Supplementary Information

Hydrogen-Bond-Supported Dimeric Boron Complexes of Potentially Tetradentate β-Diketiminate Ligands

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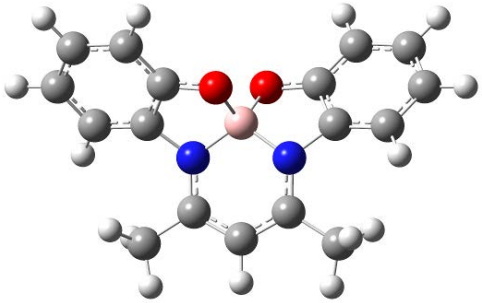
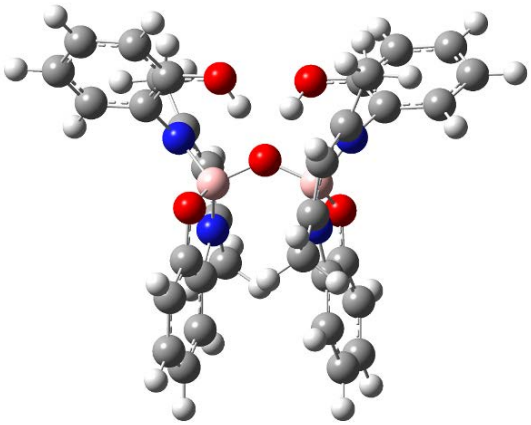
Gas-phase molecular geometry of 10 optimized at the PBE0/6-31G* level. All nuclear coordinates are given in Å.



C	0.688642	2.975737	-2.046962
C	0.367572	1.997061	-1.116676
C	-0.605624	2.252041	-0.126615
C	-1.300037	3.451699	-0.088137
C	-0.985669	4.426072	-1.039293
C	0.000000	4.188923	-1.995355
O	0.909739	0.773533	-1.036492
B	0.000000	0.000000	-0.162768
N	-0.632384	1.102623	0.702115
C	-0.572639	1.088316	2.036917
C	0.000000	0.000000	2.700896
C	0.572639	-1.088316	2.036917
C	1.075749	-2.257590	2.819818
N	0.632384	-1.102623	0.702115
C	0.605624	-2.252041	-0.126615
C	1.300037	-3.451699	-0.088137
C	0.985669	-4.426072	-1.039293
C	0.000000	-4.188923	-1.995355
C	-0.688642	-2.975737	-2.046962
C	-0.367572	-1.997061	-1.116676
O	-0.909739	-0.773533	-1.036492
C	-1.075749	2.257590	2.819818
H	0.000000	0.000000	3.783747
H	-0.877586	2.124541	3.884980
H	-0.589774	3.180671	2.481735
H	-2.154429	2.388110	2.679016
H	0.877586	-2.124541	3.884980
H	0.589774	-3.180671	2.481735

H	2.154429	-2.388110	2.679016
H	-2.082427	3.629331	0.642012
H	-1.522108	5.370111	-1.034180
H	0.229709	4.958240	-2.727818
H	1.446757	2.780160	-2.798439
H	-1.446757	-2.780160	-2.798439
H	-0.229709	-4.958240	-2.727818
H	1.522108	-5.370111	-1.034180
H	2.082427	-3.629331	0.642012

Gas-phase molecular geometry of 7a optimized at the PBE0/6-31G* level. All nuclear coordinates are given in Å.



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C	2.646112	-2.533252	2.702793
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H	-2.639530	-1.835495	3.691177
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C	2.595836	-2.416045	-1.110491
O	2.558987	-1.111738	-1.424833
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C	3.394697	-3.248547	-1.902651
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C	3.487191	-4.607554	-1.642871
H	4.111982	-5.231064	-2.276931
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C	-3.726228	-1.603261	1.011064
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N	1.089264	2.165220	-0.819574
N	-1.203571	1.302779	-1.302080
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H	3.464278	2.391245	-2.005936
C	-1.974306	0.959574	-3.617839
H	-2.577022	0.086325	-3.345756
H	-1.528999	0.792524	-4.600991
H	-2.647085	1.823164	-3.691682
C	1.887583	2.991529	0.022623
C	2.583018	2.428842	1.111953
O	2.551405	1.124738	1.427712

H	1.854628	0.647792	0.918239
C	3.377268	3.265623	1.904217
H	3.916636	2.812193	2.730287
C	3.464381	4.624711	1.642981
H	4.085695	5.251576	2.277149
C	2.751825	5.187656	0.584677
H	2.799228	6.254444	0.388287
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H	1.380379	4.781351	-1.026850
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C	-2.031050	1.952347	0.688814
O	-0.712167	1.888268	0.922124
C	-2.989626	2.346392	1.610585
H	-2.685586	2.650931	2.607480
C	-4.328817	2.351360	1.212801
H	-5.093441	2.656446	1.922310
C	-4.696039	1.971696	-0.075584
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H	-4.039667	1.276502	-2.002940

NMR Spectra

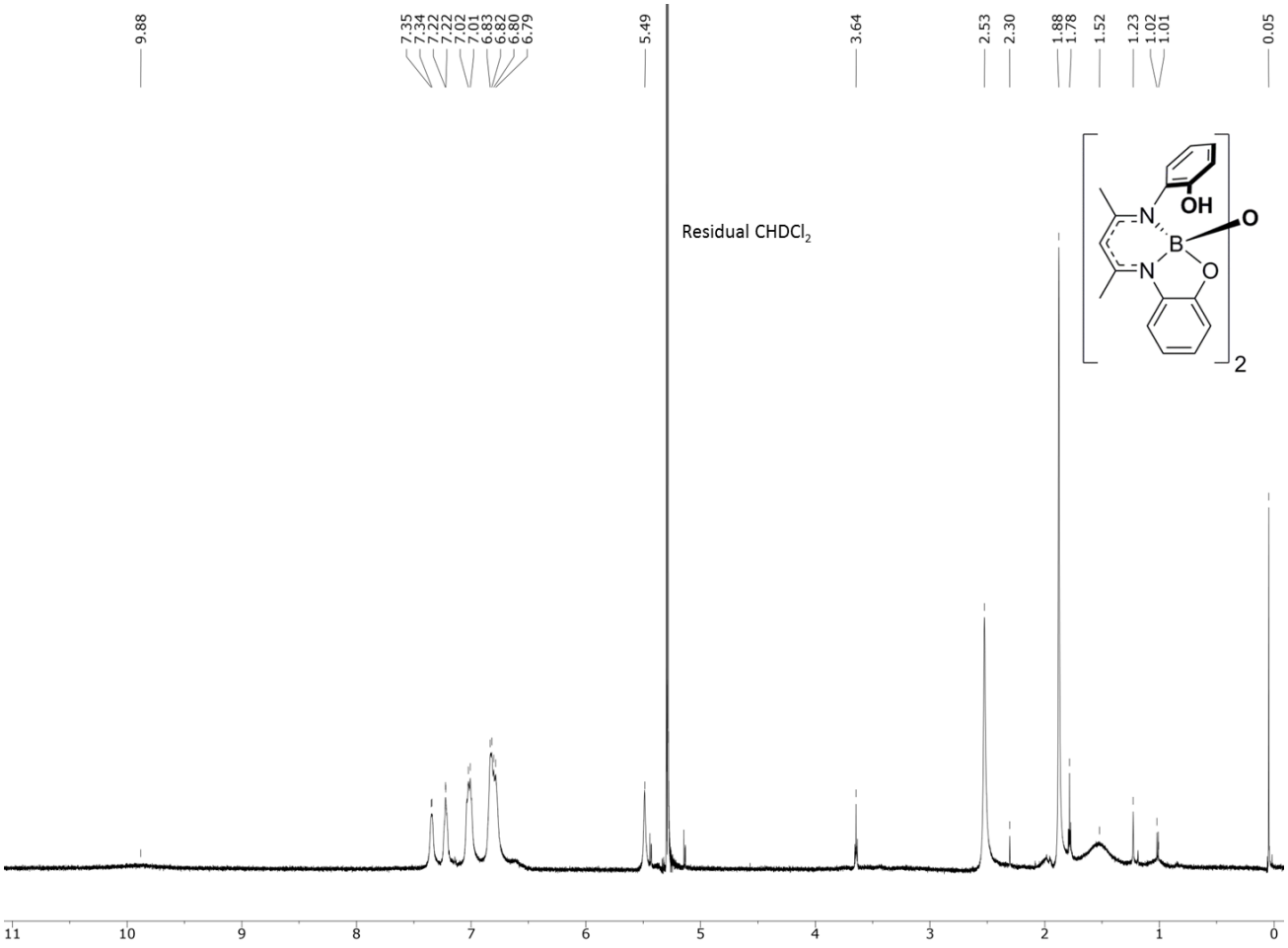

Fig. S1. ^{1}H NMR spectrum of crude **7a** in CD_2Cl_2.

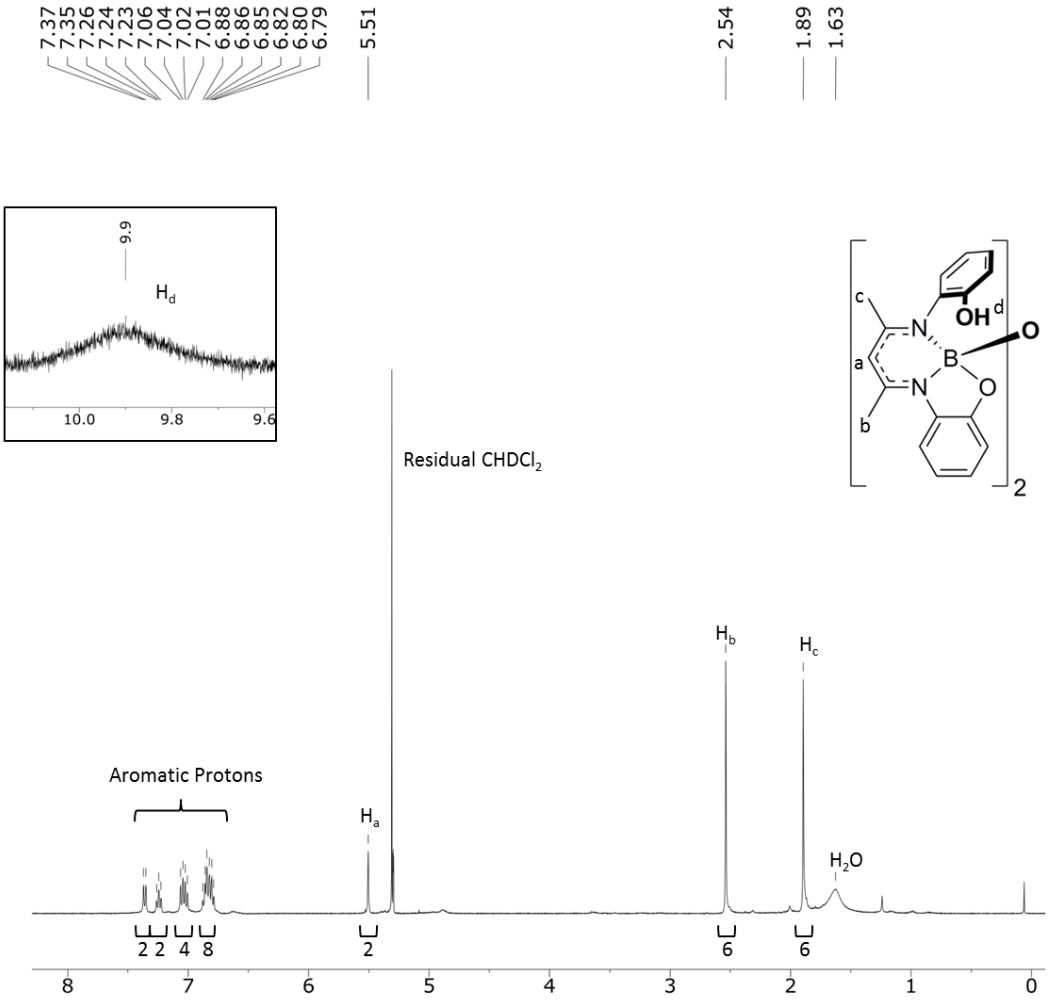

Fig. S2. ^{1}H NMR spectrum of **7a** in CD_2Cl_2.

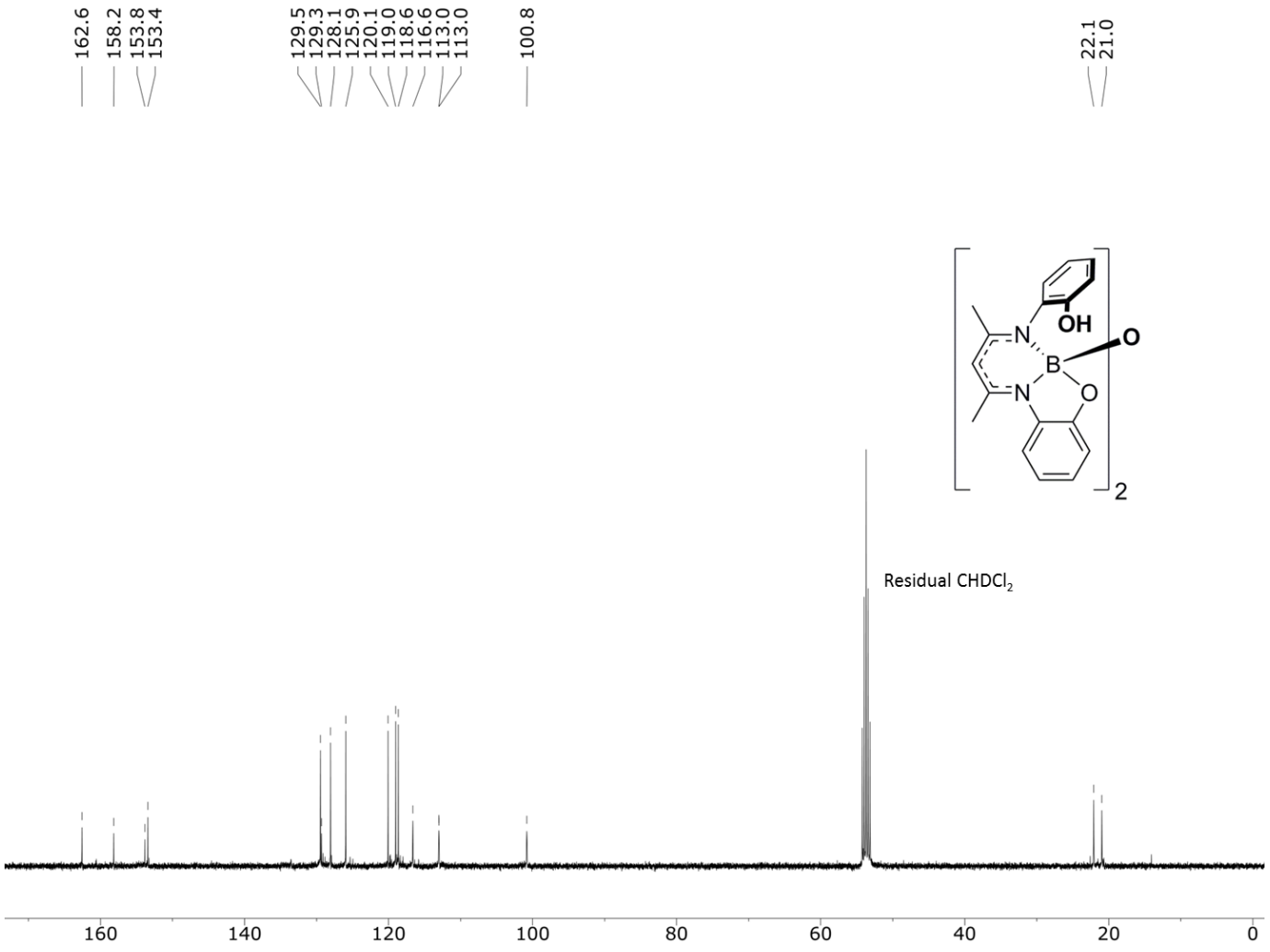

Fig. S3. ^{13}C NMR spectrum of **7a** in CD_2Cl_2.

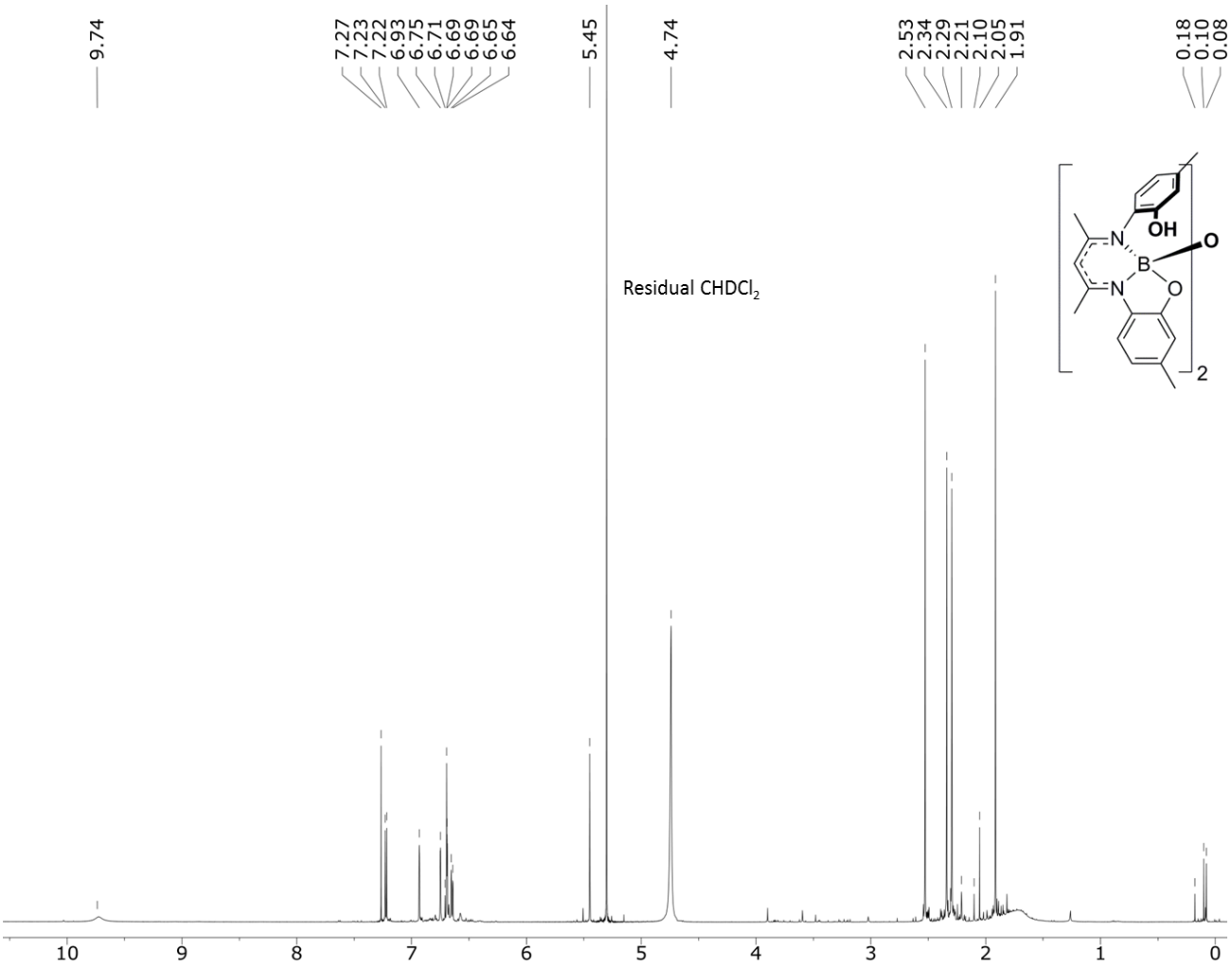

Fig. S4. ^{1}H NMR spectrum of crude **7b** in CD_2Cl_2.

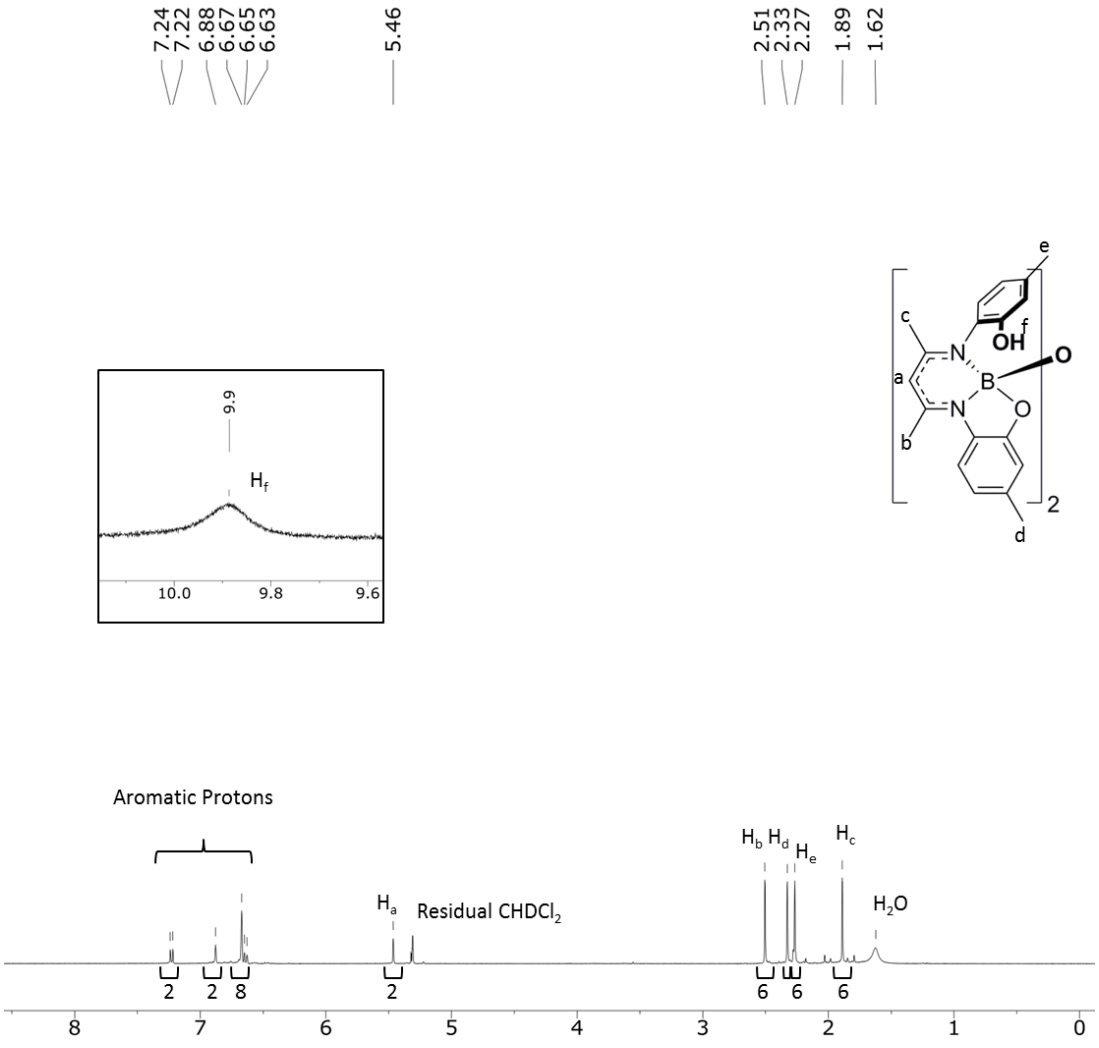

Fig. S5. ^{1}H NMR spectrum of **7b** in CD_2Cl_2. The inset shows the broadened OH signal.

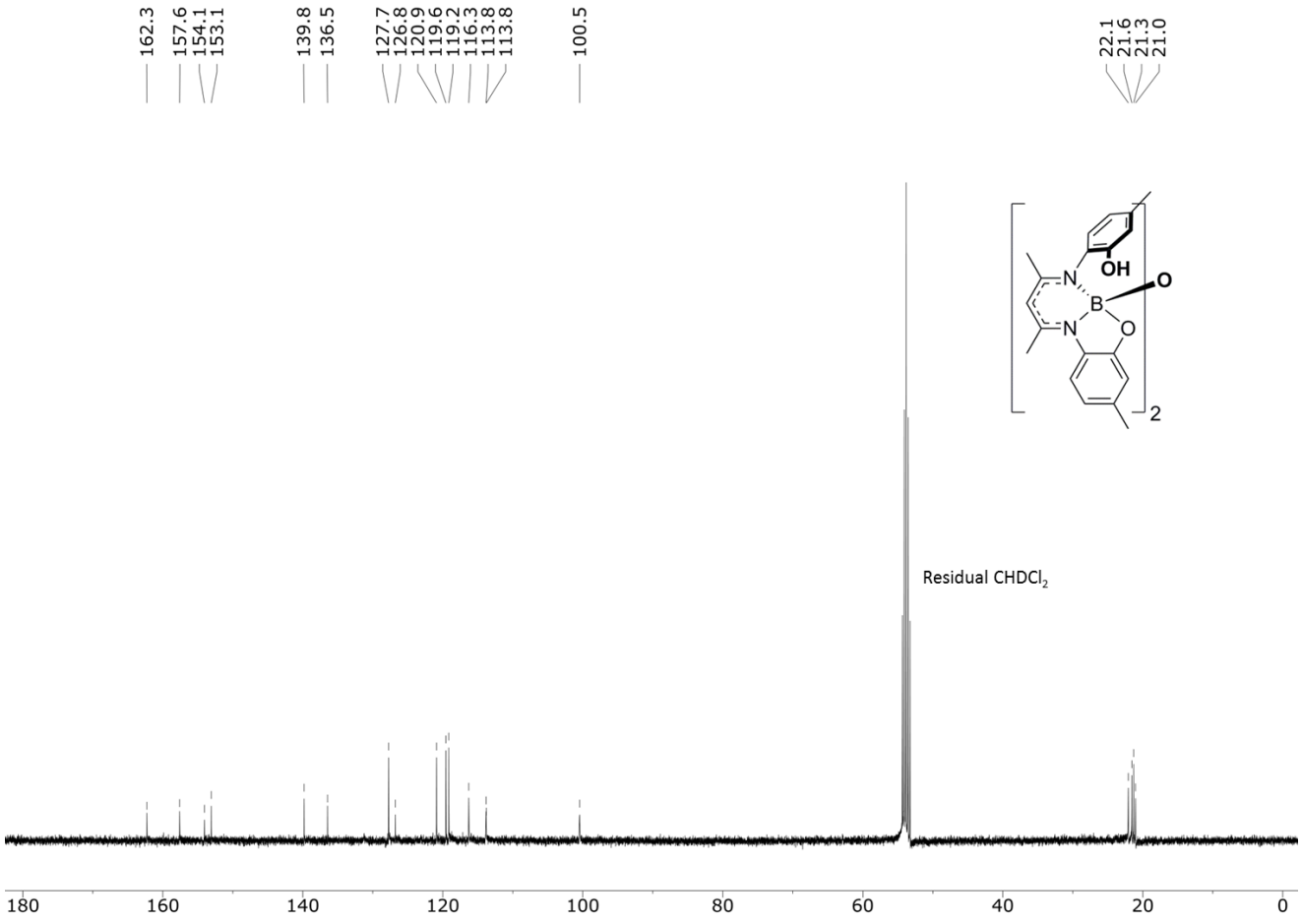

Fig. S6. ^{13}C NMR spectrum of **7b** in CD_2Cl_2.

Cyclic Voltammetry

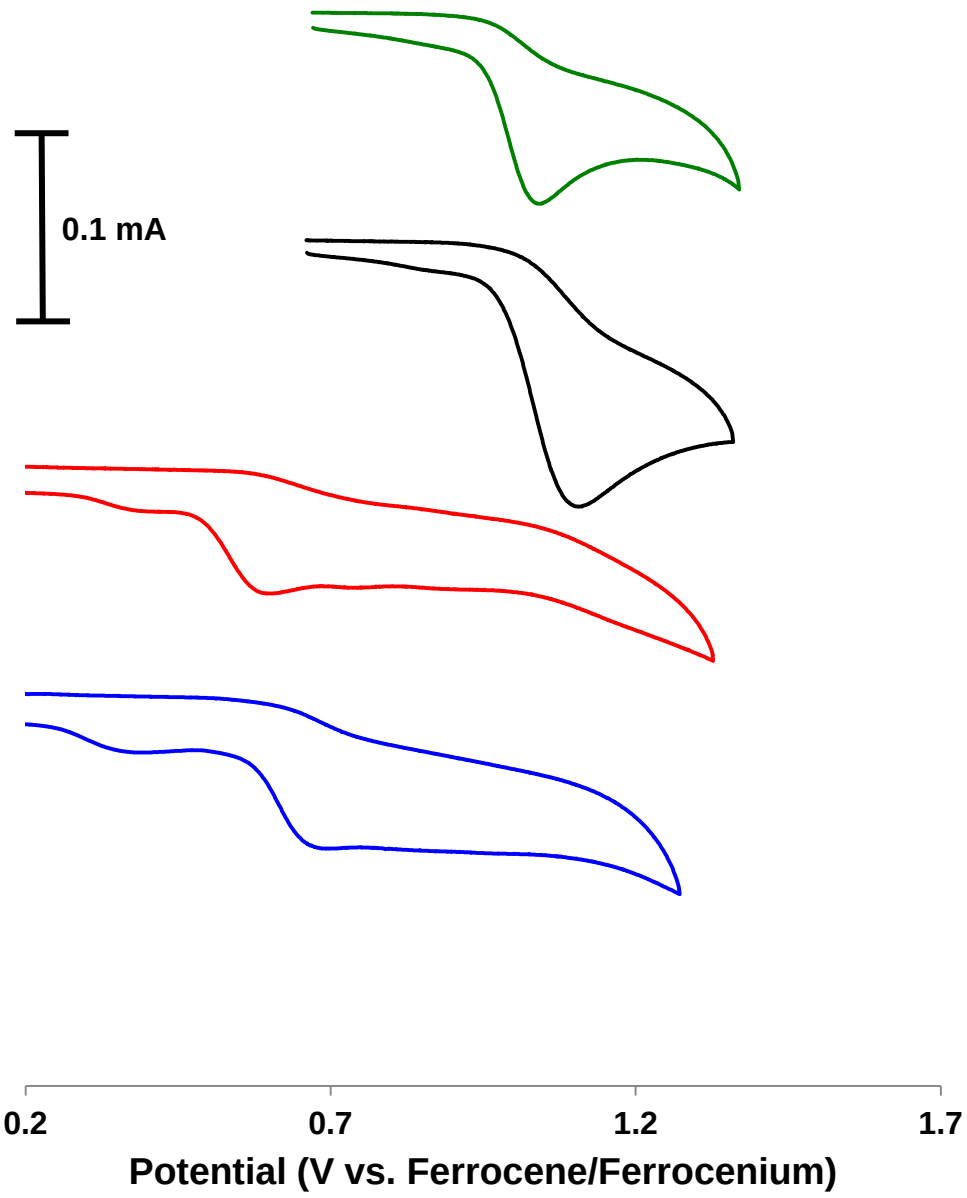

Fig. S7. Cyclic voltammograms showing the oxidation of complexes **7a** (blue), **7b** (red), **8a** (black) and **8b** (green) recorded at 250 mV/s scan rates in acetonitrile solutions. The concentrations of supporting electrolyte ($Bu_4N^+PF_6^-$) and analyte were 0.1 M and 1 mM respectively. Complexes **7a,b** and **8a,b** were not electrochemically active between -2.3 V and 0.2 V under the conditions employed.

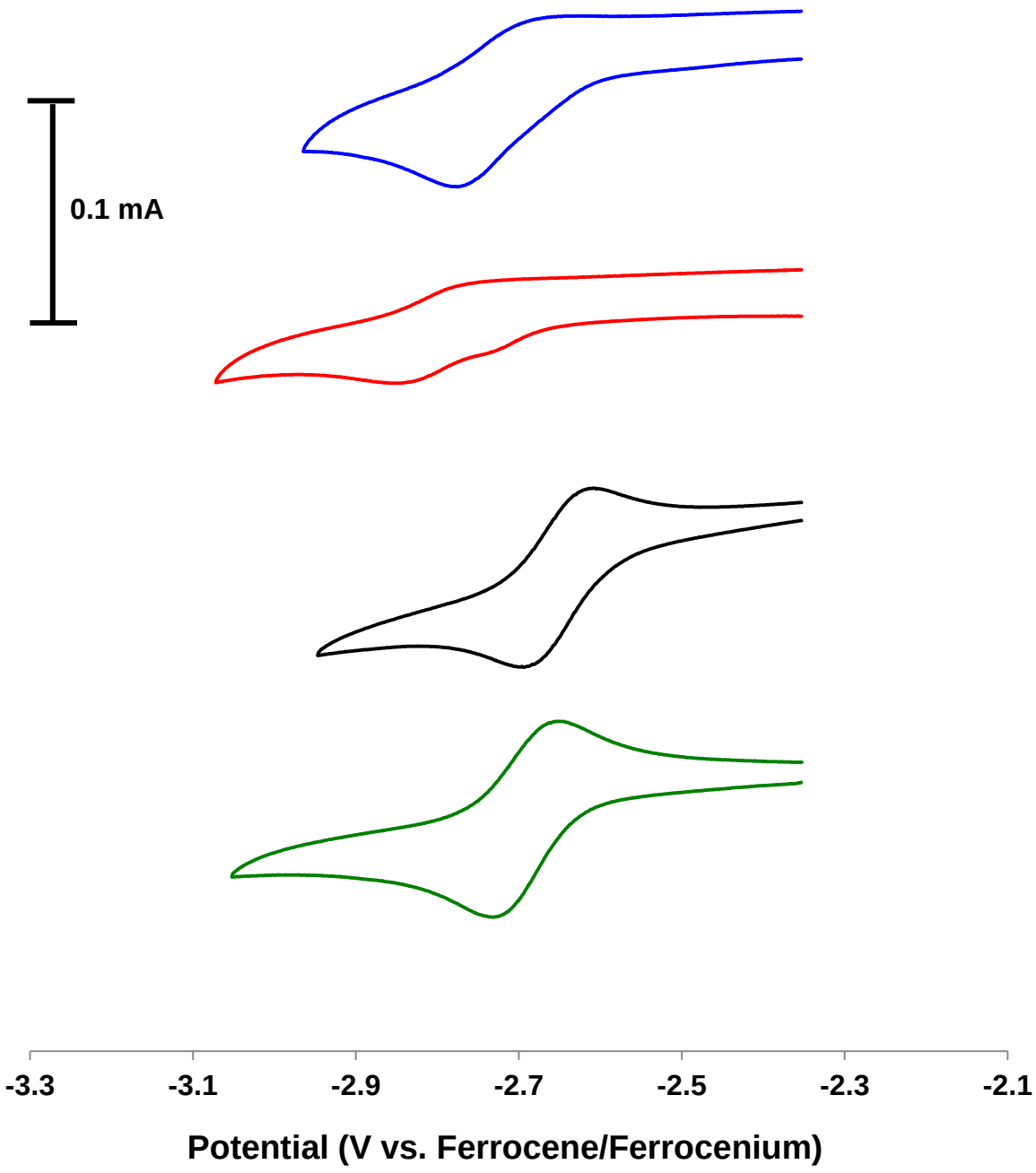

Fig. S8. Cyclic voltammograms showing the reduction of complexes **7a** (blue), **7b** (red), **8a** (black) and **8b** (green) recorded at 250 mV/s scan rates in acetonitrile solutions. The concentrations of supporting electrolyte ($Bu_4N^+PF_6^-$) and analyte were 0.1 M and 1 mM respectively. Complexes **7a,b** and **8a,b** were not electrochemically active between -2.3 V and 0.2 V under the conditions employed.