Supporting Information

Aminotroponiminates: ligand-centred, reversible redox events under oxidative conditions in sodium and bismuth complexes

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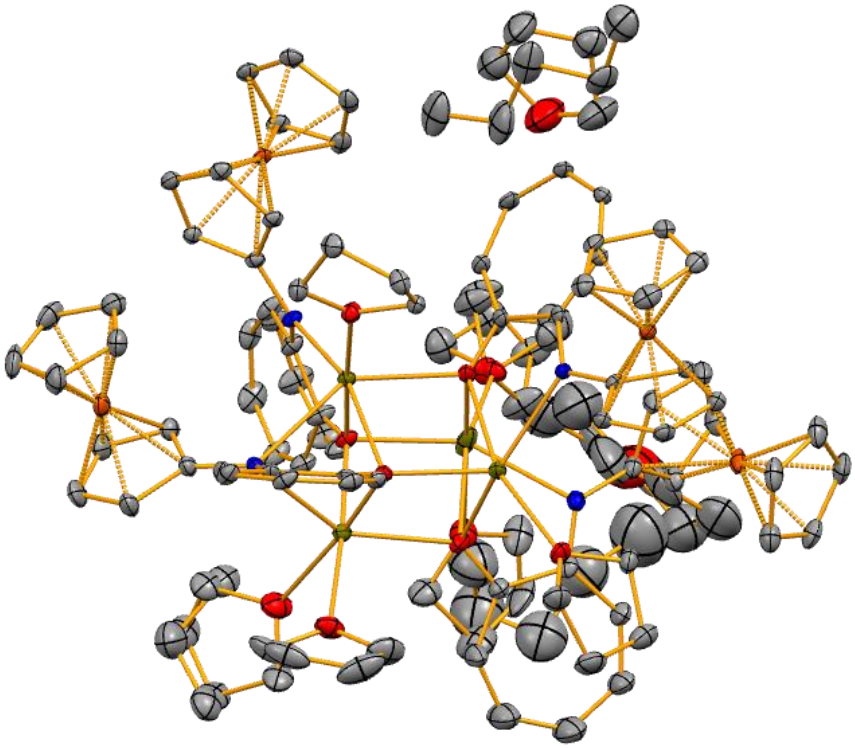
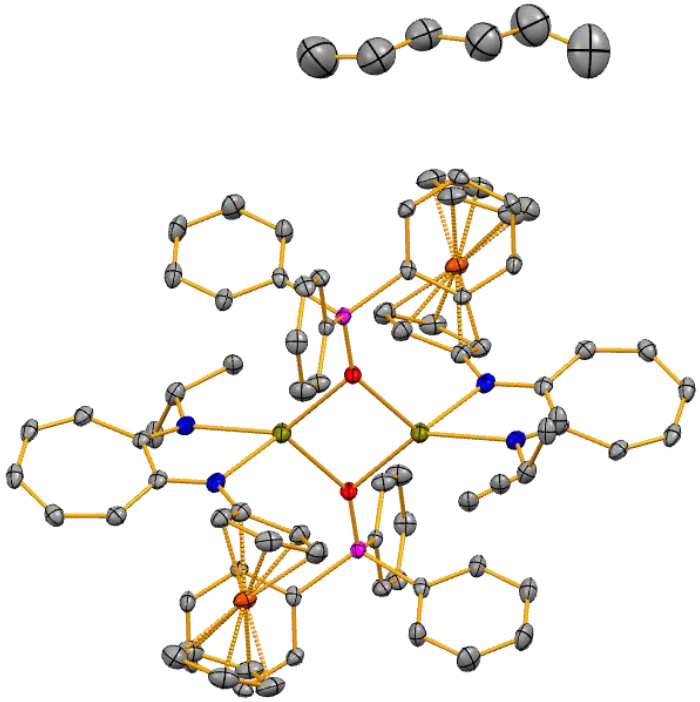
Single Crystal X-ray Analysis

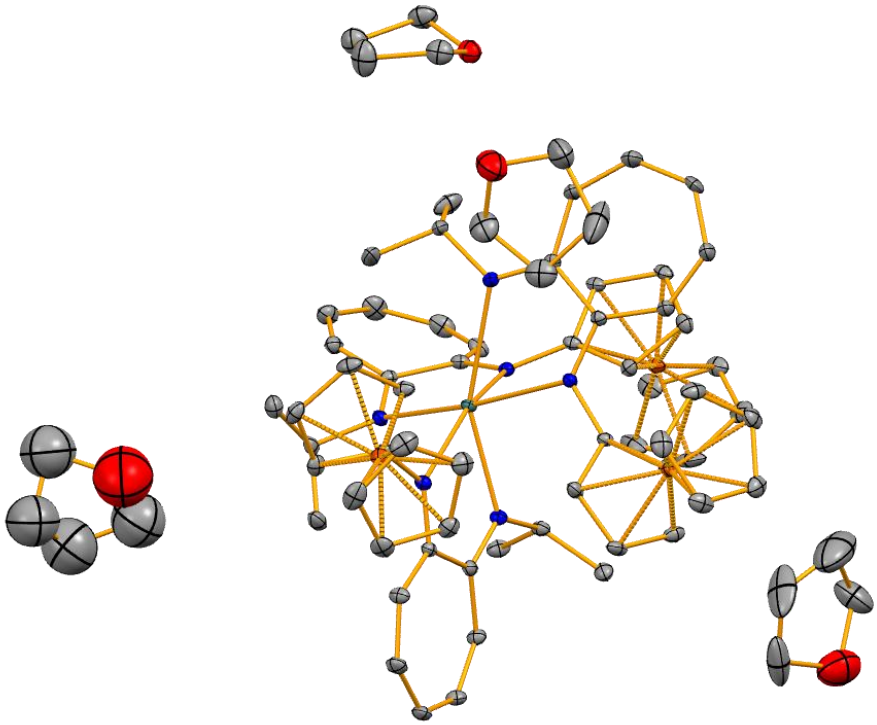
The full asymmetric units of compounds **3·(thf)$_{1.5}$**, **6-OPPh$_3$**, and **8** are not depicted in the main part, because they result in very crowded representations. They are shown in Schemes S1-S3 for completeness.



Scheme S1. Asymmetric unit of **3·(thf)$_{1.5}$** with displacement ellipsoids shown at the 50% probability level. Hydrogen atoms are omitted for clarity.



Scheme S2. Asymmetric unit of **6-OPPh$_3$** with displacement ellipsoids shown at the 50% probability level. Hydrogen atoms are omitted for clarity.



Scheme S3. Asymmetric unit of **8** with displacement ellipsoids shown at the 50% probability level. Hydrogen atoms are omitted for clarity.

Solid state structure of [$BiCl_2(ATI^{Fc/iPr})$] (7).

As described in the main text, compound **7** forms a coordination polymer in the solid state, in which the repeating unit **7** shows intermolecular Bi···Cl and C_7^{ATI}···C_7^{ATI} interactions. A cut out of this one-dimensional coordination polymer is shown in Scheme S4a. Furthermore, every second ATI backbone (namely C1-C7) shows additional C_7^{ATI}···C_7^{ATI} (arene-arene) interactions with an ATI backbone that belongs to a neighbouring polymer strand (C3–centroid^{ATI}, 3.427(17) Å; C3–plane(C1-7), 3.346(17) Å; a centroid is defined here as the centre of an ATI ligand backbone, calculated from the positions of the seven carbon atoms C1-C7 and C21-C27, respectively.). Thus a linear double strand structure is formed in the solid state due to interaction of one ATI ligand backbone with two other ATI ligand backbones in parallel-displaced arene···arene bonding (Figure S4).

Bonding parameters for the description of π-stacking between ATI ligand backbones are summarised in Table S1.

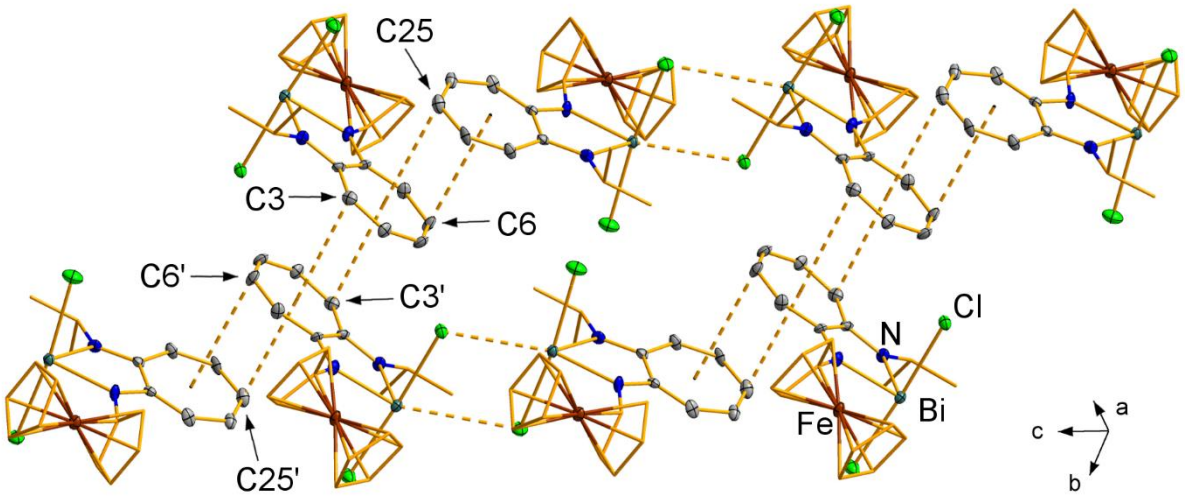


Figure S4. Cut out of coordination polymer $(\mathbf{7})_\infty$ in the solid state.

Table S1. Distances for description of π-stacking between ATI ligand backbones in [$BiCl_2(ATI^{Fc/iPr})$] (**7**).

	Centroid		plane	
Atom	**ct(C1-7)**	**ct(C21-27)**	**plane(C1-7)**	**plane(C21-27)**
C3	3.427(17) Å	-	3.346(17) Å	-
C6	-	3.758(17) Å	-	3.625(17) Å
C25	3.369(17) Å	-	3.301(17) Å	-

Table S2. Crystallographic data.

Data	**Compound 2**	**Compound 3·(thf)$_{1.5}$**	**Compound 5**	**Compound 6·OPPh$_3$**	**Compound 7**	**Compound 8**
Empirical formula	$C_{17}H_{15}FeNO$	$C_{98.96}H_{119.35}Fe_4N_4Na_4O_{10.27}$	$C_{20}H_{22}FeN_2$	$C_{88}H_{100}Fe_2N_4Na_2O_2P_2$	$C_{40}H_{42}Bi_2Cl_4Fe_2N_4$	$C_{76}H_{95}BiFe_3N_6O_4$
Formula weight (g·mol^{-1})	305.15	1844.51	346.24	1465.33	1250.23	1533.10
Temperature (K)	101(2)	100(2)	100(2)	105(2)	101(2)	100(2)
Radiation, λ (Å)	$Mo_{K\alpha}$ 0.71073	$Mo_{K\alpha}$ 0.71073	$Mo_{K\alpha}$ 0.71073	$Mo_{K\alpha}$ 0.71073	$Mo_{K\alpha}$ 0.71073	$Mo_{K\alpha}$ 0.71073
Crystal system	Monoclinic	Triclinic	Orthorhombic	Monoclinic	Triclinic	Triclinic
Space group	$P12_1/c1$	$P\ \bar{1}$	$P2_12_12_1$	$P\ 1\ 2_1/c\ 1$	$P\ \bar{1}$	$P\ \bar{1}$
Unit cell dimensions						
a (Å)	9.478(3)	15.062(3)	28.5012(14)	13.8101(5)	12.3954(8)	13.4649(19)
b (Å)	10.500(4)	15.807(3)	5.7094(3)	15.5735(4)	12.5471(8)	14.607(2)
c (Å)	13.271(5)	21.488(4)	10.1021(5)	18.4473(5)	14.5794(9)	18.529(3)
α (°)	90	85.773(6)	90	90	64.945(2)	93.978(2)
β (°)	94.603(6)	87.331(6)	90	98.746(3)	75.396(2)	107.059(2)
γ (°)	90	62.126(5)	90	90	84.677(2)	105.219(2)
Volume (Å^3)	1316.5(8)	4509.9(15)	1643.86(14)	3921.4(2)	1987.5(2)	3319.2(8)
Z	4	2	4	2	2	2
Calculated density (mg·m^{-3})	1.540	1.358	1.399	1.241	2.089	1.534
Absorbtion coefficient (mm^{-1})	1.138	0.712	0.918	0.472	9.847	3.341
F(000)	632	1943	728	1552	1192	1572
Theta range for collection	2.900 to 26.948°	2.328 to 25.058°	1.429 to 28.756°	2.814 to 29.182	2.253 to 26.750°	1.689 to 26.810°
Reflections collected	27828	78926	12552	27402	25022	31442
Independent reflections	2844	15892	4047	9267	8337	14110
Minimum/maximum transmission	0.5306/0.7454	0.6838/0.7452	0.6807/0.7458	0.95936/1.0000	0.6078/0.7454	0.6295/0.7461
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / parameters / restraints	2844 / 185 / 0	15892 / 1321 / 486	4047 / 191 / 84	9267 / 464 / 78	8337 / 467 / 171	14110 / 825 / 104
Goodness-of-fit on F^2	0.985	1.024	1.063	1.072	1.116	1.069
Final R indices [I>2σ(I)]	R_1 = 0.0446, wR^2 = 0.1115	R_1 = 0.0548, wR^2 = 0.1233	R_1 = 0.0970, wR^2 = 0.2235	R_1 = 0.0913, wR^2 = 0.2150	R_1 = 0.0445, wR^2 = 0.0852	R_1 = 0.0379, wR^2 = 0.0981
R indices (all data)	R_1 = 0.0666, wR^2 = 0.1274	R_1 = 0.0940, wR^2 = 0.1435	R_1 = 0.1127, wR^2 = 0.2314	R_1 =0.1463, wR^2 = 0.2458	R_1 = 0.0689, wR^2 = 0.0903	R_1 = 0.0438, wR^2 = 0.1014
Maximum/minimum residual electron density (e·Å^{-3})	0.607 / –0.775	0.963 / –0.610	1.429 / –1.732	0.930 / –0.590	1.731 / –1.566	2.346 / –1.015

DFT Calculations

DFT calculations on ATI ligand H-ATI$^{Fc/iPr}$ (5).

Geometry optimisations of two tautomers of compound H-ATI$^{Fc/iPr}$ (**5**) in the gas phase were performed. The experimentally observed tautomer with an HN*i*PrR amine group (Figure S5a) was found to be lower in energy (H^{rel} = –2.6 kcal·mol^{-1}; G^{rel} = –2.6 kcal·mol^{-1}) than the hypothetical tautomer with an HNFcR amine group (Figure S5b).

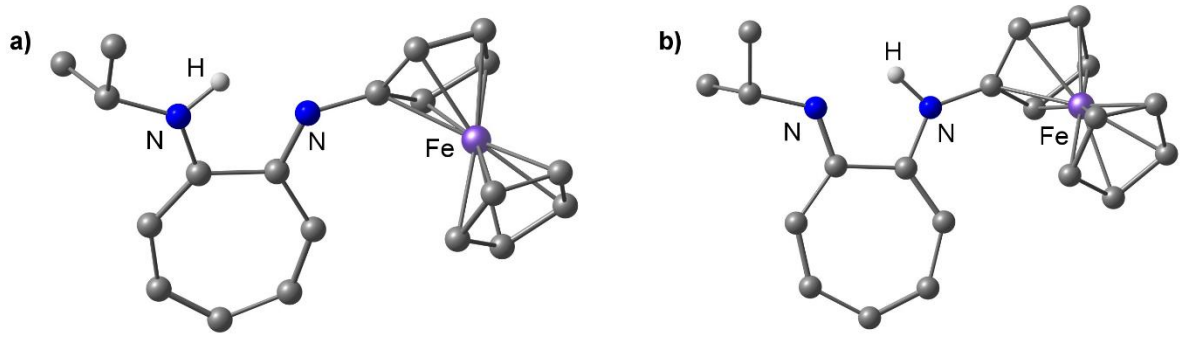


Figure S5. Molecular structures of two tautomers of H-ATI$^{Fc/iPr}$ (**5**) with an HN*i*Pr amine / NFc imine groups (a, left) or N*i*Pr imine / HNFc amine groups (b, right), as determined by DFT calculations. Carbon-bound hydrogen atoms are omitted for clarity.

Spin densities of reduced and oxidised forms of AT ligand 2 and ATI ligand 5.

The spin density plots of the non-isolated radical cations [H-AT^{Fc}]$^{\bullet+}$ (**2-ox**) and [H-ATI$^{Fc/iPr}$]$^{\bullet+}$ (**5-ox**) as well as the non-isolated radical anions [H-AT^{Fc}]$^{\bullet-}$ (**2-red**) and [H-ATI$^{Fc/iPr}$]$^{\bullet-}$ (**5-red**) are shown in the main part. Further details of the spin density distributions in these species as determined by DFT calculations are given below.

[H-AT^{Fc}]$^{\bullet+}$ (2-ox). The Mulliken spin density for the iron atom amounts to Fe: +1.31. For all other atoms of this compound, the absolute value of the Mulliken spin densities was ≤ 0.05.

[H-AT^{Fc}]$^{\bullet-}$ (2-red). The Mulliken spin densities for the carbon atoms in the C_7 backbone amount to C1: –0.07, C2: +0.36, C3: –0.11, C4: +0.24, C5: +0.12, C6: –0.01, C7: +0.32 and for the Fe atom to Fe: +0.22. For all other atoms of this compound, the absolute value of the Mulliken spin densities was ≤ 0.03.

[H-ATI$^{Fc/iPr}$]$^{\bullet+}$ (5-ox). The Mulliken spin density for the iron atom amounts to Fe: +1.32. For all other atoms of this compound, the absolute value of the Mulliken spin densities was ≤ 0.06.

[H-ATI$^{Fc/iPr}$]$^{\bullet-}$ (5-red). The Mulliken spin densities for the carbon atoms in the C_7 backbone amount to C1: –0.08, C2: +0.44, C3: –0.15, C4: +0.33, C5: +0.08, C6: +0.04, C7: +0.34. For all other atoms of this compound, the absolute value of the Mulliken spin densities was ≤ 0.04.

DFT calculations on Bi(ATI$^{Fc/iPr}$)$_3$ (8).

Geometry optimisations of two tautomers of compound Bi(ATI$^{Fc/iPr}$)$_3$ (**8**) in the gas phase were performed. The experimentally observed *trans* isomer (Figure S6, left) was found to be lower in energy (H^{rel} = –4.1 kcal·mol^{-1}; G^{rel} = –4.6 kcal·mol^{-1}) than the *cis* isomer (Figure S6, right).

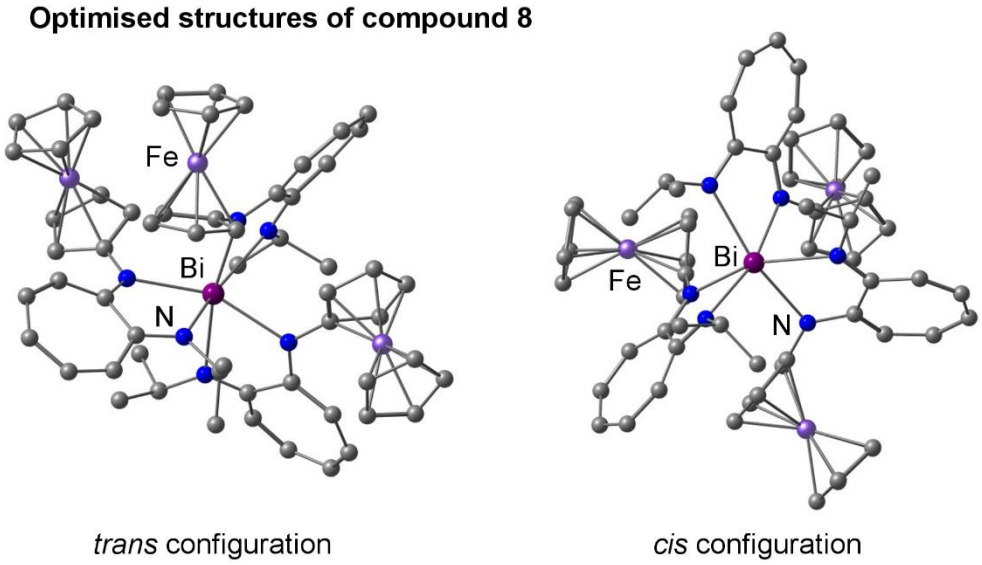


Figure S6. Molecular structures of Bi(ATI$^{Fc/iPr}$)$_3$ (**8**) in its *trans* configuration (left) and *cis* configuration (right), as determined by DFT calculations. Hydrogen atoms are omitted for clarity.

The strongly distorted coordination geometry around the bismuth atom of **8** in its experimentally observed *trans* configuration raised the question whether the bismuth-centred lone pair might exhibit a "stereochemical activity". A molecular orbital analysis revealed that the HOMO-9 indeed shows a significant contribution of a distorted s-type Bi centred atomic orbital, which is located between the nitrogen atoms with the largest N–Bi–N angles (Figure S7). This supports a possible "stereochemical activity" of the Bi lone pair in compound **8**.

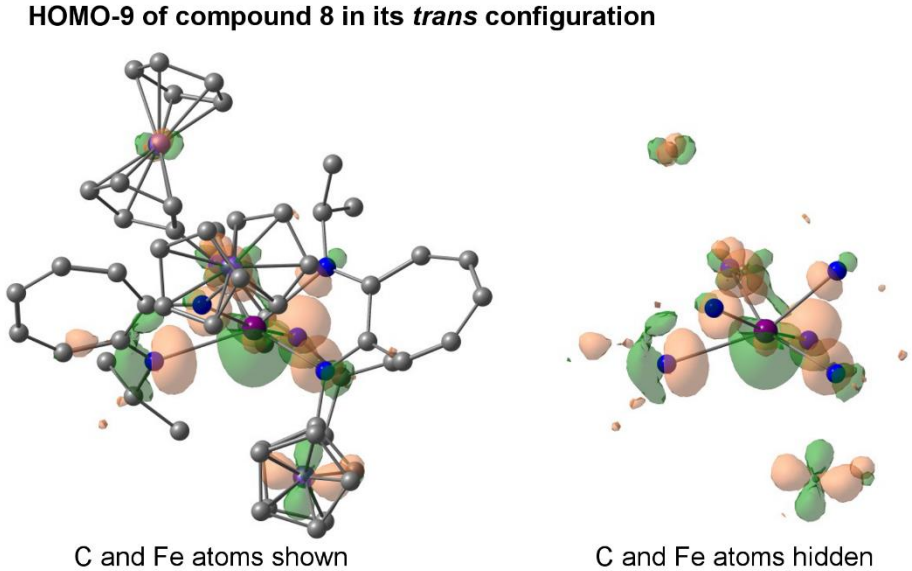


Figure S7. Plot of the HOMO-9 of compound **8** in its *trans* configuration with C and Fe atoms shown (left) and with C and Fe atoms omitted for clarity (right) at an isovalue of 0.04.

DFT calculations on $[Bi(AT^{Fc})_3]^+$ (4^+) and $[Bi(ATI^{Fc/iPr})_3]^+$ (8^+).

One electron oxidation of $[Bi(AT^{Fc})_3]$ (**4**) and $[Bi(ATI^{Fc/iPr})_3]$ (**8**) should afford the cationic species $[Bi(AT^{Fc})_3]^+$ ($\mathbf{4}^+$) and $[Bi(ATI^{Fc/iPr})_3]^+$ ($\mathbf{8}^+$). A geometry optimization and frontier orbital analysis was performed for these species. The optimized structures and singly occupied molecular orbitals (SOMOs) of $\mathbf{4}^+$ and $\mathbf{8}^+$ are shown in Figure S8. The shortest distances between the iron centres amount to 6.051 Å in $\mathbf{4}^+$ and to 5.796 Å in $\mathbf{8}^+$.

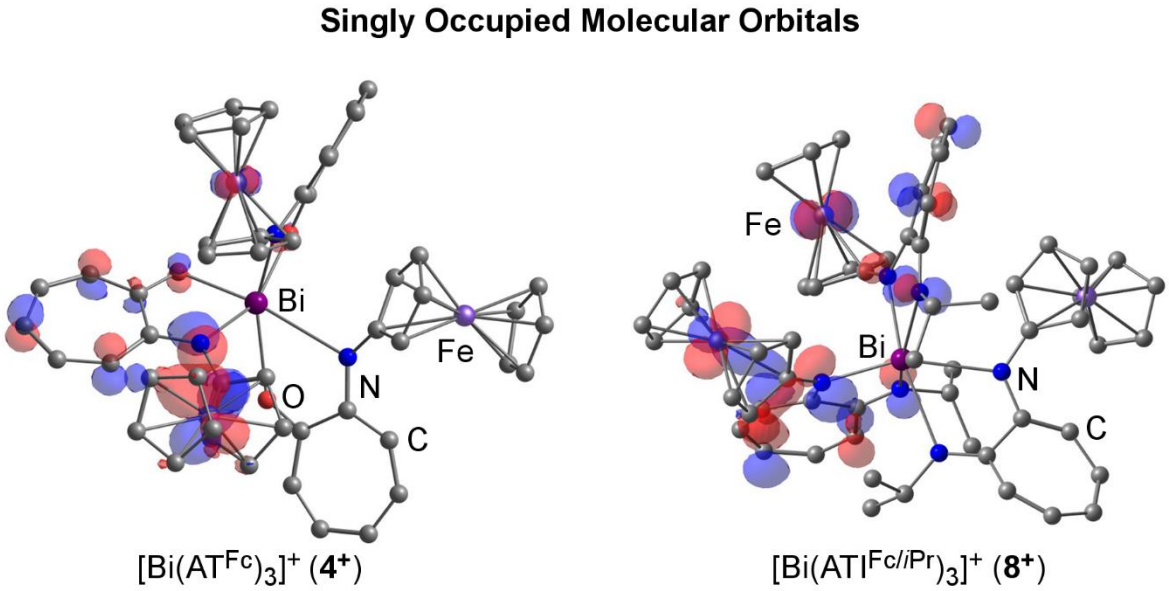


Figure S8. Plot of the SOMOs of compounds $[Bi(AT^{Fc})_3]^+$ ($\mathbf{4}^+$) (left) and $[Bi(ATI^{Fc/iPr})_3]^+$ ($\mathbf{8}^+$) (right) at an isovalue of 0.04.

Electrochemical Measurements

H-AT^{Fc} (2). The redox wave at –2.38 V is chemically reversible, when the potential window of –2.0 V to –2.7 V is scanned (Figure S10). When the full potential window from +0.50 V to –3.50 V is scanned, this redox event becomes partially reversible and a corresponding oxidation wave appears at –1.38 V (Figure S9). Moreover, an irreversible reduction wave was detected at –3.21 V.

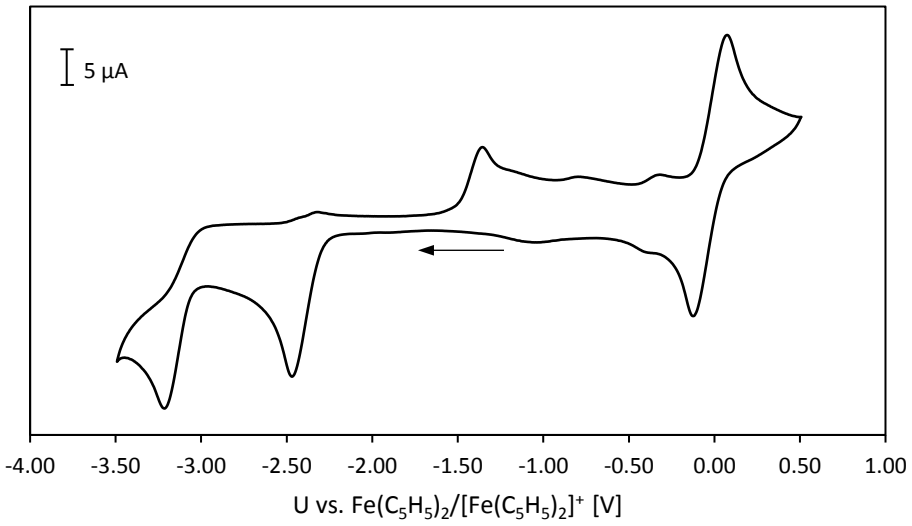


Figure S9. Cyclic voltammogram of **2** at 23 °C in THF / 0.1 M [N(*n*Bu)$_4$][PF$_6$] at a scan rate of 250 mV·s^{-1}.

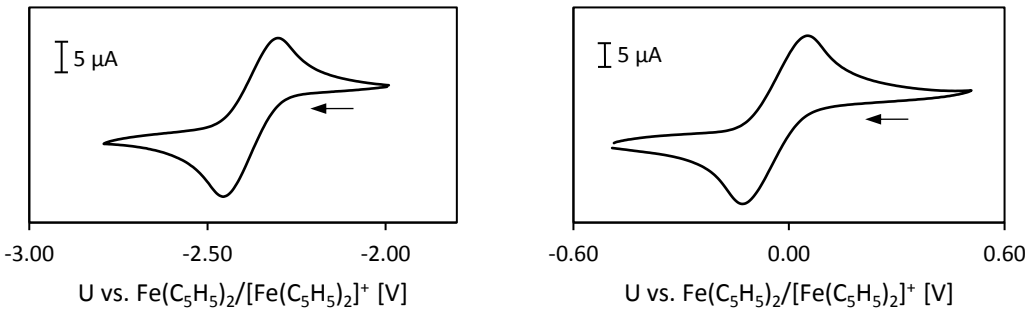


Figure S10. Cyclic voltammograms of **2** at 23 °C in THF / 0.1 M [N(*n*Bu)$_4$][PF$_6$] at scan rates of 250 mV·s^{-1} for two different potential windows.

Na(AT^{Fc}) (3).

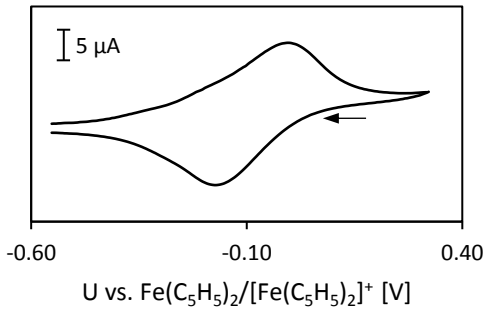


Figure S11. Cyclic voltammogram of **3** at 23 °C in THF / 0.1 M [N(*n*Bu)$_4$][PF$_6$] at a scan rate of 250 mV·s^{-1}.

Bi(AT^{Fc})$_3$ (4).

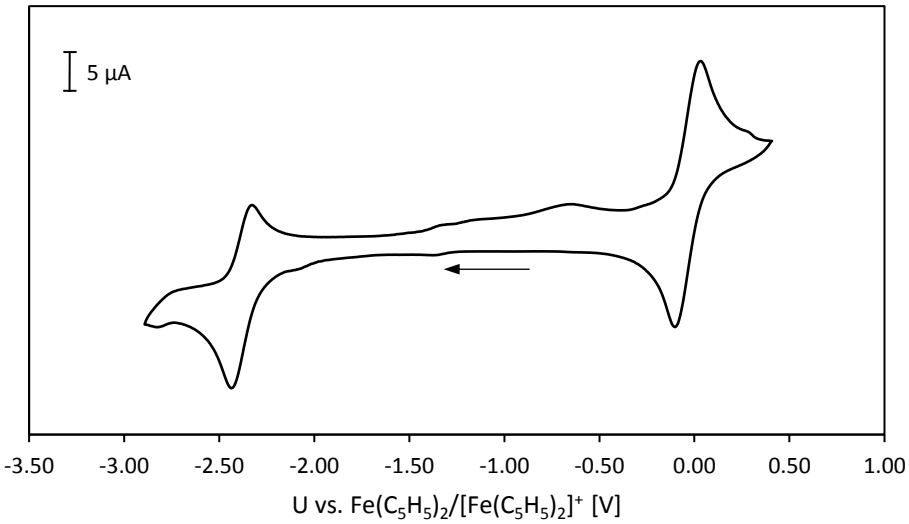


Figure S12. Cyclic voltammogram of **4** at 23 °C in THF / 0.1 M [N(*n*Bu)$_4$][PF$_6$] at a scan rate of 250 mV·s^{-1}.

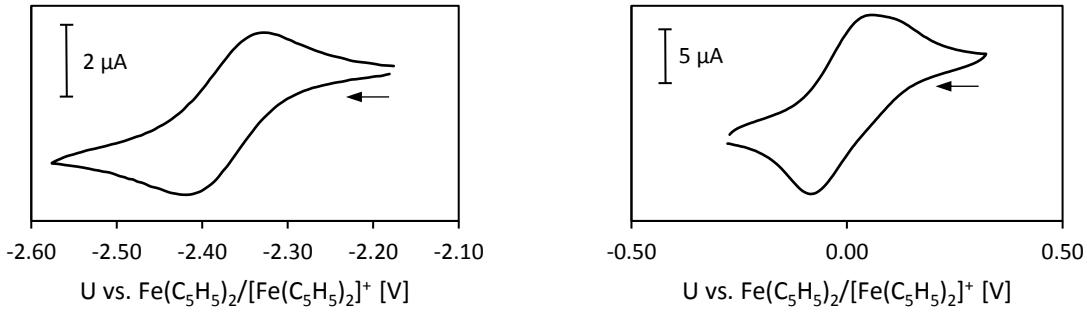


Figure S13. Cyclic voltammogram of **4** at 23 °C in THF / 0.1 M [N(*n*Bu)$_4$][PF$_6$] at scan rates of 250 mV·s^{-1}.

H-ATI$^{Fc/iPr}$ (5). The redox wave at –2.64 V is chemically reversible, when the potential window of –2.0 V to –2.5 V is scanned (Figure S15). When the full potential window from +0.30 V to –3.50 V is scanned, this redox event becomes partially reversible and a corresponding oxidation wave appears at –1.63 V (Figure S14).

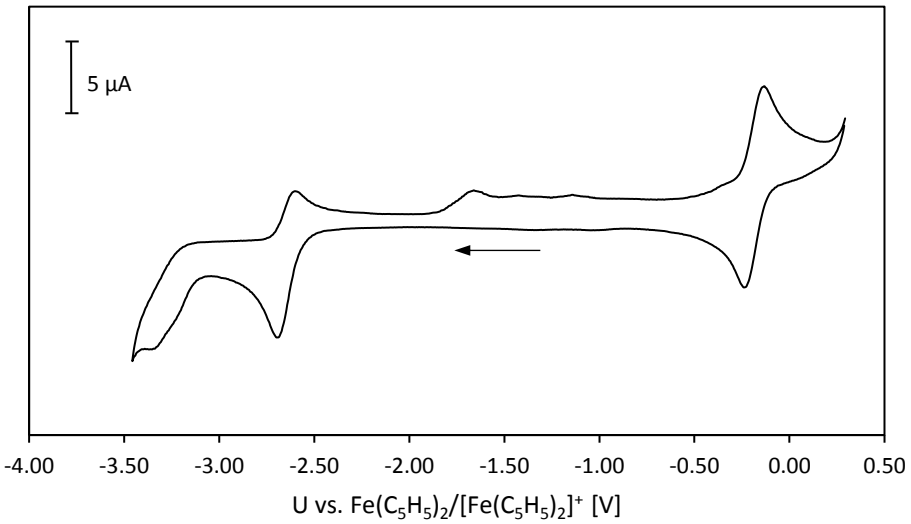


Figure S14. Cyclic voltammogram of **5** at 23 °C in THF / 0.1 M [N(*n*Bu)$_4$][PF$_6$] at a scan rate of 250 mV·s^{-1}.

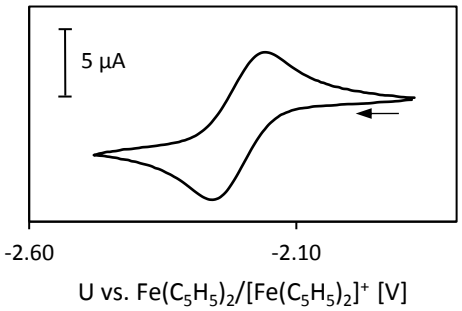


Figure S15. Cyclic voltammogram of **5** at 23 °C in THF / 0.1 M [N(*n*Bu)$_4$][PF$_6$] at a scan rate of 250 mV·s^{-1}.

[Na(ATI$^{Fc/iPr}$)(OPPh$_3$)] (6-OPPh$_3$). In addition to the redox events described in the main part of this document, a chemically reversible redox event was detected at potentials of –3.07 V, where beginning solvent decomposition can play a role (Figure S16).

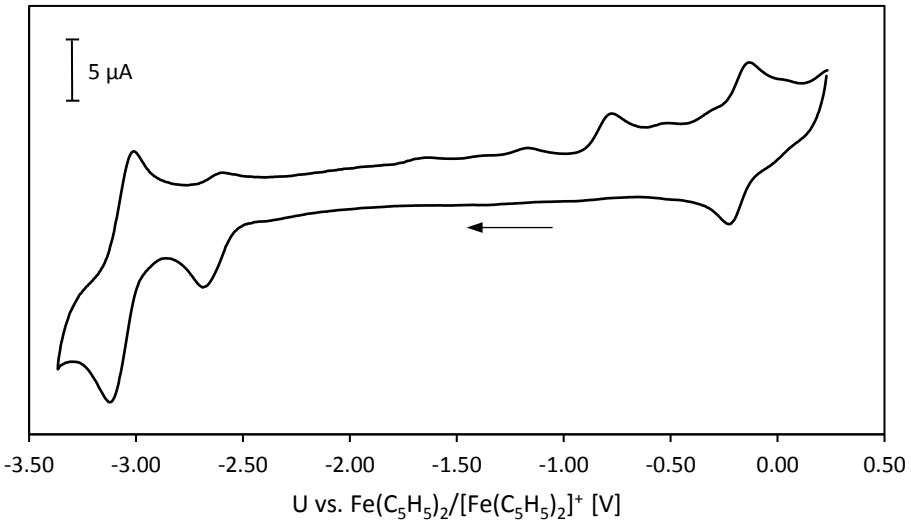


Figure S16. Cyclic voltammogram of **6-OPPh$_3$** at 23 °C in THF / 0.1 M [N(*n*Bu)$_4$][PF$_6$] at a scan rate of 250 mV·s^{-1}.

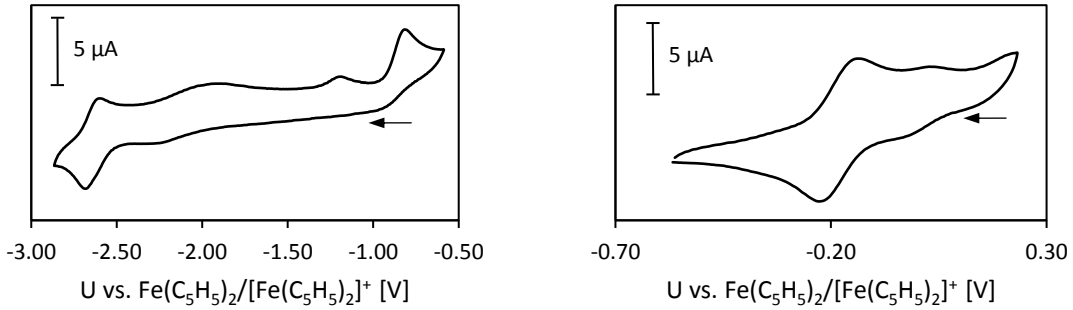


Figure S17. Cyclic voltammogram of **6-OPPh$_3$** at 23 °C in THF / 0.1 M [N(*n*Bu)$_4$][PF$_6$] at scan rates of 250 mV·s^{-1}.

Bi(ATI$^{Fc/iPr}$)Cl$_2$ (7). In addition to the redox events discussed in the main part, a redox event was detected at –2.67 V. The nature of the species associated with this redox event is not discussed due to the ill-defined redox events that take place at –1.08 V and –1.31 V.

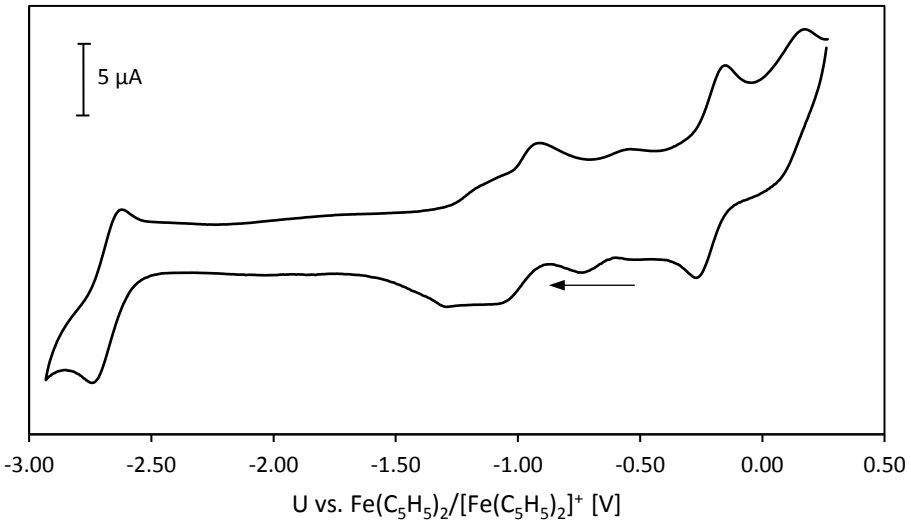


Figure S18. Cyclic voltammogram of **7** at 23 °C in THF / 0.1 M [N(*n*Bu)$_4$][PF$_6$] at a scan rate of 250 mV·s^{-1}.

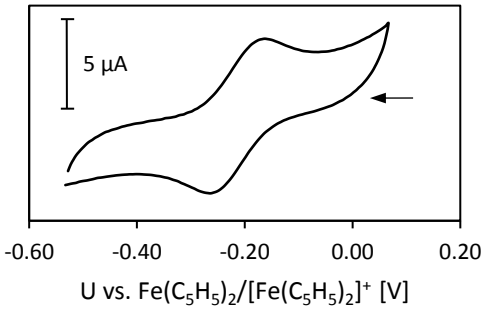


Figure S19. Cyclic voltammogram of **7** at 23 °C in THF / 0.1 M [N(*n*Bu)$_4$][PF$_6$] at a scan rate of 250 mV·s^{-1}.

Bi(ATI$^{Fc/iPr}$)$_3$ (8).

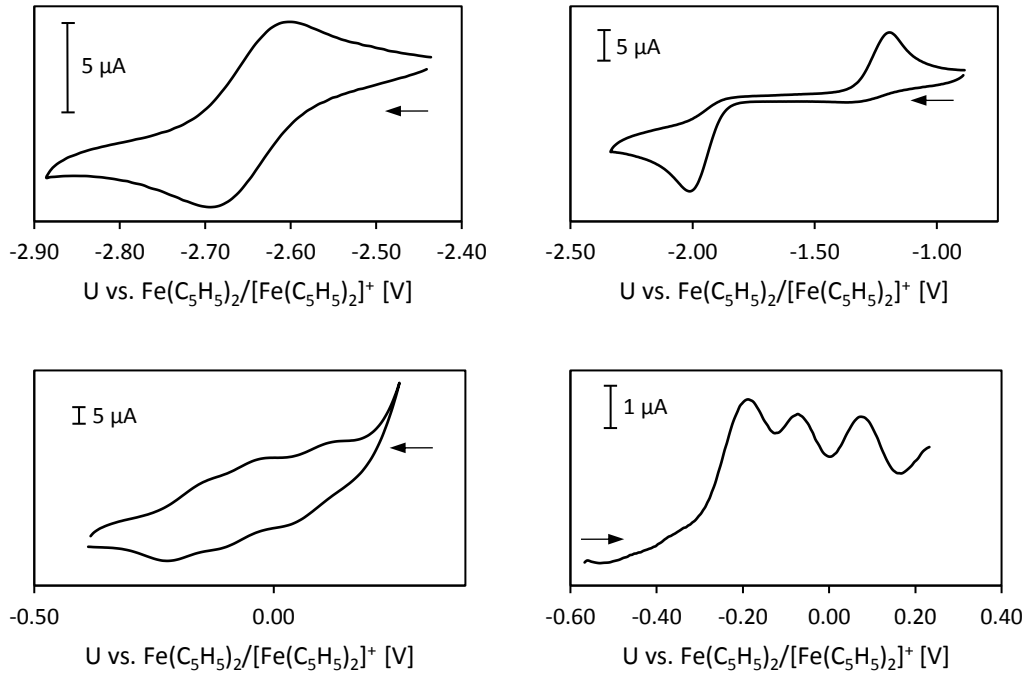


Figure S20. Electrochemical measurements of **8** at 23 °C in THF / 0.1 M [N(*n*Bu)$_4$][PF$_6$]. Top row and bottom left: cyclic voltammograms at scan rates of 250 mV·s^{-1}. Bottom right: differential pulse voltammogram with step size of 5 mV, pulse size of 25 mV, sample period of 0.2 s and pulse time of 0.1 s.

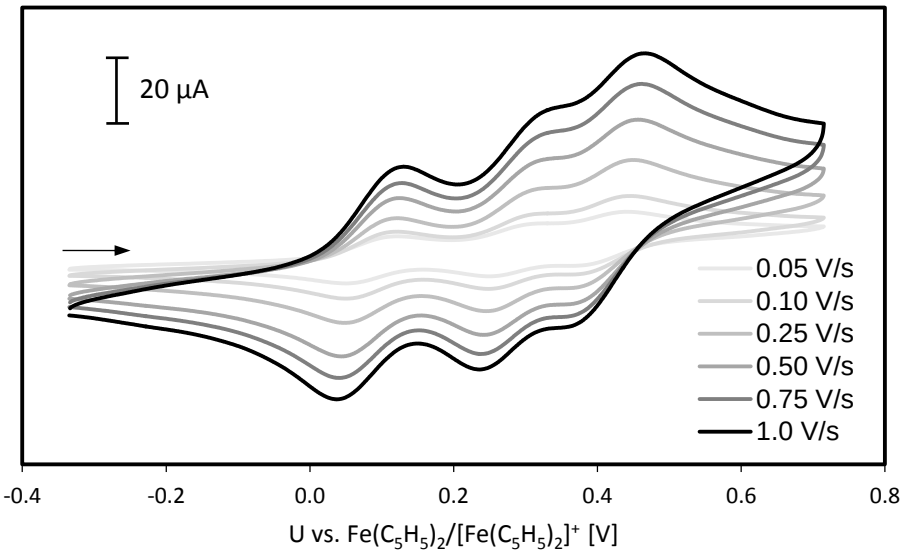


Figure S21. Cyclic voltammogram of **8** at 23 °C in CH_2Cl_2 / 0.1 M [N(*n*Bu)$_4$][PF$_6$] at scan rates ranging from 50 to 1000 mV·s^{-1}.

A plot of the square root of the anodic peak current vs. the scan rate is shown for the redox event at –0.23 V as a representative example for results obtained from cyclic voltammograms of **8** at 23 °C in CH_2Cl_2 / 0.1 M $[N(nBu)_4][PF_6]$ (Figure S22).

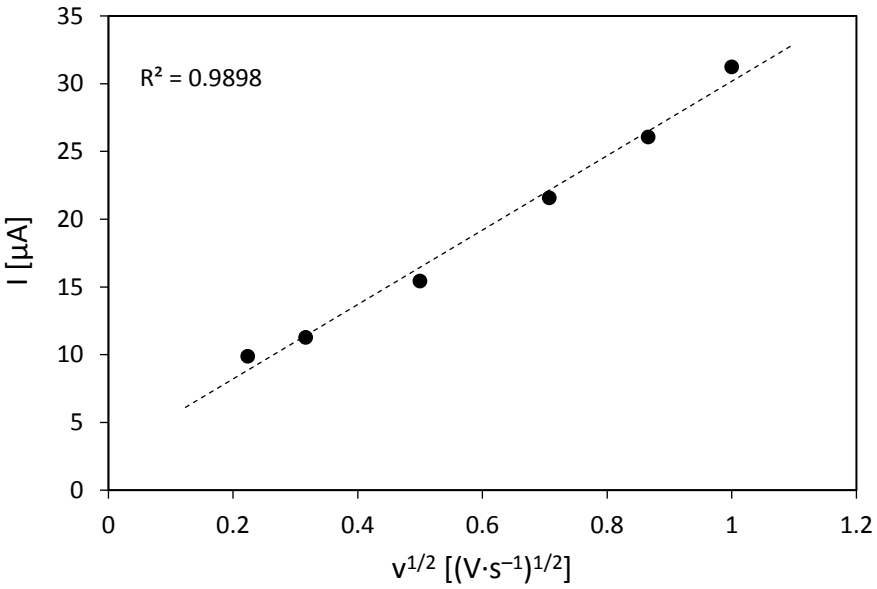


Figure S22. Plot of anodic peak current vs. square root of scan rate for the redox event at –0.23 V in cyclic voltammograms of **8** at 23 °C in CH_2Cl_2 / 0.1 M $[N(nBu)_4][PF_6]$.

UV/vis spectroscopy

The coloured compounds **2-8** were investigated by UV/vis spectroscopy in THF solution. The starting material H_2NFc shows a broad absorption band at 442 nm. This band is shifted to 476 nm, 500 nm, and 482 nm for compounds **2**, **3**, and **4**, respectively (Figure S23). The aminotroponates show two additional absorption maxima, which could thus be ascribed to the presence of the troponate moiety. These maxima are similar for the free ligand **2** (346 nm, 409 nm) and the bismuth compound **4** (348 nm, 410 nm) and red-shifted for the sodium compound **3** (415 nm, 500 nm).

For the aminotroponiminate compounds **5-8**, the UV-vis spectra show features in the range of 360-410 nm and 420-510 nm, some of which consist of more than one individual band (Figure S24). The bismuth compounds and the free ligand show considerable similarities with respect to intensity and wavelength of the maxima. For the sodium compounds, the bands in the range of 420-510 nm exhibit higher intensities.

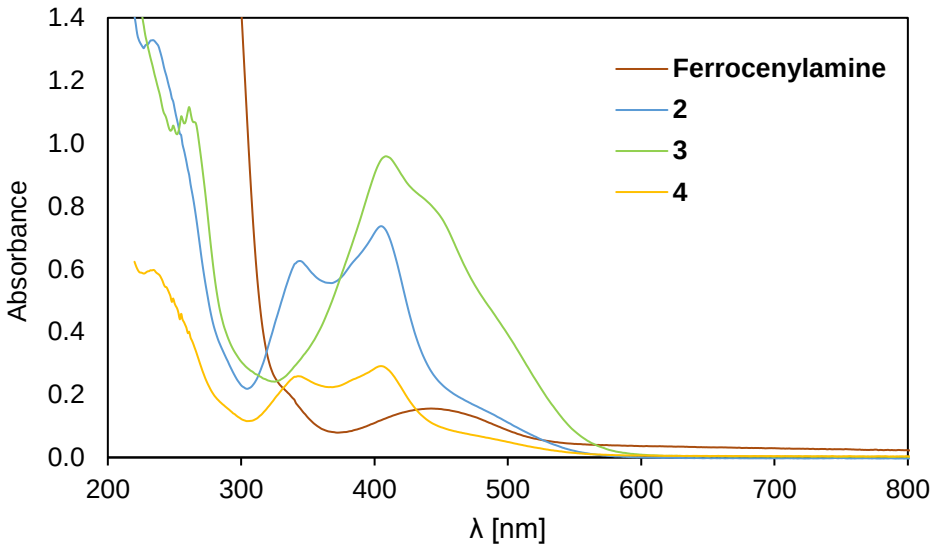


Figure S23. UV-vis spectra of compounds **2**, **3**, **4**, and H_2NFc in THF.

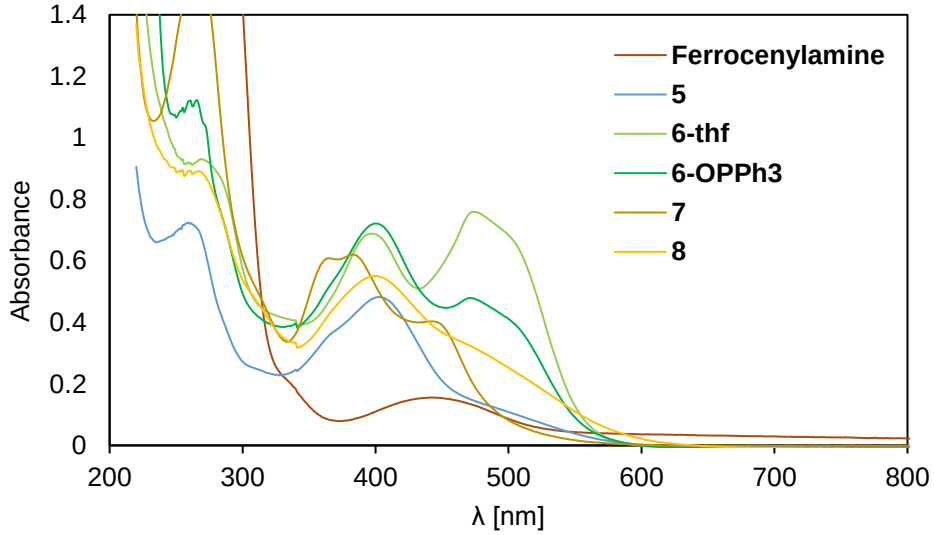


Figure S24. UV-vis spectra of compounds **5**, **6-thf**, **6-OPPh$_3$**, **7**, **8**, and H_2NFc in THF.

NMR Spectra

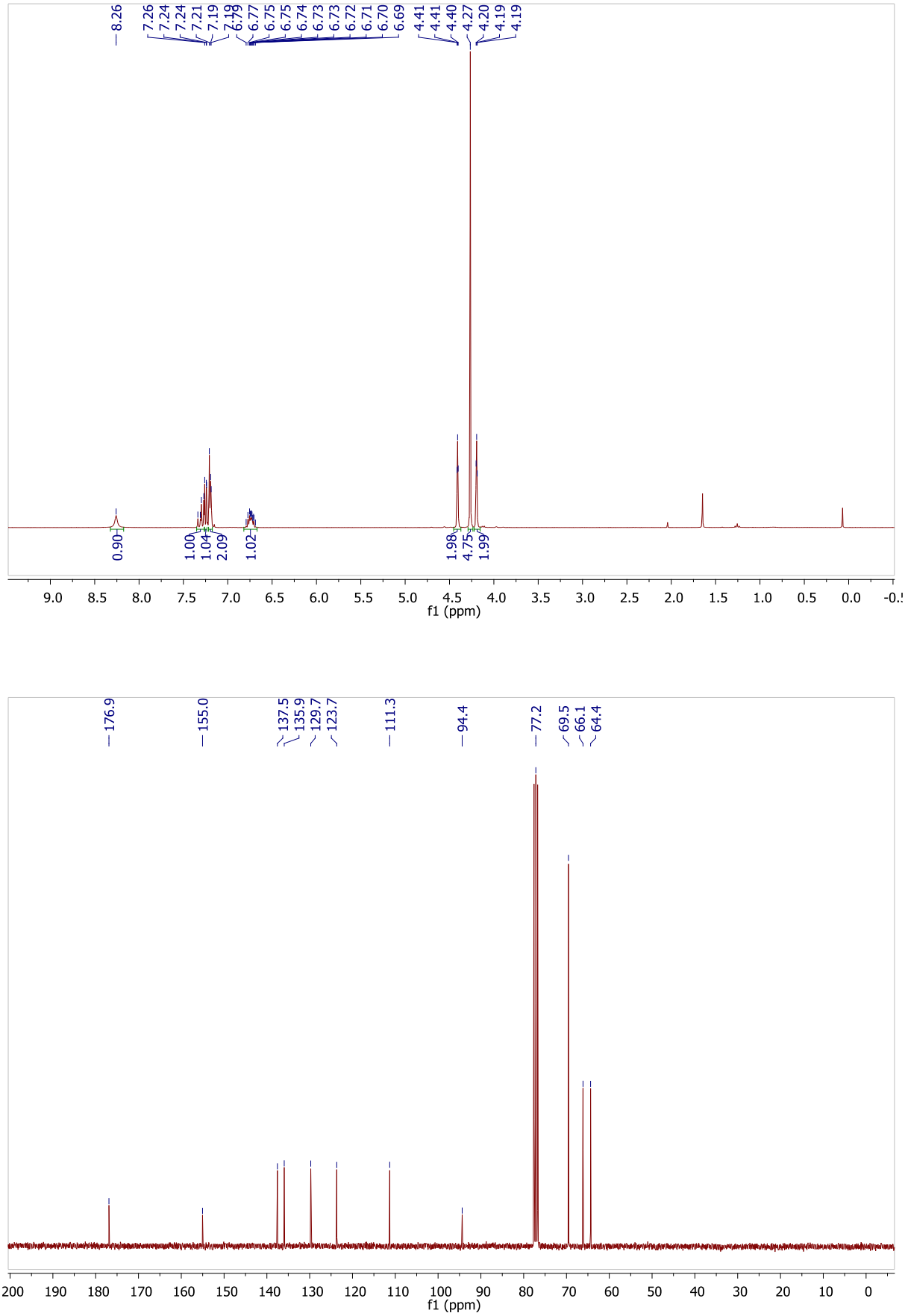


Figure S25. ^{1}H and ^{13}C NMR spectra of **2** in $CDCl_3$.

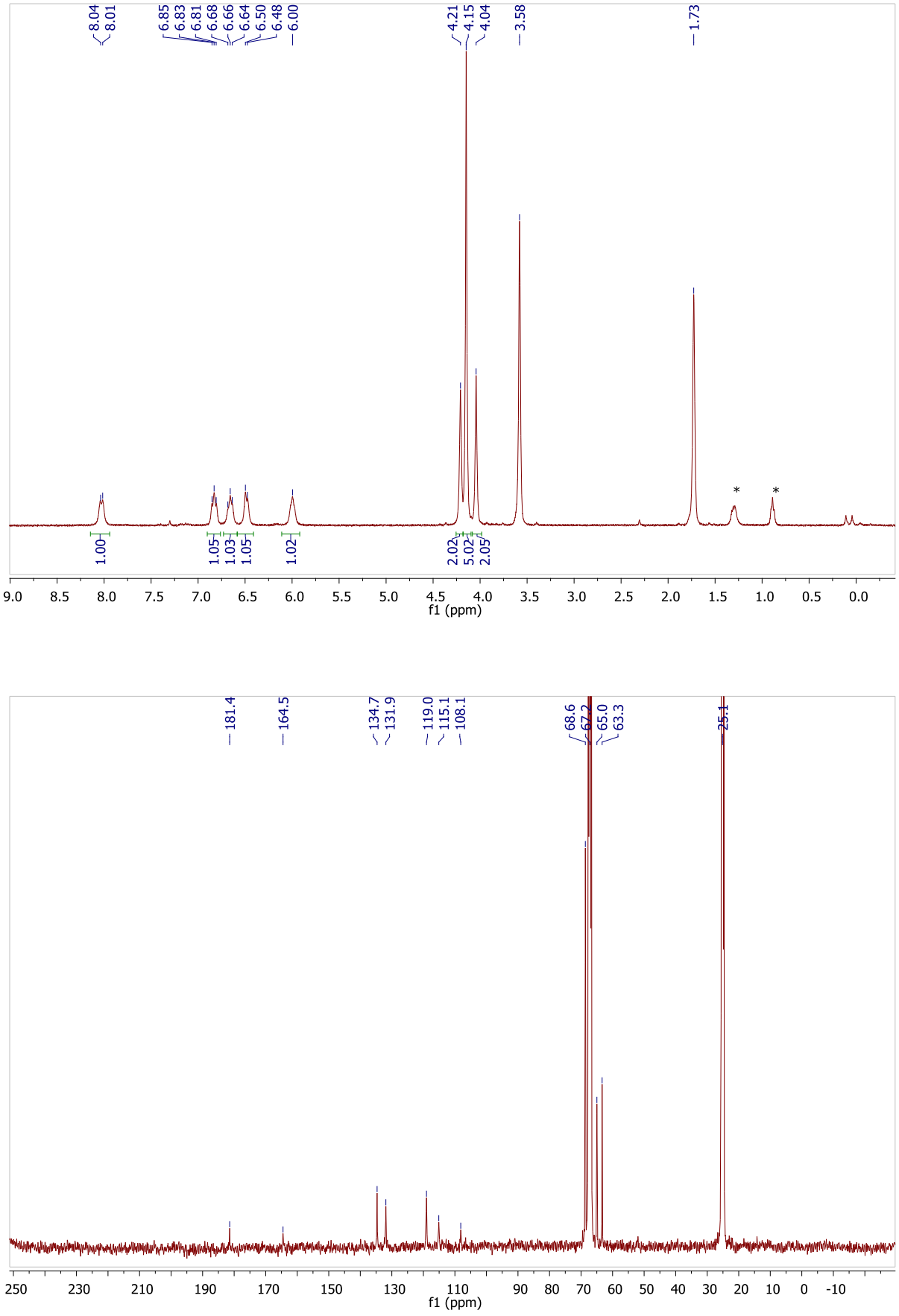


Figure S26. ^{1}H and ^{13}C NMR spectra of **3** in THF-d_8; asterisks denote resonances due to residual amounts of hexanes.

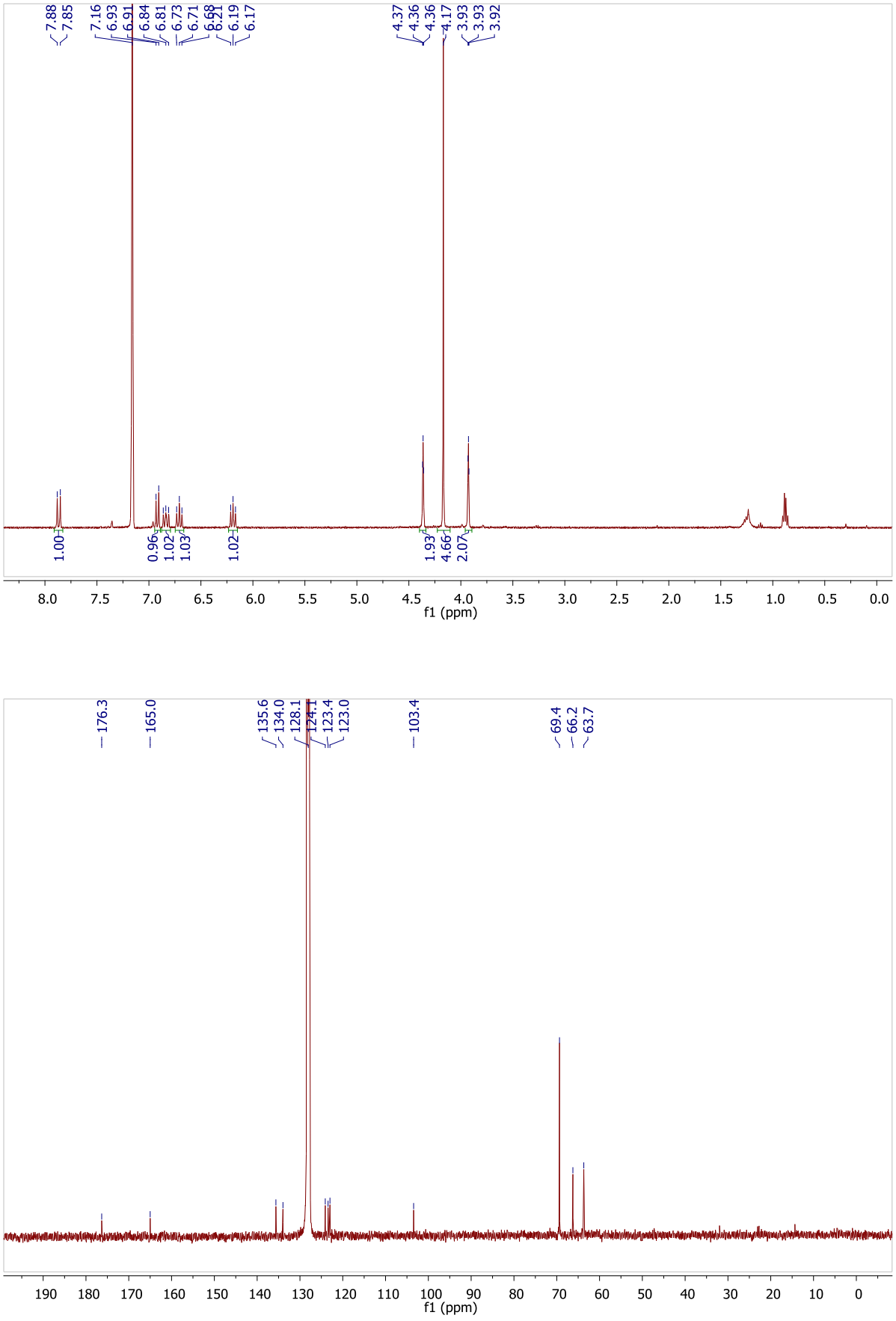


Figure S27. ^{1}H and ^{13}C NMR spectra of **4** in C_6D_6.

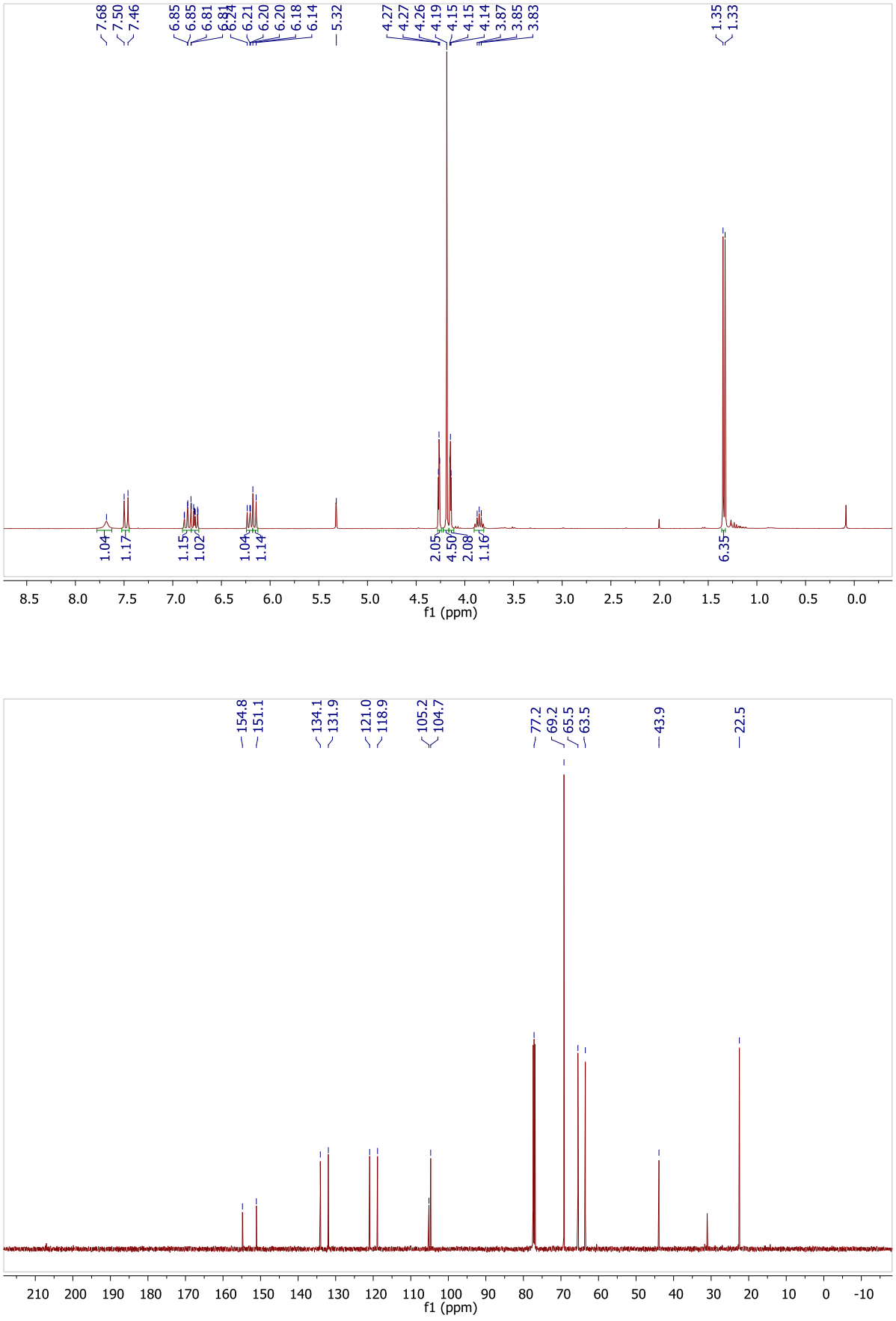


Figure S28. ^{1}H and ^{13}C NMR spectra of **5** in CD_2Cl_2 and $CDCl_3$, respectively.

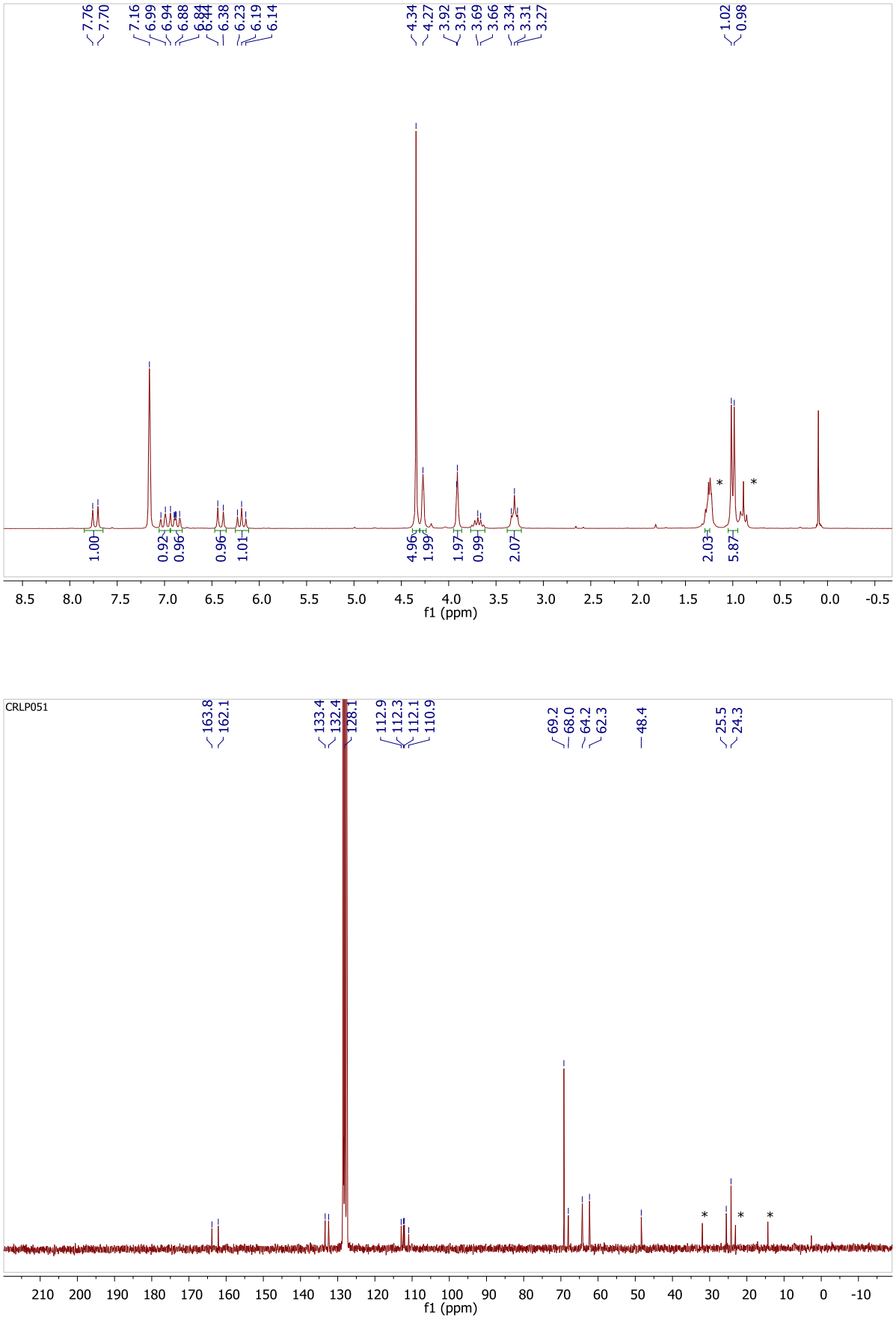


Figure S29. ^{1}H and ^{13}C NMR spectra of **6-thf** in C_6D_6; asterisks denote residual amounts of hexanes.

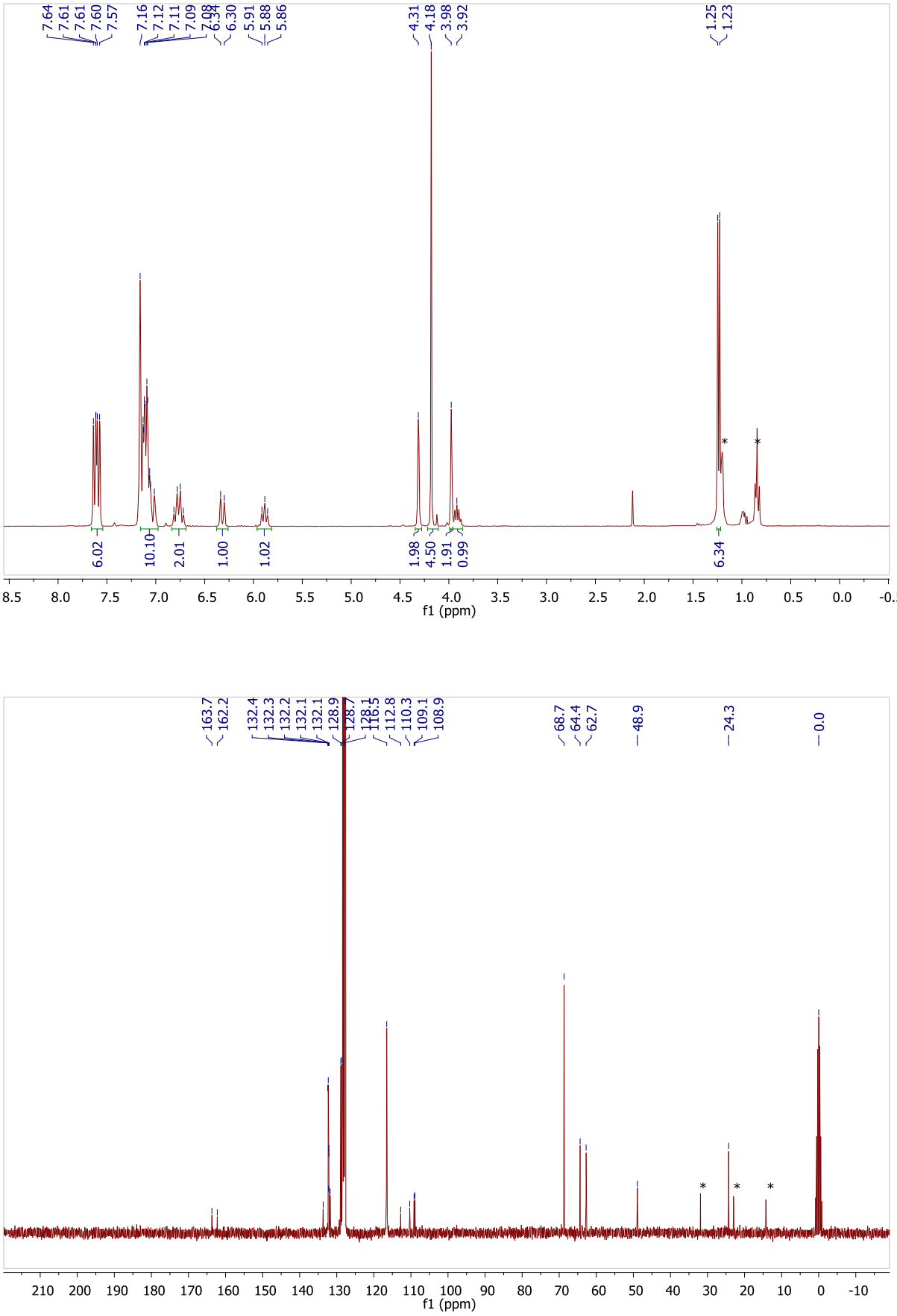


Figure S30. ^{1}H and ^{13}C NMR spectra of **6-OPPh$_3$** in C_6D_6/MeCN-d_3 (10:1)); asterisks denote residual amounts of hexanes.

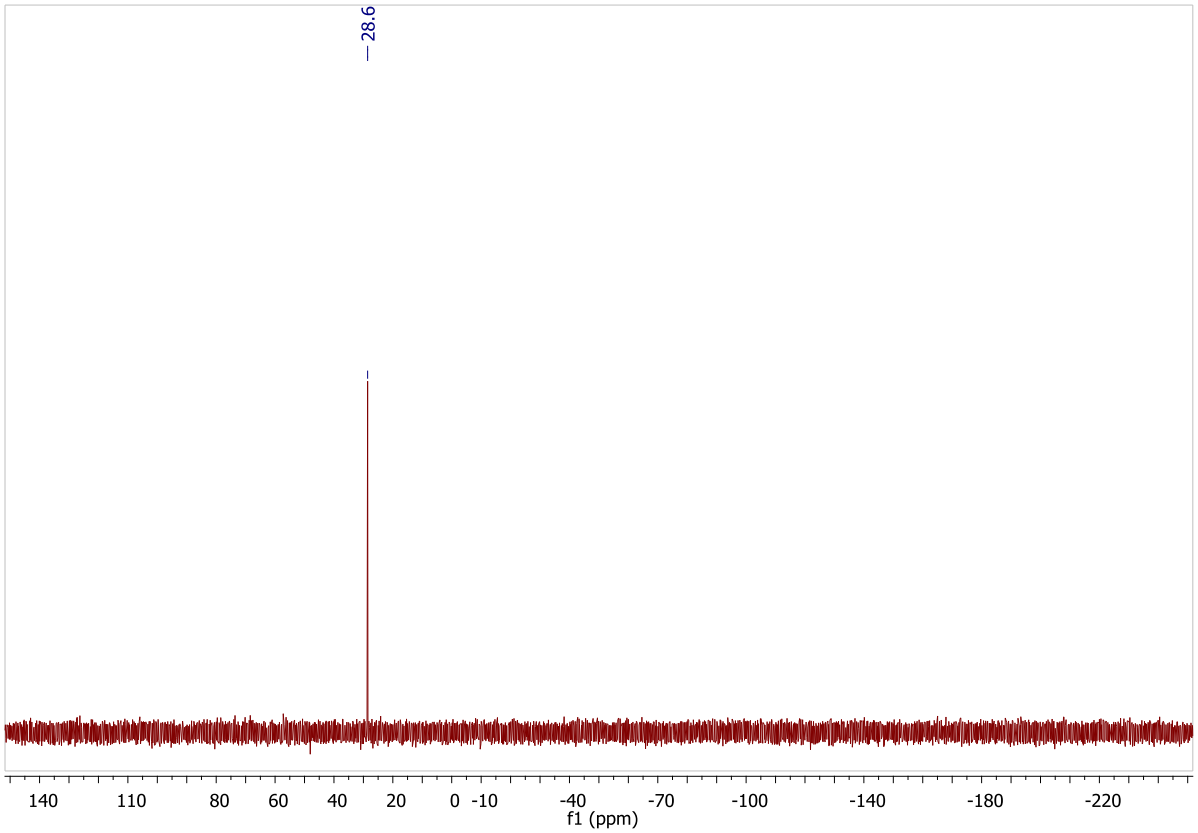


Figure S31. ^{31}P NMR spectrum of **6-OPPh$_3$** in C_6D_6/MeCN-d_3 (10:1)).

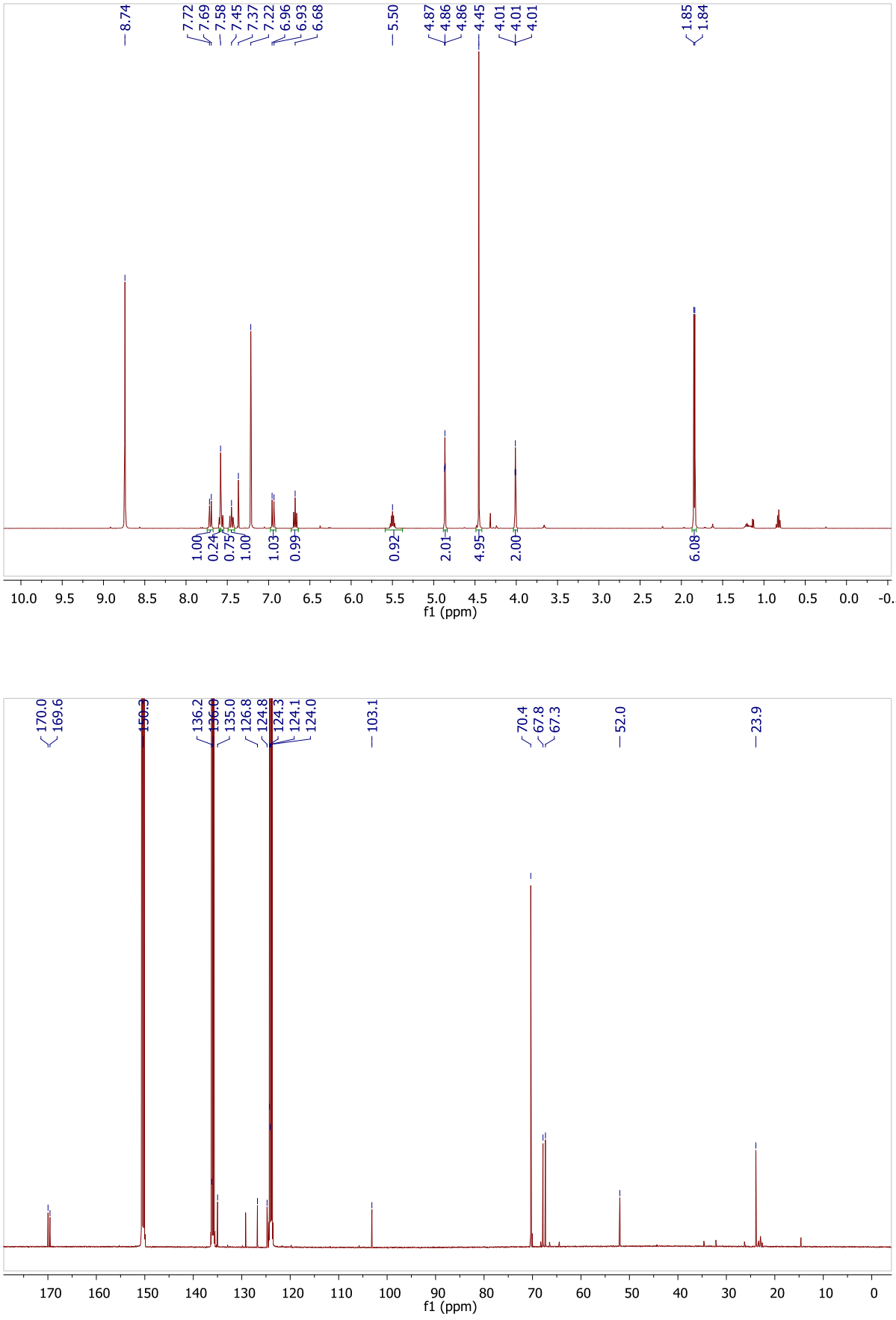


Figure S32. ^{1}H and ^{13}C NMR spectra of **7** in NC_5D_5.

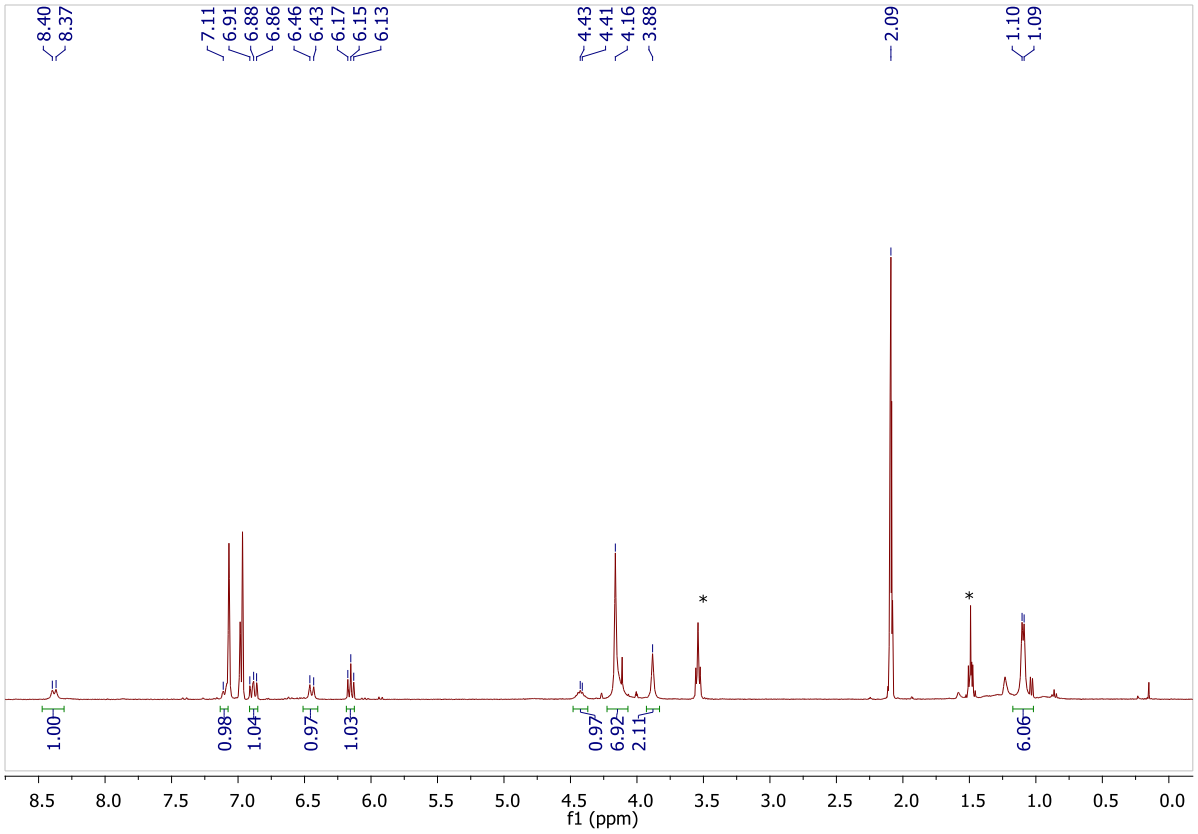


Figure S33. ^{1}H NMR spectrum of **8** in toluene-d_8 at 353 K; asterisks indicate resonances due to THF.

Free energies (G^0, hartree), enthalpies (H^0, hartree), and cartesian coordinates (Å) of optimized structures. Calculations were performed with the Gaussian16 program suite.[1]

[H-AT^{Fc}]$^{\bullet+}$ (2-ox)
H^0 = –909.761506
G^0 = –909.826358

Fe	-2.069332	-0.021119	0.055429
C	4.391041	1.777362	0.578047
H	5.005710	2.621890	0.876694
C	5.069002	0.732877	-0.111559
H	6.135752	0.892957	-0.250383
C	4.580489	-0.430029	-0.641700
C	-0.217155	-1.213039	0.517976
C	-1.316495	-1.993222	0.000197
H	-1.269301	-2.611629	-0.886078
C	-1.685674	1.773708	-0.996316
H	-0.702733	2.219005	-1.066551
C	3.058776	1.844445	0.899650
H	2.733232	2.744916	1.414331
C	-2.416093	-1.885607	0.900103
H	-3.361915	-2.401000	0.807927
C	-0.734376	-0.480759	1.644422
H	-0.193976	0.223906	2.255537
C	-2.663877	2.054039	0.006371
H	-2.542397	2.733807	0.838720
C	3.242397	-0.981020	-0.650657
C	2.091425	-0.336290	0.056039
C	-2.059542	-0.945736	1.909954
H	-2.680788	-0.621022	2.733271
C	2.028814	0.894904	0.664970
H	1.049361	1.208839	1.008024
C	-3.810576	1.256622	-0.254097
H	-4.705875	1.216165	0.350973
C	-3.537051	0.454409	-1.399772
H	-4.203301	-0.277439	-1.835492
C	-2.225370	0.783871	-1.871143
H	-1.732502	0.353828	-2.732123
H	5.281421	-1.084383	-1.152611
O	3.004028	-2.045227	-1.248890
N	0.990677	-1.173528	-0.084893
H	1.248579	-1.933462	-0.732941

[H-AT^{Fc}]$^{\bullet-}$ (2-red)
H^0 = –909.998460
G^0 = –910.062177

Fe	-2.031509	-0.001760	0.035784
C	4.176087	1.830937	0.616930
H	4.732340	2.710418	0.940377
C	4.902608	0.824041	0.001557
H	5.973228	1.022026	-0.093638
C	4.497238	-0.408253	-0.549303
C	-0.320782	-1.316376	0.479078
C	-1.447387	-1.988182	-0.118184
H	-1.406549	-2.543735	-1.045894
C	-1.316423	1.465692	-1.256411
H	-0.278973	1.515256	-1.556634
C	2.770894	1.851873	0.845356
H	2.365335	2.770890	1.268229
C	-2.587365	-1.846797	0.735967
H	-3.564983	-2.279511	0.569988
C	-0.837454	-0.622387	1.630291
H	-0.269810	0.024797	2.280449
C	-1.877044	2.062148	-0.083515
H	-1.335923	2.661205	0.636624
C	3.211561	-1.037193	-0.569944
C	2.005552	-0.444513	0.069476
C	-2.209529	-0.993443	1.815438
H	-2.846071	-0.663006	2.625852
C	1.840381	0.849313	0.593699
H	0.811819	1.112006	0.825835
C	-3.256752	1.696659	-0.004740
H	-3.944173	1.972420	0.783863
C	-3.548590	0.851570	-1.119122
H	-4.498382	0.377695	-1.328743
C	-2.349115	0.707253	-1.887035
H	-2.233791	0.097246	-2.773038
H	5.260040	-1.012077	-1.035262
O	3.052593	-2.151827	-1.147965
N	0.930517	-1.330592	-0.050856
H	1.197474	-2.085158	-0.685913

[H-ATI$^{Fc/iPr}$] (5) (HN^{iPr} group)
H^0 = –1007.959605
G^0 = –1008.030978

Fe	-2.540323	-0.321911	-0.023545
N	0.633309	-0.690676	-0.385409
C	-2.685210	-1.020213	-1.959574
H	-3.494689	-0.774508	-2.633131
C	-1.475393	-0.279998	-1.807117
H	-1.202018	0.602189	-2.366596
C	1.019516	3.037469	-0.401477
H	0.248325	3.795739	-0.532842
C	-4.152163	-0.272037	1.276431
H	-4.883936	-1.063686	1.358521
C	-2.926528	-0.183827	2.004841
H	-2.568780	-0.896958	2.734390
C	4.185635	-2.821110	1.256649
H	3.583708	-2.739916	2.166371
H	5.161258	-3.239310	1.520058
H	3.691041	-3.525473	0.577467
C	-1.426550	-2.050649	-0.325572
H	-1.101375	-2.714481	0.463099
C	2.329446	3.538172	-0.235539
H	2.451446	4.616353	-0.293089

C	-4.212491	0.836830	0.378541
H	-4.999278	1.034470	-0.336139
C	4.352853	-1.454658	0.585271
H	4.834772	-0.778455	1.304069
C	-0.670510	-0.924748	-0.796212
C	-2.229857	0.980655	1.561789
H	-1.252390	1.302707	1.891889
C	0.556582	1.742340	-0.429832
H	-0.513337	1.640341	-0.560309
C	-2.658282	-2.111144	-1.038574
H	-3.449731	-2.830801	-0.881726
C	5.226262	-1.546302	-0.677256
H	4.785149	-2.251742	-1.389135
H	6.234252	-1.892736	-0.426122
H	5.307046	-0.574546	-1.171832
C	3.459315	2.787322	0.010112
H	4.386518	3.346991	0.121947
C	1.223885	0.476823	-0.289046
C	-3.024376	1.609542	0.553905
H	-2.761890	2.500673	0.000341
C	3.607893	1.394630	0.155848
H	4.623329	1.080621	0.373414
C	2.676807	0.359287	0.063415
N	3.032553	-0.923869	0.280533
H	2.246931	-1.556259	0.106039

[H-ATI$^{Fc/iPr}$] (5-isom) (HN^{Fc} group)

H^0 = –1007.955491

G^0 = –1008.026793

Fe	-2.528440	-0.306287	-0.009766
N	2.950368	-0.985567	0.221678
C	-2.764818	-0.986139	-1.945552
H	-3.599271	-0.724218	-2.580878
C	-1.540782	-0.259162	-1.842914
H	-1.280970	0.627763	-2.399952
C	1.121741	3.072714	-0.421228
H	0.368048	3.844280	-0.571076
C	-4.075005	-0.230557	1.364565
H	-4.815422	-1.009313	1.483826
C	-2.814857	-0.161370	2.034127
H	-2.435049	-0.879096	2.747925
C	4.084148	-2.800077	1.354275
H	3.469916	-2.648116	2.247050
H	5.051347	-3.210610	1.663754
H	3.581154	-3.536658	0.718329
C	-1.456135	-2.038247	-0.363271
H	-1.111742	-2.708096	0.412350
C	2.403705	3.517977	-0.196793
H	2.566077	4.592415	-0.200071
C	-4.160954	0.879638	0.470460
H	-4.977853	1.089932	-0.205717
C	4.265402	-1.481453	0.593024
H	4.787756	-0.779705	1.264449
C	-0.722396	-0.913238	-0.862563
C	-2.121072	0.990816	1.556190
H	-1.122675	1.296185	1.835280
C	0.620704	1.755154	-0.502020
H	-0.443323	1.687626	-0.690917
C	-2.710181	-2.087652	-1.040508
H	-3.497992	-2.805545	-0.861718
C	5.127492	-1.684416	-0.665792
H	4.632324	-2.385822	-1.345388
H	6.111251	-2.089359	-0.405002
H	5.272030	-0.741980	-1.202823
C	3.541871	2.707831	0.036329
H	4.474749	3.254934	0.166561
C	1.257550	0.532107	-0.344829
C	-2.952995	1.631834	0.587214
H	-2.700512	2.516301	0.018720
C	3.661888	1.344114	0.133270
H	4.671510	0.995345	0.321274
C	2.690644	0.277594	0.031809
N	0.591375	-0.643793	-0.478829
H	1.210184	-1.422084	-0.216746

[H-ATI$^{Fc/iPr}$]$^{\bullet+}$ (5-ox)

H^0 = –1007.758885

G^0 = –1007.834232

Fe	-2.647215	-0.363023	-0.069864
N	0.679594	-0.670407	-0.059235
C	-2.406746	-1.151951	-1.956192
H	-3.113972	-0.986260	-2.757590
C	-1.268938	-0.341706	-1.670483
H	-0.964241	0.525310	-2.237846
C	1.103461	3.061289	-0.294203
H	0.319856	3.808930	-0.398940
C	-4.451308	-0.330615	1.030976
H	-5.122711	-1.175089	1.098606
C	-3.361224	-0.051432	1.915656
H	-3.054691	-0.657386	2.756807
C	4.409420	-2.725609	1.309957
H	3.873100	-2.597005	2.254427
H	5.404473	-3.119595	1.530281
H	3.882178	-3.472426	0.705083
C	-1.352592	-2.033238	-0.106495
H	-1.111302	-2.649863	0.747928
C	2.402090	3.553578	-0.238745
H	2.526172	4.629019	-0.321964
C	-4.489687	0.700392	0.044864
H	-5.189236	0.774873	-0.775797
C	4.526985	-1.400195	0.553255
H	5.047350	-0.681752	1.198120
C	-0.505926	-0.962635	-0.595550
C	-2.739290	1.151969	1.483197
H	-1.859010	1.602526	1.920969
C	0.646423	1.743013	-0.246902
H	-0.432695	1.641775	-0.300754
C	-2.461872	-2.198069	-0.983717
H	-3.223921	-2.961721	-0.910445
C	5.296366	-1.556786	-0.766580
H	4.804018	-2.294750	-1.407565
H	6.316456	-1.898580	-0.569503

H	5.351046	-0.613129	-1.316639
C	3.566017	2.796328	-0.079223
H	4.494460	3.362436	-0.063492
C	1.320482	0.512852	-0.114514
C	-3.420942	1.606744	0.320046
H	-3.166348	2.478968	-0.266273
C	3.727407	1.425640	0.074791
H	4.757503	1.108738	0.188604
C	2.780711	0.376382	0.101586
N	3.172910	-0.886090	0.311439
H	2.396539	-1.546641	0.286680

[H-ATI$^{Fc/iPr}$]$^{\bullet -}$ (5-red)

H^0 = – 1007.968676

G^0 = – 1008.041553

Fe	2.527655	-0.324666	0.015572
N	-0.719734	-0.685977	-0.211557
C	2.338823	-1.494361	1.682703
H	3.029279	-1.466380	2.516284
C	1.160070	-0.695666	1.543430
H	0.805810	0.034379	2.255417
C	-1.219738	2.950245	0.744563
H	-0.484784	3.633139	1.177754
C	4.292620	0.054875	-1.006771
H	5.043085	-0.694702	-1.220603
C	3.162224	0.370395	-1.824377
H	2.902666	-0.107611	-2.759296
C	-4.641517	-2.774496	-0.862037
H	-5.046026	-2.515058	-1.845485
H	-5.406954	-3.313243	-0.290494
H	-3.796914	-3.458558	-1.015810
C	1.354269	-2.000807	-0.338023
H	1.158548	-2.417568	-1.316748
C	-2.466999	3.494504	0.526361
H	-2.605464	4.537934	0.810108
C	4.223227	0.865582	0.169501
H	4.912833	0.839093	1.002778
C	-4.176144	-1.513493	-0.126589
H	-5.046782	-0.856537	0.009122
C	0.489441	-1.042877	0.306680
C	2.396019	1.377651	-1.161842
H	1.444940	1.779097	-1.482099
C	-0.707958	1.645805	0.504599
H	0.338689	1.517489	0.744229
C	2.460975	-2.305820	0.512616
H	3.265752	-2.995844	0.293820
C	-3.613993	-1.851244	1.266127
H	-2.743437	-2.510017	1.174901
H	-4.365666	-2.344829	1.896708
H	-3.282857	-0.936509	1.766147
C	-3.594351	2.838531	-0.054887
H	-4.493194	3.439278	-0.188426
C	-1.344230	0.489408	-0.027404
C	3.050322	1.676594	0.073818
H	2.690493	2.366053	0.825344
C	-3.665237	1.522457	-0.500693
H	-4.620375	1.239080	-0.946735
C	-2.745826	0.462402	-0.488051
N	-3.216923	-0.795998	-0.986135
H	-2.374053	-1.371674	-1.066287

[Bi(ATI$^{Fc/iPr}$)$_3$] (*trans*-8)

H^0 = –3027.615368

G^0 = –3027.782415

Bi	0.307541	-0.996097	-0.262857
Fe	4.550081	1.916633	0.548587
Fe	-2.546113	3.396029	0.866769
Fe	-4.614002	-1.553198	-1.140799
N	-0.484596	1.292379	-0.643747
C	0.649808	4.336456	-3.898497
H	0.814913	5.258426	-4.448981
C	0.840250	3.129265	-4.583156
H	1.109406	3.222994	-5.634546
N	-1.845410	-1.663137	0.602661
N	1.564341	-3.150892	0.128699
C	0.757018	1.826781	-4.131291
C	-1.105026	1.860583	0.489829
N	2.715958	-0.703515	-0.198189
N	0.597539	-0.075318	-2.653494
N	0.181705	-0.805644	2.091565
C	-2.335136	1.346923	1.008242
H	-2.945803	0.629144	0.488697
C	4.208562	2.442556	-1.419919
H	4.881828	3.054527	-2.003895
C	0.701266	-2.409273	-3.436863
H	1.205698	-2.796138	-2.547050
H	0.995207	-3.047559	-4.276769
H	-0.379153	-2.507178	-3.295062
C	-6.362413	-1.095122	-0.108308
H	-6.736534	-1.647071	0.743033
C	-3.201814	4.304180	-0.886564
H	-2.894481	3.995121	-1.875097
C	-1.920120	-1.690527	5.072141
H	-1.564413	-1.828622	6.092157
C	4.255523	1.021963	-1.318909
H	4.953237	0.373957	-1.826037
C	5.963104	-2.577283	-0.217424
H	6.941437	-2.172887	0.039717
C	5.298381	3.334505	1.857571
H	5.004112	4.374740	1.842259
C	1.104821	-0.956557	-3.712750
C	4.645569	2.290369	2.580231
H	3.774337	2.405835	3.208285
C	-3.305933	-1.710300	4.911423
H	-3.913143	-1.802343	5.807534
C	0.250556	4.432273	-2.577430
H	0.137878	5.443212	-2.186700
C	-2.575521	1.917242	2.290986
H	-3.426471	1.715704	2.925886
C	0.092539	-4.425213	1.632994
H	0.720053	-4.109018	2.469663
H	-0.295051	-5.426645	1.848909

H	-0.755233	-3.743459	1.562118
C	-0.623450	2.823056	1.448111
H	0.265319	3.429846	1.354857
C	-3.962857	-1.652174	3.686948
H	-5.051315	-1.668549	3.724134
C	2.634901	-0.849706	-3.846475
H	2.952013	0.183251	-4.009091
H	2.993350	-1.462566	-4.680823
H	3.112104	-1.205288	-2.929445
C	2.560462	1.781782	0.045053
H	1.751447	1.810876	0.755999
C	-3.665527	-3.223875	-0.317668
H	-3.966419	-3.751598	0.574780
C	-3.428497	-1.630905	2.403145
H	-4.166261	-1.658704	1.609794
C	5.953398	-3.865293	-0.736017
H	6.910647	-4.354104	-0.894385
C	6.365570	2.753317	1.107985
H	7.024298	3.275927	0.428494
C	0.893137	-4.448710	0.324320
H	1.657598	-5.229726	0.434728
C	-2.524913	5.254993	-0.062507
H	-1.629817	5.801109	-0.325293
C	-2.723409	-2.136730	-0.370478
C	0.472545	1.226531	-2.855018
C	-0.037516	2.019893	-1.694248
C	-1.521545	2.839952	2.559539
H	-1.429300	3.468653	3.434486
C	2.273738	-1.611884	3.268854
H	1.825120	-2.144049	4.111402
H	3.258055	-1.256268	3.591529
H	2.412434	-2.323392	2.453043
C	3.202410	0.592733	-0.436650
C	5.311441	1.062454	2.282666
H	5.035877	0.083899	2.649533
C	-2.644015	-1.716275	-1.745410
H	-2.063261	-0.878882	-2.109890
C	-0.052317	3.429194	-1.651983
H	-0.379389	3.821154	-0.702565
C	-0.906409	-1.487821	4.144775
H	0.077815	-1.505297	4.584773
C	4.907651	-1.683806	-0.033194
H	5.208745	-0.699679	0.299897
C	3.157940	2.913801	-0.580750
H	2.879601	3.944884	-0.420489
C	-0.012545	-4.828646	-0.859029
H	-0.810499	-4.091787	-0.994768
H	-0.487059	-5.798429	-0.674613
H	0.547400	-4.896651	-1.795913
C	-3.484259	-2.563970	-2.526488
H	-3.654745	-2.478925	-3.590563
C	-6.649793	-1.373053	-1.478787
H	-7.268357	-2.179560	-1.847407
C	-0.906730	-1.229115	2.741000
C	1.285548	0.709718	3.813554
H	0.762115	1.559141	3.370149
H	2.282061	1.036796	4.126544
H	0.739821	0.414313	4.710752
C	-2.104303	-1.548759	1.909181
C	4.799708	-4.573670	-1.089497
H	4.962627	-5.537657	-1.569383
C	-4.116482	-3.490360	-1.644168
H	-4.844509	-4.239688	-1.923063
C	3.510320	-1.792759	-0.207828
C	-5.470448	0.018794	-0.060469
H	-5.063217	0.469636	0.831720
C	1.441739	-0.413120	2.773811
H	2.051612	0.019509	1.980759
C	6.374278	1.350519	1.371047
H	7.052795	0.631251	0.933308
C	3.469559	-4.250172	-0.883118
H	2.774128	-5.002927	-1.237268
C	-3.214952	5.335433	1.184010
H	-2.925507	5.938711	2.033313
C	-5.926623	-0.436344	-2.278858
H	-5.900229	-0.411169	-3.359402
C	-4.319280	4.432144	1.132098
H	-5.013116	4.229175	1.936245
C	2.823406	-3.115721	-0.282864
C	-4.312436	3.797258	-0.146680
H	-5.007864	3.039216	-0.475034
C	-5.190043	0.417649	-1.402921
H	-4.500394	1.195083	-1.699163
H	0.645146	-0.691696	-4.677270
H	0.974465	1.103211	-4.906105

[Bi(ATI$^{Fc/iPr}$)$_3$] (*cis*-8)

H^0 = –3027.608795

G^0 = –3027.775106

Bi	0.016848	0.122797	1.437342
Fe	2.762446	-2.340522	-2.394055
Fe	-4.267682	-1.263503	-1.489635
Fe	1.229538	3.606947	-2.212331
N	-1.567568	-1.360152	0.393984
C	-1.522970	-5.941842	0.210910
H	-1.669741	-6.973530	-0.096535
C	-1.076611	-5.713905	1.519815
H	-0.969285	-6.601211	2.142357
N	-0.538286	1.909245	-0.046920
N	2.157700	1.315031	2.088960
C	-0.724070	-4.532496	2.142235
C	-2.423026	-0.754651	-0.556162
N	2.064030	-0.735871	0.388281
N	-0.051411	-2.229754	2.421836
N	-1.724316	1.563477	2.290743
C	-3.498524	0.109939	-0.166751
H	-3.844401	0.235185	0.845335
C	1.493581	-3.773437	-1.630057
H	1.545029	-4.826228	-1.868784
C	0.988449	-1.350724	4.478642
H	1.601004	-0.614588	3.950763
H	1.530501	-1.632170	5.387230
H	0.050056	-0.875440	4.781888

C	0.387287	5.467676	-2.609893
H	-0.636224	5.630743	-2.918311
C	-4.976011	-3.115329	-0.852076
H	-4.482408	-3.728064	-0.112959
C	-4.459925	3.864095	1.141550
H	-5.409538	4.032402	1.647578
C	2.159785	-3.134041	-0.546066
H	2.793523	-3.615547	0.182878
C	5.688493	-1.339260	1.132970
H	6.342134	-2.004969	0.569839
C	3.281011	-2.452202	-4.394655
H	2.594851	-2.764916	-5.169624
C	0.729423	-2.588257	3.613628
C	3.449485	-1.118109	-3.914368
H	2.906910	-0.249271	-4.255921
C	-4.245717	4.618610	-0.012374
H	-5.018086	5.324803	-0.303623
C	-1.815026	-4.945839	-0.704130
H	-2.156740	-5.281942	-1.682269
C	-4.009349	0.764635	-1.323952
H	-4.820419	1.478308	-1.341598
C	1.275881	3.608805	2.209597
H	1.570050	3.739248	1.165811
H	1.383454	4.567330	2.729342
H	0.220998	3.327773	2.225686
C	-2.320295	-0.666917	-1.987056
H	-1.622894	-1.210473	-2.604182
C	-3.109067	4.535860	-0.807003
H	-3.072924	5.218582	-1.655287
C	2.061996	-3.258410	3.230942
H	1.896885	-4.138588	2.604277
H	2.608381	-3.569402	4.127867
H	2.690717	-2.558524	2.674338
C	0.989971	-1.523954	-1.715458
H	0.615818	-0.564396	-2.035391
C	-0.117919	2.041518	-2.590109
H	-1.128007	2.128914	-2.958868
C	-2.009472	3.686803	-0.717539
H	-1.295492	3.829824	-1.512882
C	6.251669	-0.746323	2.257473
H	7.274292	-1.010430	2.511618
C	4.125665	-3.309524	-3.626623
H	4.195814	-4.384346	-3.719965
C	2.140902	2.543030	2.897760
H	3.161919	2.948302	2.953339
C	-4.728792	-3.140101	-2.258711
H	-4.028112	-3.785688	-2.769330
C	0.265902	2.008569	-1.202503
C	-0.662646	-3.162693	1.708737
C	-1.367367	-2.697158	0.477474
C	-3.286654	0.274767	-2.452121
H	-3.460584	0.540158	-3.486048
C	-3.331807	0.174182	3.648360
H	-4.270207	0.607950	3.292252
H	-3.499731	-0.193148	4.666457
H	-3.087307	-0.680440	3.010403
C	1.834789	-1.732163	-0.575283
C	4.401106	-1.147691	-2.850934
H	4.712252	-0.305835	-2.249222
C	1.697361	1.891773	-1.167573
H	2.285139	1.866083	-0.265714
C	-1.772000	-3.556008	-0.562277
H	-2.123963	-3.028688	-1.434668
C	-3.636616	2.941439	1.768663
H	-4.071625	2.530953	2.667389
C	4.399142	-1.244036	0.618741
H	4.238305	-1.849229	-0.260349
C	0.765364	-2.780283	-2.350535
H	0.182885	-2.944774	-3.246347
C	1.640469	2.295212	4.332423
H	0.609067	1.931075	4.314762
H	1.656170	3.224953	4.911386
H	2.247150	1.553083	4.858648
C	2.180416	1.816903	-2.503696
H	3.217672	1.741136	-2.795584
C	1.492351	5.228997	-3.481420
H	1.449028	5.163711	-4.559701
C	-2.350147	2.398103	1.468298
C	-2.356819	2.356203	4.622020
H	-1.518096	3.053550	4.541363
H	-2.383914	1.969621	5.646302
H	-3.276952	2.919753	4.457405
C	-1.633682	2.662524	0.182069
C	5.595114	0.167896	3.081071
H	6.164303	0.523122	3.939235
C	1.060302	1.916024	-3.383991
H	1.094658	1.928285	-4.464839
C	3.236671	-0.530664	1.008008
C	0.865042	5.423236	-1.263694
H	0.263071	5.523104	-0.372091
C	-2.166901	1.183126	3.642151
H	-1.310366	0.623722	4.043800
C	4.818370	-2.503395	-2.674096
H	5.517988	-2.864312	-1.932829
C	4.326208	0.719363	2.972736
H	4.107330	1.422650	3.765487
C	-5.543558	-2.140718	-2.870847
H	-5.558550	-1.887832	-3.921967
C	2.654108	5.035304	-2.674340
H	3.644410	4.792336	-3.033875
C	-6.292764	-1.494090	-1.841068
H	-6.969524	-0.661521	-1.975373
C	3.245560	0.546633	2.048542
C	-5.940228	-2.096104	-0.594661
H	-6.306641	-1.801276	0.378863
C	2.265701	5.153414	-1.304955
H	2.911795	5.020031	-0.448734
H	0.156345	-3.283972	4.245669
H	-0.397076	-4.673780	3.165281

$[Bi(AT^{Fc})_3]^+$ (4^+)

H^0 = –2733.501477

G^0 = –2733.648408

Bi	-0.087911	0.050426	-2.019850
Fe	-2.377143	-2.784198	1.795114
Fe	4.628249	-0.150694	1.076553
Fe	-1.756053	3.234427	1.836659
N	2.010605	-1.296335	-0.673987
C	2.607253	-5.849872	-0.525899
H	2.961697	-6.847160	-0.281331
C	1.578025	-5.760584	-1.486499
H	1.235275	-6.708948	-1.895216
N	-0.020976	1.867172	-0.562136
C	0.951872	-4.646381	-1.990783
C	2.499045	-0.551855	0.318168
N	-1.878145	-0.982558	-0.909864
C	3.019162	0.789398	0.108874
H	3.090379	1.263130	-0.858870
C	-1.029162	-4.067830	0.910409
H	-1.005938	-5.133613	1.087560
C	-1.051989	5.127621	2.345129
H	-0.027652	5.370399	2.591735
C	6.103466	-1.412020	0.100284
H	5.834482	-2.164085	-0.628792
C	2.602472	5.077070	-2.437873
H	3.132815	5.663174	-3.185256
C	-1.782731	-3.410839	-0.104175
H	-2.396489	-3.888341	-0.853479
C	-5.561685	-1.444147	-1.439575
H	-6.215944	-2.147024	-0.927019
C	-2.821171	-3.068122	3.799546
H	-2.086335	-3.348690	4.541205
C	-3.149187	-1.736023	3.407212
H	-2.702368	-0.833057	3.793700
C	2.573854	5.609496	-1.148861
H	3.088250	6.552806	-0.990105
C	3.218704	-4.790646	0.111251
H	4.021432	-5.051153	0.798793
C	3.309607	1.394056	1.363148
H	3.630588	2.414837	1.515290
C	2.734231	-0.815178	1.733774
H	2.518640	-1.743521	2.240237
C	1.942639	5.038741	-0.046253
H	2.037929	5.594226	0.885264
C	-0.680678	-1.794853	1.130799
H	-0.369449	-0.831780	1.506460
C	-0.286652	1.749418	2.002990
H	0.733932	1.887273	2.325423
C	1.190868	3.870518	0.066498
H	0.801505	3.697618	1.058472
C	-6.194024	-0.609127	-2.371700
H	-7.265204	-0.738291	-2.496119
C	-3.587632	-3.967160	2.999507
H	-3.538091	-5.046548	3.029545
C	6.156857	-1.597447	1.510119
H	5.970921	-2.523696	2.036195
C	-0.759685	1.806068	0.644456
C	1.083572	-3.238455	-1.710839
C	2.034311	-2.665783	-0.716470
C	3.130926	0.396826	2.372311
H	3.290109	0.525311	3.434529
C	-1.555738	-1.997114	0.013365
C	-4.122479	-1.809442	2.366628
H	-4.549519	-0.972458	1.834372
C	-2.175120	1.579129	0.679765
H	-2.827198	1.611134	-0.177891
C	2.966024	-3.408912	0.014944
H	3.636970	-2.811254	0.620828
C	2.058535	3.887532	-2.903910
H	2.219698	3.659164	-3.953982
C	-4.233965	-1.520090	-1.054242
H	-4.025796	-2.259585	-0.294015
C	-0.347596	-3.071688	1.673038
H	0.266569	-3.251609	2.544235
C	-2.564001	1.360643	2.030984
H	-3.571694	1.193337	2.381430
C	-2.052942	4.707457	3.270986
H	-1.915014	4.555811	4.332352
C	1.313172	2.864293	-2.267377
C	0.810439	2.890999	-0.878368
C	-5.578634	0.358688	-3.150150
H	-6.225376	0.913734	-3.825796
C	-1.400385	1.472942	2.850044
H	-1.369021	1.399234	3.928220
C	-3.086274	-0.786351	-1.458347
C	-1.637394	5.158786	1.042305
H	-1.131718	5.413102	0.122744
C	-4.392236	-3.189704	2.114287
H	-5.073602	-3.585093	1.373416
C	-4.229102	0.721645	-3.201746
H	-3.967271	1.503054	-3.909749
C	6.480575	-0.344235	2.114922
H	6.595273	-0.161441	3.174021
C	-3.256452	4.475610	2.540053
H	-4.187490	4.110446	2.950579
C	6.601490	0.622745	1.072733
H	6.829476	1.671939	1.197847
C	-3.107211	0.254535	-2.503347
C	6.358584	-0.040531	-0.172266
H	6.351527	0.423583	-1.148597
C	-2.998474	4.752238	1.163402
H	-3.700612	4.637870	0.349518
H	0.186503	-4.814939	-2.743419
O	-1.967226	0.816632	-2.809111
O	0.336340	-2.457600	-2.351462
O	1.038907	1.825658	-2.970785

[Bi(ATI$^{Fc/iPr}$)$_3$]$^+$ (8$^+$)

H^0 = –3027.425646

G^0 = –3027.596553

Bi	0.203731	-0.906283	-0.296706
Fe	4.738459	1.910525	0.293221
Fe	-2.535411	3.397343	1.069661
Fe	-4.633734	-1.528323	-1.149073
N	-0.527358	1.313196	-0.478997
C	0.525390	4.572817	-3.542362

H	0.705704	5.528557	-4.025800
C	0.463616	3.434161	-4.365966
H	0.537179	3.621765	-5.435598
N	-1.824051	-1.576951	0.496802
N	1.579278	-3.287568	-0.033909
C	0.352443	2.105829	-4.019830
C	-1.178334	1.820593	0.675781
N	2.874241	-0.829959	-0.307807
N	0.467114	0.117217	-2.649513
N	0.198136	-0.805344	2.005486
C	-2.457554	1.337452	1.098614
H	-3.082652	0.691217	0.505558
C	4.753296	1.946757	-1.761902
H	5.541482	2.413120	-2.337312
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H	-0.793641	-3.848928	1.236485
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H	-0.765599	-4.006135	-1.339543
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C	-4.002073	-3.356023	-1.884875
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H	0.313341	-0.424948	-4.691547
H	0.352665	1.435976	-4.871787

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