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Electronic Supplementary Information

A Homobimetallic Complex of Chromium(0) with a σ-borane Component

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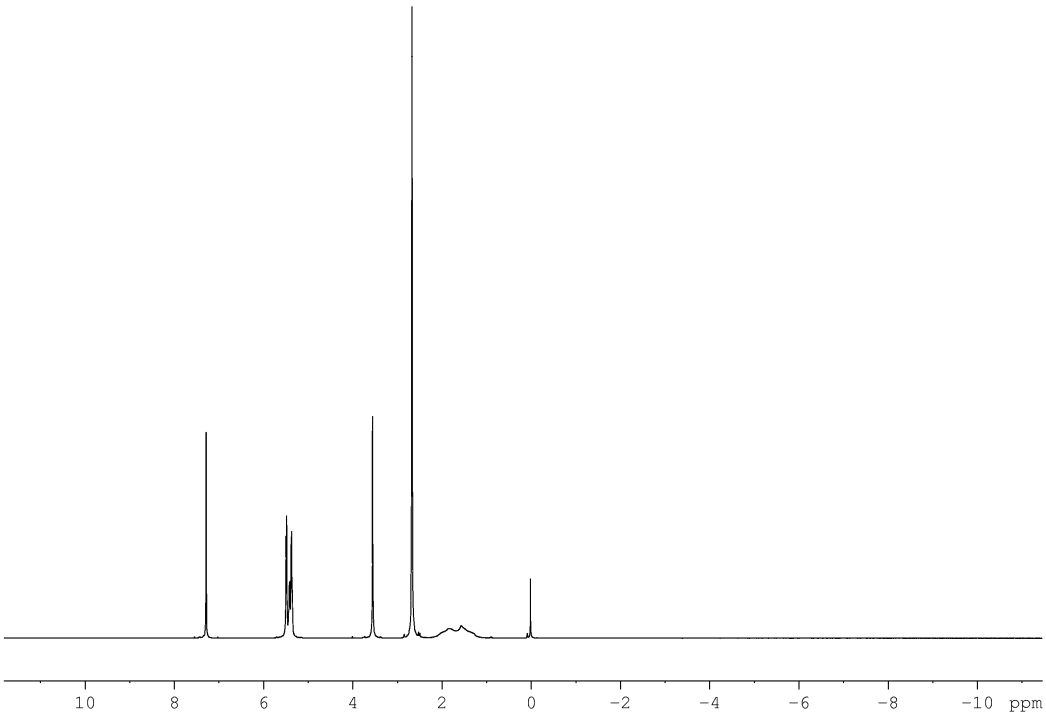

Figure S1. ^{1}H NMR spectrum ($CDCl_3$, 293 K) of (η^6-$C_6H_5CH_2NMe_2{\cdot}BH_3$)$Cr(CO)_3$ (**2**)

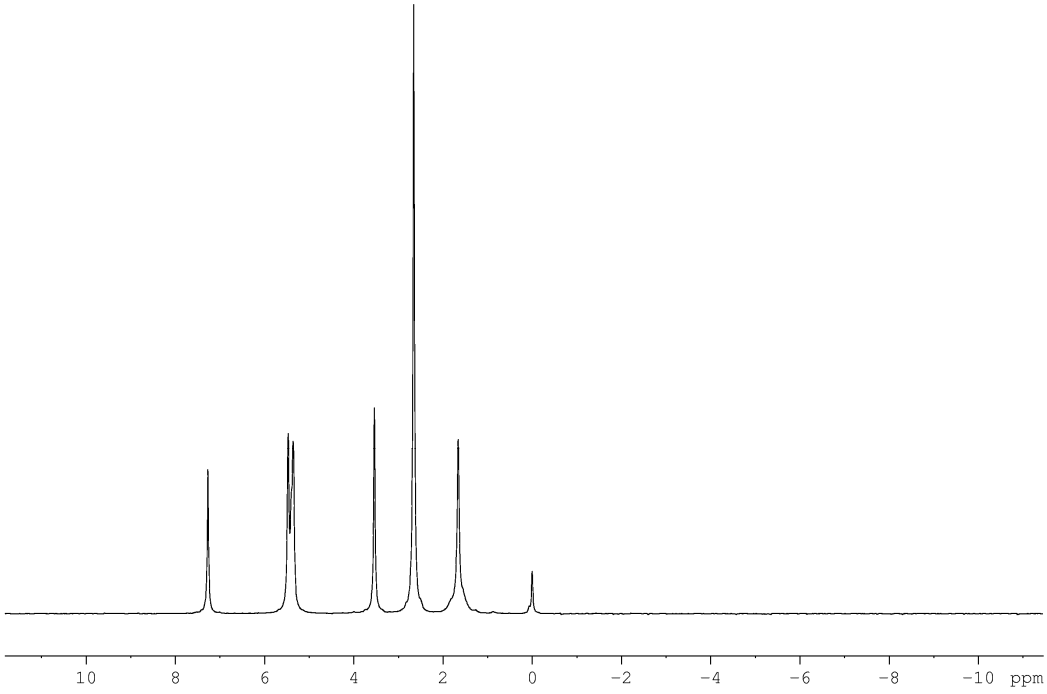

Figure S2. $^{1}H\{^{11}B\}$ NMR spectrum($CDCl_3$, 293 K) of (η^6-$C_6H_5CH_2NMe_2 \cdot BH_3$)$Cr(CO)_3$ (**2**)

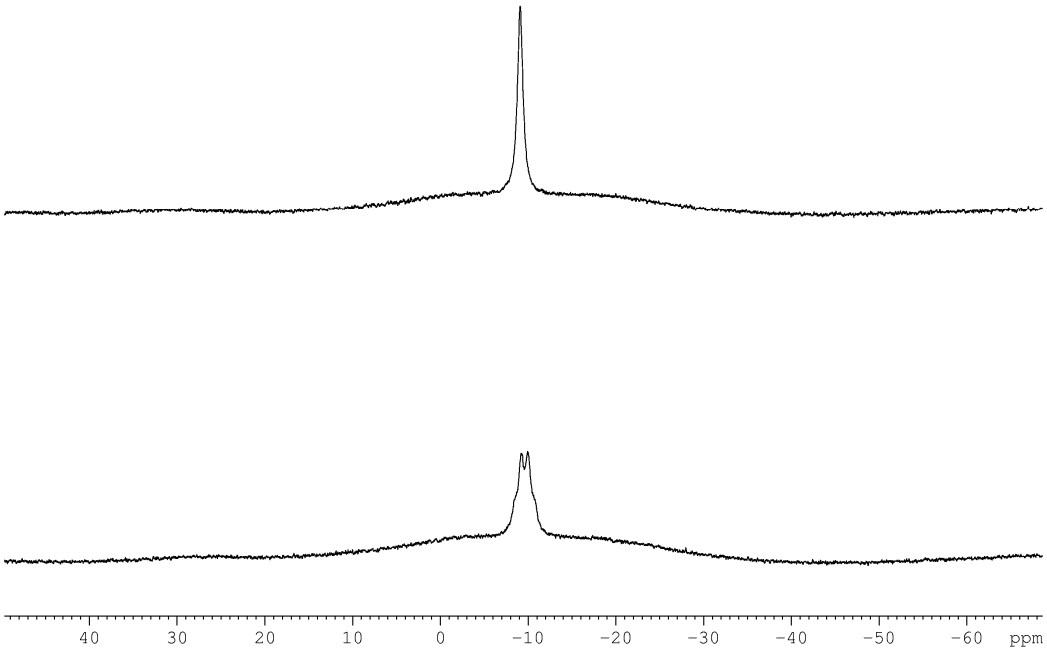

Figure S3. ^{11}B (bottom) and $^{11}B\{^{1}H\}$ (top) NMR spectra ($CDCl_3$, 293 K) of (η^6-$C_6H_5CH_2NMe_2{\cdot}BH_3$)$Cr(CO)_3$ (**2**)

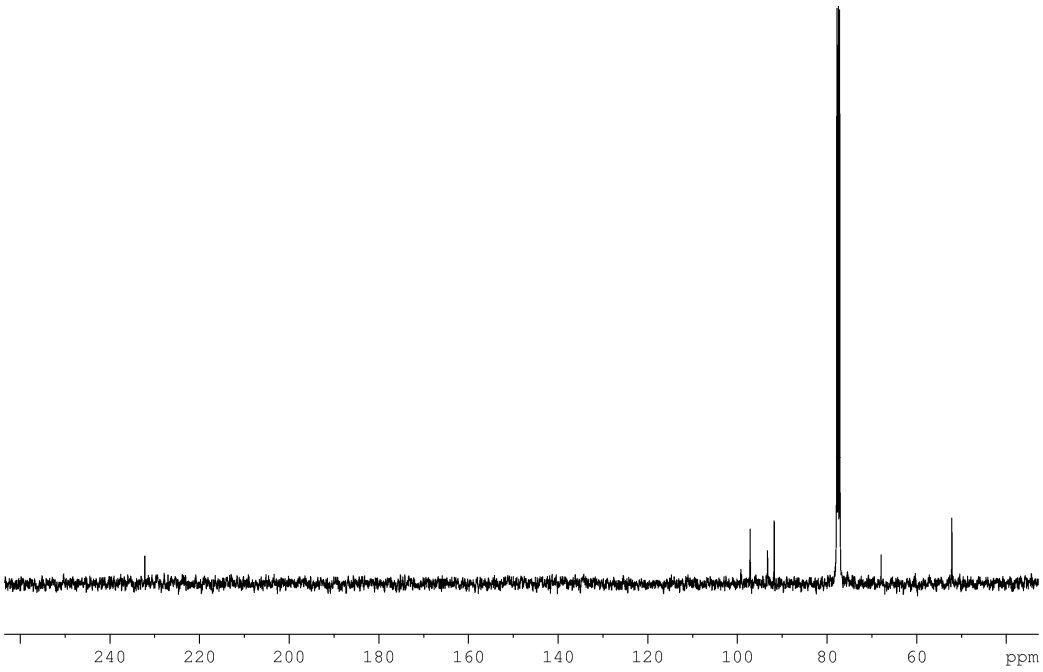

Figure S4. ^{13}C NMR spectrum ($CDCl_3$, 293 K) of (η^6-$C_6H_5CH_2NMe_2 \cdot BH_3$)$Cr(CO)_3$ (**2**)

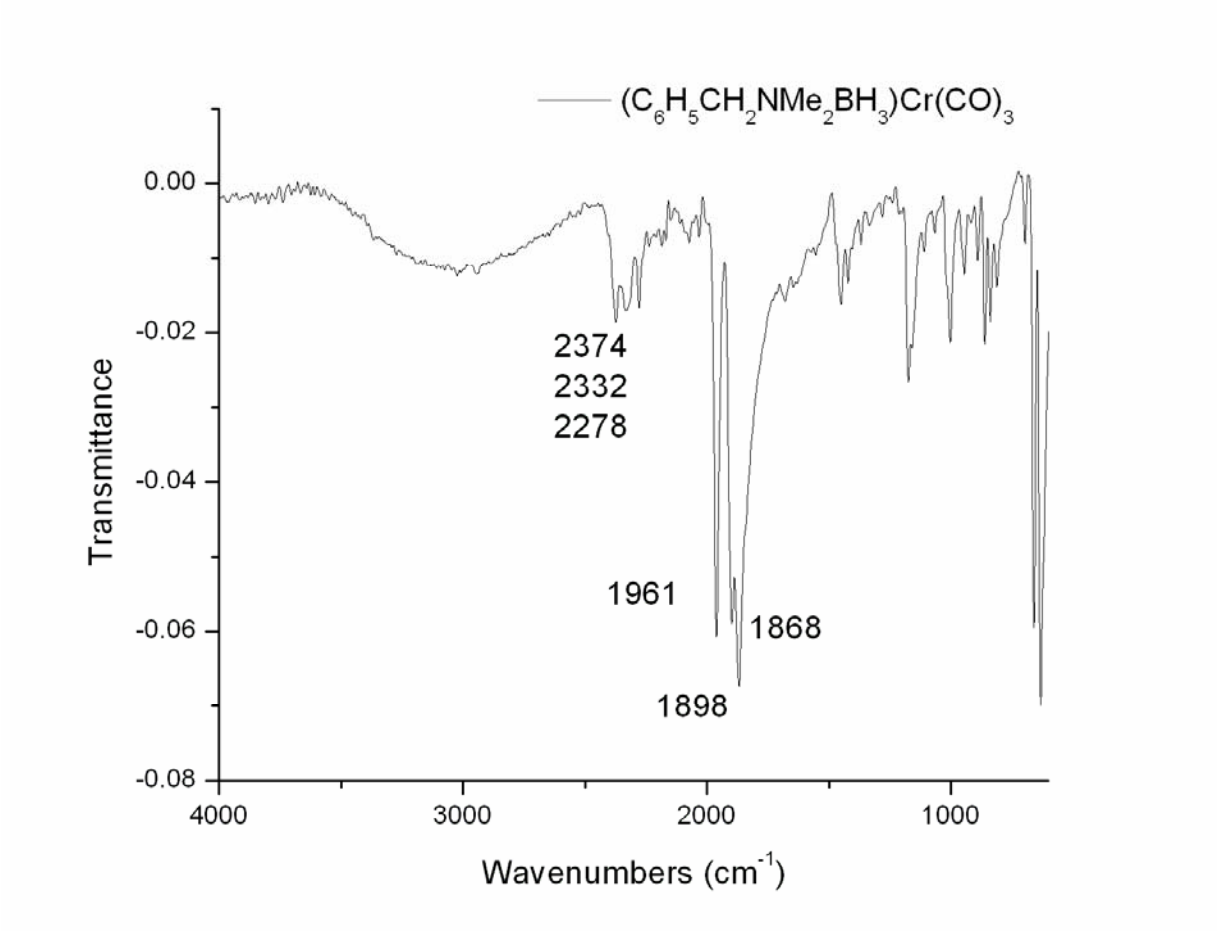

Figure S5. IR spectrum of (η^6-$C_6H_5CH_2NMe_2 \cdot BH_3$)$Cr(CO)_3$ (**2**)

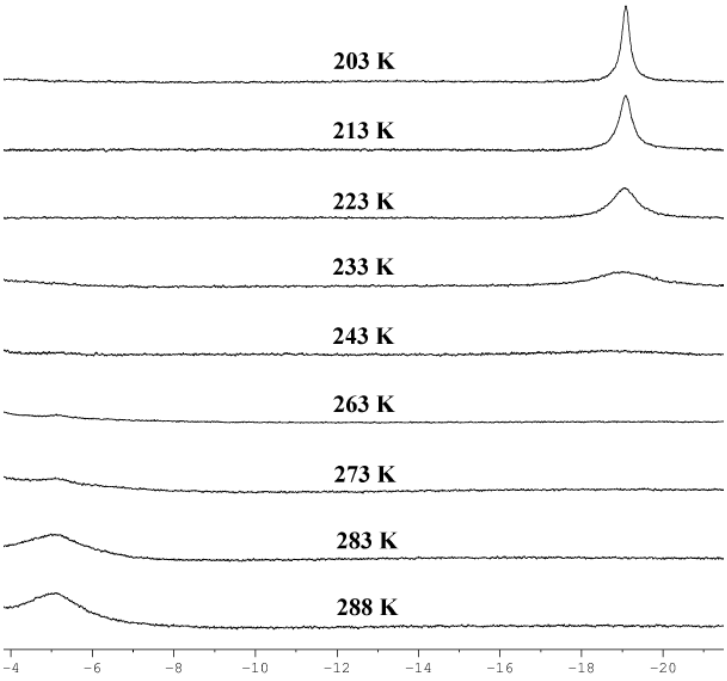

Figure S6. VT ^{1}H NMR spectral stack plot of the σ-borane region of (η^{1}-(η^{6}-$C_6H_5CH_2NMe_2{\cdot}BH_2$–H))$Cr(CO)_2$ (**3**) in toluene-d_8

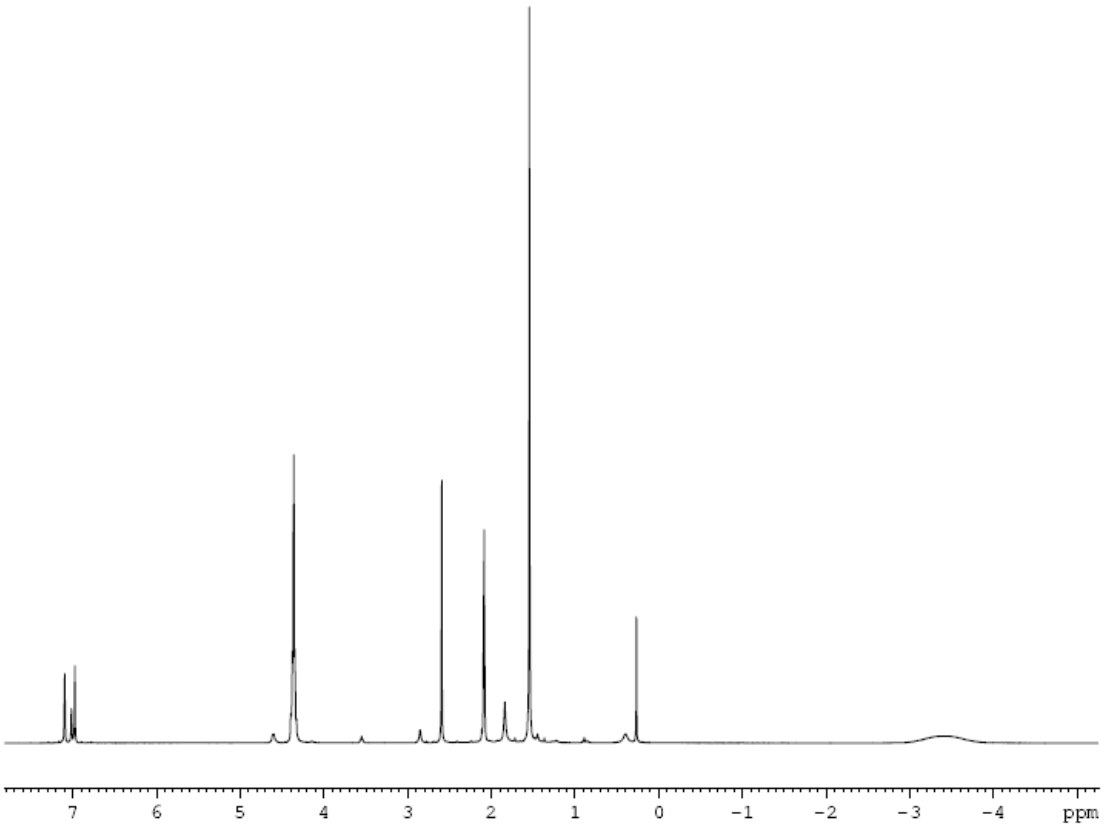

Figure S7. ^{1}H NMR spectrum (toluene-d_8, 288 K) of (η^6-$C_6H_5CH_2NMe_2 \cdot BH_2HCr(CO)_5$)$Cr(CO)_3$ (**4**)

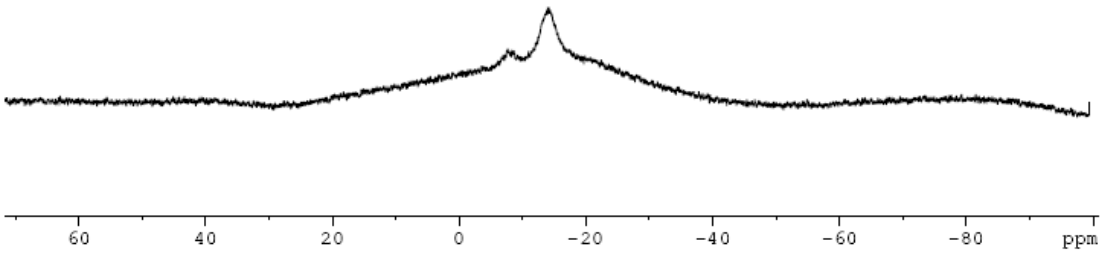

Figure S8. ^{11}B NMR spectrum (toluene-d_8, 288 K) of (η^6-$C_6H_5CH_2NMe_2 \cdot BH_2HCr(CO)_5)Cr(CO)_3$ (**4**)

^{13}C NMR spectrum of 4

In the ^{13}C NMR spectrum of the σ-borane complex **4**, recorded at 263 K, two carbonyl signals at δ 216 ppm and δ 224 ppm were assigned to the *cis*- and *trans*-*C*O ligands respectively, of the Cr(*C*O)$_5$ unit. The –N*Me*$_2$ group appears at δ 50.3 ppm which was upfield shifted from that of the starting complex **2**. The –*C*H$_2$– group appears at δ 67.1 ppm. In the ^{11}B NMR spectrum of the σ-borane complex **4**, the presence of a broad signal at δ –14.9 ppm, which is about 6 ppm upfield shifted from that of the starting complex **2**, fulfils the typical ^{11}B NMR spectral characteristics of a σ-borane complex.

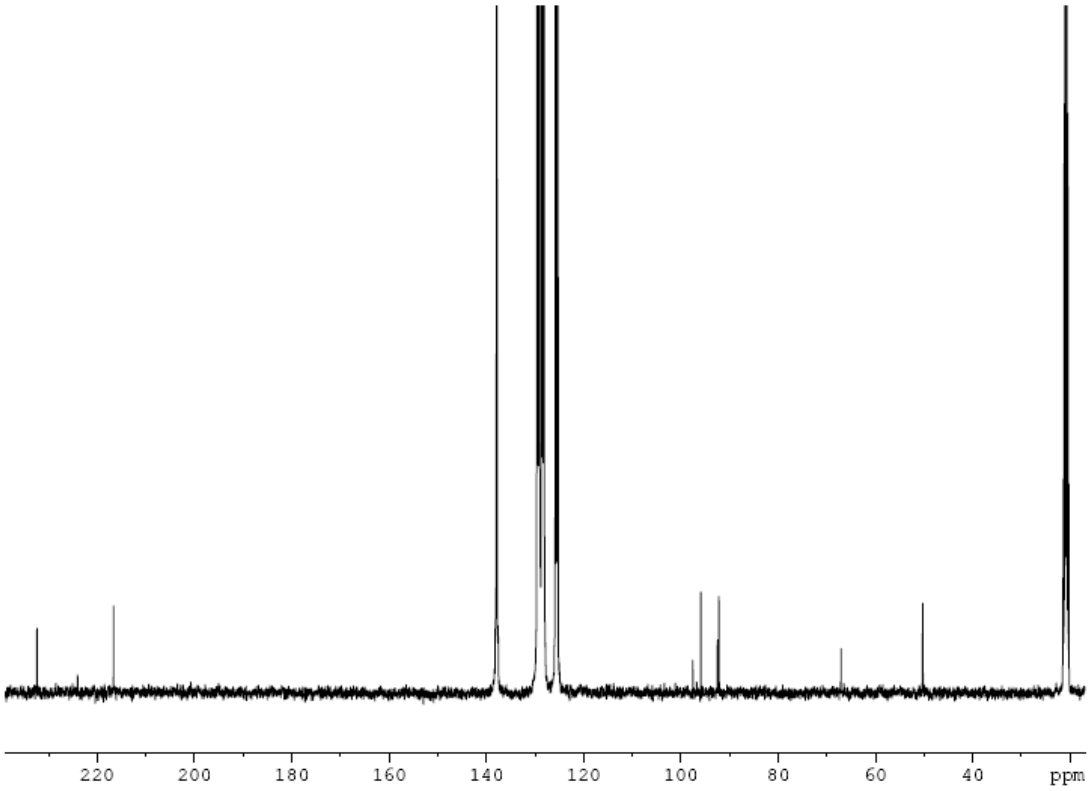

Figure S9. ^{13}C NMR spectrum (toluene-d_8, 288 K) of (η^6-$C_6H_5CH_2NMe_2{\cdot}BH_2HCr(CO)_5$)$Cr(CO)_3$ (**4**)

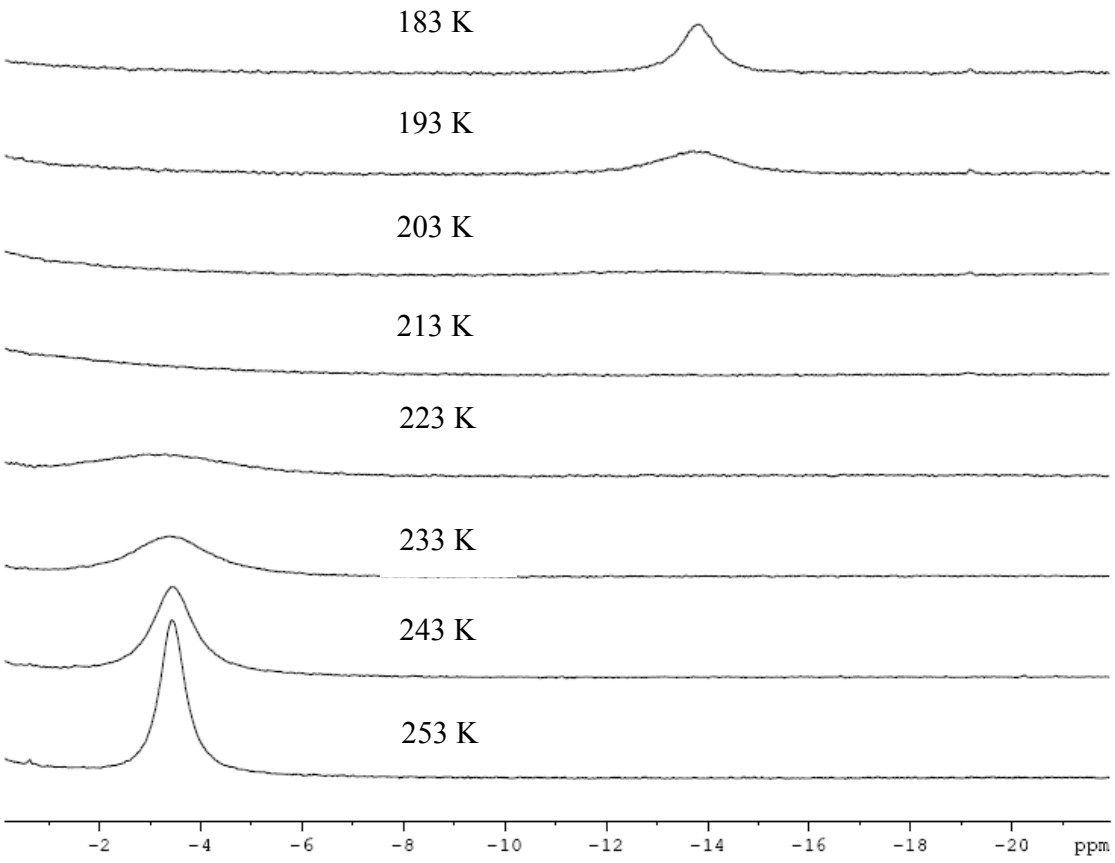

Figure S10. Variable temperature ^{1}H NMR spectral stack plot (toluene-d_8) (high field region) of (η^6-$C_6H_5CH_2NMe_2 \cdot BH_2HCr(CO)_5$)$Cr(CO)_3$ (**4**)

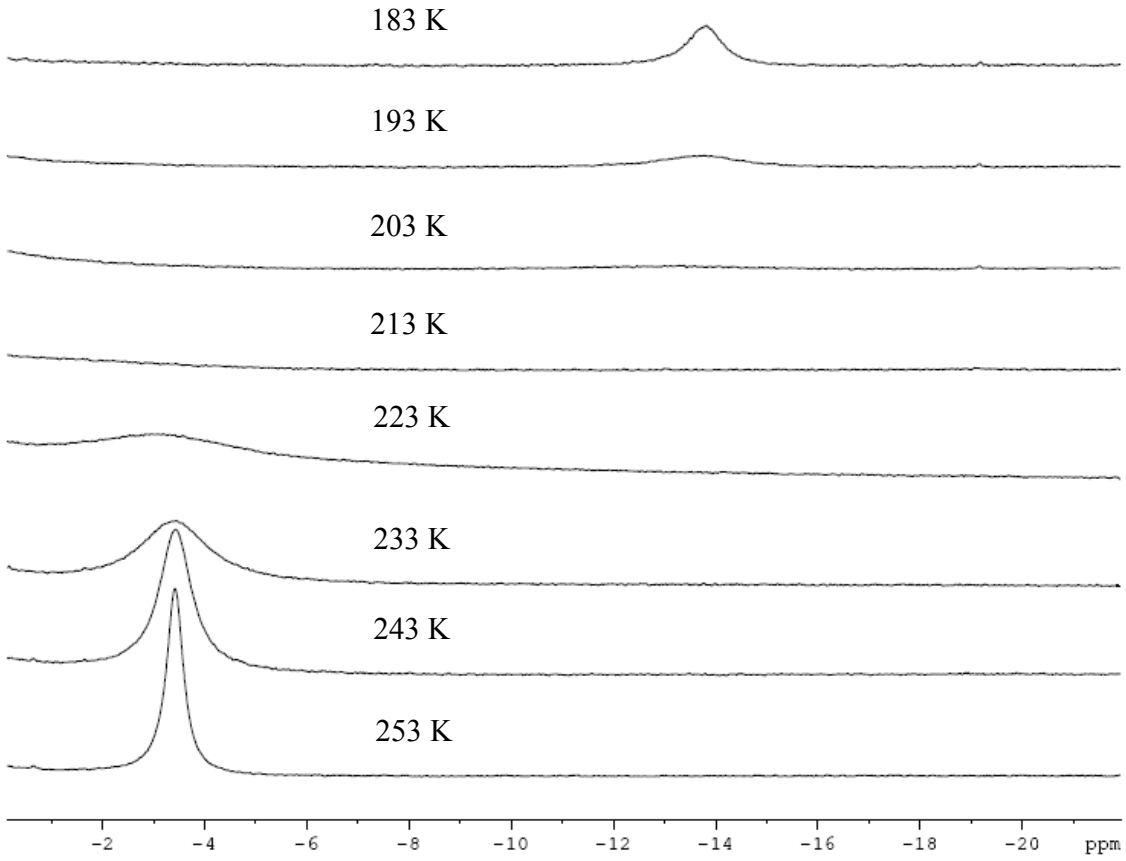

Figure S11. VT $^{1}H\{^{11}B\}$ NMR spectral stack plot (toluene-d_8) (high field region) of (η^6-$C_6H_5CH_2NMe_2 \cdot BH_2HCr(CO)_5)Cr(CO)_3$ (**4**)

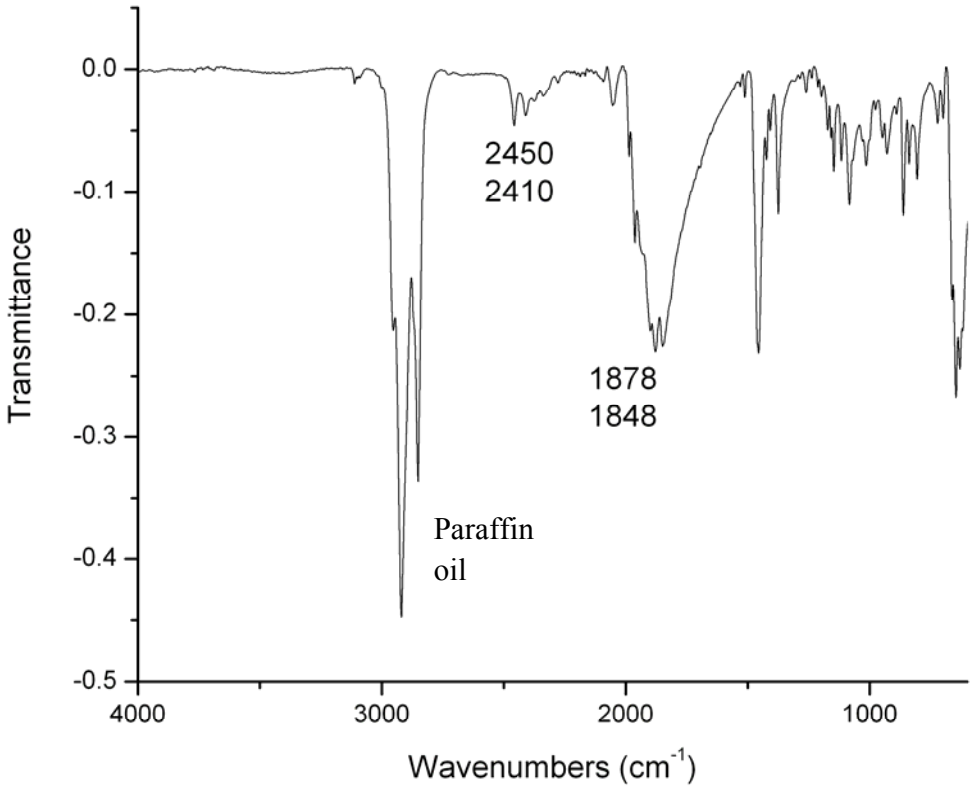

Figure S12. IR spectrum of (η^6-$C_6H_5CH_2NMe_2 \cdot BH_2HCr(CO)_5$)$Cr(CO)_3$ (**4**)

Table S1. List of Cr–H bond lengths (Å) and Cr–H–B bond angles (°) of σ-borane complexes of chromium(0) reported to date

Complex	Cr–H Length (Å)	Angle (Cr–H–B) (°)
$[HCr(CO)_5][PPh_4]$[1]	1.66(5)	
$(OC)_5Cr(\eta^1\text{-}B_2H_4\cdot 2PMe_3)$[2]	1.76(8)	141(8)
$(OC)_5Cr(\eta^1\text{-}HBHPh\cdot PMe_3)$[3]	1.77(2)	133(2)
$(OC)_5Cr(\eta^1\text{-}HBHMe\cdot PMe_3)$[3]	1.78(3)	138.4(16)
$(OC)_4Cr(\eta^1\text{-}HBH_2\cdot dppm)$[4]	1.78(3)	136(3)
$(OC)_5Cr(\eta^1\text{-}HBH_2\cdot NMe_3)$[5]	1.83	158
$(OC)_5Cr(\eta^1\text{-}HBH_2\cdot PMe_3)$[5]	1.94(10)	130(8)
$(OC)_3Cr(HC_6H_{10}PCy_2)(PCy_3)$[6]	2.240(1)	

References

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