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Electronic Supplementary Information

for

Sulfinyl-Aminotroponiminates: Alkali- (Li, Na, K) and heavy-metal (Bi) complexes

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Plots of NMR Spectra

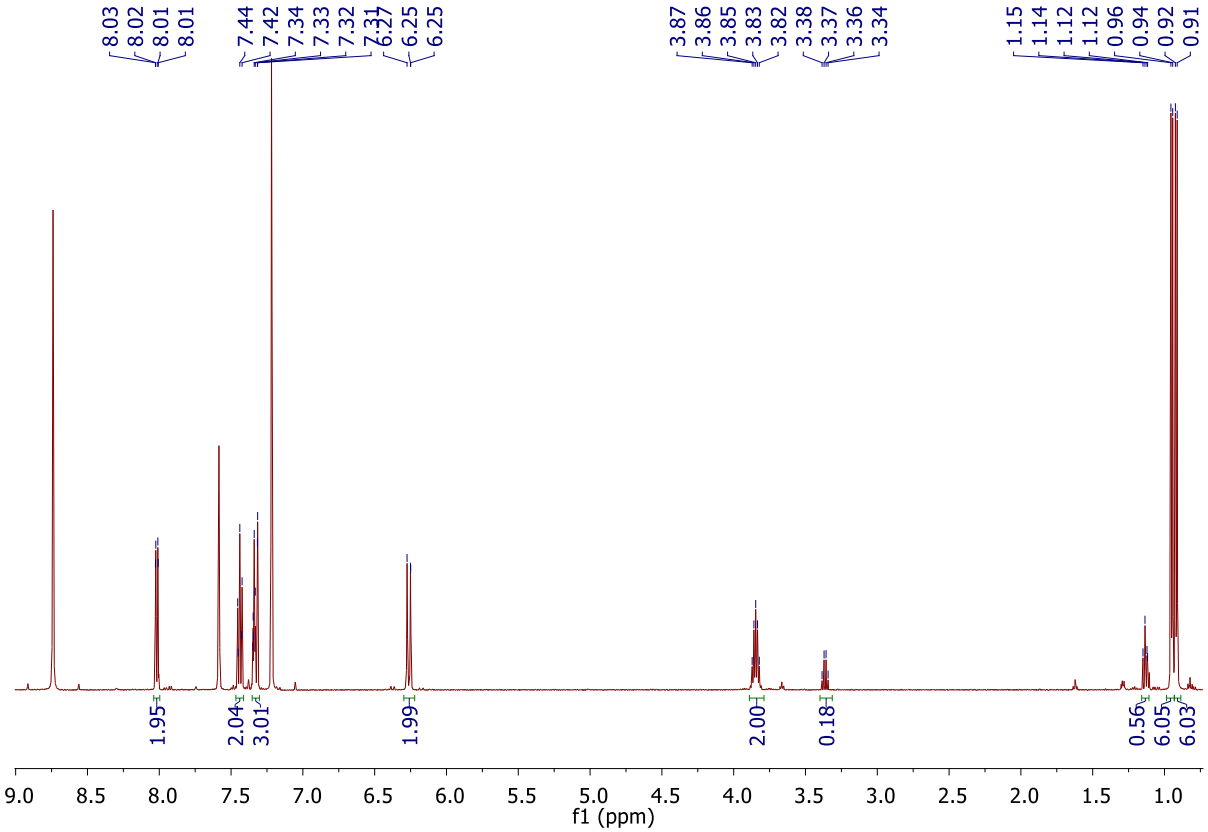

Figure S1. ^{1}H NMR spectrum (400 MHz, 298 K, pyridine-d_5) of compound **2-Li**.

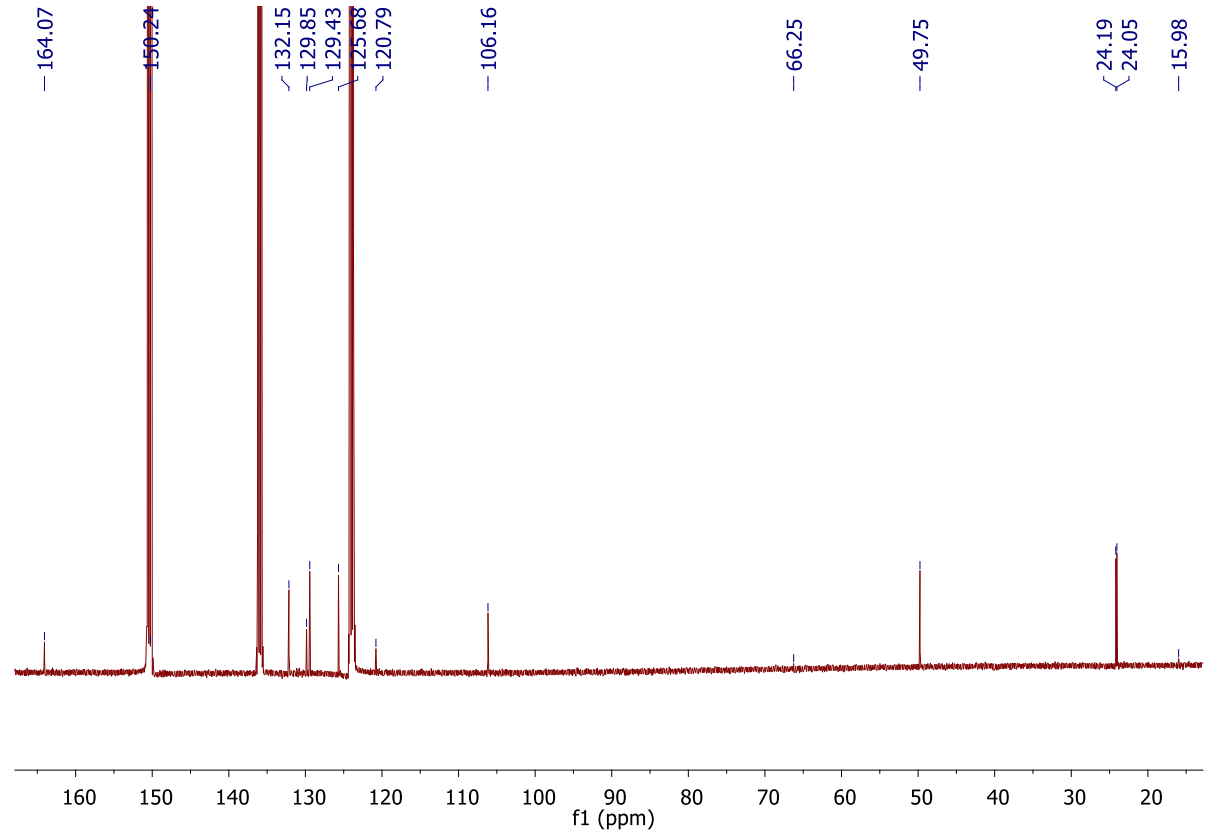

Figure S2. ^{13}C{^{1}H} NMR spectrum (100 MHz, 298 K, pyridine-d_5) of compound **2-Li**.

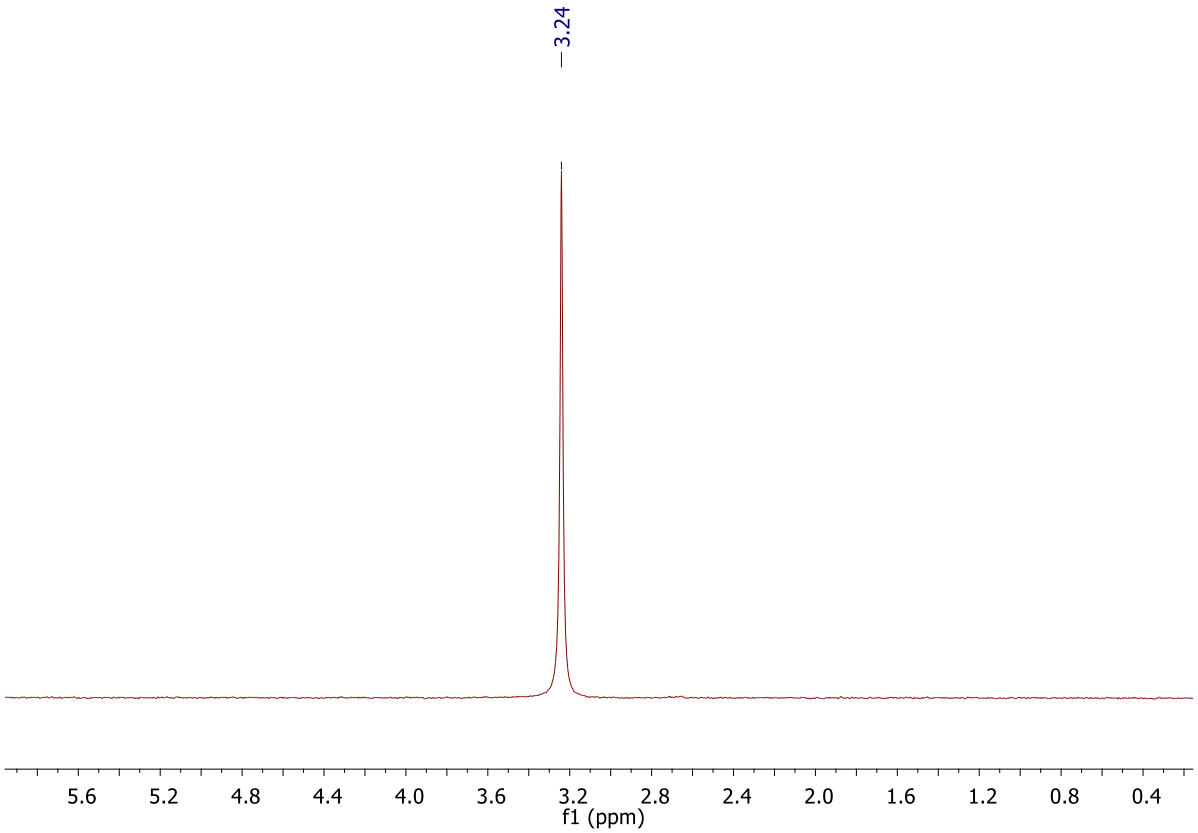

Figure S3. ^{7}Li NMR spectrum (194 MHz, 298 K, pyridine-d_5) of compound **2-Li**.

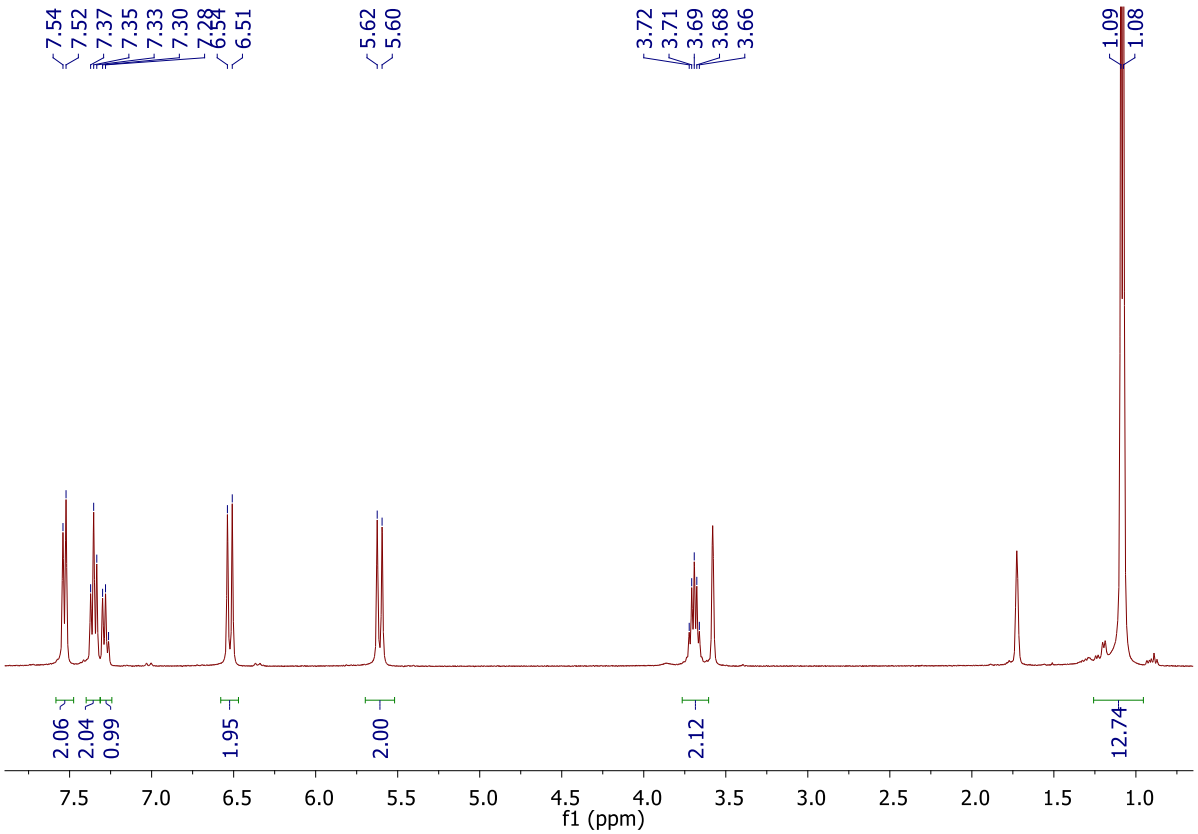

Figure S4. ^{1}H NMR spectrum (400 MHz, 298 K, pyridine-d_5) of compound **2-Na**.

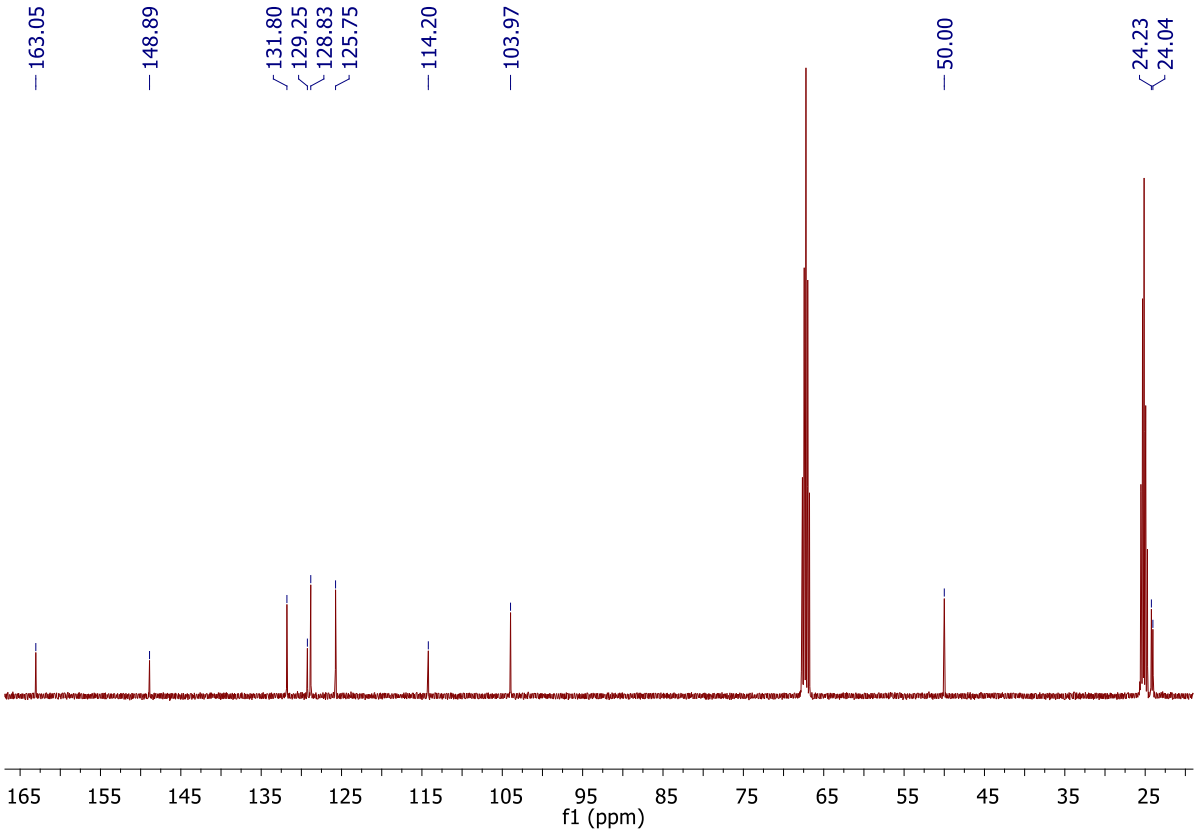

Figure S5. $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, 298 K, pyridine-d_5) of compound **2-Na**.

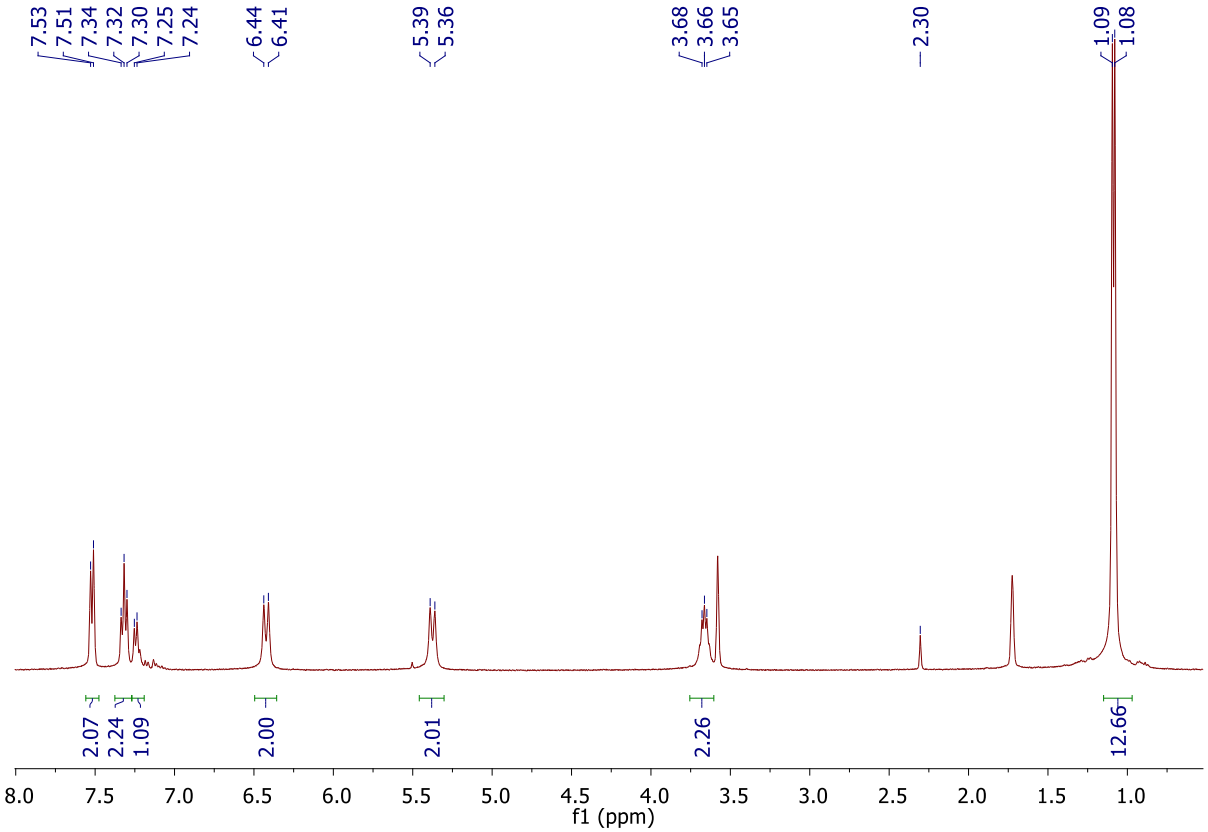

Figure S6. ^{1}H NMR spectrum (400 MHz, 298 K, THF-d_5) of compound **2-K**.

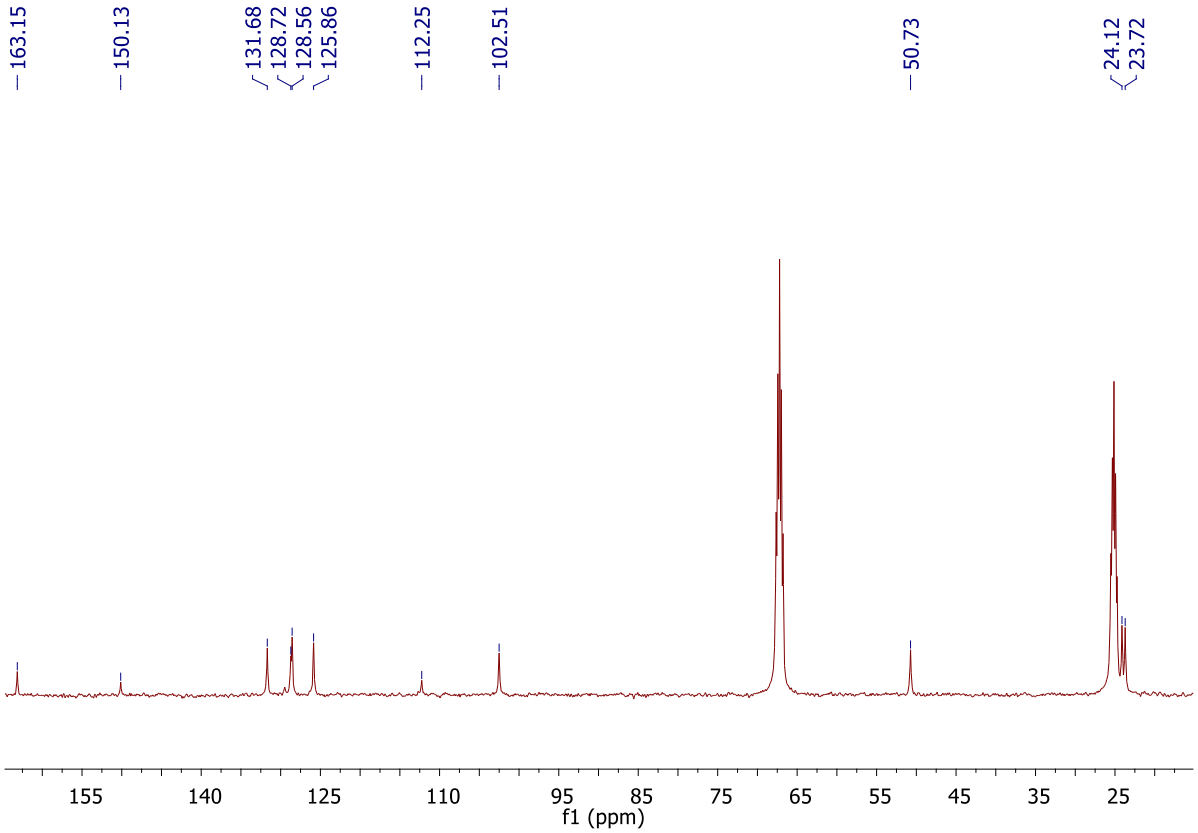

Figure S7. $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, 298 K, THF-d_5) of compound **2-K**.

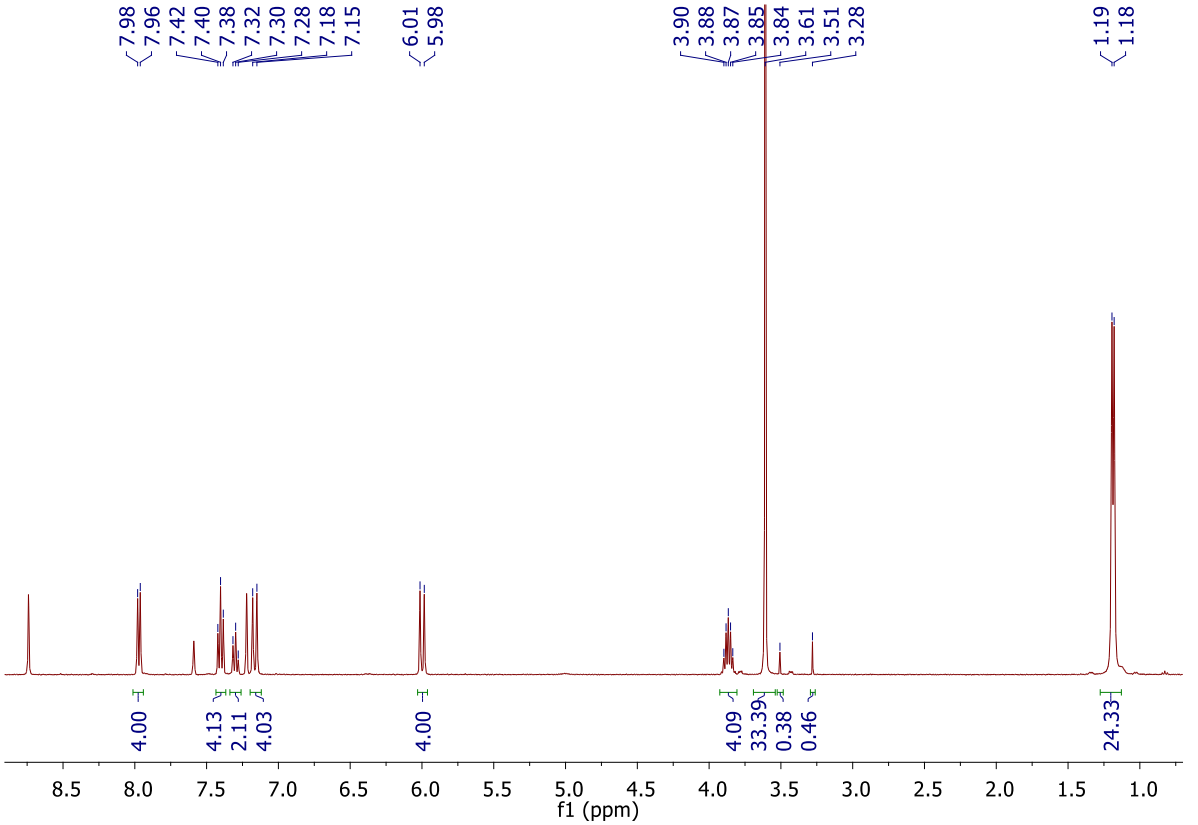

Figure S8. ^{1}H NMR spectrum (400 MHz, 298 K, pyridine-d_5) of compound **3**.

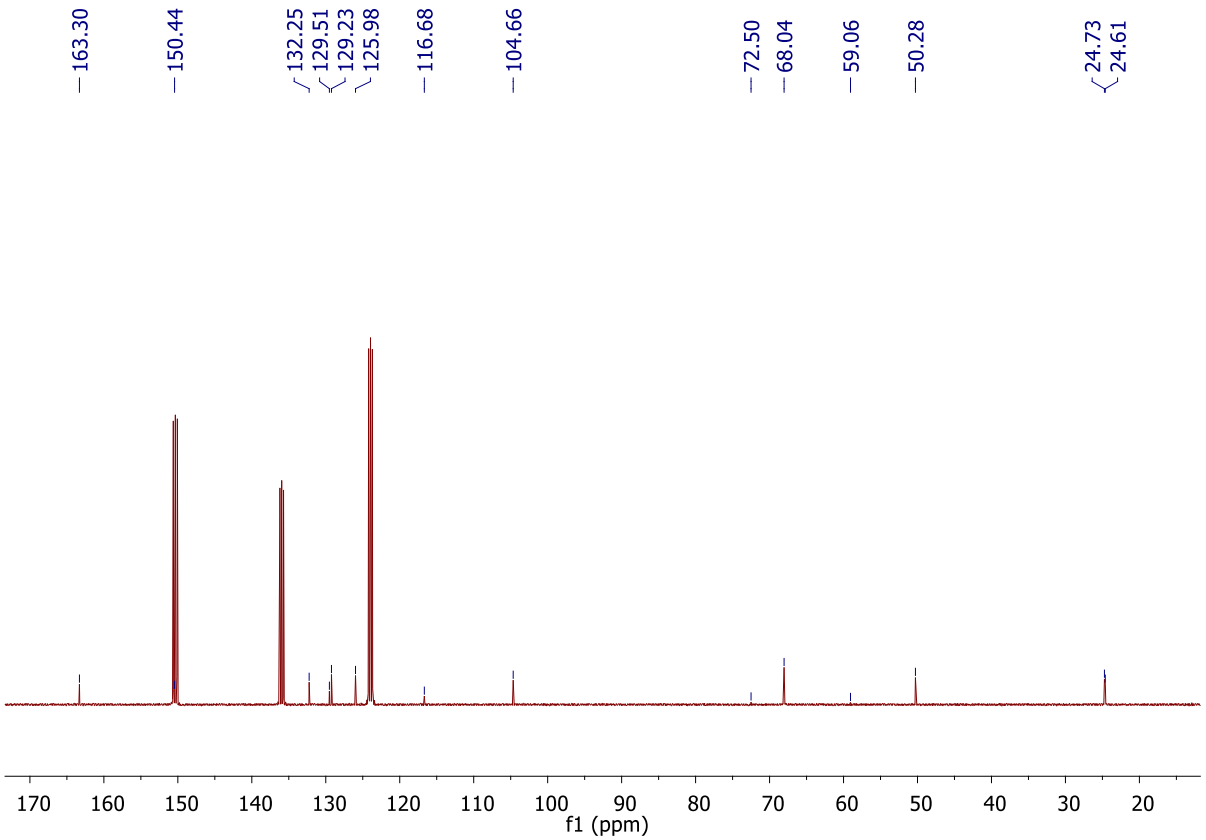

Figure S9. $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, 298 K, pyridine-d_5) of compound **3**.

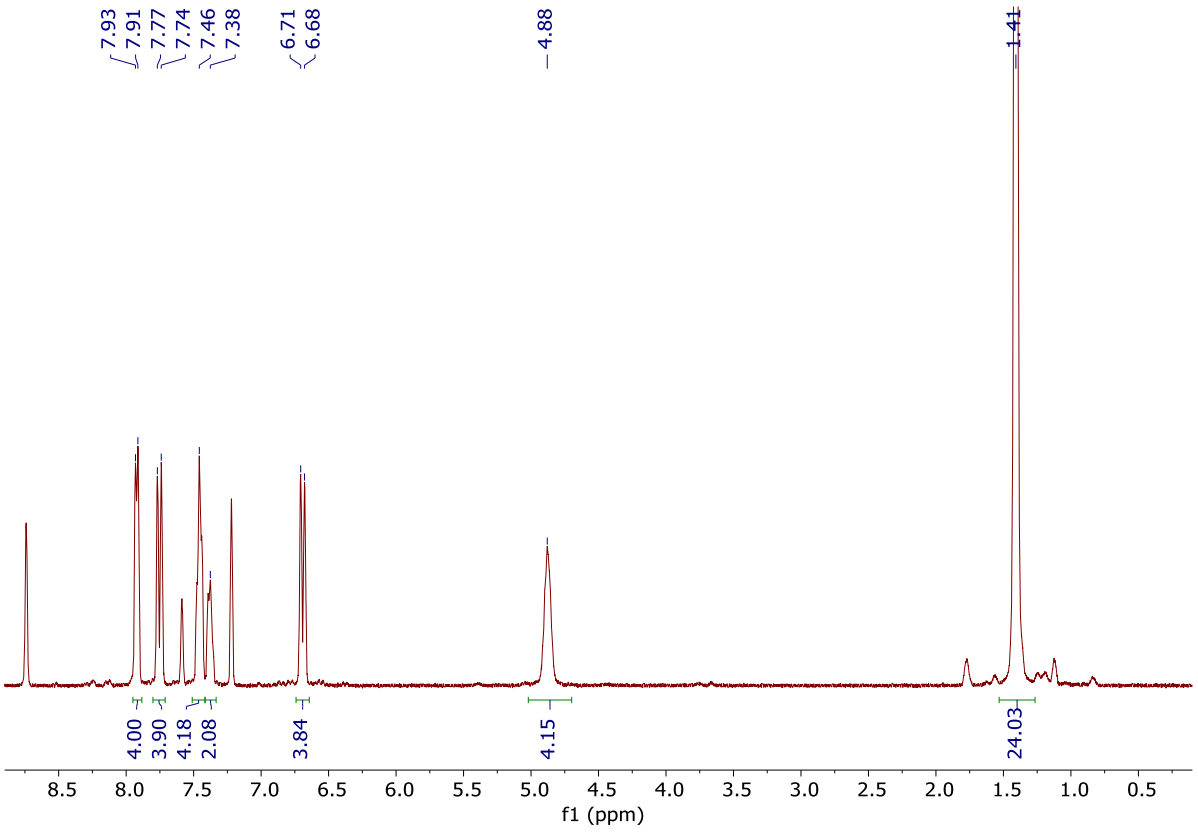

Figure S10. ^{1}H NMR spectrum (400 MHz, 298 K, pyridine-d_5) of compound **5-Cl**.

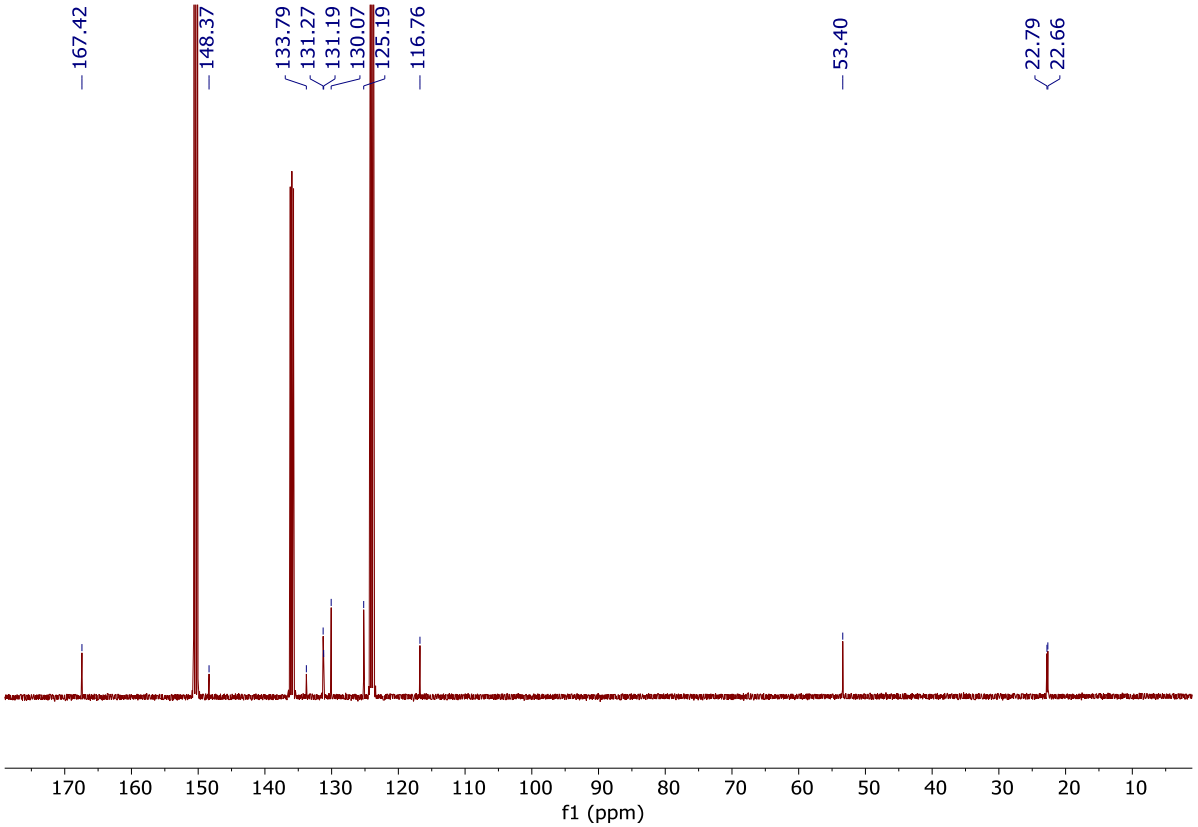

Figure S11. $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, 298 K, pyridine-d_5) of compound **5-Cl**.

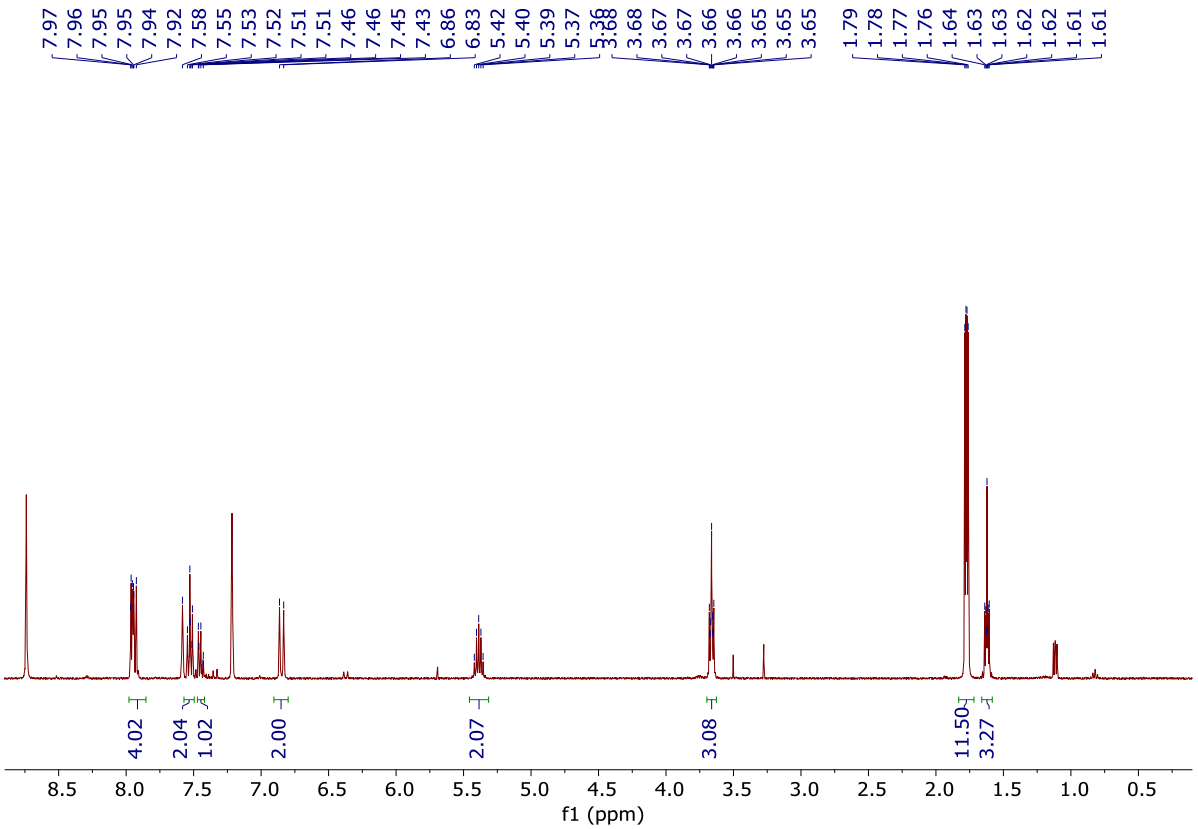

Figure S12. ^{1}H NMR spectrum (400 MHz, 298 K, pyridine-d_5) of compound **6-Cl** (a crude product (prior to recrystallisation from pyridine/pentane) was analysed, revealing residual amounts of THF).

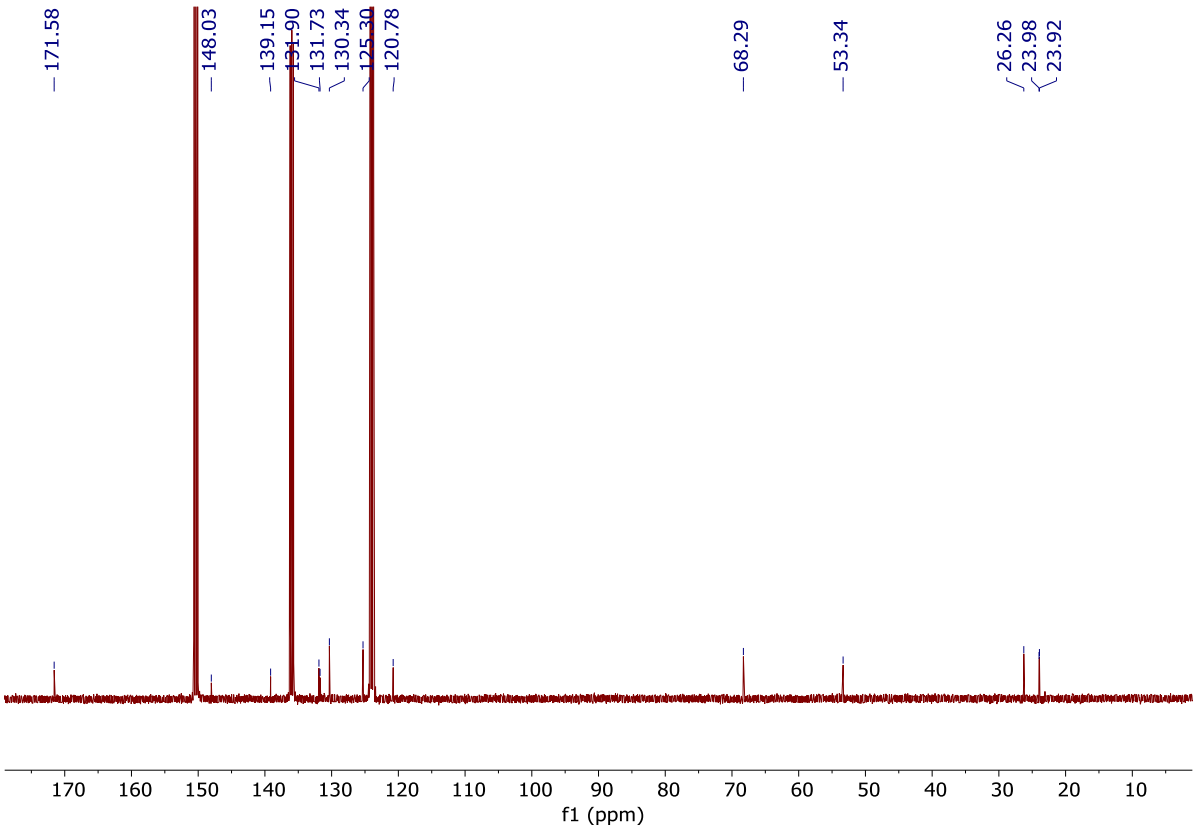

Figure S13. $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, 298 K, pyridine-d_5) of compound **6-Cl** (a crude product (prior to recrystallisation from pyridine/pentane) was analysed, revealing residual amounts of THF).

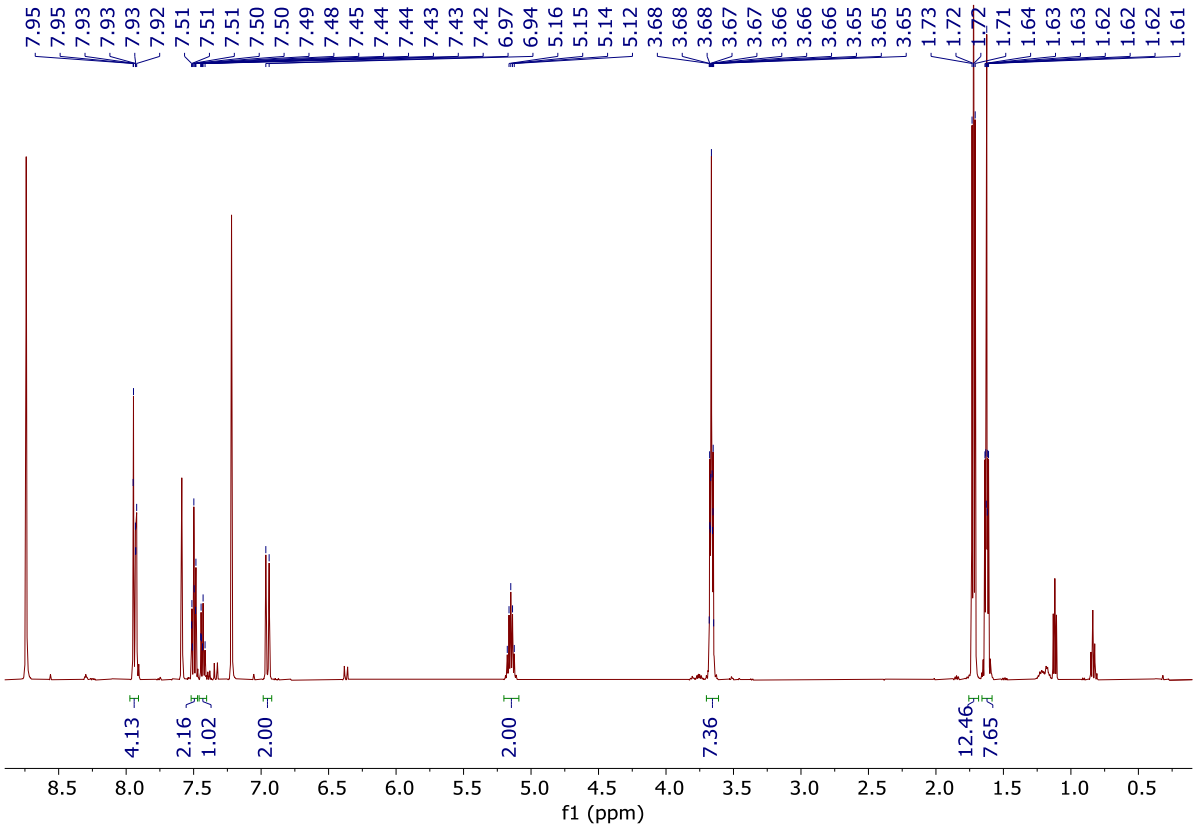

Figure S14. ^{1}H NMR spectrum (400 MHz, 298 K, pyridine-d_5) of compound **6-I**.

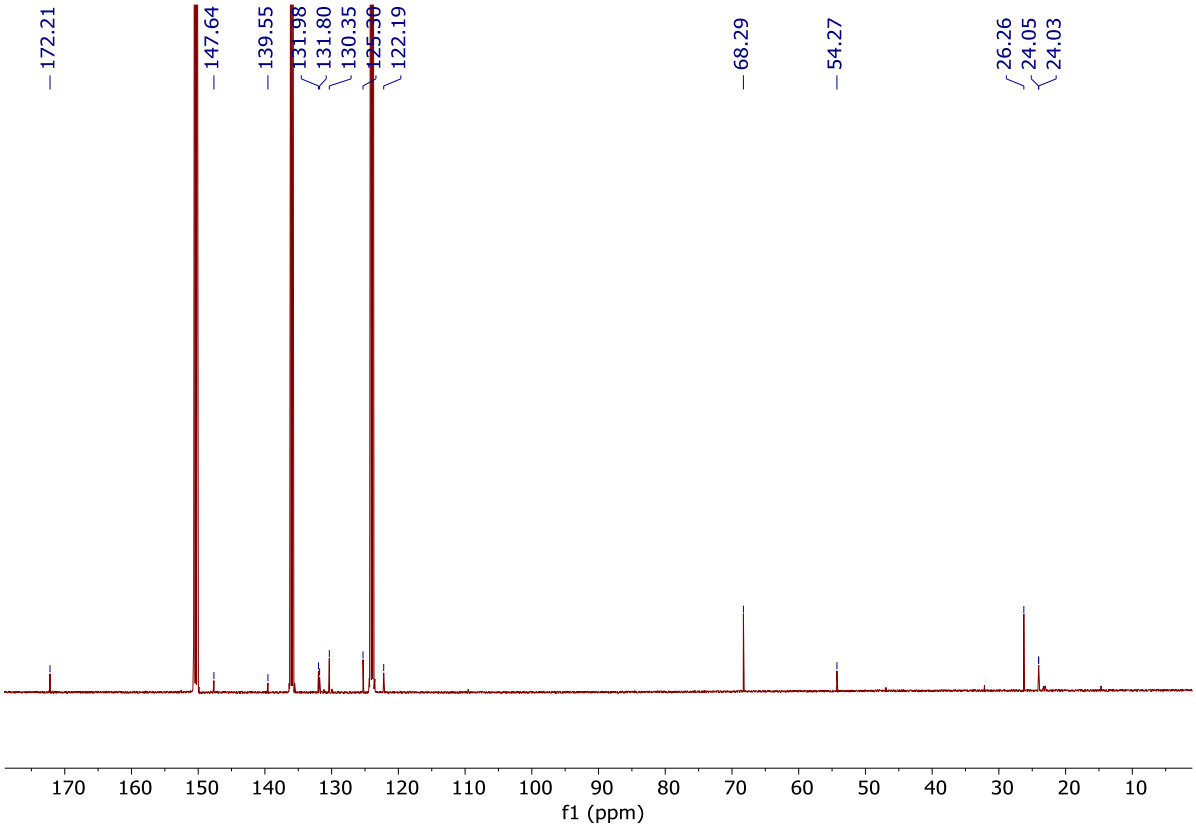

Figure S15. $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, 298 K, pyridine-d_5) of compound **6-I**.

Single-Crystal X-Ray Diffraction Analysis

Crystal data were collected on a Bruker D8 Quest diffractometer equipped with a CMOS area detector or a Bruker X8-APEX II diffractometer equipped with a CCD area detector (**2-Li-py**, **2-K-thf**, **6-Cl**, **6-I**) using multi-layer mirror monochromated $Mo_{K\alpha}$ radiation or with a Rigaku XtaLAB Synergy Dualflex diffractometer equipped with a HyPix hybrid photon counting detector using monochromated $Cu_{K\alpha}$ radiation (**3**). Crystals were kept at 100(2) K during data collection. The structures were solved with the ShelXT program[1] using the intrinsic phasing method, refined with the ShelXL program,[2] and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in structure factors calculations. All hydrogen atoms were assigned to idealised geometric positions.

2-Li-py: The displacement parameters of atoms Li1_5 and Li1_15 (of the residues 1 and 15) were constrained to the same value with EADP keyword.
The displacement parameters of atoms Li1_5 and Li1_15 (of the residues 1 and 15), atoms N3_4, C20_4-C24_4 and N3_14, C20_14-C24_14 (of the residues 4 and 14), atoms C14_3-C19_3 and C14_13-C19_13 (of the residues 3 and 13), atoms S1_2, O1_2 and S1_12, O1_12 (of the residues 2 and 12), and atoms N1_1, N2_1, C1_1-C13_1 and N1_11, N2_11, C1_11-C13_11 (of the residues 1 and 11) were restrained to the same value with the similarity restraint SIMU.
The distances between atoms C5_11, S1_12 and C5_1, S1_2, atoms O1_12, S1_12 and O1_2, S1_2, atoms O1_12, Li1_15 and O1_2, Li1_5, and atoms C14_3-C19_3 and C14_13-C19_13 were restrained during refinement to the same value with the SADI restraint.
The atomic displacement parameters of atoms Li1_5 and Li1_15 (of the residues 1 and 15), atoms N3_14, C20_14-C24_14 (of the residue 14), atoms C14_3-C19_3 and C14_13-C19_13 (of the residues 3 and 13), atoms S1_2, O1_2 and S1_12, O1_12 (of the residues 2 and 12), and atoms N1_1, N2_1, C1_1-C13_1 and N1_11, N2_11, C1_11-C13_11 (of the residues 1 and 11) were restraint with the RIGU keyword in the ShelXL input ('enhanced rigid bond' restraint for all bonds in the connectivity list. Standard values of 0.005 for both parameters s1 and s2 were used).

Crystal data for **2-Li-py**: $C_{24}H_{28}LiN_3OS$, M_r = 413.49, yellow block, 0.24×0.205×0.104 mm^3, Monoclinic space group $P2_1/n$, a = 10.0549(17) Å, b = 13.985(4) Å, c = 16.726(4) Å, β = 103.829(8)°, V = 2283.9(9) Å^3, Z = 4, ρ_{calcd} = 1.203 g·cm^{-3}, μ = 0.161 mm^{-1}, $F(000)$ = 880, T = 100(2) K, R_1 = 0.0494, wR^2 = 0.1095, 4347 independent reflections [$2\theta \leq 51.44°$] and 544 parameters.

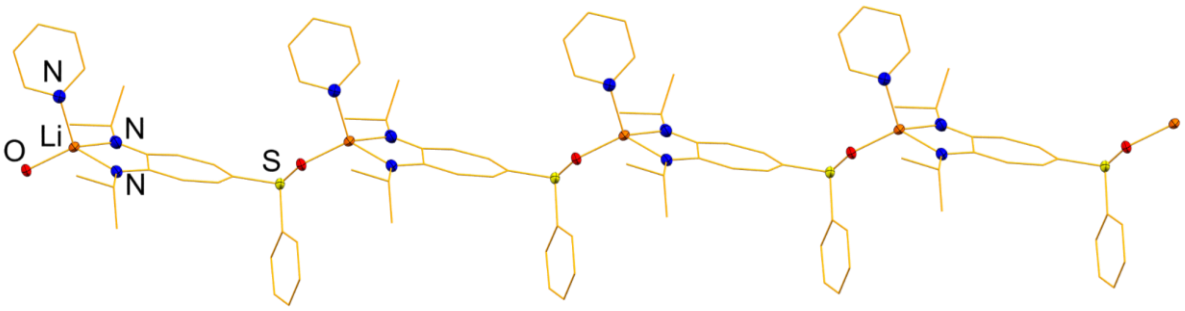

Figure S16. Coordination polymer of **2-Li-py**. Hydrogen atoms are omitted and carbon atoms are displayed in the wire-frame model for clarity. Thermal displacement ellipsoids are shown at the 50% probability level.

2-K-thf: The displacement parameters of atoms O1_2, C1_2-C4_2 and O1_21, C1_21-C4_21 (of the residues 2 and 21) were restrained to the same value with similarity restraint SIMU.

The distances between atoms C1_2-C4_2 (in residue 2) were restrained during refinement to the same value with SADI restraint.

The atomic displacement parameters of atoms O1_2, C1_2-C4_2 and O1_21, C1_21-C4_21 (of the residues 2 and 21) were restraint with the RIGU keyword in the ShelXL input ('enhanced rigid bond' restraint for all bonds in the connectivity list. Standard values of 0.003 for both parameters s1 and s2 were used).

The 1-2 and 1-3 distances in residues 2 (O1_2, C1_2-C4_2) and 21 (O1_21, C1_21-C4_21) were restrained to the same values with the restraint SAME.

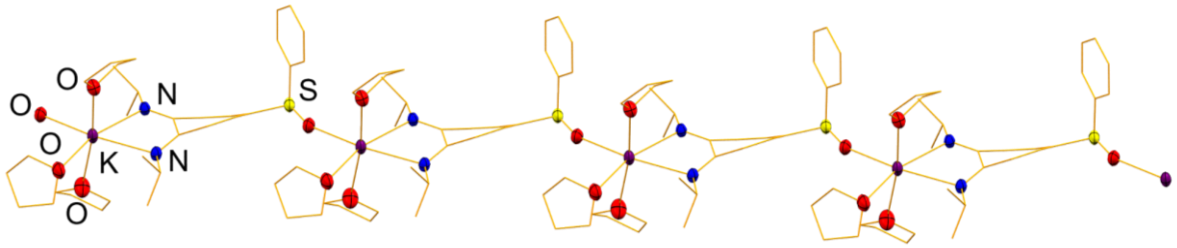

Figure S17. Coordination polymer of **2-K-thf**. Hydrogen atoms are omitted and carbon atoms are displayed as wire-frames for clarity. Thermal displacement ellipsoids are shown at the 50% probability level.

Crystal data for **2-K-thf**: $C_{35}H_{55}KN_2O_5S$, M_r = 654.97, yellow block, 0.254×0.185×0.181 mm^3, Monoclinic space group $P2_1/c$, a = 17.397(11) Å, b = 11.350(7) Å, c = 18.379(11) Å, β = 92.661(8)°, V = 3625(4) Å^3, Z = 4, ρ_{calcd} = 1.200 g·cm^{-3}, μ = 0.245 mm^{-1}, $F(000)$ = 1416.0, T = 100(2) K, R_1 = 0.0556, wR^2 = 0.1481, 6414 independent reflections [$2\theta \leq 50.12°$] and 447 parameters.

3: The displacement parameters of atoms O1_10-O4_10, C1_10-C8_10 and O1_110-O4_110, C1_110-C8_110 (of the residues 10 and 110), atoms C1_4-C3_4 and C1_14-C3_14 (of the residues 4 and 14), atoms S1_7, S1B_7 and O1_7, O1B_7 (in the residue 7), and atoms S1_3, S1B_3 and O1_3, O2B_3 (in the residue 3) were restrained to the same value with the similarity restraint SIMU.

The distances between atoms Na2 and O1_9-O4_9 and Na2 and O1_10-O4_10 and Na2 and O1_110-O4_110 and atoms O1_9-O4_9 and C1_9-C8_9 and atoms N2_1, C1_4 and N2_1, C1_14 and atoms C1_4-C3_4 and C1_14-C3_14 were restrained during refinement to the same value with the SADI restraint.

The atomic displacement parameters of atoms C5_5, C6_5 (of the residue 5), atoms O1_10-O4_10, C1_10-C8_10 and O1_110-O4_110, C1_110-C8_110 (of the residues 10 and 110), atoms S1_7, S1B_7 and O1_7, O1B_7 (in the residue 7), and atoms S1_3, S1B_3 and O1_3, O2B_3 (in the residue 3) were restraint with the RIGU keyword in the ShelXL input ('enhanced rigid bond' restraint for all bonds in the connectivity list. Standard values of 0.005 for both parameters s1 and s2 were used).

The 1-2 and 1-3 distances in residues 4 (C1_4-C3_4) and 14 (C1_14-C3_14) and residue 9 (O1_9-O4_9, C1_9-C8_9) and 10 (O1_10-O4_10, C1_10-C8_10) were restrained to the same values with the restraint SAME.

The U_{ii} displacement parameters of atoms C5, and C6 were restrained with the ISOR keyword to approximate isotropic behavior and with the DELU keyword to apply a rigid bond restraint.

Crystal data for **3**: $C_{58}H_{86}N_4Na_2O_{11}S_2$, M_r = 1125.40, yellow block, 0.173×0.115×0.032 mm^3, Triclinic space group $P\bar{1}$, a = 9.80150(10) Å, b = 15.37580(10) Å, c = 20.2757(2) Å, α α = 98.6750(10)°, β = 95.3650(10)°, γ = 98.1400(10)°, V = 2969.61(5) Å^3, Z = 2, ρ_{calcd} = 1.259 g·cm^{-3}, μ = 1.450 mm^{-1}, F(000) = 1208.0, T = 100(2) K, R_1 = 0.0792, wR^2 = 0.1710, 12420 independent reflections [$2\theta \leq 77.39°$] and 879 parameters.

6-Cl-py: The quality of the data does not allow for a discussion of bonding parameters, but the connectivity is definite.

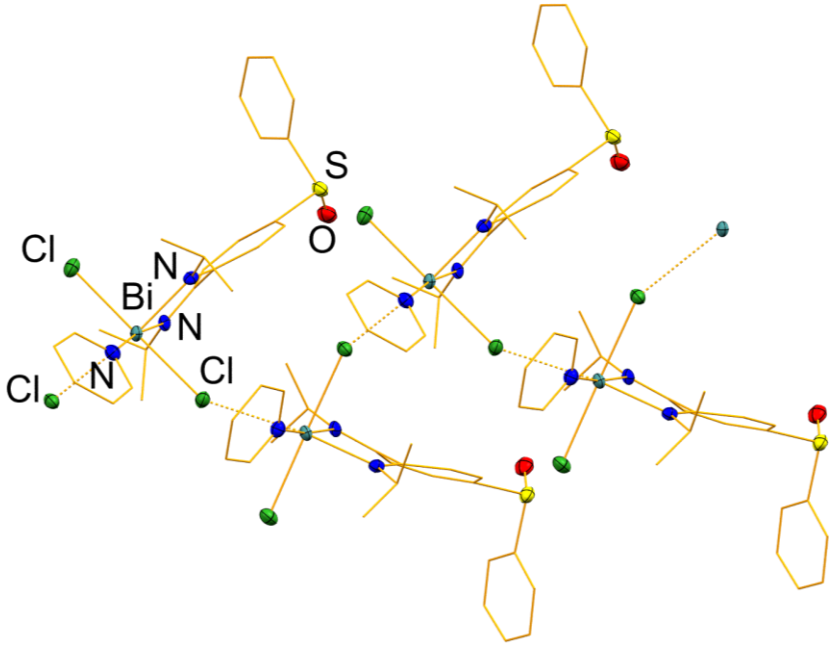

Figure S18. Coordination polymer of **6-Cl-py**. Hydrogen atoms are omitted and carbon atoms are displayed as wire-frames for clarity. Thermal displacement ellipsoids are shown at the 50% probability level.

6-I: The displacement parameters of atoms N1_4, C1_4-C5_4 (of the residue 4) were restrained to the same value with the similarity restraint SIMU.

The atomic displacement parameters of atoms N1_4, C1_4-C5_4 (of the residue 4) were restrained with the RIGU keyword in the ShelXL input ('enhanced rigid bond' restraint for all bonds in the connectivity list. Standard values of 0.003 for both parameters s1 and s2 were used).

The unit cell contains one molecule which has been treated as a diffuse contribution to the overall scattering without specific atom positions by SQUEEZE/PLATON.[3]

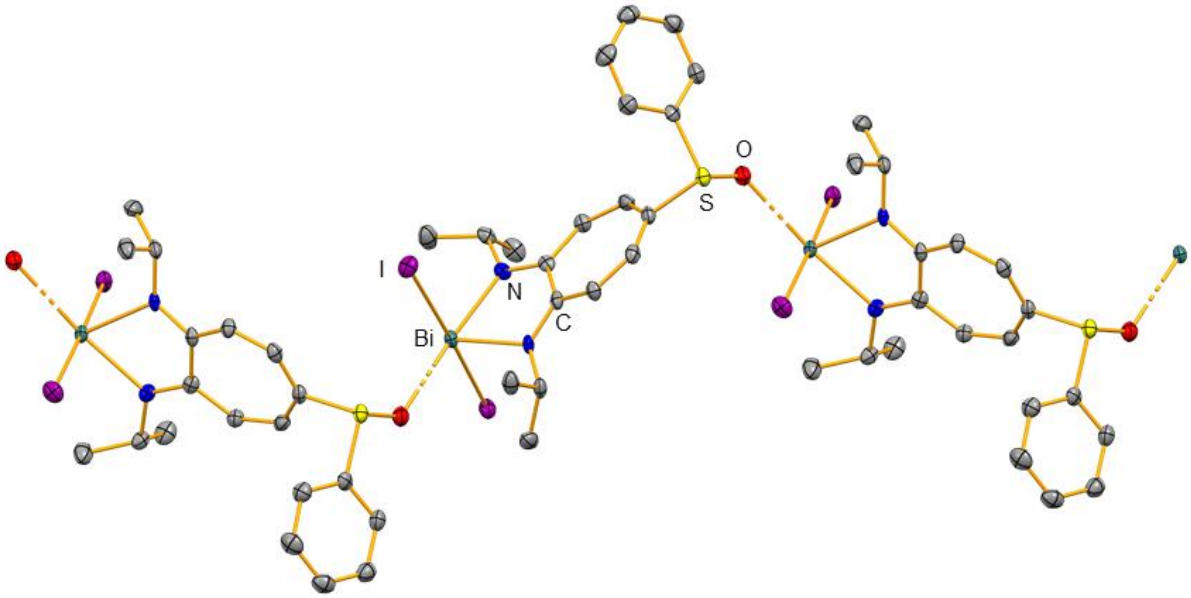

Figure S19. Coordination polymer of **6-I-py**. Hydrogen atoms and lattice-bound pyridine molecules are omitted for clarity. Co-crystallized pyridine solvent molecules are not depicted. Thermal displacement ellipsoids are shown at the 50% probability level.

Crystal data for **6-I-py**: $C_{29}H_{33}BiI_2N_4OS$, M_r = 948.43, red plate, 0.156×0.137×0.058 mm^3, Orthorhombic space group *Pnna*, a = 18.727(12) Å, b = 16.981(4) Å, c = 21.579(7) Å, V = 6862(5) Å^3, Z = 8, ρ_{calcd} = 1.836 g·cm^{-3}, μ = 7.025 mm^{-1}, F(000) = 3584, T = 100(2) K, R_1 = 0.0275, wR^2 = 0.0619, 6111 independent reflections [$2\theta \leq 50.208°$] and 347 parameters.

Electrochemical analyses

Table S1. Redox properties of compounds **1**, **2-Li**, **2-Na** and **2-K** under oxidative conditions, determined by cyclic voltammetry (0.1 M [nBu$_4$N][PF$_6$], THF, *vs.* Fc/Fc$^+$)

entry	compound	E_{pa} or E_{pa}/E_{pc} / V [a]	classification [b]	reversibility [b]
I	**1**	0.46	E	irrev
II	**2-Li**	0.45	E	irrev
III	**2-Li**	–0.26	E	irrev
IV	**2-Na**	0.42	E	irrev
V	**2-Na**	–0.55/–1.96	ECEC	pr
VI	**2-K**	0.45	E	irrev
VII	**2-K**	–0.77	E	irrev

a: E_{pa} for I-IV and VI-VII; E_{pa}/E_{pc} for V; b: E = electron transfer, C = chemical reaction; c: irrev = irreversible, pr = partially reversible.

The oxidation events described in Table S1, entries I-IV and VI-VII are irreversible. The oxidation that is related to a potential of –0.55 V (entry V, compound 2-Na) proved to show a partially reversible character. At the same time, reduction event associated with this oxidation event is strongly cathodically shifted, showing a peak potential of –1.96 V. This points towards an ECEC series of transformations (E = electron transfer; C = chemical reaction), as reported for related ATI complexes under reducing conditions.[4–7] Products related to these redox events could not be isolated to date. Selected cyclic voltammograms are depicted in Figures S20-S23.

Table S2. Redox properties of compounds **1**, **2-Li**, **2-Na** and **2-K** under reductive conditions, determined by cyclic voltammetry (0.1 M [nBu$_4$N][PF$_6$], THF, *vs.* Fc/Fc$^+$).

entry	compound	$E_{1/2}$ *or* E_{pc} [V][a]	classification[b]	reversibility[c]
I	**1**	–2.38	EE	rev
II	**2-Li**	–2.38	E	qr
III	**2-Na**	–2.44	E	irrev
IV	**2-K**	–2.37	EE	rev

a: $E_{1/2}$ for entries I, II, and IV, E_{pc} for entry III, b: E = electron transfer; c: rev = reversible; irrev = irreversible, qr = quasi-reversible.

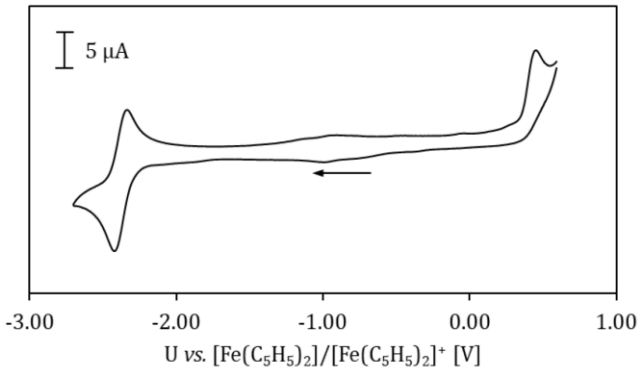

Figure S20. Cyclic voltammogram of compound **1** at room temperature in THF containing 0.1 M [(*n*Bu)$_4$N][PF$_6$] at a scan rate of 250 mV·s^{-1}.

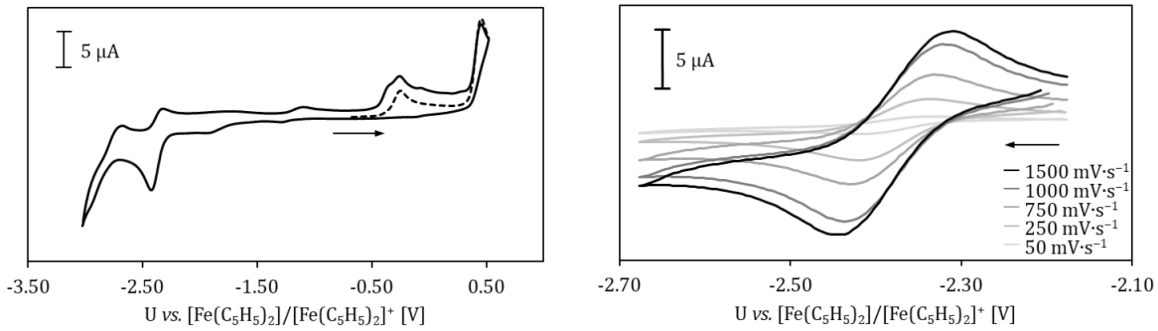

Figure S21. Cyclic voltammograms of compound **2-Li** at room temperature in THF containing 0.1 M [(*n*Bu)$_4$N][PF$_6$]. Left: full potential window at a scan rate of 250 mV·s^{-1} (dotted line indicates starting point). Right: analysis of the redox event at $E_{1/2}$ = –2.38 V at varying scan rates.

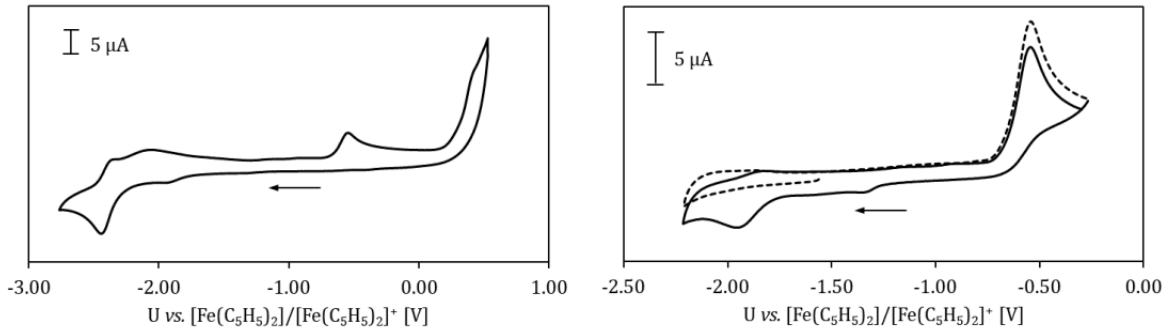

Figure S22. Cyclic voltammogram of compound **2-Na** at room temperature in THF containing 0.1 M [(*n*Bu)$_4$N][PF$_6$]. Left: full potential window at a scan rate of 250 mV·s^{-1}. Right: analysis of the redox event at E_{pa} / E_{pa} = –0.55 / –1.96 V (dotted line indicates starting point).

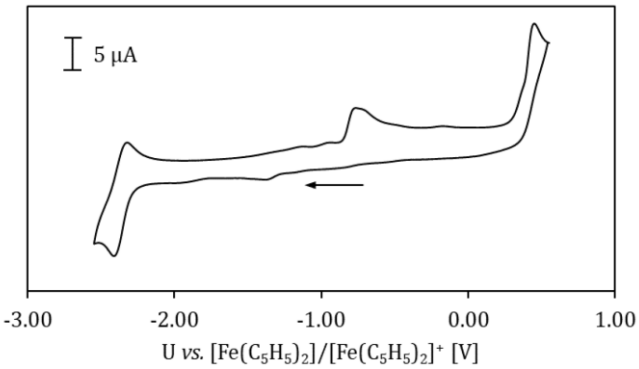

Figure S23. Cyclic voltammogram of compound **2-K** at room temperature in THF containing 0.1 M [(*n*Bu)$_4$N][PF$_6$] at a scan rate of 250 mV·s^{-1}.

DOSY NMR Spectroscopic Studies

In a pulsed field gradient (PFG) diffusion experiment, a pair of pulsed field gradients is implemented into a spin-echo with an echo delay. Due to changes in the molecules spatial position caused by their translational diffusion, incomplete re-focusing of the signal occurs. Such incomplete refocusing results in an attenuation in the signal intensity, which can be correlated to the duration of the delay, the strength of the applied gradients, and the diffusion coefficient of the molecule, as described by the Stejskel-Tanner relation in equation (1)

$$I = I_0 exp\left[-D\gamma^2\delta^2 g^2(\Delta - \frac{\delta}{3})\right] \qquad (1)$$

I_0 is the signal intensity in the absence of an applied gradient, γ is the gyromagnetic ratio of the investigated nucleus, δ the duration of the gradient pulses, g the strength of the applied gradient, and Δ is the total delay where diffusion occurs. In a typical DOSY experiment, the signal attenuation is detected by varying the gradient strength g while holding the gradient duration δ and the diffusion delay Δ constant. By fitting the experimental data to a non-linear exponential decay using equation (1), the diffusion coefficient D can be extracted.

Based on the Stokes-Einstein theory, as shown in equation (2), where k is the Boltzmann constant, T is the absolute temperature, and η the viscosity of the sample solution, the hydrodynamic radius R_H can be obtained from the experimentally determined diffusion coefficient D.

$$D = \frac{kT}{6\pi\eta R_H} \qquad (2)$$

In a DOSY experiment, it is necessary to know the accurate viscosity of the sample solution at the measurement temperature. In order to confirm a constant viscosity of the samples throughout our experiments, the diffusion coefficient of the solvent was measured and normalised with the true viscosity of the solvent.[8]

Furthermore, assuming a spherical shape of the molecules in concern, aggregation of the molecules in solution can be studied by a comparison of the experimentally obtained hydrodynamic radius R_H (Table S3) with the van der Waals radii R_W and molecular volumes V_W.[9,10] The van der Waals radii R_W and molecular volumes V_W can be obtained by the empirical method of hard-sphere increments (HSI).[11,12] Taking solvent molecules coordinated to the alkali metal atom into consideration, theoretical hydrodynamic radii R_H^{HSI} were obtained. For the monomeric subunits, the species [Li(Ph(O)S−ATI$^{iPr/iPr}$)(py)], [Na(Ph(O)S−ATI$^{iPr/iPr}$)(py)$_2$], and [K(Ph(O)S−ATI$^{iPr/iPr}$)(py)$_3$] were employed. The degree of oligomerisation n was thus calculated as (R_H / R_H^{HSI})^3, giving compounds of type [Li(Ph(O)S−ATI$^{iPr/iPr}$)(py)]$_n$,

$[Na(Ph(O)S{-}ATI^{iPr/iPr})(py)_2]_n$, and $[K(Ph(O)S{-}ATI^{iPr/iPr})(py)_3]_n$, which reflect the mean degree of oligomerisation for oligomerisation reactions in equilibrium. The free ligand **1** was used as a reference compound and was found to be present as a monomer in pyridine solution according to the procedure described above, justifying its applicability for the compounds investigated in this work.

Table S3. Diffusion coefficients and hydrodynamic radii of compounds **1**, **2-Li**, **2-Na**, and **2-K** in pyridine-d_5 at 298 K as determined by DOSY NMR spectroscopy and Stokes-Einstein theory.

Compound	D $\times 10^{-9}$ [$m^2 \cdot s^{-1}$]	R_H [Å]
H-ATI-(S=O)Ph (**1**)	0.58	4.7
2-Li	0.44	5.8
2-Na	0.41	6.3
2-K	0.42	6.1

Experimental details. About 3 mg of the samples were dissolved in about 0.5 mL pyridine-d_5 or THF-d_8. NMR spectroscopic measurements were performed on a Bruker AVIII 500 spectrometer with a cryo probe Prodigy BB-H&F with a z-gradient at 298 K. The temperature was calibrated with a Bruker standard 4% methanol in methanol-d_4. The DOSY experiments were carried out a using pulse sequence with a long delay for the recovery of the eddy current and bipolar gradients. The pulse sequence was ledbpgp3s from the Bruker pulse program library. The gradient shape used was smoothed using square SMSQ10.100, and the gradient length was between 2 and 3 ms. The optimized diffusion delays (Δ) were between 30 and 50 ms. The diffusion attenuation was realized with 9 steps in a gradient ramp. The DOSY 2D spectra were recorded with 9 experiments and each with 16 to 32 transients. The relaxation delays were 3 s.

DFT Calculations

DFT calculations were performed with the Gaussian 16, Revision A.03 program package[13] using the B3LYP[14–17] functional and the 6-311++G(d,p).[18,19] The D3 version of Grimme's dispersion model with the original D3 damping function was applied.[20] Frequency analyses of the reported structures showed no imaginary frequencies for minimum energy structures and only one imaginary frequency for transition states.

The results of geometry optimization are shown in Figure S24 using the lithium species [Li(Ph(O)S−ATI$^{iPr/iPr}$)(thf)$_2$] and [Li(Ph(O)S−ATI$^{iPr/iPr}$)(thf)]$_2$ as examples. For model compound [Li(Ph(O)S−ATI$^{iPr/iPr}$)(thf)$_2$], the HOMO-1 is also depicted, showing a significant contribution by a p(O) atomic orbital and antibonding character with respect to the S-O moiety of the sulfinyl group.

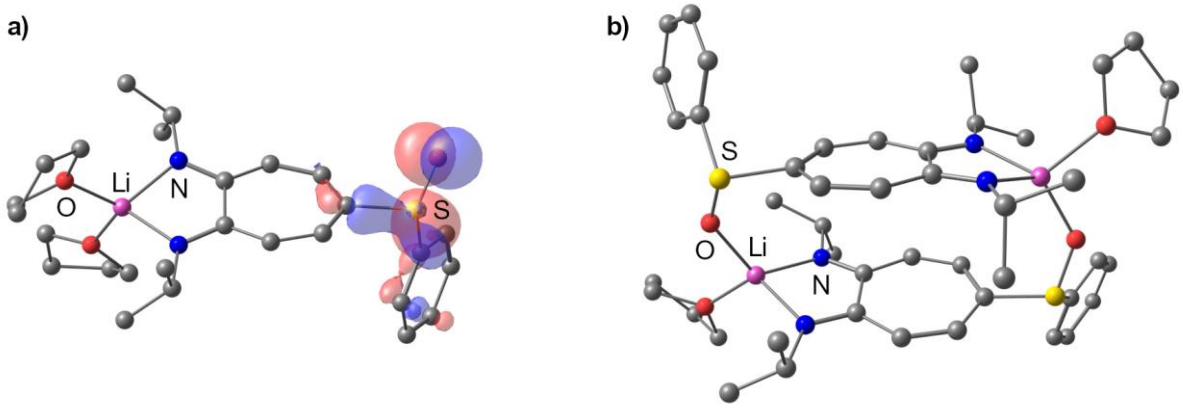

Figure S24. Molecular structures of [Li(Ph(O)S−ATI$^{iPr/iPr}$)(thf)$_2$] and [Li(Ph(O)S−ATI$^{iPr/iPr}$)(thf)]$_2$ as obtained by geometry optimization. The HOMO-1 of [Li(Ph(O)S−ATI$^{iPr/iPr}$)(thf)$_2$] is shown at an iso-value of 0.05. Hydrogen atoms are omitted for clarity.

The energies of compounds investigated by DFT calculations are given in Table S4. Their Cartesian coordinates are given in Table S5.

Table S4 Energies of calculated species.

#	Compound	*ΔH* [hartree]	*ΔG* [hartree]	Imaginary frequencies
1	[Li(Ph(O)S−ATI$^{iPr/iPr}$)(thf)$_2$]	–1793.080953	–1793.194673	none
2	[Li(Ph(O)S−ATI$^{iPr/iPr}$)(thf)]$_2$	–3121.389831	–3121.555835	none
3	[Na(Ph(O)S−ATI$^{iPr/iPr}$)(thf)$_3$]	–2180.255667	–2180.388502	none
4	[Na(Ph(O)S−ATI$^{iPr/iPr}$)(thf)$_2$]$_2$	–3895.738116	–3895.938149	none
5	[K(Ph(O)S−ATI$^{iPr/iPr}$)(thf)$_4$]	–2850.310466	–2850.462398	none
6	[K(Ph(O)S−ATI$^{iPr/iPr}$)(thf)$_3$]$_2$	–5235.853037	–5236.089143	none
7	THF	–232.403972	–232.438308	none

Table S5. Cartesian coordinates of compounds investigated by DFT calculations.

Compound [Li(Ph(O)S−ATI$^{iPr/iPr}$)(thf)$_2$]

N	-1.242709919	-0.920137692	-0.912410328
N	-1.135631120	0.169792854	1.460757648
C	-0.089875853	-1.058099583	-0.290740123
C	0.018651348	-0.260878399	0.999479110
C	1.274433153	0.057614533	1.621198078
H	1.204291021	0.798579979	2.406315544
C	2.561969608	-0.385427673	1.407290282
H	3.321758555	0.055939883	2.048918893
C	3.027636120	-1.359047701	0.524552421
C	2.271473455	-2.089774938	-0.386465010
H	2.805811801	-2.869737006	-0.926874029
C	0.938997326	-1.951940124	-0.735388585
H	0.625799236	-2.648184859	-1.501415257
C	-1.506880837	-1.615642336	-2.168946231
H	-0.591053998	-1.714186115	-2.768892586
C	-2.066914369	-3.025270756	-1.905095110
H	-2.247827445	-3.559664767	-2.842975163
H	-3.014333107	-2.954635097	-1.364193029
H	-1.381130336	-3.618500106	-1.296632128
C	-2.499597544	-0.791133270	-2.997549372
H	-2.727534183	-1.291029538	-3.943679658
H	-2.090797260	0.196805490	-3.220370142
H	-3.436662002	-0.649772378	-2.450766041
C	-1.225718429	0.875478085	2.737177946
H	-0.445176594	0.539789317	3.432769734
C	-2.576810670	0.548811027	3.385707679
H	-2.685782347	1.069361480	4.341913240
H	-2.661194835	-0.525253095	3.567595017
H	-3.403357015	0.846498704	2.732671118
C	-1.077489611	2.393326629	2.535661688
H	-1.110539910	2.922278359	3.492916957
H	-1.894482037	2.765044785	1.911742449
H	-0.135609512	2.637760802	2.038761113
O	5.307121541	-1.599964295	1.988801754
S	4.799224546	-1.732777858	0.562068261
C	5.386001548	-0.211891016	-0.288463656
C	5.024887390	0.042471829	-1.610650750
H	4.357088488	-0.632322944	-2.135433674
C	5.510976863	1.184910142	-2.240376603
H	5.232302942	1.394051458	-3.267374306
C	6.352786474	2.060964486	-1.550558027
H	6.730152825	2.949631097	-2.044149360
C	6.708725803	1.791332537	-0.230528165
H	7.363611965	2.469901710	0.305120979
C	6.229727046	0.645316097	0.407063903
H	6.491600726	0.405453736	1.431466555
C	-3.320861568	4.246722222	-0.977872930
H	-3.665088389	5.128074175	-0.434203478
H	-3.646144347	4.338066280	-2.018291500
C	-3.846814022	2.946207907	-0.368557214
H	-3.932060016	3.015287081	0.721907466
H	-4.812240470	2.634622178	-0.773739039
O	-2.868829340	1.936100002	-0.694732177
C	-1.799349790	4.042750566	-0.908916409
H	-1.250072314	4.662665859	-1.619250483
H	-1.428600150	4.262627782	0.095213944
C	-1.659829456	2.553177100	-1.213071966
H	-1.612189555	2.361070704	-2.289639951
H	-0.808058496	2.074026199	-0.730083334
O	-4.304054132	-0.579758746	0.483250161
C	-5.375050013	-2.726667734	0.505189848
H	-6.206930301	-2.854432782	1.201862653
H	-5.017028028	-3.719448376	0.229041010
C	-4.261882166	-1.871828001	1.144875470
H	-4.415252270	-1.721126581	2.216058812
H	-3.259627585	-2.272682487	0.987025887
C	-5.821012288	-1.901853053	-0.717793028
H	-5.216333765	-2.147452654	-1.593547889
H	-6.871439869	-2.052744617	-0.972819229
C	-5.522087627	-0.475050278	-0.269839630
H	-5.344427055	0.223814758	-1.088630866
H	-6.319956794	-0.077708224	0.371898801
Li	-2.550383161	0.165301307	0.085125986

Compound [Li(Ph(O)S−ATI$^{iPr/iPr}$)(thf)]$_2$

N	-2.117784882	-1.533008874	-0.789302591
N	-2.316583931	-1.828953378	1.779323521
C	-0.973236031	-1.710079853	-0.181773982
C	-1.089031136	-1.875516541	1.333431320
C	0.043851572	-2.068601101	2.201314611
H	-0.217794851	-2.165666983	3.245803454
C	1.400398315	-2.110017470	1.985709078
H	1.996515121	-2.232283403	2.886876750
C	2.130365018	-2.013163730	0.791729483
C	1.587850650	-1.851439426	-0.491898414

H	2.307424699	-1.807765835	-1.303247542	C	-6.567765631	-1.767547867	-0.023566868
C	0.279680378	-1.748949985	-0.892135034	H	-6.535891433	-0.679767806	0.015366654
H	0.179121614	-1.640837248	-1.962867226	H	-7.185718502	-2.138461446	0.805783986
C	-2.207412485	-1.400941494	-2.242888072	N	2.117814696	1.532999423	-0.789311275
H	-1.394111885	-0.772744646	-2.633476710	N	2.316590350	1.828811161	1.779334814
C	-2.134038471	-2.781283912	-2.920294579	C	0.973260119	1.710025993	-0.181779238
H	-2.187310470	-2.683856623	-4.009004652	C	1.089041513	1.875387575	1.333436109
H	-2.974899093	-3.399204016	-2.591624256	C	-0.043856233	2.068398944	2.201320072
H	-1.212484240	-3.307022996	-2.663567099	H	0.217776558	2.165379264	3.245819879
C	-3.526347899	-0.708497866	-2.604595618	C	-1.400399760	2.109812404	1.985700145
H	-3.608324694	-0.576515324	-3.687654762	H	-1.996533118	2.231993519	2.886868124
H	-3.601470214	0.269627444	-2.129711590	C	-2.130344438	2.013060773	0.791699193
H	-4.375589313	-1.305517464	-2.263232990	C	-1.587815910	1.851437590	-0.491933248
C	-2.639676948	-2.000517182	3.193990328	H	-2.307380867	1.807833946	-1.303294983
H	-1.971335243	-2.731247536	3.670614757	C	-0.279641151	1.748949149	-0.892158085
C	-4.064771753	-2.554965958	3.311505524	H	-0.179065196	1.640910909	-1.962896982
H	-4.329553940	-2.713752322	4.361397647	C	2.207428572	1.401012716	-2.242905604
H	-4.150767898	-3.508497835	2.784270673	H	1.394197294	0.772733771	-2.633506201
H	-4.786770714	-1.861598238	2.871965678	C	2.133851100	2.781372232	-2.920251303
C	-2.514489047	-0.662636894	3.941152662	H	2.187061238	2.683991849	-4.008968563
H	-2.732185021	-0.790415499	5.006036884	H	2.974659625	3.399382704	-2.591619700
H	-3.226174629	0.057640784	3.528476890	H	1.212249249	3.306988700	-2.663442494
H	-1.512426684	-0.243044995	3.833648303	C	3.526448750	0.708762280	-2.604670031
O	4.455453177	-0.569450532	0.635336068	H	3.608448077	0.576876223	-3.687739181
S	3.891144777	-1.960229331	1.019023992	H	3.601692738	-0.269398098	-2.129876640
C	4.440657641	-3.023010931	-0.357600035	H	4.375612025	1.305866906	-2.263259984
C	4.006926198	-4.346824598	-0.421596628	C	2.639670450	2.000318693	3.194011913
H	3.302450058	-4.725489697	0.310468506	H	1.971335401	2.731043528	3.670654482
C	4.463215954	-5.160710907	-1.454090750	C	4.064773431	2.554735511	3.311574560
H	4.125040893	-6.188803864	-1.517070674	H	4.329530022	2.713487369	4.361478574
C	5.345598336	-4.653148612	-2.410894356	H	4.150802850	3.508278983	2.784366883
H	5.695496736	-5.289887746	-3.215538251	H	4.786765597	1.861363579	2.872033259
C	5.773478253	-3.329762488	-2.332126428	C	2.514449782	0.662415185	3.941126817
H	6.455442468	-2.933142161	-3.076032263	H	2.732133331	0.790157837	5.006017961
C	5.326019201	-2.507470982	-1.296765385	H	3.226130940	-0.057856575	3.528435165
H	5.637450172	-1.474016348	-1.213647150	H	1.512381645	0.242844076	3.833596254
O	-5.224498985	-2.234545450	0.147485305	O	-4.455405461	0.569364387	0.634931168
C	-6.133428746	-3.632296768	-1.526958992	S	-3.891128965	1.960069969	1.018935979
H	-6.722551564	-4.550834900	-1.550964551	C	-4.440624435	3.023142114	-0.357475540
H	-5.555149510	-3.585219106	-2.451250164	C	-4.007021910	4.347016255	-0.421096349
C	-5.202391674	-3.594610526	-0.298817204	H	-3.302658511	4.725568963	0.311135480
H	-5.574005577	-4.242586268	0.506016708	C	-4.463286662	5.161114801	-1.453434105
H	-4.164054893	-3.850522364	-0.508090166	H	-4.125209685	6.189257898	-1.516122188
C	-7.018835313	-2.363690010	-1.366835825	C	-5.345516261	4.653701448	-2.410457552
H	-6.827193613	-1.658611872	-2.177868842	H	-5.695395822	5.290606369	-3.214978466
H	-8.086002570	-2.592942405	-1.370042522	C	-5.773265418	3.330250744	-2.332067584

H	-6.455108028	2.933745624	-3.076146365
C	-5.325831819	2.507745604	-1.296864569
H	-5.637158966	1.474235972	-1.214043430
O	5.224392959	2.234551155	0.147638563
C	6.133509498	3.632112783	-1.526919504
H	6.722742227	4.550586287	-1.550718722
H	5.555491200	3.585143381	-2.451379236
C	5.202150386	3.594508871	-0.298995586
H	5.573417661	4.242740963	0.505787425
H	4.163817256	3.850162142	-0.508596409
C	7.018764826	2.363429210	-1.366593372
H	6.826905053	1.658170491	-2.177419306
H	8.085966427	2.592517920	-1.369997018
C	6.567732399	1.767678896	-0.023158620
H	6.536012615	0.679905943	0.016143736
H	7.185589436	2.138968287	0.806098360
Li	-3.637248994	-1.147258382	0.459720845
Li	3.637254518	1.147100703	0.459717535

Compound [Na(Ph(O)S−ATI$^{iPr/iPr}$)(thf)$_3$]

N	-0.68138910	-0.35191282	-1.07293425
N	-0.48878901	-0.86070778	1.61214102
C	0.41090840	-0.90524214	-0.60758778
C	0.60456501	-0.82769669	0.89773144
C	1.92142918	-0.62057403	1.45627372
H	1.91693341	-0.17447642	2.44395593
C	3.17740280	-0.88928985	0.96433616
H	4.00570431	-0.61910312	1.61571262
C	3.53644278	-1.53388705	-0.22445556
C	2.67379027	-1.95231057	-1.23724490
H	3.12719943	-2.54095350	-2.03316750
C	1.33051744	-1.67067895	-1.40927446
H	0.90419649	-2.07487264	-2.31953476
C	-0.93539090	-0.32080745	-2.51107533
H	-0.00179241	-0.39145994	-3.08632318
C	-1.84571077	-1.49055321	-2.91877133
H	-2.05605284	-1.47383215	-3.99274048
H	-2.79662830	-1.42789118	-2.38073913
H	-1.38747206	-2.45179479	-2.67369770
C	-1.59279389	1.01955266	-2.86560336
H	-1.83572931	1.06724611	-3.93174986
H	-0.92671122	1.85245381	-2.62920302
H	-2.51409522	1.15285077	-2.29280407
C	-0.41391559	-0.97735239	3.06814530
H	0.54888205	-1.40118897	3.38473448
C	-1.51205435	-1.94282675	3.53371492
H	-1.51551155	-2.03373759	4.62433761
H	-1.34915157	-2.93555962	3.10829279
H	-2.49669532	-1.59375099	3.20734662
C	-0.57851045	0.39168196	3.74579645
H	-0.53260705	0.29604415	4.83483634
H	-1.54573632	0.83371577	3.48569637
H	0.20137316	1.08556750	3.42872771
O	5.93729179	-2.31990471	0.80500693
S	5.28542741	-1.87363246	-0.49537143
C	5.83798951	-0.13392181	-0.71859309
C	5.33273854	0.64056763	-1.76220355
H	4.57249887	0.23696440	-2.42240829
C	5.79433821	1.94328325	-1.92841233
H	5.40426367	2.55459129	-2.73497657
C	6.75434136	2.46363973	-1.05642071
H	7.11182869	3.47887425	-1.18854820
C	7.25229990	1.67750822	-0.01921781
H	7.99771051	2.08014763	0.65804645
C	6.79907620	0.36766150	0.15063035
H	7.16791476	-0.27009952	0.94614767
C	-0.28662801	3.86069088	2.37305271
H	-0.07868928	3.51464518	3.38615862
H	-0.18446411	4.94775650	2.36761418
C	-1.70414199	3.44438604	1.91158273
H	-2.30480631	2.98933987	2.70086483
H	-2.25645699	4.30227944	1.50462409
O	-1.52759798	2.46402468	0.88013878
C	0.65473270	3.19217827	1.34030507
H	1.44685228	3.85881812	0.99543919
H	1.12584380	2.29957457	1.75388947
C	-0.29213553	2.78530244	0.21335087
H	-0.46602151	3.61519636	-0.48787519
H	0.01561146	1.90116492	-0.34058725
O	-3.63048576	-1.76272192	0.63487563
C	-3.85584644	-3.77349707	-0.58554842
H	-3.75535355	-4.84341498	-0.39546196
H	-3.64723082	-3.60358401	-1.64273493
C	-2.89672981	-2.95616947	0.29722679
H	-2.64877830	-3.49188555	1.22025489
H	-1.97168018	-2.64573069	-0.18337497
C	-5.26445997	-3.23439511	-0.20654954
H	-5.73839952	-2.75506245	-1.06595149
H	-5.93662905	-4.01784434	0.14803919
C	-4.96742352	-2.19811570	0.89031257
H	-5.61597865	-1.32229006	0.87242955

H	-5.01833266	-2.65386721	1.88936308
O	-4.29390801	1.26906251	-0.36857280
H	-3.37447335	3.03261290	-0.91864811
C	-4.35678597	2.70377800	-0.57213023
H	-4.56065218	3.18226038	0.38884752
C	-5.45880639	2.94377475	-1.61142610
H	-6.41751840	3.13289242	-1.11998782
C	-5.50591147	1.60583701	-2.36643496
H	-6.46033947	1.42505549	-2.86411109
H	-6.15293247	0.38813236	-0.68434128
H	-5.23693367	3.79475419	-2.25735551
H	-4.78476108	-0.32710346	-1.56734390
C	-5.23381200	0.61203329	-1.24152358
H	-4.71111315	1.55635521	-3.11486690
Na	-2.34565167	0.21687677	0.53665136

Compound [Na(Ph(O)S−ATI$^{iPr/iPr}$)(thf)$_2$]$_2$

N	1.67310639	-1.55418418	1.04340676
N	2.25842530	-2.38420609	-1.47908064
C	0.70158583	-1.94559865	0.27727500
C	1.02319754	-2.07582650	-1.20314648
C	0.02310485	-1.78823623	-2.20677643
H	0.43169415	-1.55124743	-3.18011459
C	-1.34521987	-1.69966894	-2.14508821
H	-1.82529562	-1.40315559	-3.07461313
C	-2.21943671	-1.98775196	-1.08198788
C	-1.83563736	-2.37439875	0.21646082
H	-2.64201412	-2.69401872	0.87218852
C	-0.59009696	-2.37944030	0.78330483
H	-0.57099687	-2.72400077	1.80944606
C	1.47454727	-1.41129787	2.48570690
H	0.42813417	-1.18742334	2.72739579
C	1.87205478	-2.71903773	3.18960091
H	1.79384673	-2.62022897	4.27705987
H	2.90373814	-2.98013394	2.93694698
H	1.23855339	-3.55048929	2.87164173
C	2.32133824	-0.23673170	2.98582715
H	2.20729125	-0.10794912	4.06710856
H	2.01878157	0.68457126	2.48905601
H	3.37684019	-0.40410589	2.76486557
C	2.65231536	-2.69176954	-2.85384865
H	1.79474404	-3.05504658	-3.43792664
C	3.69173021	-3.81947877	-2.81830992
H	3.99583719	-4.09853893	-3.83256240
H	3.27665257	-4.70288774	-2.32644086
H	4.57465983	-3.50170720	-2.26002470
C	3.21813820	-1.44418454	-3.55109049
H	3.56132237	-1.68376640	-4.56250873
H	4.06275199	-1.04152885	-2.98708777
H	2.46384567	-0.65837273	-3.62093673
O	-4.59066440	-0.69850011	-0.59282008
S	-3.93114673	-1.79401305	-1.47045825
C	-4.61213426	-3.34343908	-0.78475861
C	-4.09829687	-4.56970900	-1.20683384
H	-3.25608621	-4.59977294	-1.88887318
C	-4.65460387	-5.74606163	-0.71318049
H	-4.25439140	-6.70282733	-1.02923011
C	-5.71555171	-5.69575169	0.19440229
H	-6.14232199	-6.61489458	0.57970906
C	-6.22114908	-4.46465399	0.60589772
H	-7.04168603	-4.42204816	1.31381676
C	-5.67331114	-3.28010046	0.11071023
H	-6.04382766	-2.31143689	0.41700382
O	5.96502772	-2.12578619	-0.83119376
C	8.25208543	-2.70967487	-0.48559017
H	8.86182764	-3.46386594	-0.98722674
H	8.70563309	-2.51479400	0.48776021
C	6.78848329	-3.19192734	-0.34133976
H	6.60733147	-4.09458206	-0.93913931
H	6.48730010	-3.37581375	0.68935503
C	8.13995156	-1.41183126	-1.32558129
H	8.26780988	-0.53209646	-0.69186866
H	8.87970648	-1.35982127	-2.12660572
C	6.70573966	-1.45735940	-1.85969895
H	6.24526967	-0.48047463	-1.99789357
H	6.64236290	-2.03285191	-2.79441257
O	5.61997393	-1.41840335	2.08612596
H	6.26620482	0.03180651	0.79482078
C	6.49735669	-0.31862220	1.79771256
H	7.54190009	-0.66300914	1.83668058
C	6.20256274	0.69152175	2.90687569
H	7.03360698	1.37777778	3.08262664
C	5.89403092	-0.21012534	4.12901087
H	6.71877879	-0.22014114	4.84465546
H	6.53685723	-2.27400615	3.73631155
H	5.32636851	1.28148691	2.63153796
H	4.76973400	-2.10332403	3.81961902
C	5.69035610	-1.61310151	3.50571127
H	5.00014813	0.12705889	4.65511244
N	-1.66424532	1.50535063	1.08949478
N	-2.27065046	2.38740014	-1.41152764

C	-0.69909918	1.91006877	0.32213583
C	-1.03466572	2.06871336	-1.15237887
C	-0.04514544	1.79328326	-2.17040921
H	-0.46426045	1.56716571	-3.14188990
C	1.32389188	1.71084910	-2.12565527
H	1.79482562	1.43111949	-3.06500814
C	2.20899468	1.98604448	-1.06765000
C	1.83770271	2.34261477	0.24303184
H	2.64991080	2.65085191	0.89698660
C	0.59838900	2.33136258	0.82370930
H	0.59035738	2.65265501	1.85753714
C	-1.45177369	1.33060741	2.52626437
H	-0.40294811	1.10203941	2.75288041
C	-1.84176106	2.62275435	3.26242463
H	-1.75378247	2.50003472	4.34670379
H	-2.87525498	2.89082781	3.02501856
H	-1.21002011	3.46028261	2.95705033
C	-2.29238895	0.14405741	3.00892848
H	-2.17126259	-0.00468626	4.08692009
H	-1.98931149	-0.76648123	2.49317987
H	-3.34984502	0.31023599	2.79654433
C	-2.67604735	2.71628418	-2.77810630
H	-1.82096687	3.07626096	-3.36765306
C	-3.70195608	3.85537413	-2.71922288
H	-4.00748027	4.15335287	-3.72770685
H	-3.27319459	4.72631540	-2.21684887
H	-4.58572847	3.53869046	-2.16178202
C	-3.26357729	1.48266344	-3.48219495
H	-3.61736024	1.73747562	-4.48626018
H	-4.10473395	1.08111796	-2.91196590
H	-2.51786332	0.69061459	-3.57122750
O	4.59079398	0.68793475	-0.65076153
S	3.91681560	1.81085476	-1.48192218
C	4.60060816	3.33861083	-0.75269660
C	4.08828029	4.57713022	-1.13932734
H	3.24677906	4.62795078	-1.82102243
C	4.64542017	5.73799925	-0.61123663
H	4.24667191	6.70401136	-0.89981521
C	5.70552983	5.66012785	0.29543624
H	6.13303043	6.56721968	0.70755598
C	6.20942733	4.41704382	0.67139658
H	7.02937351	4.35298841	1.37838426
C	5.66083457	3.24798575	0.14145338
H	6.03022489	2.27029750	0.41899673
O	-5.95908590	2.17968223	-0.75568121
C	-8.15316680	3.12832593	-0.82037256
H	-8.26567222	3.81569591	-1.66339276
H	-8.94222808	3.35032233	-0.09953479
C	-6.74834282	3.25547364	-0.20384513
H	-6.26951398	4.20933205	-0.44646110
C	-8.17925212	1.67397855	-1.32039222
H	-8.43238215	0.98931193	-0.50613008
H	-8.88496470	1.51311046	-2.13765694
C	-6.72808993	1.46768967	-1.74182644
H	-6.38450673	0.43370827	-1.72607614
H	-6.53924568	1.89674622	-2.73543897
H	-6.74844611	3.12701471	0.88094129
O	-5.58441989	1.34139211	2.14492290
H	-6.28270330	-0.05881621	0.82494591
C	-6.49963835	0.27940903	1.83524956
H	-7.53163685	0.65948313	1.88514337
C	-6.23691793	-0.76383359	2.92210485
H	-7.09177843	-1.42262475	3.08845528
C	-5.88790998	0.09971188	4.16123684
H	-6.70239563	0.11663712	4.88837341
H	-6.48151450	2.18566310	3.81163270
H	-5.38410768	-1.37900861	2.62931602
H	-4.71904201	1.97191215	3.89161898
C	-5.65051466	1.50977702	3.56796921
H	-4.99717918	-0.27526654	4.66677577
Na	3.85670625	-1.36329498	0.05318246
Na	-3.86350130	1.35551809	0.12201772

Compound [K(Ph(O)S−ATI$^{iPr/iPr}$)(thf)$_4$]

K	1.99706608	0.14456444	-0.25790547
N	-0.18973447	-0.72126640	1.20609752
N	-0.14621251	-1.08844959	-1.54183328
C	-1.23781271	-1.19858351	0.58983051
C	-1.28892174	-0.99424661	-0.91454282
C	-2.53321741	-0.62067788	-1.54957169
H	-2.41474612	-0.10200428	-2.49367121
C	-3.84186150	-0.80470052	-1.16606080
H	-4.59199110	-0.39646587	-1.84011921
C	-4.34668897	-1.52007647	-0.07499966
C	-3.60192241	-2.13705836	0.93380105
H	-4.16387057	-2.76913612	1.61974852
C	-2.25798434	-2.00460319	1.22197999
H	-1.92789119	-2.55502514	2.09484107
C	-0.06135240	-0.88532508	2.65205900
H	-1.04250854	-0.98420394	3.13796804
C	0.76323290	-2.14493705	2.96394506

H	0.88412253	-2.28741993	4.04271609
H	1.75729150	-2.05890327	2.51406024
H	0.28801322	-3.03682738	2.54923121
C	0.61896880	0.35668344	3.24269638
H	0.77009716	0.24216501	4.32094941
H	0.01156610	1.24980478	3.07974340
H	1.59365500	0.52128017	2.77531476
C	-0.11864338	-1.06806780	-3.00532031
H	-1.08476895	-1.38171681	-3.42471812
C	0.93337374	-2.07562202	-3.48673313
H	0.98398020	-2.09398857	-4.57995240
H	0.68868570	-3.08089370	-3.13603438
H	1.92367312	-1.81544007	-3.10139017
C	0.20482346	0.33769198	-3.54156318
H	0.19002763	0.34691174	-4.63611040
H	1.20112324	0.65689050	-3.22004934
H	-0.52037554	1.07355066	-3.18733125
O	-6.75432585	-1.90107515	-1.30526946
S	-6.13333265	-1.67756363	0.06651410
C	-6.49949282	0.08264569	0.45673864
C	-5.96218942	0.68159598	1.59566156
H	-5.28548849	0.12559899	2.23567471
C	-6.27972683	2.00615003	1.88301978
H	-5.86294355	2.48131935	2.76454937
C	-7.12892244	2.72346084	1.03605814
H	-7.37427092	3.75526374	1.26250729
C	-7.66034133	2.11190167	-0.09772854
H	-8.31939493	2.66745012	-0.75620711
C	-7.35167992	0.78160541	-0.38955320
H	-7.74876833	0.27718806	-1.26336106
C	-0.51350372	3.83059025	-1.78598375
H	-0.75683332	3.65491937	-2.83516419
H	-0.72679138	4.87978022	-1.56498147
C	0.96145788	3.50228949	-1.47374513
H	1.42751979	2.88802004	-2.24777552
H	1.56391181	4.40770756	-1.33808491
O	0.97379026	2.73724556	-0.24762157
C	-1.29631661	2.91096054	-0.83217046
H	-2.26822203	3.31705877	-0.54686266
H	-1.46081041	1.92625210	-1.27170516
C	-0.34070762	2.78377515	0.34716537
H	-0.40860311	3.65021698	1.02055620
H	-0.47560999	1.86421355	0.91586772
O	3.66229919	1.09570582	-2.31503847
C	5.90875194	0.28458338	-2.11504447
H	6.70268175	0.41278393	-2.85374879
H	6.17746730	-0.56456663	-1.48510594
C	4.54235084	0.06800047	-2.81289931
H	4.62683724	0.16402190	-3.90153988
H	4.08613746	-0.89243655	-2.57318654
C	5.70281896	1.57255129	-1.28231276
H	5.45086926	1.32555686	-0.24897188
H	6.57822577	2.22506357	-1.28468928
C	4.48648224	2.20937914	-1.95522740
H	3.89928806	2.86063702	-1.30618288
H	4.77160216	2.77329393	-2.85564545
O	3.41537859	-2.19214001	-0.43900426
C	2.89416290	-4.26520312	0.63686753
H	3.09233727	-5.28044364	0.28802188
H	2.08045437	-4.31592446	1.35985188
C	2.54100430	-3.33904054	-0.54971264
H	2.72869736	-3.83242005	-1.51036048
H	1.51808635	-2.96132065	-0.54769608
C	4.16052700	-3.62393161	1.25804783
H	3.90362469	-3.07129400	2.16472526
H	4.92731346	-4.35637742	1.51733595
C	4.62226372	-2.64972068	0.17173266
H	5.15706348	-1.77621482	0.54931055
H	5.25351450	-3.15553018	-0.57448614
O	3.86488457	1.03448084	1.62402625
H	2.71629799	2.69506173	2.08762680
C	3.77396577	2.43331666	1.98978118
H	4.20063255	3.02824477	1.17869514
C	4.53402252	2.57588592	3.31080207
H	5.59125972	2.78674702	3.12442155
C	4.37076422	1.18070269	3.93354827
H	5.13605331	0.94553480	4.67515981
H	5.49156664	0.03959610	2.44883931
H	4.13295734	3.37589793	3.93504097
H	3.89195805	-0.65357284	2.80709883
C	4.45058863	0.27919628	2.70248414
H	3.39013117	1.08563317	4.40636528

Compound [K(Ph(O)S−ATI$^{iPr/iPr}$)(thf)$_3$]$_2$

K	-4.06792400	0.69953400	-0.28951000
N	-1.58855400	1.42030400	0.82743100
N	-2.05764500	2.20115800	-1.76176000
C	-0.63601600	1.97874800	0.14657100
C	-0.83583800	2.02964600	-1.35950900
C	0.29002600	1.81469300	-2.25327800
H	0.01976400	1.38981400	-3.21194600

C	1.62358000	2.08735500	-2.10477900
H	2.24171300	1.85443100	-2.96917400
C	2.30460300	2.66911800	-1.01398300
C	1.75018300	2.94691600	0.25059500
H	2.41114400	3.44613400	0.95476100
C	0.50558500	2.64969300	0.74422000
H	0.35277800	2.95960500	1.77054500
C	-1.50378400	1.31421800	2.28270800
H	-0.46330300	1.23930800	2.62522600
C	-2.15106100	2.54748700	2.93419100
H	-2.16676000	2.45573800	4.02500500
H	-3.17868200	2.65300100	2.57747000
H	-1.61655700	3.46389700	2.67338600
C	-2.22615100	0.03594800	2.72173400
H	-2.13283300	-0.11354800	3.80231500
H	-1.81350400	-0.83286200	2.20897800
H	-3.29095200	0.09049000	2.48091000
C	-2.33814300	2.40485300	-3.18306500
H	-1.44623100	2.75953600	-3.71854600
C	-3.41066800	3.49271700	-3.31164500
H	-3.65897400	3.67098500	-4.36281800
H	-3.05780400	4.43102900	-2.87617100
H	-4.32025000	3.19432300	-2.78745700
C	-2.80479300	1.09610900	-3.83937400
H	-2.98039300	1.24312000	-4.90983500
H	-3.74313300	0.75216400	-3.39334500
H	-2.05413800	0.31299400	-3.71649400
O	4.87130100	1.91564800	-0.45524500
S	4.03416600	2.91188500	-1.29751800
C	4.29164400	4.51416400	-0.46593800
C	3.61537700	5.64586100	-0.92136800
H	2.89792800	5.56163900	-1.72995500
C	3.84952700	6.87115700	-0.30464300
H	3.32291800	7.75463100	-0.64771700
C	4.75241300	6.96215600	0.75791600
H	4.92940200	7.91840900	1.23721600
C	5.42334100	5.82442200	1.20071900
H	6.12273700	5.89226500	2.02684100
C	5.19904100	4.59238200	0.58378600
H	5.70388300	3.69153400	0.90765000
O	-6.19717900	0.99438500	-2.16011600
C	-8.29195300	2.00952000	-1.57346700
H	-9.08994200	2.11451800	-2.31273900
H	-8.48897800	2.72039000	-0.76904600
C	-6.90816600	2.24492700	-2.22850000
H	-7.00332400	2.55154800	-3.27673900
H	-6.30664600	2.98271800	-1.69761400
C	-8.20647600	0.55679300	-1.06189800
H	-7.82466000	0.53690800	-0.03939700
H	-9.16636600	0.03647600	-1.08898900
C	-7.16793100	-0.05225800	-2.00096000
H	-6.64611500	-0.92294100	-1.60296200
H	-7.61144100	-0.30338600	-2.97646700
O	-4.96091200	3.23085600	0.39209800
C	-4.25488100	5.21515000	1.51641600
H	-4.41205100	6.25808600	1.23342300
H	-3.39230000	5.17931400	2.18216700
C	-4.04333400	4.33316100	0.26256600
H	-4.27905400	4.88582400	-0.65498200
H	-3.04709200	3.90558400	0.15907400
C	-5.51446800	4.61517200	2.19261400
H	-5.23261600	4.00416500	3.05312800
H	-6.21850300	5.37582500	2.53612800
C	-6.10064700	3.72228200	1.09559500
H	-6.66092700	2.85920300	1.45475000
H	-6.74052200	4.30591400	0.41484900
O	-6.13589300	0.37686100	1.89098700
H	-6.50856900	-1.41571500	0.97176700
C	-6.63985100	-0.96774400	1.95428800
H	-7.70707800	-0.95155600	2.22404500
C	-5.79730700	-1.62051400	3.04621700
H	-6.26453000	-2.51166900	3.47068200
C	-5.63480300	-0.47779800	4.07457600
H	-6.35466900	-0.57521500	4.89037900
H	-6.81791200	1.31838900	3.61346700
H	-4.83228200	-1.90579900	2.62241200
H	-5.09276600	1.50914900	3.23962800
C	-5.92153000	0.80090400	3.24682400
H	-4.63572400	-0.46272600	4.51101100
K	4.06792400	-0.69953400	-0.28951100
N	1.58855500	-1.42030300	0.82743000
N	2.05764500	-2.20115600	-1.76176100
C	0.63601600	-1.97874600	0.14657000
C	0.83583800	-2.02964300	-1.35950900
C	-0.29002600	-1.81469000	-2.25327800
H	-0.01976500	-1.38981000	-3.21194600
C	-1.62358000	-2.08735300	-2.10477900
H	-2.24171300	-1.85442800	-2.96917300
C	-2.30460200	-2.66911700	-1.01398300
C	-1.75018200	-2.94691600	0.25059400
H	-2.41114300	-3.44613500	0.95476100
C	-0.50558400	-2.64969200	0.74422000

H	-0.35277700	-2.95960500	1.77054400
C	1.50378500	-1.31421700	2.28270800
H	0.46330400	-1.23930700	2.62522600
C	2.15106200	-2.54748700	2.93418900
H	2.16676300	-2.45573800	4.02500300
H	3.17868300	-2.65300100	2.57746800
H	1.61655800	-3.46389700	2.67338400
C	2.22615200	-0.03594800	2.72173500
H	2.13283400	0.11354800	3.80231600
H	1.81350600	0.83286300	2.20897900
H	3.29095400	-0.09049000	2.48091200
C	2.33814200	-2.40484900	-3.18306600
H	1.44623000	-2.75953300	-3.71854700
C	3.41066800	-3.49271300	-3.31164700
H	3.65897300	-3.67098000	-4.36282000
H	3.05780400	-4.43102600	-2.87617300
H	4.32024900	-3.19432000	-2.78746000
C	2.80479200	-1.09610500	-3.83937500
H	2.98039100	-1.24311500	-4.90983600
H	3.74313200	-0.75216000	-3.39334600
H	2.05413600	-0.31299000	-3.71649500
O	-4.87130100	-1.91564700	-0.45524500
S	-4.03416500	-2.91188500	-1.29751800
C	-4.29164300	-4.51416400	-0.46593900
C	-3.61537600	-5.64586100	-0.92136800
H	-2.89792500	-5.56163800	-1.72995400
C	-3.84952600	-6.87115700	-0.30464300
H	-3.32291600	-7.75463100	-0.64771600
C	-4.75241300	-6.96215600	0.75791500
H	-4.92940200	-7.91840900	1.23721500
C	-5.42334200	-5.82442300	1.20071800
H	-6.12273900	-5.89226500	2.02683900
C	-5.19904100	-4.59238300	0.58378400
H	-5.70388500	-3.69153400	0.90764800
O	6.19718000	-0.99438500	-2.16011600
C	8.29195300	-2.00952100	-1.57346800
H	9.08994200	-2.11451800	-2.31274000
H	8.48897800	-2.72039200	-0.76904800
C	6.90816600	-2.24492700	-2.22850100
H	7.00332300	-2.55154900	-3.27674000
H	6.30664500	-2.98271800	-1.69761500
C	8.20647600	-0.55679500	-1.06189600
H	7.82466000	-0.53691100	-0.03939600
H	9.16636600	-0.03647800	-1.08898600
C	7.16793200	0.05225700	-2.00095800
H	6.64611700	0.92294000	-1.60296000
H	7.61144300	0.30338600	-2.97646500
O	4.96091000	-3.23085700	0.39209700
C	4.25487700	-5.21515200	1.51641300
H	4.41204600	-6.25808800	1.23341800
H	3.39229600	-5.17931600	2.18216300
C	4.04333100	-4.33316100	0.26256300
H	4.27905200	-4.88582400	-0.65498500
H	3.04709000	-3.90558300	0.15907000
C	5.51446500	-4.61517600	2.19261100
H	5.23261300	-4.00416900	3.05312600
H	6.21849900	-5.37582900	2.53612500
C	6.10064500	-3.72228400	1.09559300
H	6.66092600	-2.85920700	1.45474900
H	6.74051900	-4.30591600	0.41484700
O	6.13589300	-0.37686200	1.89098700
H	6.50856700	1.41571400	0.97176900
C	6.63985100	0.96774200	1.95428900
H	7.70707800	0.95155300	2.22404400
C	5.79730900	1.62051100	3.04622000
H	6.26453300	2.51166500	3.47068500
C	5.63480600	0.47779400	4.07457800
H	6.35467400	0.57520900	4.89038000
H	6.81791400	-1.31839300	3.61346500
H	4.83228300	1.90579700	2.62241700
H	5.09276700	-1.50915300	3.23962800
C	5.92153100	-0.80090700	3.24682300
H	4.63572800	0.46272200	4.51101400

THF

O	0.000012879	-1.252287366	0.000126355
C	-0.732704867	0.994963493	0.230228160
H	-0.790216163	1.147461406	1.312345189
H	-1.342093846	1.759676387	-0.255375746
C	-1.168730098	-0.427845916	-0.133498106
H	-1.949818721	-0.823106551	0.521194753
H	-1.527042311	-0.478215519	-1.170248101
C	0.732618067	0.995044229	-0.230153891
H	0.790085239	1.147730689	-1.312247117
H	1.341971998	1.759725357	0.255544298
C	1.168797394	-0.427787423	0.133338453
H	1.949669202	-0.822964890	-0.521665475
H	1.527458598	-0.478254234	1.169953662

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