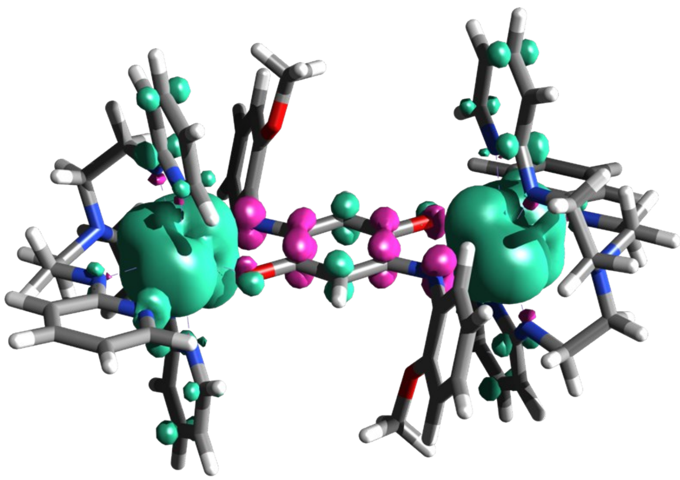


Figure S66. Spin-density plot for **6**⁻ (quartet), ρ(α)-ρ(β).

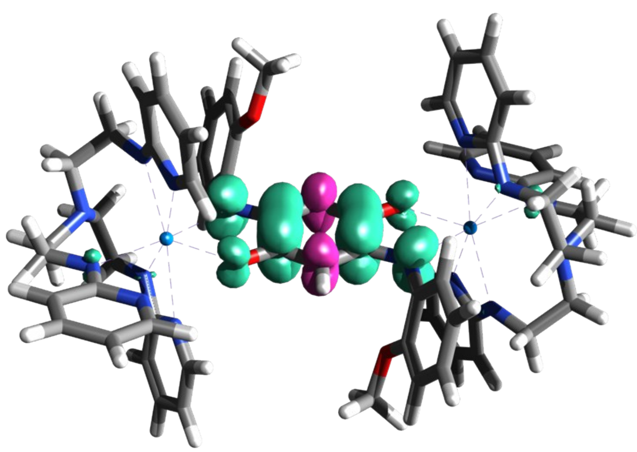


Figure S67. Spin-density difference-plot for ρ(**6**⁻)-ρ(**6**).

Optimised coordinates for 6 (*E* = –3678.46007669 Ha). Charge = 0; multiplicity = 5.

C	-1.340713	-0.721588	0.355875	C	-1.286498	0.542851	-0.335737
C	1.078332	-0.815320	0.457337	C	-0.040147	1.091872	-0.649980
C	-0.189619	-1.373287	0.747307	H	0.036515	2.023008	-1.199434
H	-0.267027	-2.313134	1.282602	C	-2.608562	2.327538	-1.268849
C	-7.586147	0.840722	-1.494424	C	-2.206686	3.506293	-0.587758
H	-8.376735	1.536746	-1.821665	C	-2.343721	4.751844	-1.205993
H	-8.064649	-0.106384	-1.232055	H	-2.028791	5.652734	-0.690397
C	-6.597516	0.567856	-2.620851	C	-2.890636	4.849228	-2.487859
H	-7.117722	-0.013259	-3.397042	H	-2.987748	5.826633	-2.952395
H	-6.276459	1.507997	-3.100830	C	-3.296055	3.703534	-3.162800
C	-4.671513	-0.918776	-2.810526	H	-3.704664	3.770331	-4.167065
C	-4.694690	-1.238641	-4.186172	C	-3.147423	2.456724	-2.551892
H	-5.468580	-0.845385	-4.836207	H	-3.427132	1.548225	-3.075904
C	-3.691424	-2.059426	-4.676513	C	-1.127518	4.432166	1.317106
H	-3.685061	-2.320005	-5.732083	H	-1.864932	5.215297	1.541121
C	-2.680799	-2.545326	-3.834368	H	-0.722344	4.044521	2.252246
H	-1.881943	-3.173009	-4.211487	H	-0.313224	4.865931	0.723193
C	-2.717131	-2.178601	-2.495404	N	-2.514932	1.060809	-0.658018
H	-1.954906	-2.492053	-1.787011	O	2.310469	0.955971	-0.553250
C	-6.464595	2.729250	-0.435630	O	-1.714890	3.328599	0.662008
H	-7.318464	3.420464	-0.531745	C	7.014263	-0.860680	2.214854
H	-5.876237	2.799743	-1.355613	H	7.737783	-1.581206	2.630255
C	-5.581318	3.130509	0.750430	H	7.517829	0.105546	2.129866
H	-4.950439	3.978606	0.446967	C	5.799850	-0.676037	3.128564
H	-6.199388	3.483272	1.592125	H	6.135885	-0.214429	4.067241
C	-4.230150	1.841693	2.336726	H	5.370065	-1.651260	3.396551
C	-4.091864	2.759595	3.396707	C	4.576489	1.414099	2.691593
H	-4.466914	3.772801	3.304441	C	4.777411	2.176303	3.863056
C	-3.436792	2.330201	4.541991	H	5.221887	1.729389	4.746334
H	-3.311758	3.018615	5.374312	C	4.370155	3.501195	3.860135
C	-2.921448	1.030990	4.632591	H	4.510439	4.104887	4.753949
H	-2.394784	0.689862	5.516097	C	3.776011	4.065878	2.721180
C	-3.100148	0.182311	3.547396	H	3.454061	5.101233	2.704543
H	-2.722524	-0.836092	3.538463	C	3.625007	3.261164	1.600179
C	-7.725482	1.137542	0.911197	H	3.194643	3.628579	0.673342
H	-8.738715	1.549740	0.774328	C	6.340507	-2.727866	0.816408
H	-7.253624	1.687793	1.726073	H	7.259856	-3.293498	1.039752
C	-7.795847	-0.336188	1.317221	H	5.614847	-2.943578	1.606223
H	-8.157036	-0.381107	2.357945	C	5.753241	-3.163434	-0.531134
H	-8.545737	-0.874268	0.712684	H	5.247801	-4.131830	-0.382225
C	-6.302513	-2.238419	1.087350	H	6.558412	-3.346642	-1.263182
C	-7.127492	-3.314087	1.481026	C	4.514379	-1.929329	-2.248553
H	-8.106733	-3.125446	1.907540	C	4.658120	-2.760992	-3.379949
C	-6.632939	-4.600667	1.342968	H	5.110261	-3.743246	-3.287492
H	-7.245036	-5.444604	1.651321	C	4.190240	-2.290470	-4.598325
C	-5.346228	-4.825604	0.827000	H	4.285688	-2.913482	-5.484939
H	-4.944285	-5.827076	0.726040	C	3.592888	-1.025560	-4.695327
C	-4.598595	-3.728172	0.431032	H	3.219248	-0.646024	-5.639771
H	-3.601638	-3.821384	0.012723	C	3.499453	-0.257307	-3.540509
C	2.348740	-2.578633	1.439066	H	3.064710	0.738113	-3.540325
C	2.078365	-3.781253	0.738071	C	7.623545	-0.881342	-0.141683
C	2.238015	-5.013314	1.377571	H	8.621859	-1.230094	0.171328
H	2.034600	-5.935760	0.844161	H	7.370334	-1.379035	-1.079738
C	2.659245	-5.070147	2.708631	C	7.637545	0.619681	-0.402817

H	2.774328	-6.037807	3.189538
C	2.923816	-3.897899	3.407858
H	3.241511	-3.935027	4.446218
C	2.768085	-2.665956	2.769041
H	2.967393	-1.731922	3.286274
C	1.467675	-4.801338	-1.316857
H	2.372714	-5.420895	-1.374467
H	1.209515	-4.458821	-2.319999
H	0.645061	-5.411788	-0.918633
N	-6.902919	1.334367	-0.293732
N	2.270095	-1.327251	0.805758
N	-5.485346	-0.149892	-2.067864
N	-3.684823	-1.403175	-2.008052
N	-4.810160	1.978799	1.126624
N	-3.753321	0.571913	2.454134
N	-6.492890	-0.912178	1.148975
N	-5.076737	-2.483770	0.528565
O	-2.556274	-1.242382	0.590997
O	1.677406	-3.637928	-0.551172
U	-4.427091	-0.134742	0.109093
C	1.141230	0.450083	-0.269368
H	8.314180	0.776320	-1.258778
H	8.101653	1.161586	0.442050
C	6.164082	2.279450	-1.318346
C	7.228265	3.149737	-1.681177
H	8.255215	2.910245	-1.427704
C	6.936875	4.327791	-2.348351
H	7.746120	4.999087	-2.628520
C	5.612107	4.655277	-2.650956
H	5.350210	5.569394	-3.173414
C	4.631720	3.754206	-2.240049
H	3.578657	3.959339	-2.437611
N	6.603118	-1.271491	0.854015
N	4.836365	0.118220	2.423577
N	4.018901	1.986814	1.582844
N	4.870566	-2.125300	-0.968238
N	3.950623	-0.688105	-2.363516
N	6.303126	1.088649	-0.681853
N	4.879583	2.616161	-1.600949
U	4.315339	-0.051607	0.083075

Optimised coordinates for 6⁻ (E = –3678.52443260 Ha). Charge = –1; multiplicity = 4.

U	4.361740	-0.097258	0.171150
O	2.487540	1.071719	-0.328230
N	2.358242	-1.348934	0.554213
C	0.124084	1.330036	-0.475497
H	0.238624	2.341193	-0.851340
C	1.148749	-0.761610	0.298146
C	2.389503	-2.712010	0.896558
C	1.261315	0.587463	-0.179212
O	1.702348	-3.276839	-1.278599
N	4.161982	1.691944	1.973785
N	4.893531	-0.314331	2.526547
N	4.216204	-0.252551	-2.359430
N	6.498362	1.039075	-0.307216
O	4.660729	0.923857	2.990393
N	4.932047	-1.982071	-1.202231
N	5.245069	2.742861	-1.174984
O	2.072750	-3.718691	-0.053569
N	6.621291	-1.554551	0.900849
O	2.162736	-5.067748	0.299249
H	1.923406	-5.837245	-0.427309
C	6.479570	2.196485	-1.008408
C	3.829880	2.963528	2.186019
H	3.435692	3.492383	1.323087
C	2.774502	-3.114797	2.176900
H	2.988360	-2.328409	2.894370
C	3.991405	3.574503	3.424565
H	3.714063	4.613462	3.565974
C	4.522871	2.808270	4.472426
H	4.661627	3.255556	5.454670
C	5.720512	-1.263746	3.206401
H	5.178863	-1.858227	3.963107
H	6.544576	-0.768186	3.748783
C	4.863733	1.478504	4.274033
H	5.251847	0.866731	5.082286
C	2.561334	-5.438938	1.587033
H	2.621567	-6.493903	1.842886
C	4.726755	-1.521469	-2.443956
C	3.870261	0.416144	-3.459044
H	3.460653	1.408110	-3.293295
C	7.621051	2.843663	-1.565880
H	8.608093	2.402419	-1.478138
C	6.278085	-2.238195	2.161679
H	7.153439	-2.774476	2.568467
H	5.511531	-2.982882	1.925586
C	5.121966	3.885849	-1.837480
H	4.102095	4.262747	-1.931291
C	7.457613	4.036855	-2.248957
H	8.327701	4.531422	-2.678076
C	2.866764	-4.464214	2.529406
H	3.159916	-4.743749	3.538087
C	4.034647	-0.115358	-4.731625
H	3.744857	0.453924	-5.607833
C	7.689536	-0.558888	1.094983
H	8.663246	-1.056071	1.253112

H	7.611199	-3.344793	0.303959
O	-2.487537	-1.071716	0.328231
N	-2.358239	1.348936	-0.554213
O	-0.124082	-1.330033	0.475498
H	-0.238622	-2.341190	0.851341
C	-1.148747	0.761613	-0.298145
C	-2.389499	2.712012	-0.896557
C	-1.261313	-0.587460	0.179214
O	-1.702351	3.276839	1.278602
C	-2.072749	3.718692	0.053572
C	-2.162734	5.067749	-0.299246
H	-1.923406	5.837245	0.427315
C	-2.774496	3.114800	-2.176899
H	-2.988352	2.328413	-2.894370
C	-2.561330	5.438940	-1.587029
H	-2.621562	6.493905	-1.842882
C	-2.866757	4.464217	-2.529405
H	-3.159907	4.743753	-3.538085
C	-1.277225	4.219854	2.231991
H	-2.082884	4.914211	2.510884
H	-0.981900	3.645292	3.110948
H	-0.415064	4.799245	1.874270
U	-4.361737	0.097260	-0.171152
N	-4.162001	-1.691948	-1.973775
N	-4.893527	0.314330	-2.526548
N	-4.216204	0.252549	2.359426
N	-6.498358	-1.039073	0.307212
O	-4.660733	-0.923861	-2.990389
N	-4.932045	1.982072	1.202230
N	-5.245065	-2.742857	1.174981
N	-6.621283	1.554554	-0.900854
O	-6.479566	-2.196482	1.008404
O	-3.829911	-2.963536	-2.186000
H	-3.435733	-3.492391	-1.323065
O	-3.991436	-3.574516	-3.424544
H	-3.714105	-4.613479	-3.565947
C	-4.522891	-2.808283	-4.472412
H	-4.661647	-3.255572	-5.454654
C	-5.720504	1.263747	-3.206405
H	-5.178853	1.858225	-3.963111
H	-6.544569	0.768189	-3.748786
C	-4.863740	-1.478512	-4.274027
H	-5.251845	-0.866740	-5.082284
C	-4.726759	1.521465	2.443954
C	-3.870265	-0.416149	3.459038
H	-3.460655	-1.408113	3.293289
C	-7.621046	-2.843659	1.565876
H	-8.608089	-2.402416	1.478133
C	-6.278075	2.238197	-2.161684
H	-7.153428	2.774479	-2.568472
H	-5.511521	2.982883	-1.925589
C	-5.121962	-3.885844	1.837477
H	-4.102090	-4.262742	1.931289
C	-7.457609	-4.036851	2.248953

H	7.451625	0.006923	1.998074
C	6.185062	4.595620	-2.396161
H	6.021079	5.527753	-2.927311
C	7.782571	0.438086	-0.053579
H	8.533862	1.185259	0.255258
H	8.205928	-0.044787	-0.955650
C	1.277221	-4.219855	-2.231987
H	2.082880	-4.914212	-2.510881
H	0.981893	-3.645294	-3.110943
H	0.415061	-4.799247	-1.874262
C	4.937240	-2.119969	-3.708068
H	5.343716	-3.123565	-3.783210
C	5.750124	-3.095909	-0.841263
H	5.195090	-3.776911	-0.180157
H	6.077728	-3.693320	-1.704509
C	4.584525	-1.402329	-4.839361
H	4.729286	-1.848522	-5.821386
C	6.991571	-2.542560	-0.132408
H	7.597963	-2.027018	-0.882001

H	-8.327696	-4.531419	2.678072
C	-4.034660	0.115347	4.731621
H	-3.744874	-0.453938	5.607828
C	-7.689529	0.558891	-1.094988
H	-8.663239	1.056074	-1.253119
H	-7.451617	-0.006920	-1.998079
C	-6.185057	-4.595616	2.396158
H	-6.021074	-5.527748	2.927308
C	-7.782566	-0.438083	0.053573
H	-8.533857	-1.185256	-0.255265
H	-8.205925	0.044789	0.955643
C	-4.937250	2.119961	3.708067
H	-5.343728	3.123556	3.783211
C	-5.750120	3.095910	0.841262
H	-5.195085	3.776913	0.180158
H	-6.077727	3.693320	1.704507
C	-4.584540	1.402317	4.839359
H	-4.729306	1.848506	5.821385
C	-6.991566	2.542563	0.132403
H	-7.597961	2.027021	0.881993
H	-7.611191	3.344797	-0.303967

Optimised coordinates for 6⁻ (*E* = –3678.49884636 Ha). Charge = –1; multiplicity = 6.

U	4.384548	-0.075050	0.166377
O	2.484183	1.092647	-0.350583
N	2.333165	-1.386057	0.581863
C	0.132593	1.320801	-0.486983
H	0.252499	2.327271	-0.873181
C	1.150873	-0.773480	0.306326
C	2.364916	-2.744097	0.913972
C	1.272435	0.585744	-0.187284
O	1.576893	-3.306191	-1.228349
N	4.076973	1.685422	1.989621
N	4.926253	-0.279557	2.514508
N	4.116421	-0.308397	-2.356037
N	6.481733	1.081485	-0.355129
C	4.621117	0.936979	2.996876
N	4.941079	-1.974336	-1.184039
N	5.181049	2.742835	-1.227400
C	2.000399	-3.751856	-0.020510
N	6.657363	-1.495806	0.877670
C	2.105453	-5.101565	0.322778
H	1.828701	-5.867788	-0.394078
C	6.430184	2.228934	-1.071967
C	3.670830	2.932758	2.216782
H	3.243880	3.446717	1.360280
C	2.826092	-3.156613	2.168581
H	3.079319	-2.374528	2.878114
C	3.796739	3.536655	3.463302
H	3.458089	4.555423	3.617955
C	4.373868	2.791054	4.501346
H	4.488319	3.234335	5.488462
C	5.787502	-1.198676	3.192714
H	5.273595	-1.792622	3.968805
H	6.610978	-0.677352	3.711970
C	4.793060	1.485528	4.286211
H	5.220090	0.888726	5.086019
C	2.574407	-5.479314	1.585088
H	2.646264	-6.535166	1.833988
C	4.655689	-1.564842	-2.428649
C	3.700734	0.318424	-3.455587
H	3.272893	1.304152	-3.297668
C	7.548911	2.892379	-1.653627
H	8.547135	2.475555	-1.572261
C	6.343116	-2.173788	2.150001
H	7.232017	-2.694702	2.546646
H	5.582191	-2.929498	1.930989
C	5.021182	3.872225	-1.905186
H	3.991563	4.223522	-1.989371
C	7.347602	4.070817	-2.352391
H	8.199433	4.579183	-2.801439
C	2.936142	-4.506953	2.510179
H	3.285803	-4.789868	3.499967
C	3.815523	-0.248445	-4.718888
H	3.467316	0.285500	-5.596099
C	7.715657	-0.483991	1.046226
H	8.697746	-0.967237	1.194063
H	7.667025	-3.275987	0.285126
O	-2.484130	-1.092590	0.350615
N	-2.333109	1.386111	-0.581835
C	-0.132538	-1.320742	0.487027
H	-0.252445	-2.327210	0.873228
C	-1.150818	0.773535	-0.306291
C	-2.364859	2.744152	-0.913940
C	-1.272381	-0.585686	0.187324
O	-1.576773	3.306231	1.228361
C	-2.000317	3.751905	0.020538
C	-2.105369	5.101616	-0.322744
H	-1.828592	5.867834	0.394107
C	-2.826058	3.156674	-2.168539
H	-3.079308	2.374592	-2.878067
C	-2.574347	5.479372	-1.585043
H	-2.646202	6.535225	-1.833938
C	-2.936108	4.507016	-2.510129
H	-3.285789	4.789936	-3.499909
C	-1.113767	4.246676	2.166072
H	-1.908393	4.938657	2.480464
H	-0.779954	3.670327	3.030042
H	-0.268694	4.829584	1.774631
U	-4.384481	0.075095	-0.166394
N	-4.077390	-1.685492	-1.989383
N	-4.926138	0.279606	-2.514509
N	-4.116603	0.308224	2.355910
N	-6.481676	-1.081428	0.355011
C	-4.621153	-0.936993	-2.996796
N	-4.941057	1.974310	1.184029
N	-5.181019	-2.742737	1.227381
N	-6.657209	1.495890	-0.877769
C	-6.430156	-2.228866	1.071871
C	-3.671531	-2.932948	-2.216381
H	-3.244856	-3.446950	-1.359766
C	-3.797364	-3.536903	-3.462882
H	-3.458937	-4.555765	-3.617402
C	-4.374153	-2.791247	-4.501075
H	-4.488568	-3.234583	-5.488171
C	-5.787270	1.198792	-3.192766
H	-5.273276	1.792704	-3.968825
H	-6.610762	0.677533	-3.712063
C	-4.793071	-1.485607	-4.286107
H	-5.219862	-0.888773	-5.086019
C	-4.655755	1.564712	2.428620
C	-3.701037	-0.318739	3.455425
H	-3.273282	-1.304493	3.297436
C	-7.548900	-2.892318	1.653489
H	-8.547127	-2.475514	1.572067
C	-6.342877	2.173908	-2.150061
H	-7.231736	2.694873	-2.546733
H	-5.581924	2.929575	-1.930992
C	-5.021164	-3.872110	1.905199
H	-3.991542	-4.223384	1.989443
C	-7.347604	-4.070738	2.352288

H	7.483454	0.087051	1.947625
C	6.059918	4.596918	-2.489884
H	5.866888	5.516399	-3.033207
C	7.778052	0.501884	-0.114078
H	8.522096	1.263772	0.174982
H	8.194050	0.015256	-1.017392
C	1.113933	-4.246644	-2.166074
H	1.908579	-4.938616	-2.480436
H	0.780143	-3.670303	-3.030058
H	0.268854	-4.829563	-1.774661
C	4.816921	-2.198976	-3.681622
H	5.243615	-3.194808	-3.747241
C	5.781432	-3.073054	-0.828601
H	5.251357	-3.758281	-0.151047
H	6.102661	-3.671923	-1.693099
C	4.390427	-1.524903	-4.815247
H	4.497395	-1.998121	-5.789426
C	7.026109	-2.490542	-0.150685
H	7.609548	-1.974238	-0.917624

H	-8.199447	-4.579110	2.801304
C	-3.815842	0.248022	4.718774
H	-3.467732	-0.286040	5.595953
C	-7.715492	0.484075	-1.046412
H	-8.697569	0.967327	-1.194311
H	-7.483226	-0.086952	-1.947804
C	-6.059916	-4.596811	2.489857
H	-5.866896	-5.516276	3.033209
C	-7.777977	-0.501819	0.113875
H	-8.522006	-1.263699	-0.175242
H	-8.194031	-0.015197	1.017167
H	-4.817013	2.198741	3.681644
H	-5.243632	3.194601	3.747335
C	-5.781363	3.073065	0.828598
H	-5.251236	3.758311	0.151102
H	-6.102630	3.671902	1.693104
C	-4.390640	1.524521	4.815226
H	-4.497626	1.997651	5.789446
C	-7.026010	2.490599	0.150591
H	-7.609500	1.974275	0.917478
H	-7.666890	3.276067	-0.285232

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