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Supporting Information

Unusual κ1 Coordination of a β-Diketiminate Ligand in Niobium Complexes

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A. NMR Spectroscopic Analysis

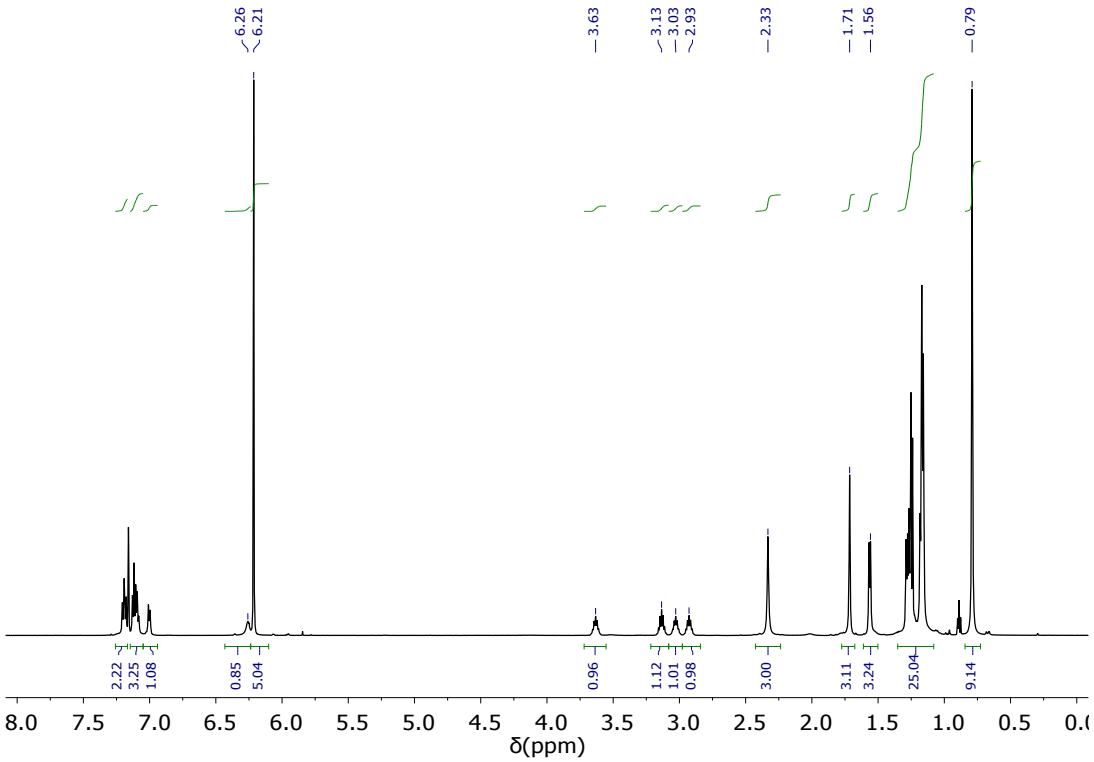

Figure S1: ^{1}H NMR spectrum of **2** in C_6D_6 at 298 K.

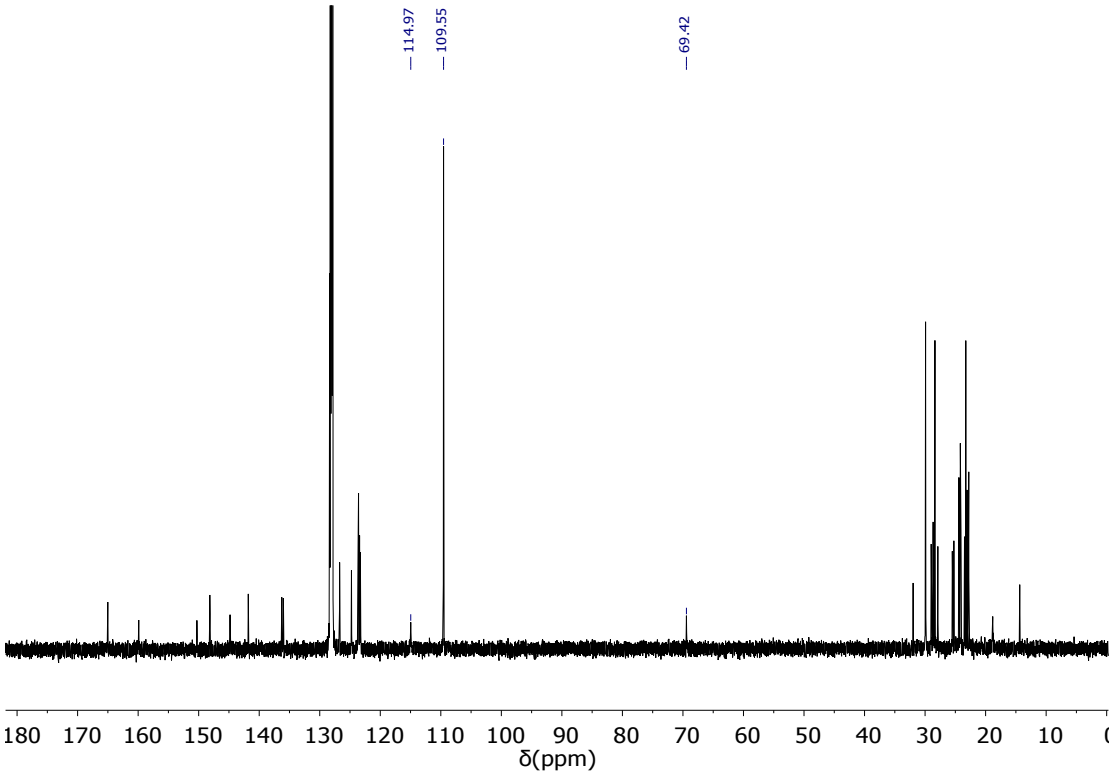

Figure S2: $^{13}C\{^{1}H\}$ NMR spectrum of **2** in C_6D_6 at 298 K.

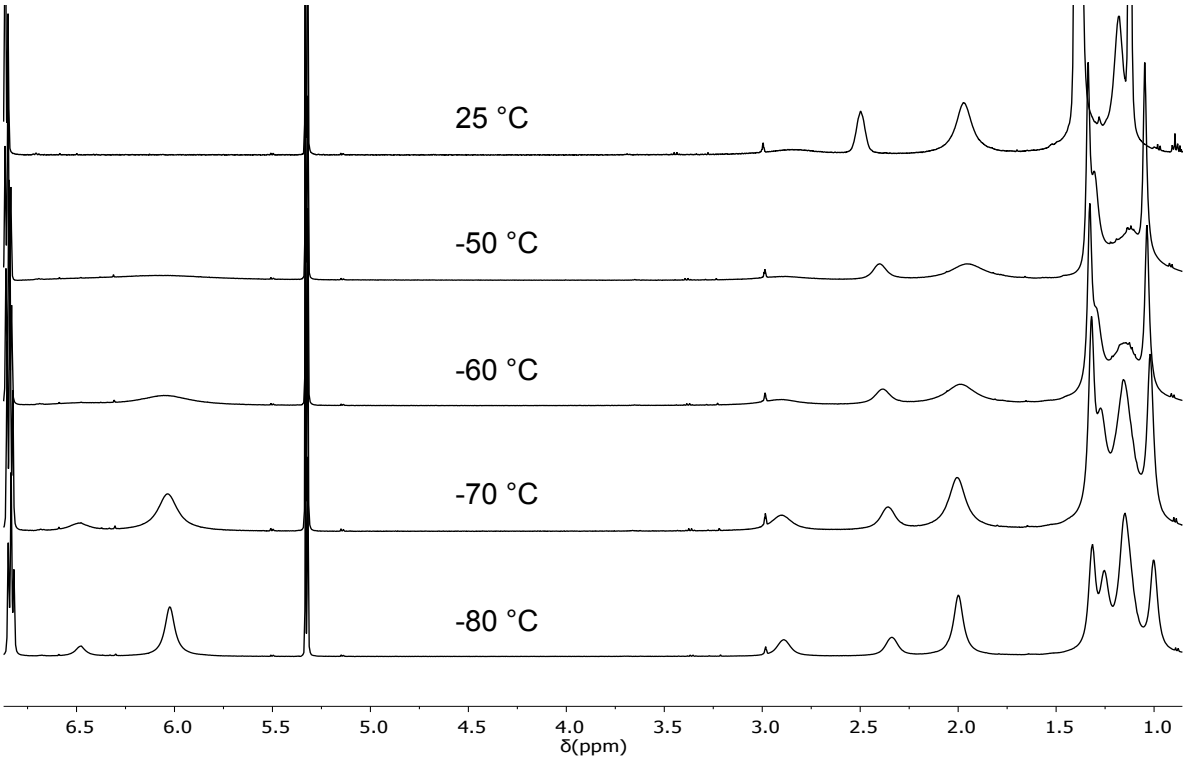

Figure S3: Low temperature ^{1}H NMR spectra of **3** in CD_2Cl_2.

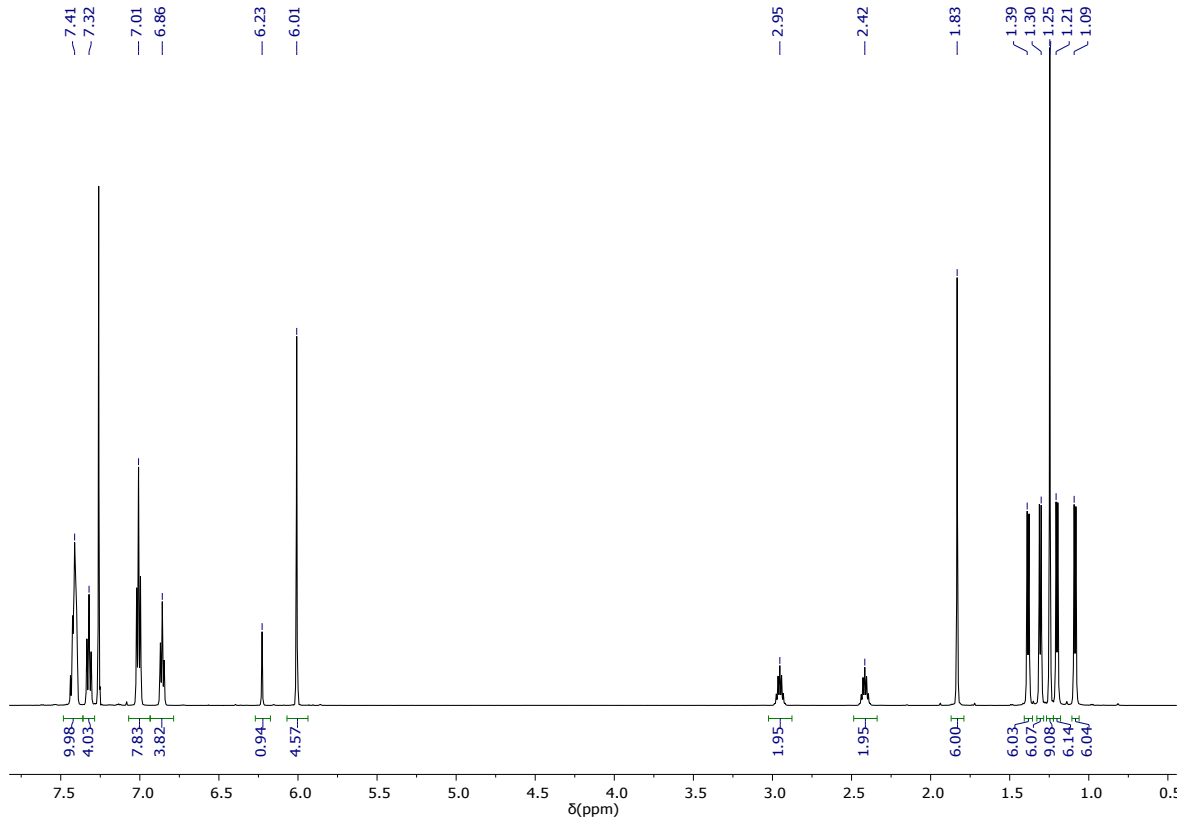

Figure S4: Representative ^{1}H NMR spectrum of **3** in $CDCl_3$ before decomposition occurs.

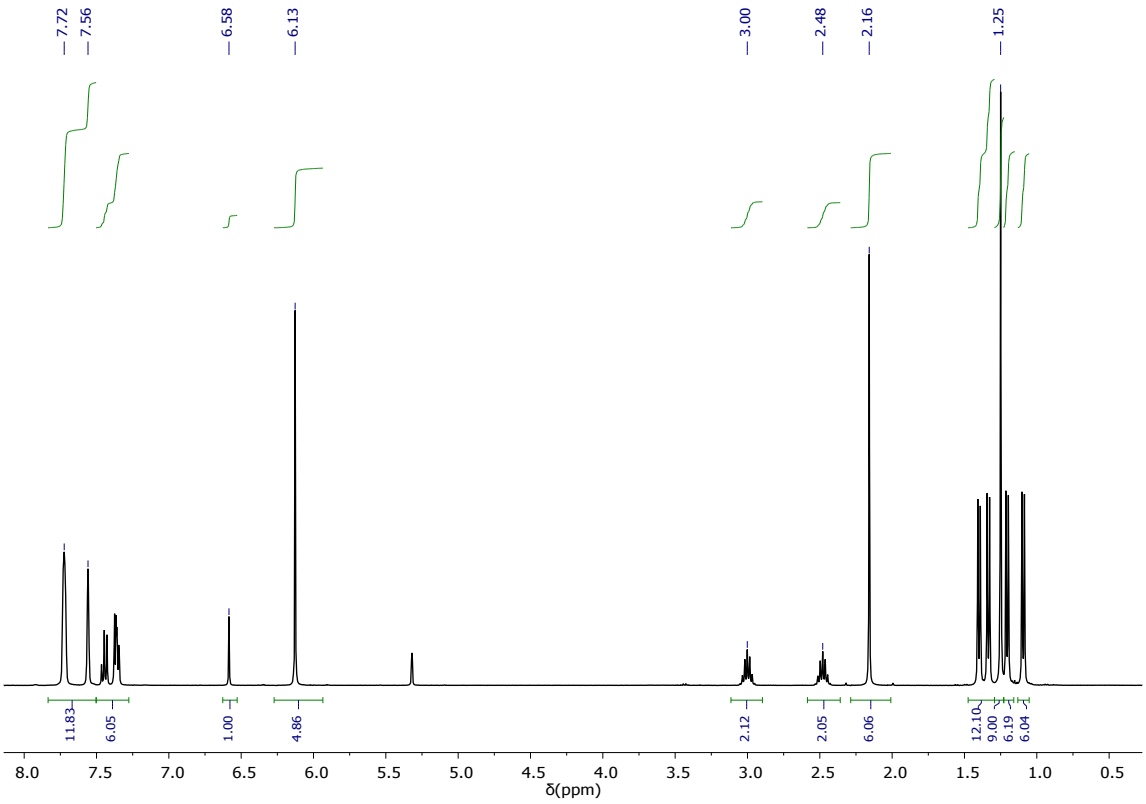

Figure S5: ^{1}H NMR spectrum of **4** in CD_2Cl_2 at 298 K.

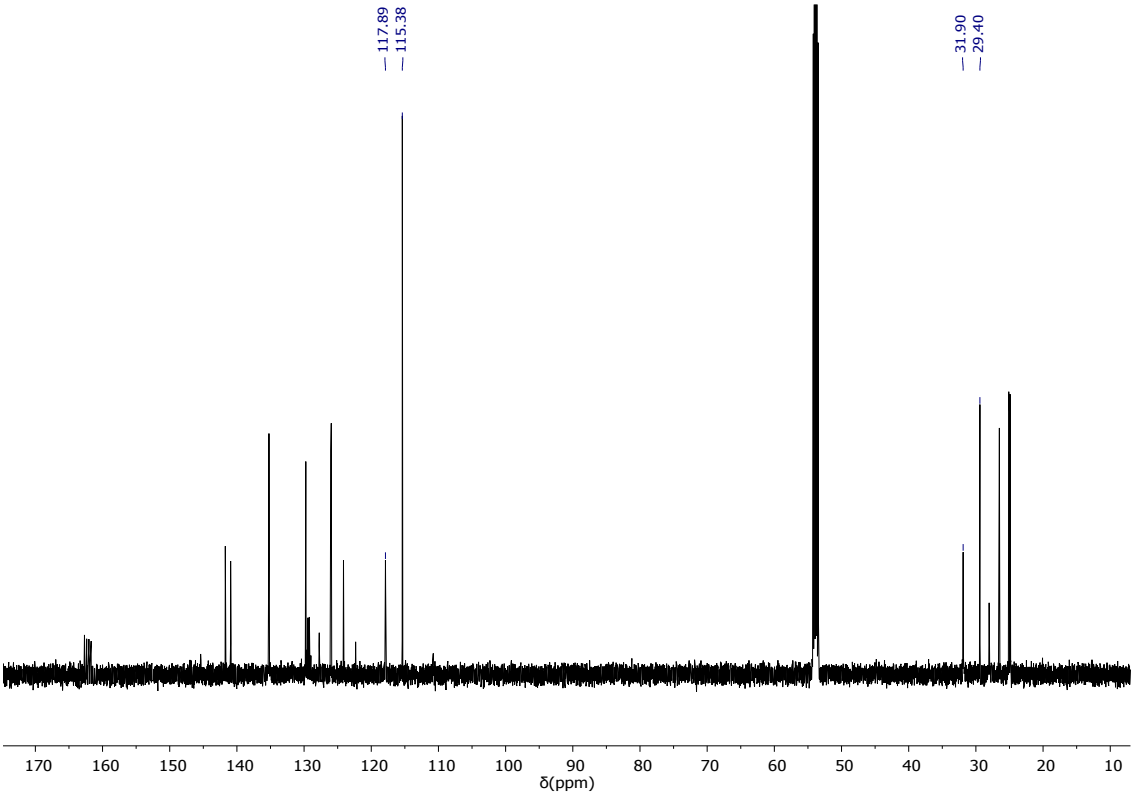

Figure S6: $^{13}C\{^{1}H\}$ NMR spectrum of **4** in CD_2Cl_2 at 298 K.

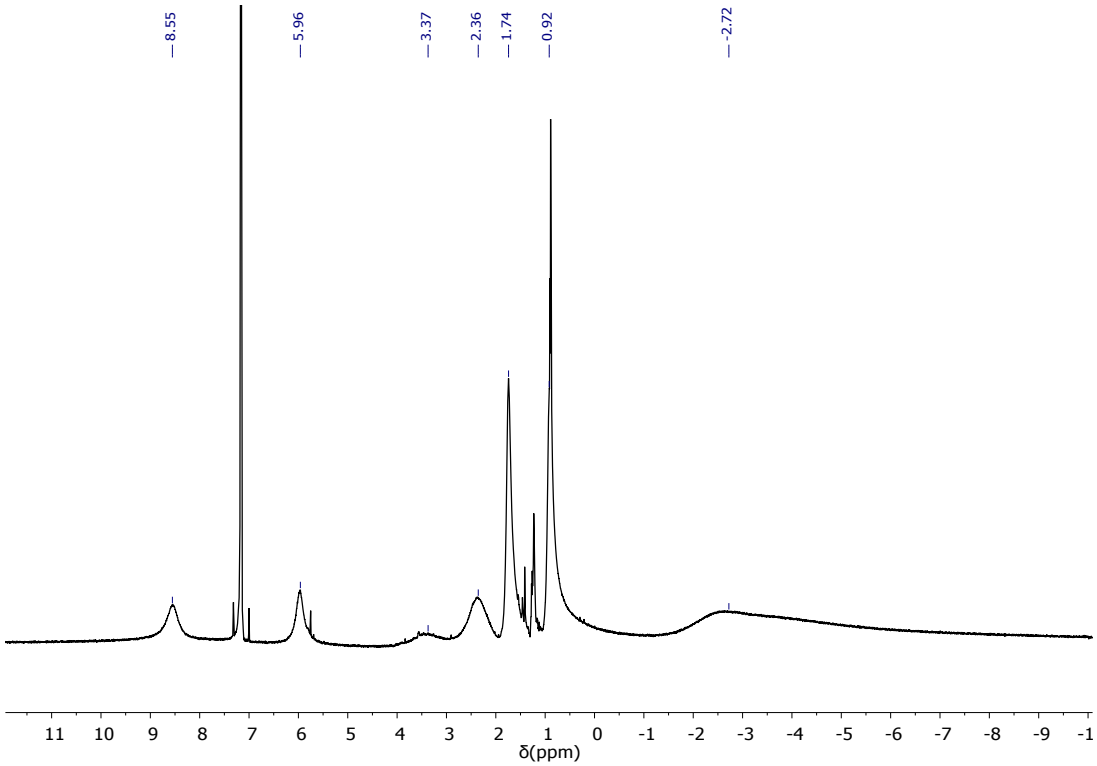

Figure S7: ^{1}H NMR spectrum of paramagnetic complex **5** in C_6D_6 at room temperature.

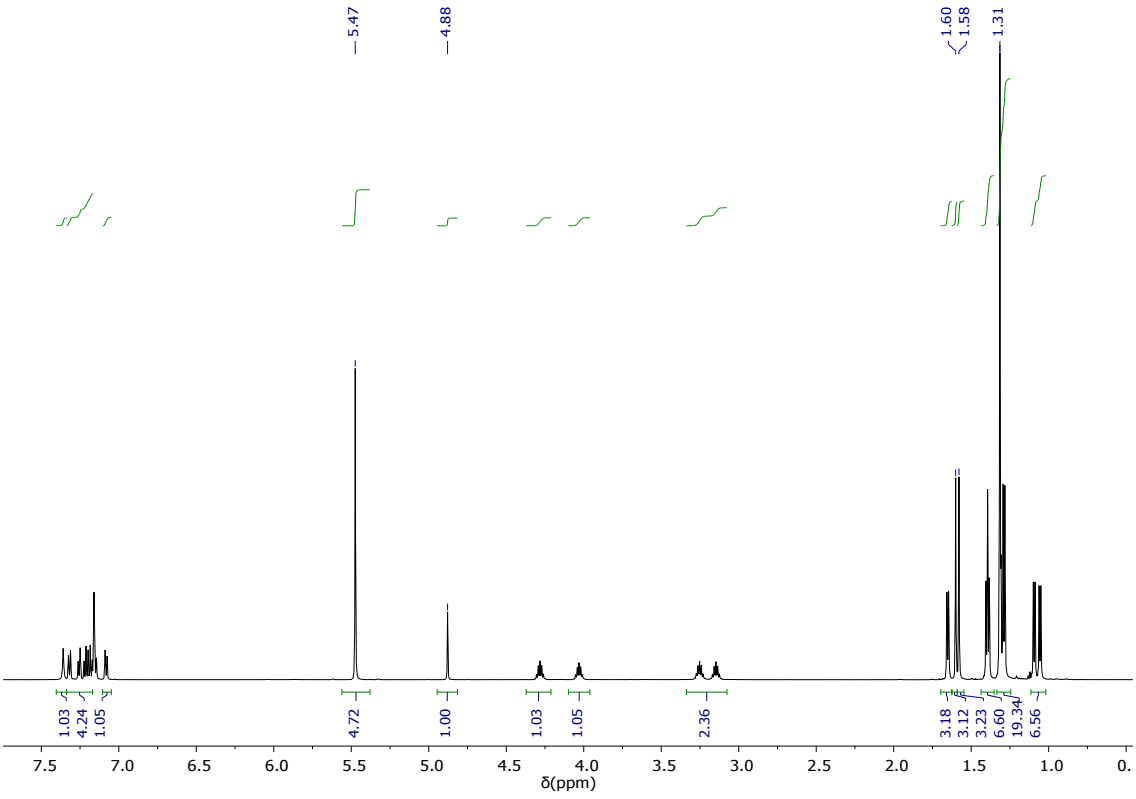

Figure S8: ^{1}H NMR spectrum of **6** in C_6D_6 at 298 K.

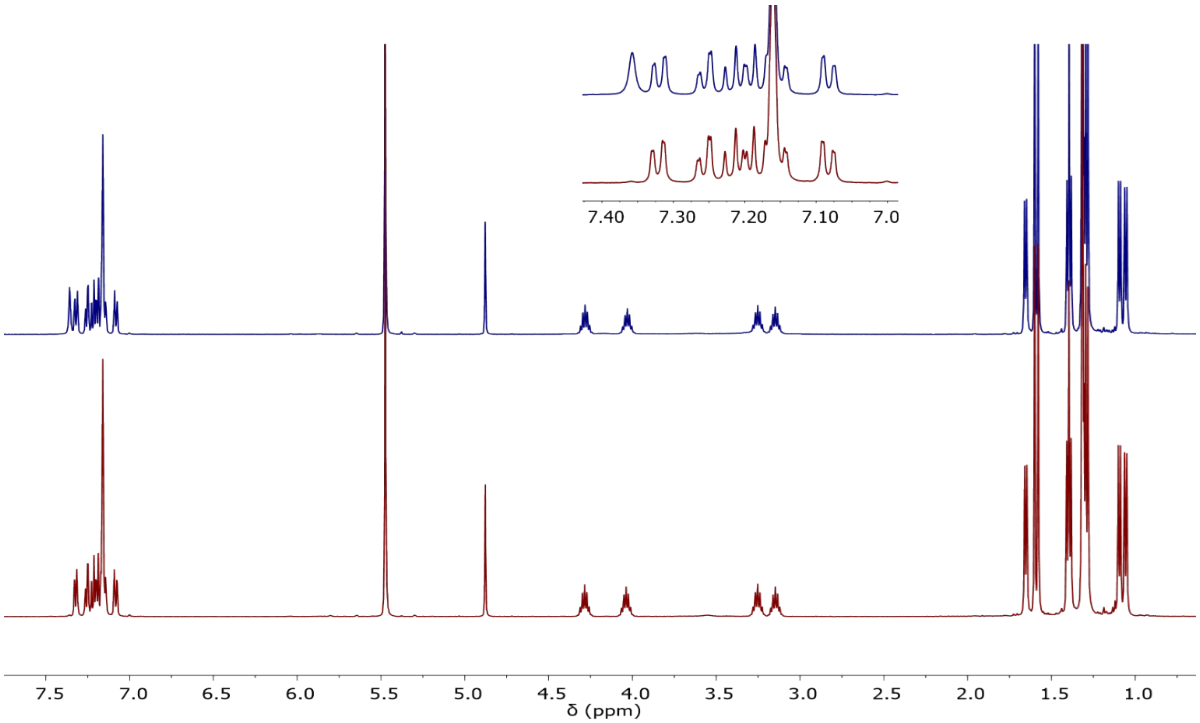

Figure S9: Stacked spectra of **6** (blue, top) and **6-D** (red, bottom) with the aromatic region enlarged, showing the chemical shift for the Nb-*H* that appears at 7.36 ppm for **6** and is absent in the spectrum of **6-D**.

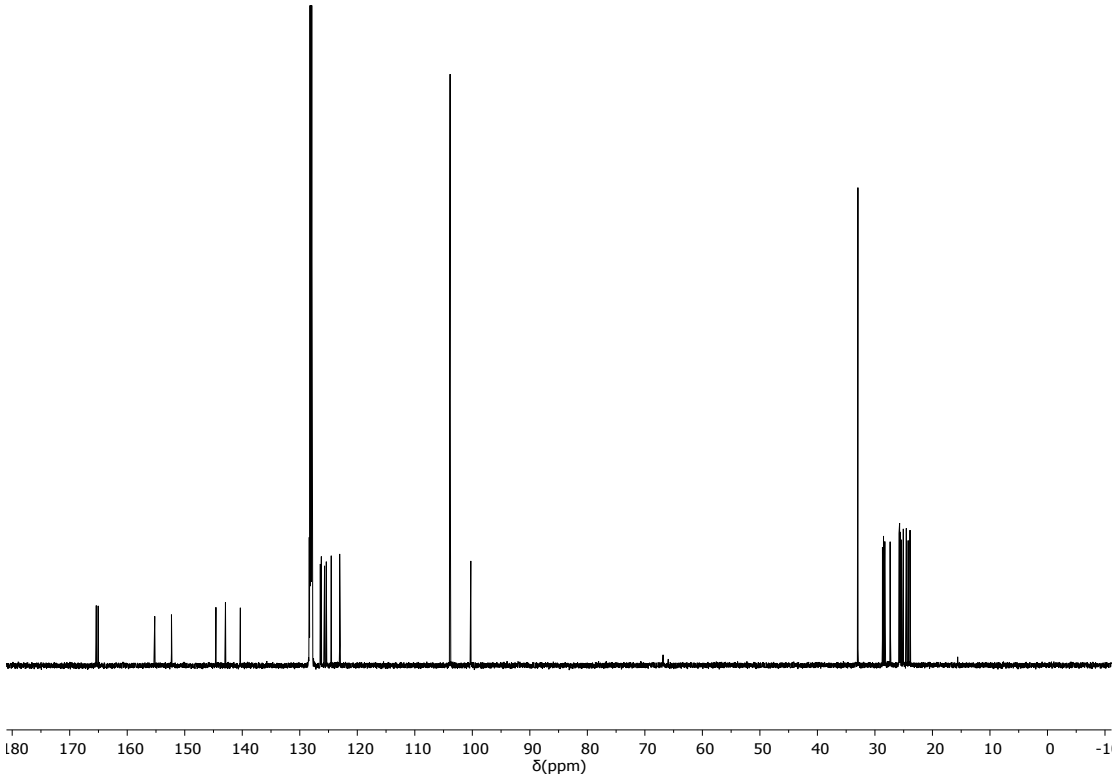

Figure S10: $^{13}C\{^{1}H\}$ NMR spectrum of **6** in C_6D_6 at 298 K.

B. Infrared Spectroscopic Analysis

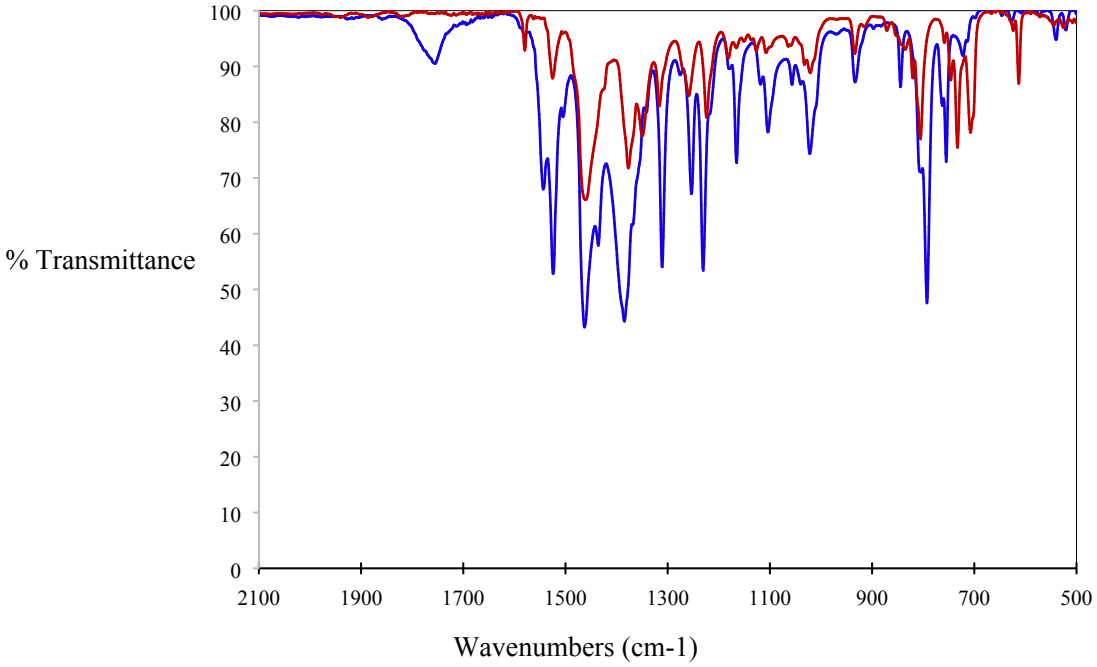

Figure S11: Overlaid IR spectra of **6** (blue) and **6-D** (red).

C. X-ray Crystallography of 5

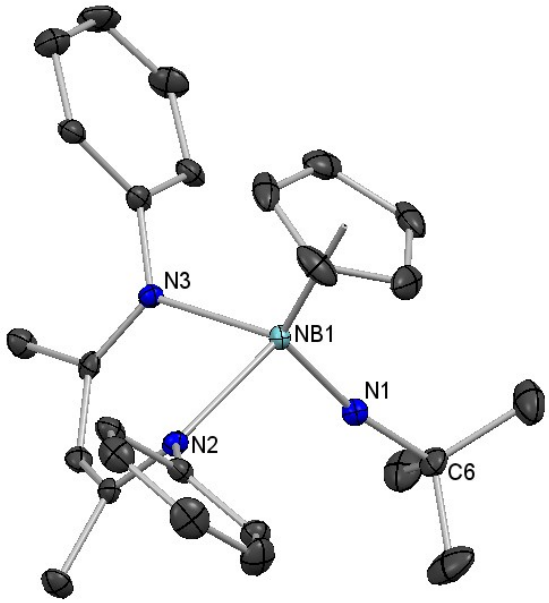

Figure S12: Molecular structure of **5** as determined by X-ray diffraction. Hydrogen atoms, a second equivalent molecule of **5**, and aryl isopropyl groups have been omitted for clarity; thermal ellipsoids are set at the 50% probability level. Selected bond lengths (Å): Nb(1)-N(1) 1.794(2), Nb(1)-N(2) 2.210(2), Nb(1)-N(3) 2.207(2). Selected bond angles (°): C(6)-N(1)-Nb(1) 168.07(2), N(2)-Nb(1)-N(3) 83.68(8).