Two Alternative Approaches to Access Mixed Hydride-Amido Zinc Complexes: Synthetic, Structural and Solution Implications

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SUPPORTING INFORMATION

Contents

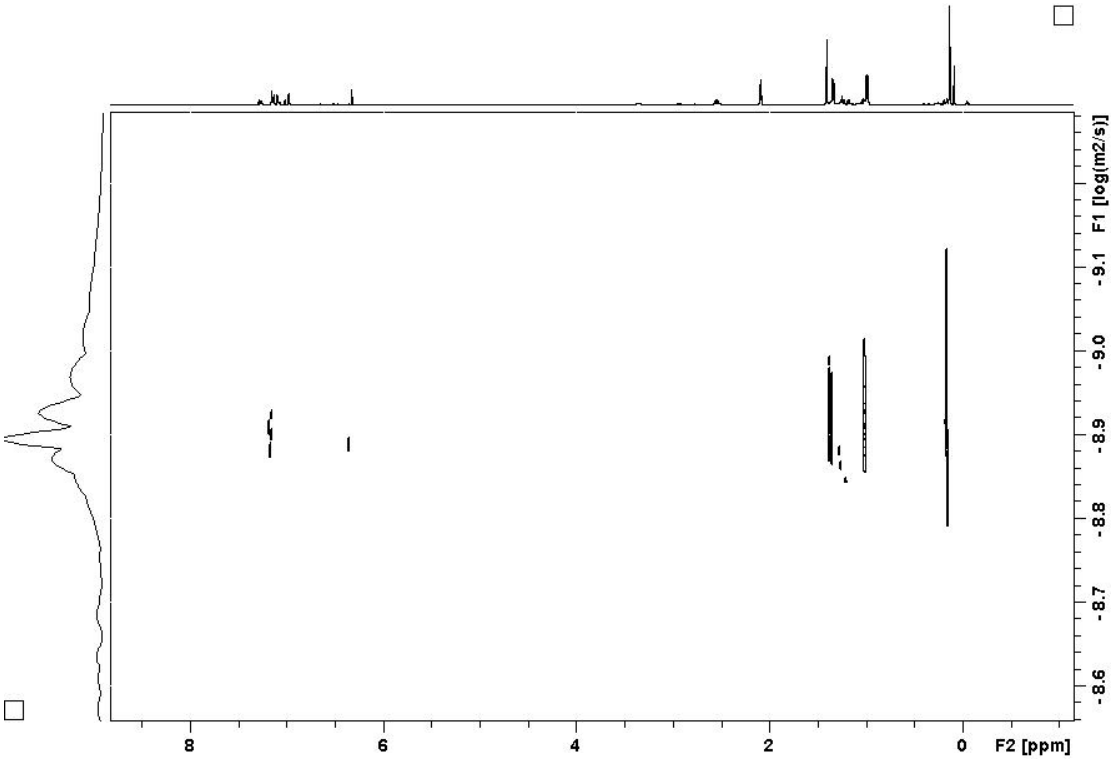

Figure S1 ^{1}H DOSY NMR spectrum of complex **1** in C_7D_8 solution.

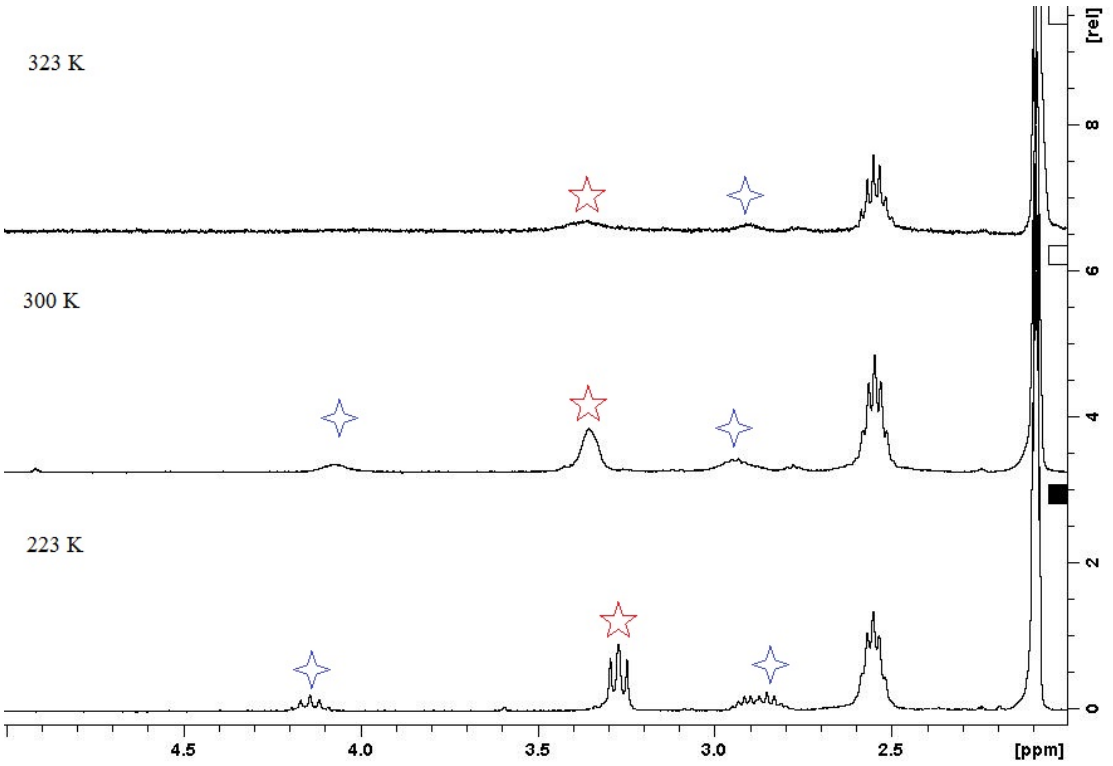

Figure S2 Region of ^{1}H NMR spectra of **1** in d_8-toluene containing the hydride resonances at 323 K (top); 300K (middle) and 223 K (bottom).

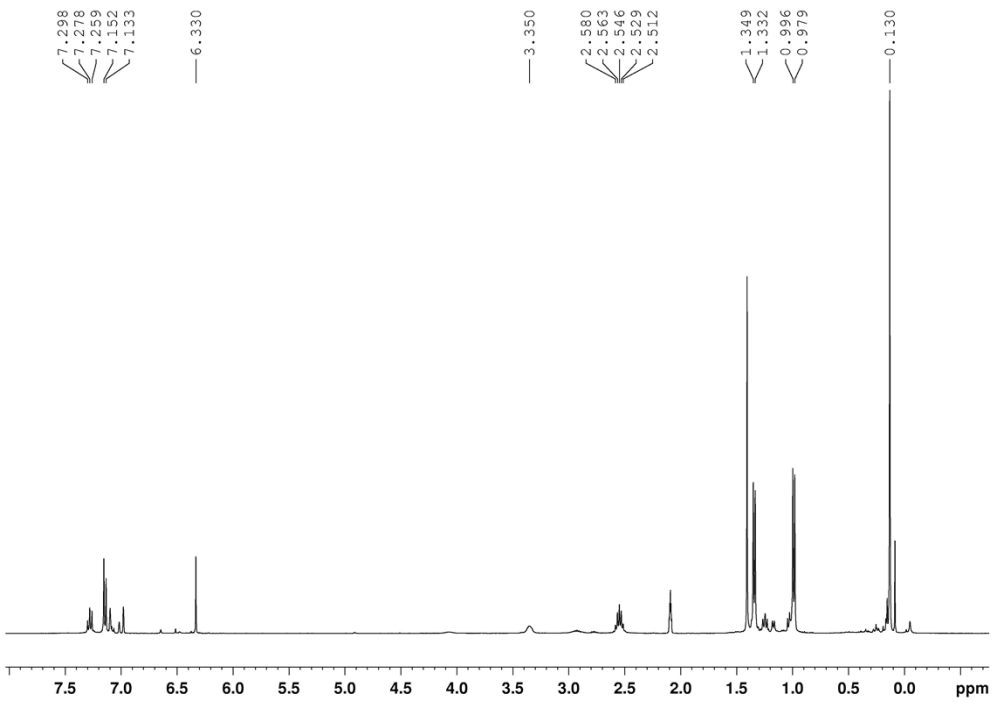

Figure S3 ^{1}H NMR spectrum of complex **1** in C_7D_8 solution.

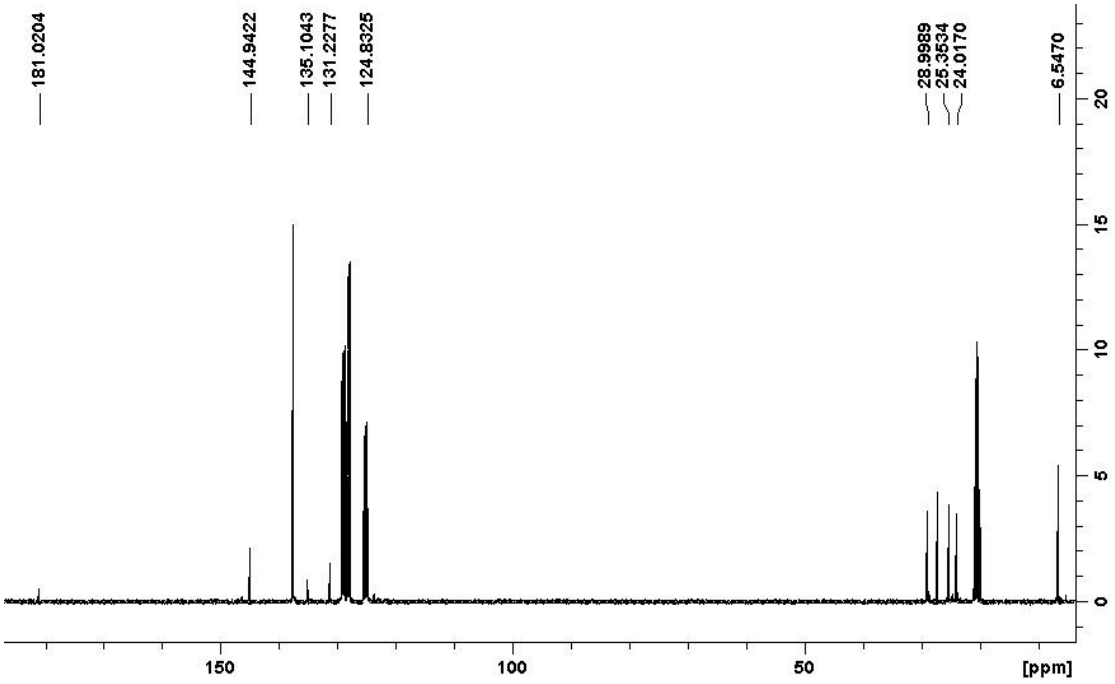

Figure S4 ^{13}C NMR spectrum of complex **1** in C_7D_8 solution.

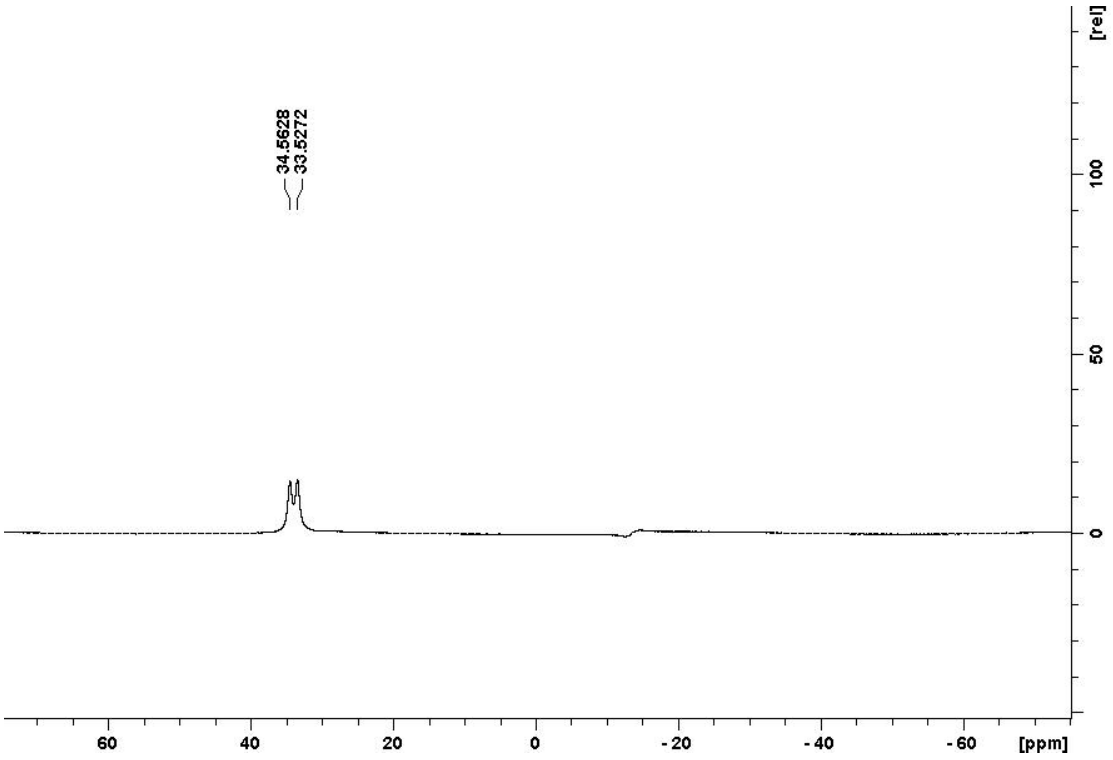

Figure S5 ^{11}B NMR spectrum of filtrate from reaction of DMAB, $Zn(HMDS)_2$ and IPr.

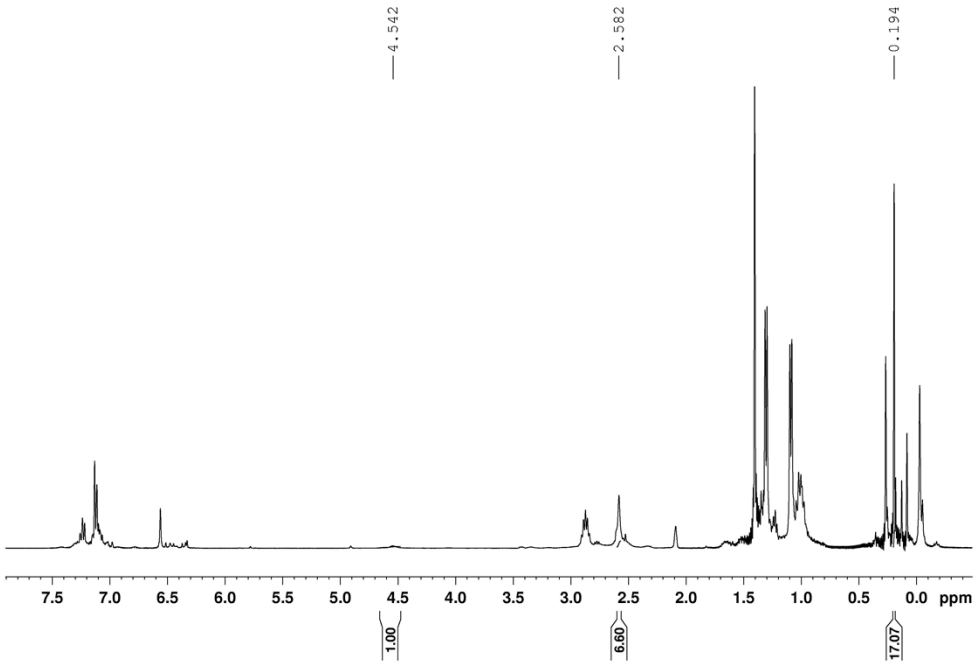

Figure S6 ^{1}H NMR spectrum of filtrate from reaction of DMAB, $Zn(HMDS)_2$ and IPr with resonances representing [$HB(NMe_2)(HMDS)$] highlighted.

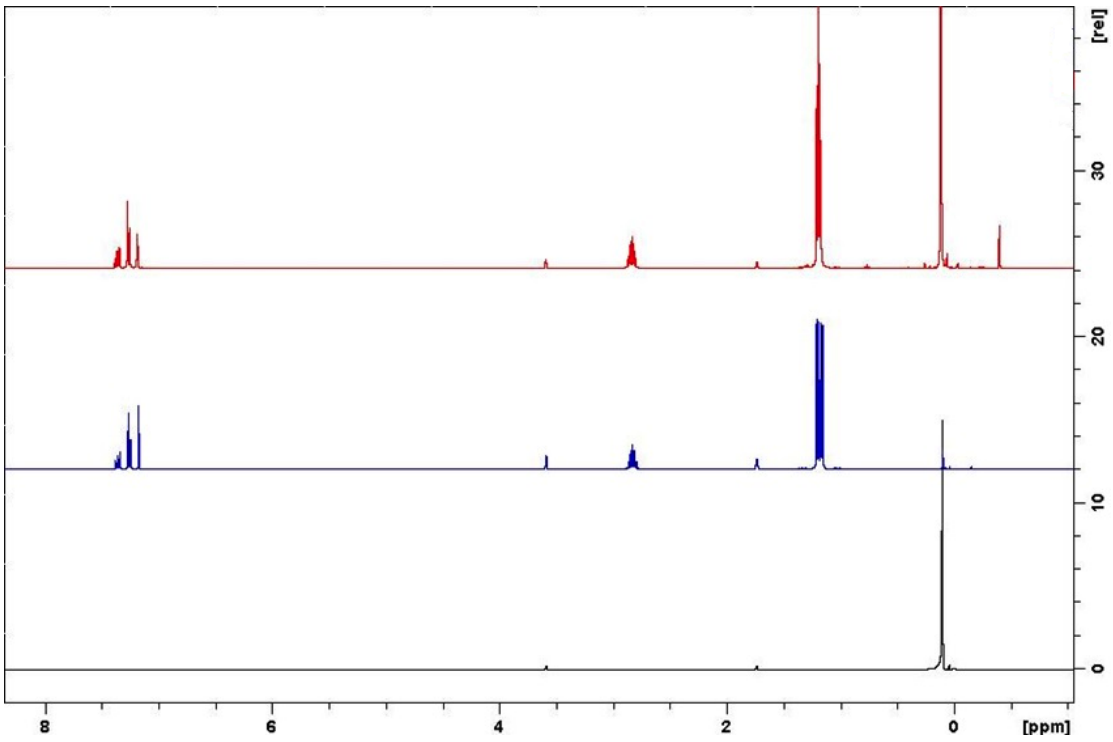

Figure S7 ^{1}H NMR spectra of $Zn(HMDS)_2$ (bottom), IPr (middle), and an equimolar amount of $Zn(HMDS)_2$ and IPr (top) confirming no interaction has occurred, in d_8-THF.

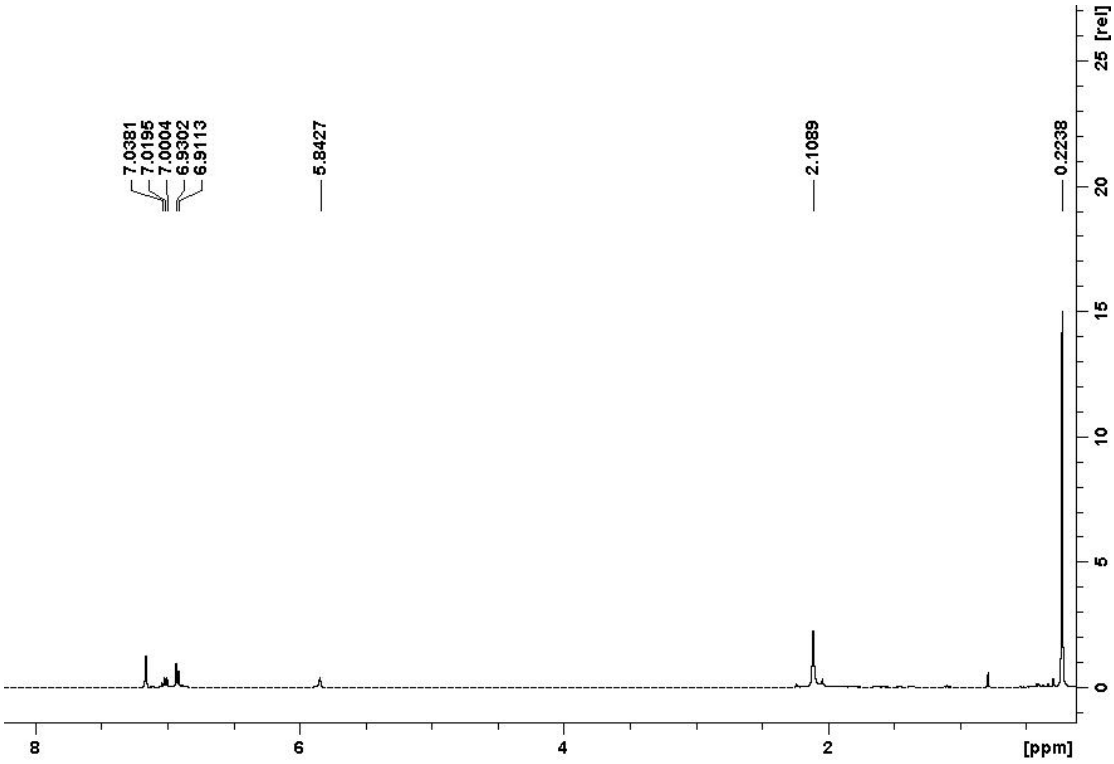

Figure S8 ^{1}H NMR spectrum of complex **2** in C_6D_6 solution.

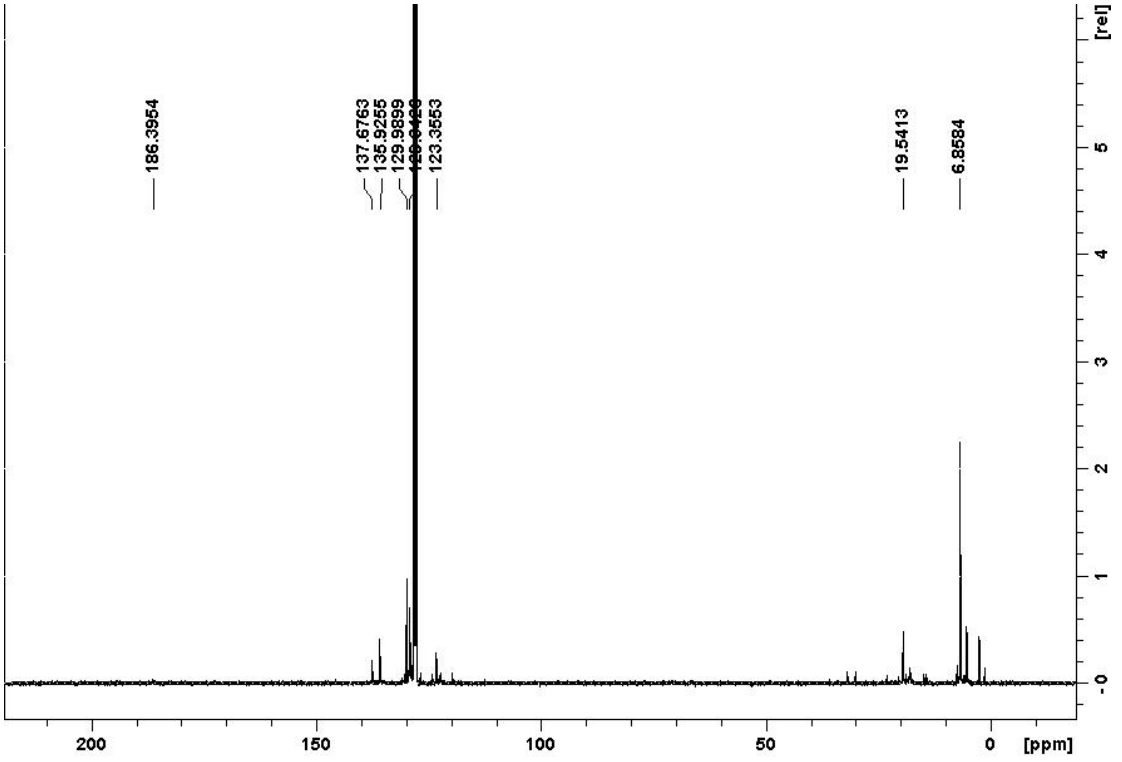

Figure S9 ^{13}C NMR spectrum of complex **2** in C_6D_6 solution.

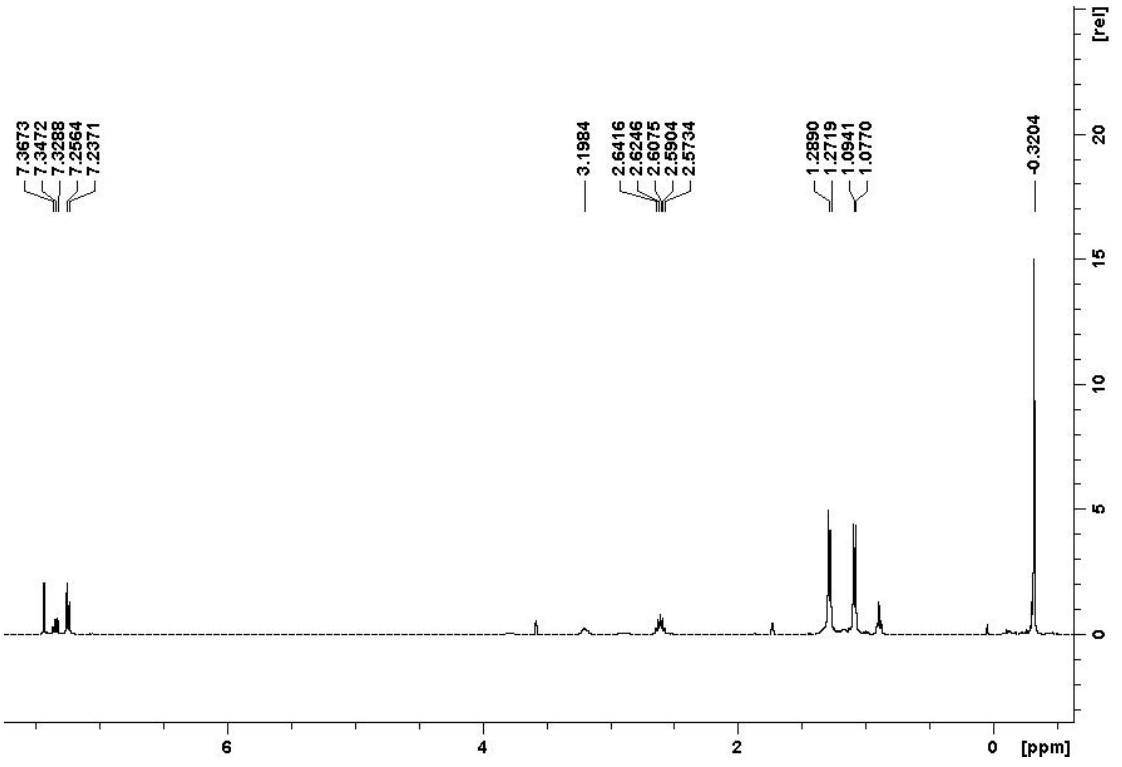

Figure S10 ^{1}H NMR spectrum of monomeric (HMDS)ZnH·IPr (**3**) in d_8-THF

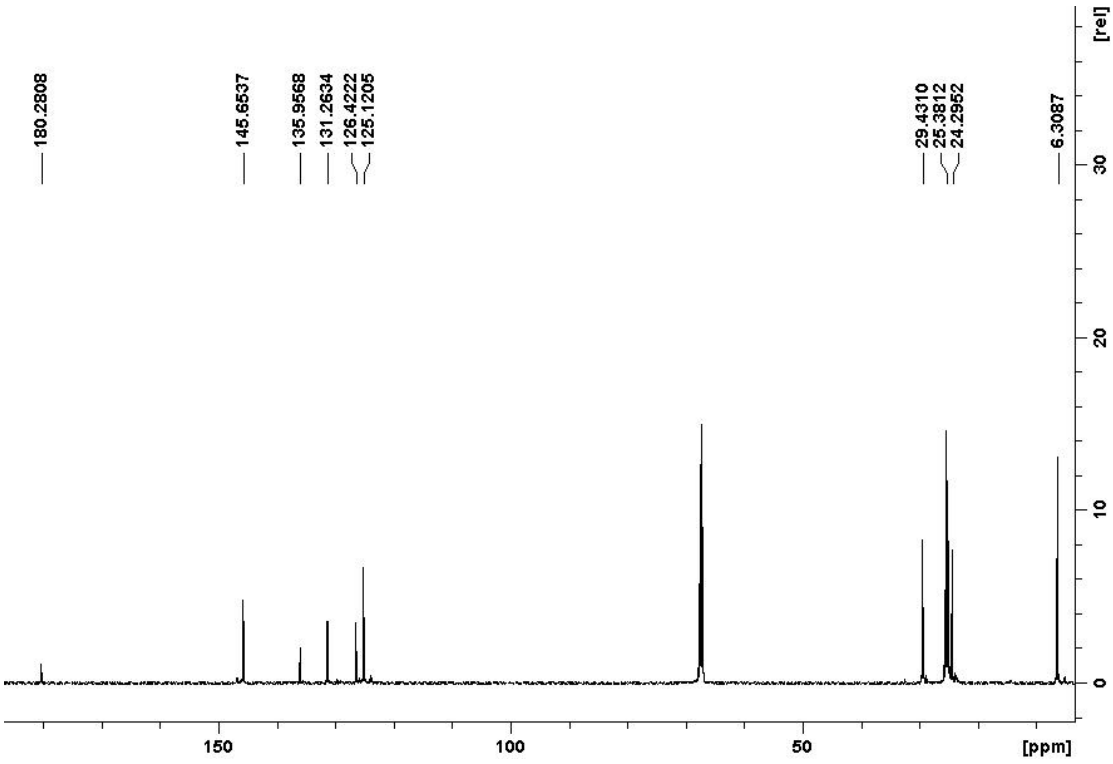

Figure S11 ^{13}C NMR spectrum of monomeric (HMDS)ZnH·IPr (**3**) in d_8-THF

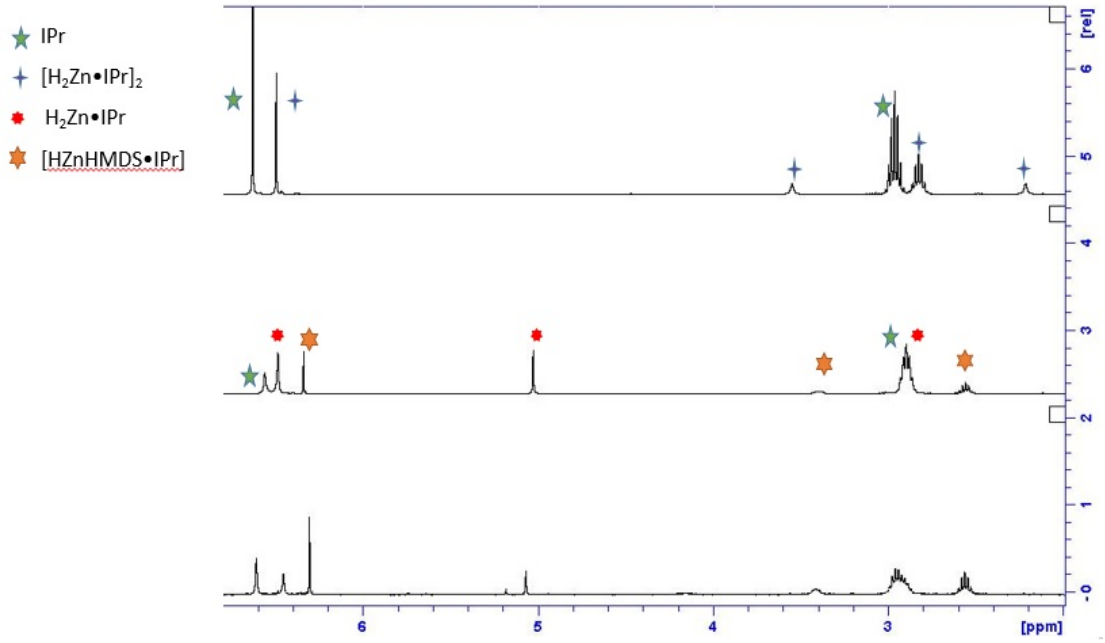

Figure S12 ^{1}H NMR spectra in C_6D_6 of (a, top) an authentic sample of $[ZnH_2{\cdot}IPr]_2$ (**B**) with two molar equivalents of IPr added; (b, middle) the same sample with two molar equivalents of $Zn(HMDS)_2$ added; (c, bottom) an authentic sample of (HMDS)ZnH·IPr (**3**) for comparison

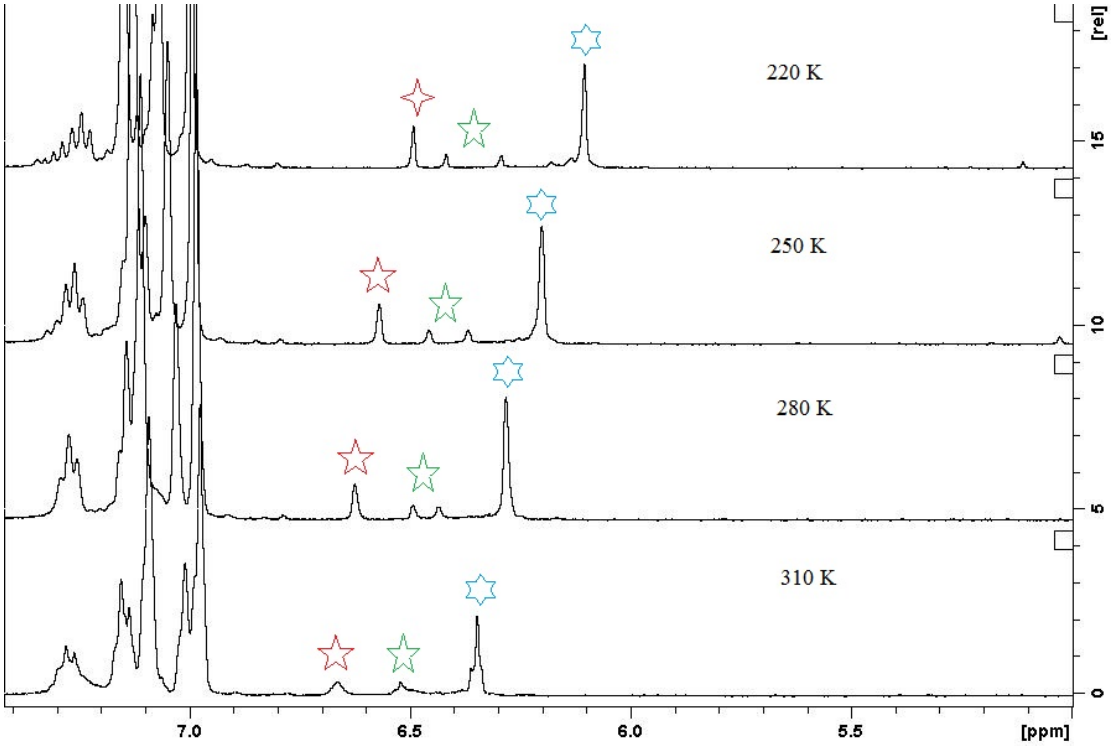

Figure S13 Aromatic region of ^{1}H NMR spectra of isolated crystals of **3** in d_8-toluene highlighting the relevant resonances of the imidazole backbone of **3** (blue), IPr (red) and ZnH_2.IPr species (green)[1] at 220 K, 250K, 280K and 310 K.

[1] In this deuterated solvent monomeric and dimeric forms of ZnH_2IPr appear also to coexist in solution.