Formation and Structures of Hafnocene Complexes in MAO and $AlBu^{i}_{3}/[CPh_3][B(C_6F_5)_4]$ Activated Systems

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Supporting Information

(SBI)HfMeCl:

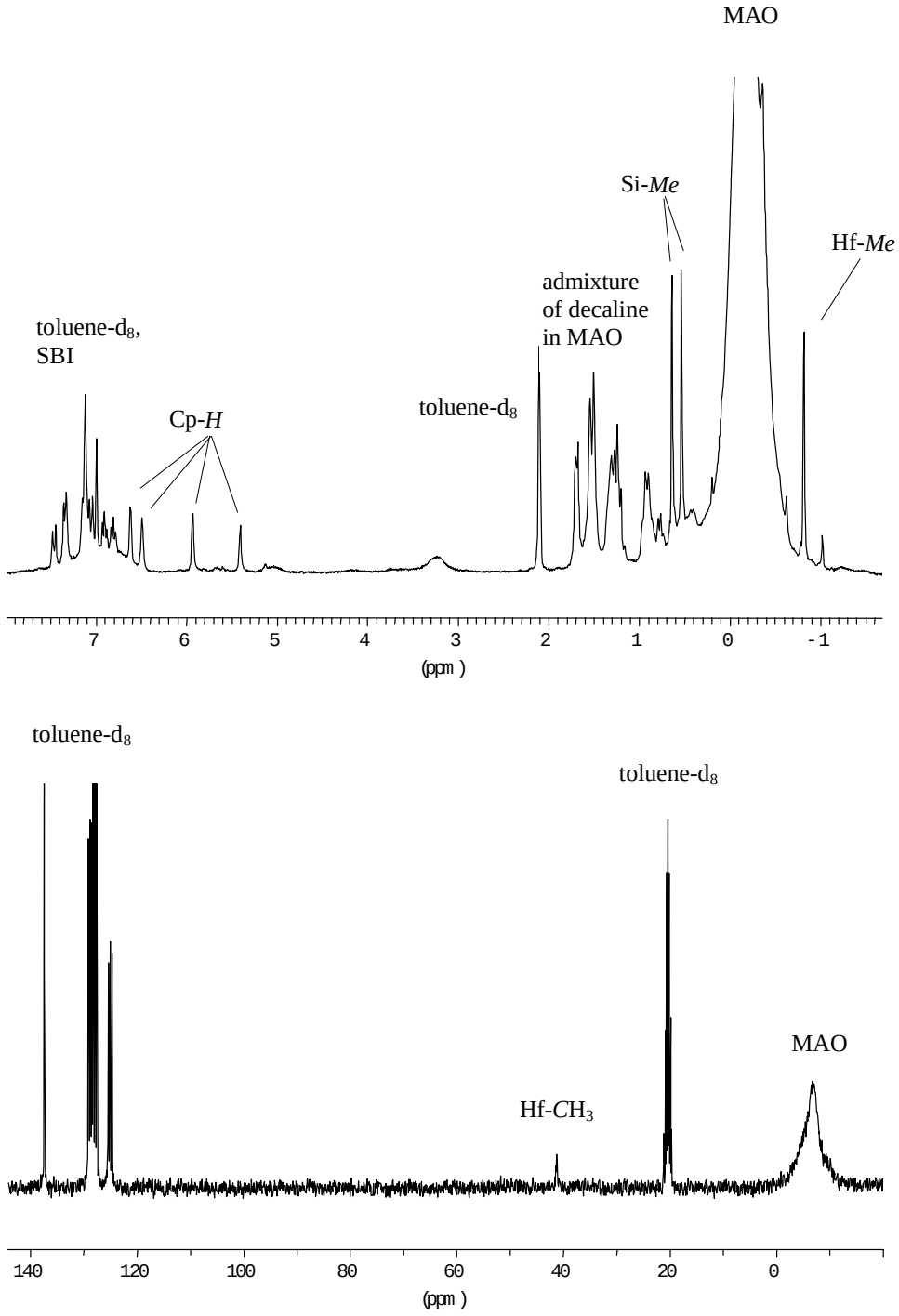


Figure S1. Upper trace: ^{1}H NMR spectrum (toluene-d_8, 20 °C) of the system **1** + MAO-^{13}C (Al:Ti = 30). Lower trace: ^{13}C NMR spectrum of the same system (toluene-d_8, 20 °C) with selective ^{1}H decoupling centered at δ –0.82.

[(SBI)Hf(μ-Me)$_2$AlMe$_2$][MeMAO] (5-MAO):

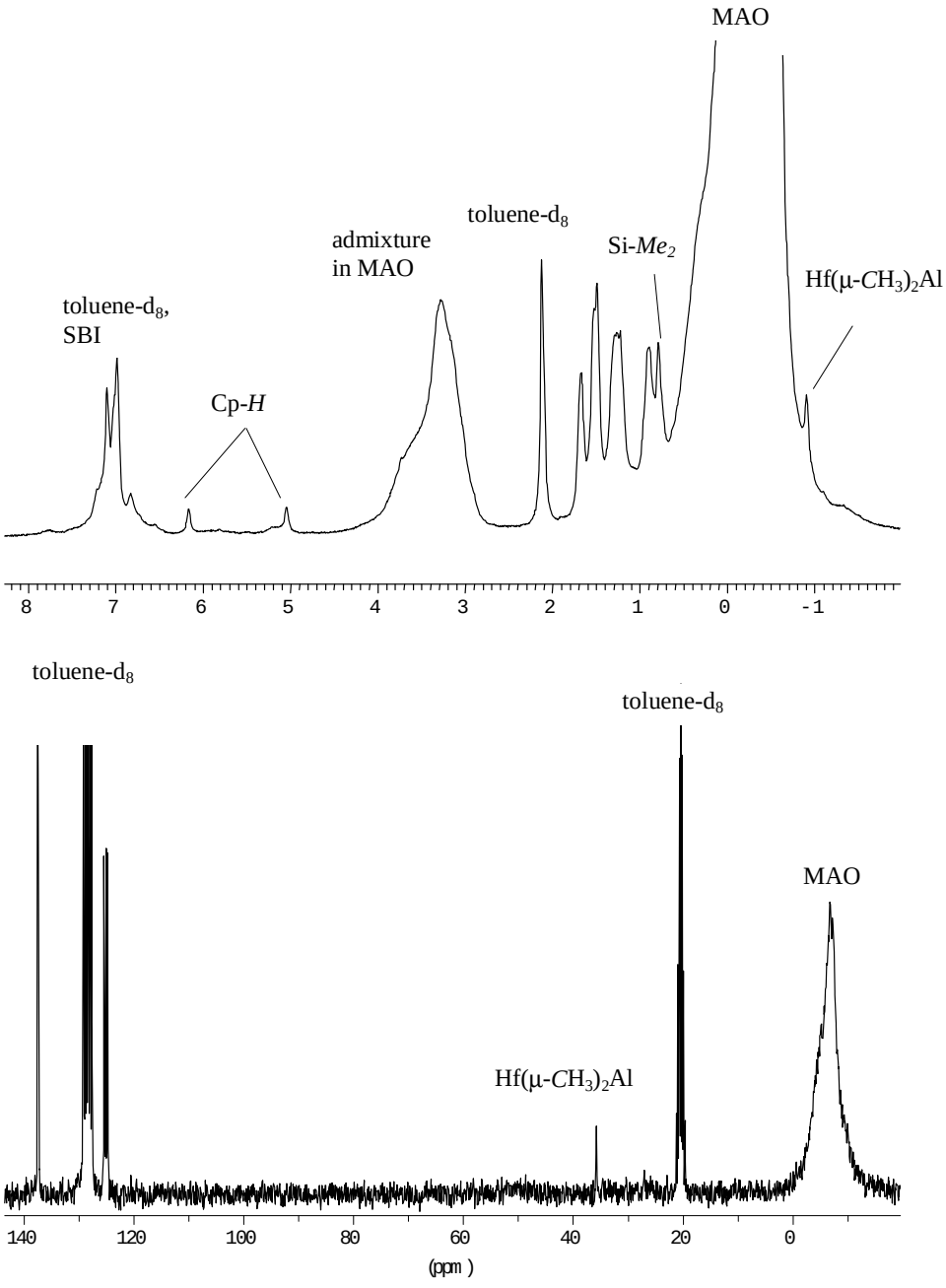


Figure S2. Upper trace: ^{1}H NMR spectrum (toluene-d$_8$, 20 °C) of the system **1** + MAO-^{13}C (Al:Ti = 240).
Lower trace: ^{13}C NMR spectrum of the same system (toluene-d$_8$, 20 °C) with selective ^{1}H decoupling centered at δ –0.91.

[(SBI)Hf(μ-Me)$_2$AlMe$_2$][B(C$_6$F$_5$)$_4$] (5-BX$_4$):

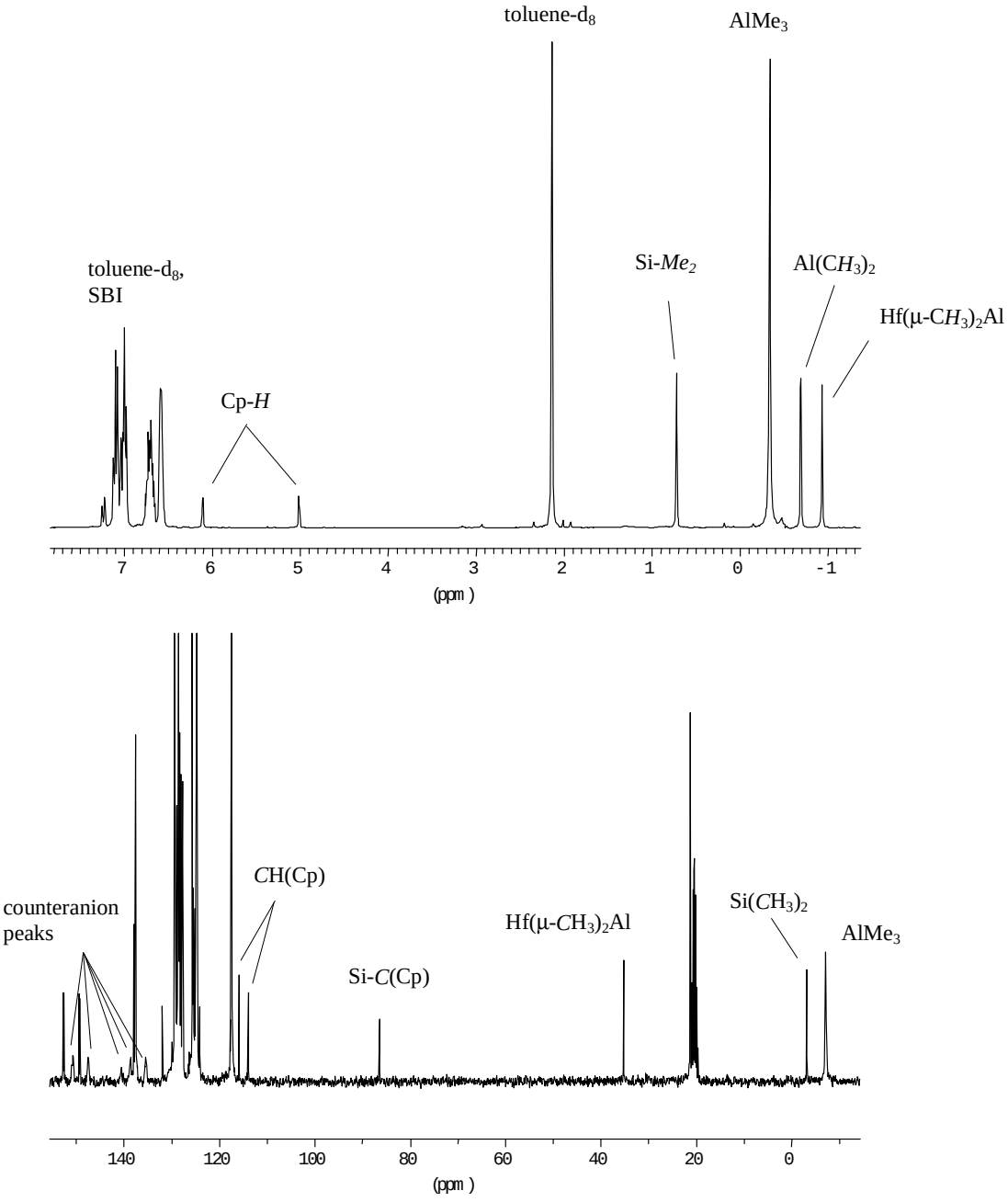


Figure S3. Upper trace: ^{1}H NMR spectrum (toluene-d$_8$/1,2-difluorobenzene, 20 °C) of the system **1** + AlMe$_3$ + CPh$_3$B(C$_6$F$_5$)$_4$, Hf:Al:B = 1:50:1.1 (oily phase + toluene-d$_8$/1,2-difluorobenzene). Lower trace: ^{13}C{^{1}H} NMR spectrum of the same system (toluene-d$_8$/1,2-difluorobenzene, 20 °C).

[$Ph_2C(Cp)(Flu)Hf(\mu\text{-}Me)_2AlMe_2][B(C_6F_5)_4]$ (7-BX_4):

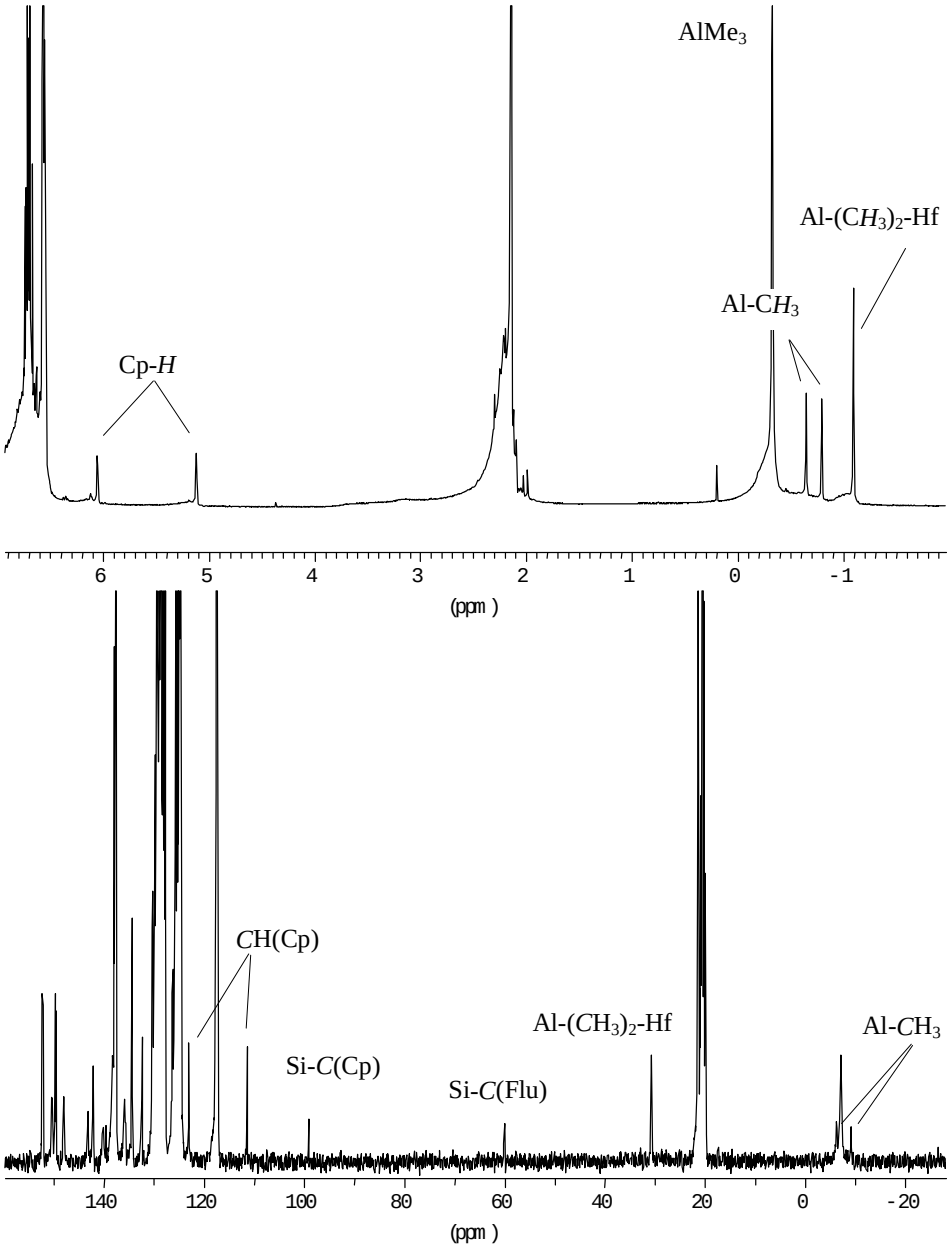


Figure S4. Upper trace: ^{1}H NMR spectrum (toluene-d_8/1,2-difluorobenzene, 20 °C) of the system **3** + $AlMe_3$ + $CPh_3B(C_6F_5)_4$, Hf:Al:B = 1:50:1.1, (oily phase + toluene-d_8/1,2-difluorobenzene). Lower trace: $^{13}C\{^{1}H\}$ NMR spectrum of the same system (toluene-d_8/1,2-difluorobenzene, 20 °C).

[(SBI)Hf(μ-H)$_2$Al(H)(*i*-Bu)]$^+$[B(C$_6$F$_5$)$_4$]$^-$ (9):

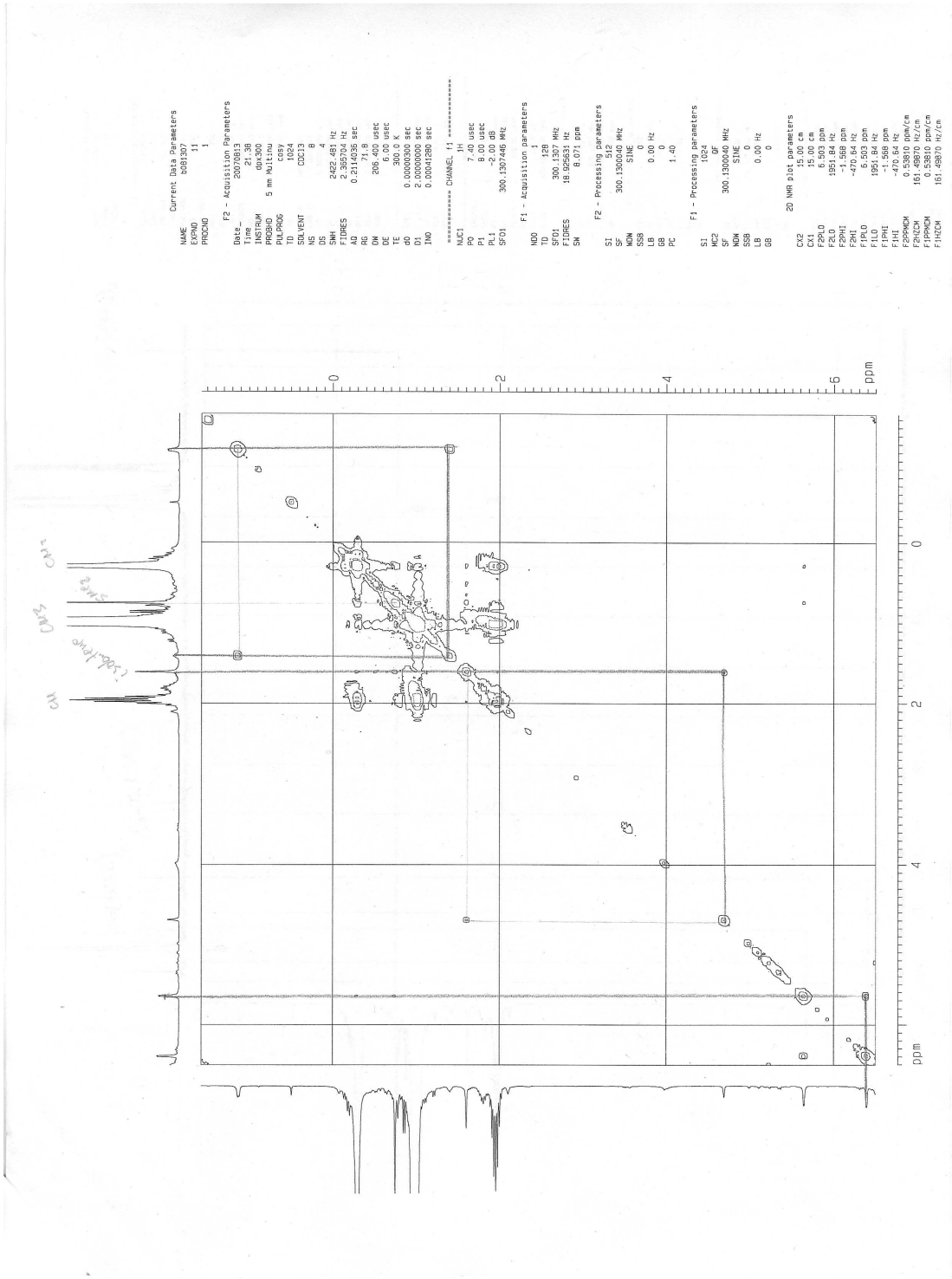


Figure S5. ^{1}H COSY NMR spectrum (toluene-d$_8$/1,2-difluorobenzene, 20 °C) of the system **1** + Al(*i*-Bu)$_3$ + CPh$_3$B(C$_6$F$_5$)$_4$, Hf:Al:B = 1:50:1.1, (oily phase + toluene-d$_8$/1,2-difluorobenzene).

[(SBI)Hf(μ-H)$_2$Al(H)(*i*-Bu)]$^+$[B(C$_6$F$_5$)$_4$]$^-$ (9):

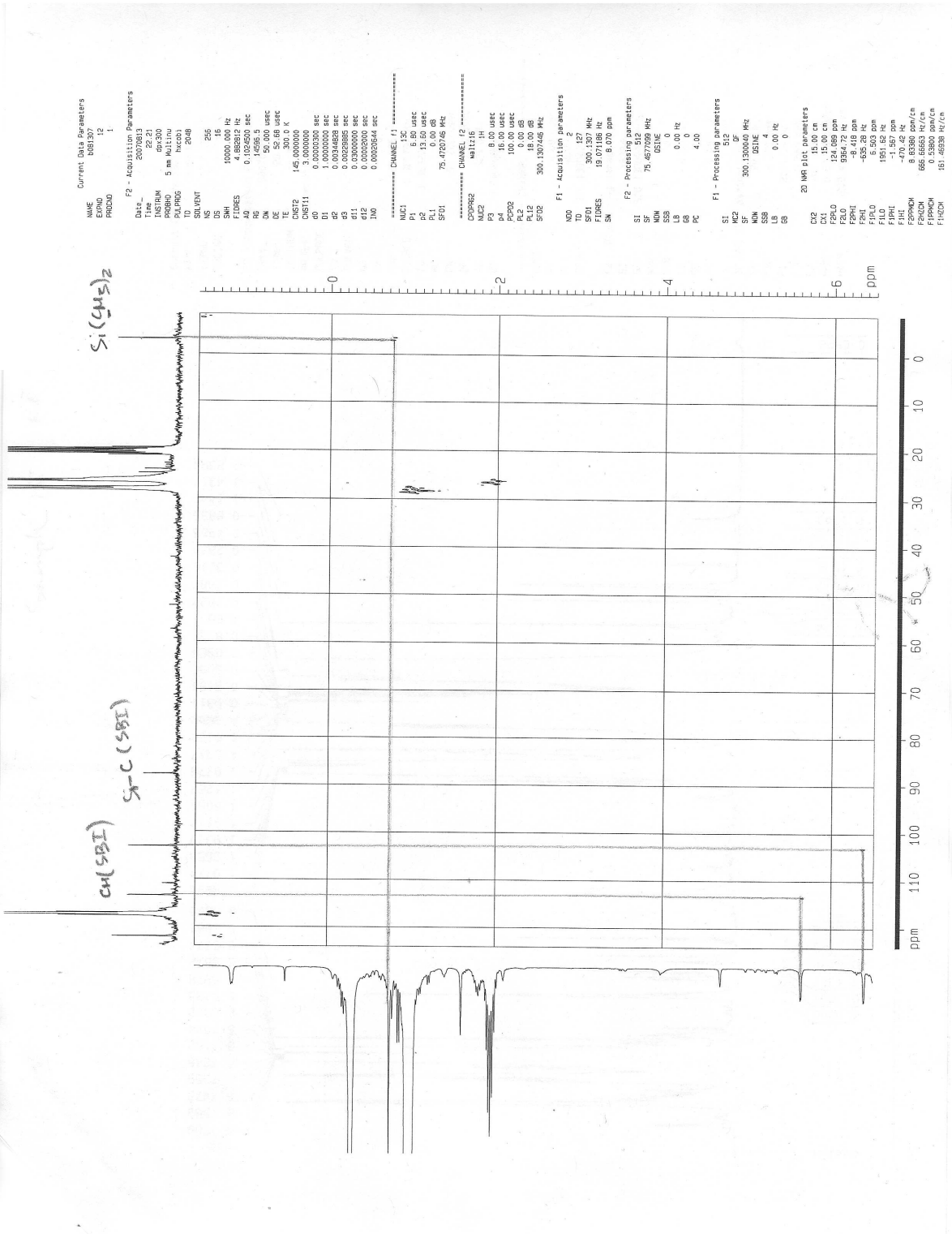
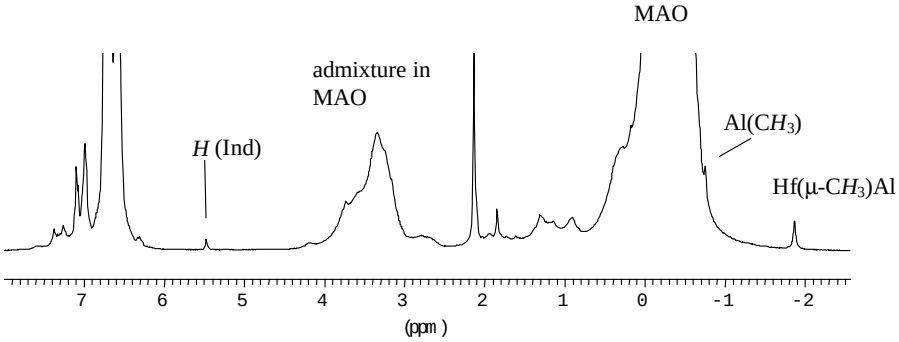


Figure S6. ^{1}H,^{13}C-correlated NMR spectrum (toluene-d$_8$/1,2-difluorobenzene, 20 °C) of the system **1** + Al(*i*-Bu)$_3$ + CPh$_3$B(C$_6$F$_5$)$_4$, Hf:Al:B = 1:50:1.1, (oily phase + toluene-d$_8$/1,2-difluorobenzene).

[C_2H_4(Flu)(5,6-C_3H_6-2-MeInd)Hf(μ-Me)$_2$AlMe$_2$][MeMAO] (11-MAO):



[C_2H_4(Flu)(5,6-C_3H_6-2-MeInd)Hf(μ-Me)$_2$AlMe$_2$]$^+$[B(C_6F_5)$_4$]$^-$ (11-BX_4):

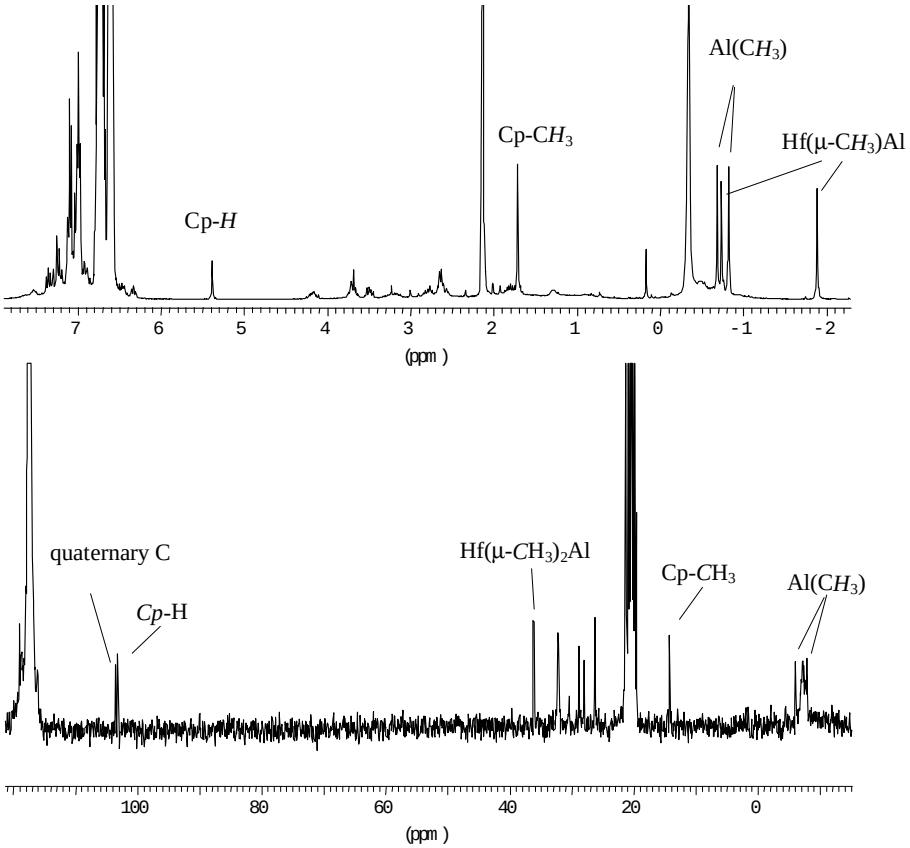


Figure S7. Upper trace: ^{1}H NMR spectrum (toluene-d_8/1,2-difluorobenzene, 20 °C) of the system **4** + MAO (Al:Hf = 140).
Middle trace: ^{1}H NMR spectrum (toluene-d_8/1,2-difluorobenzene, 20 °C) of the system **3** + $AlMe_3$ + $CPh_3B(C_6F_5)_4$, Hf:Al:B = 1:50:1.1, (oily phase + toluene-d_8/1,2-difluorobenzene).
Lower trace: $^{13}C\{^1H\}$ NMR spectrum of the system in the middle trace (toluene-d_8/1,2-difluorobenzene, 20 °C).

$[C_2H_4(Flu)(5,6\text{-}C_3H_6\text{-}2\text{-}MeInd)Hf(\mu\text{-}Me)_2AlMe_2]^+[B(C_6F_5)_4]^-$ (8-BX_4).

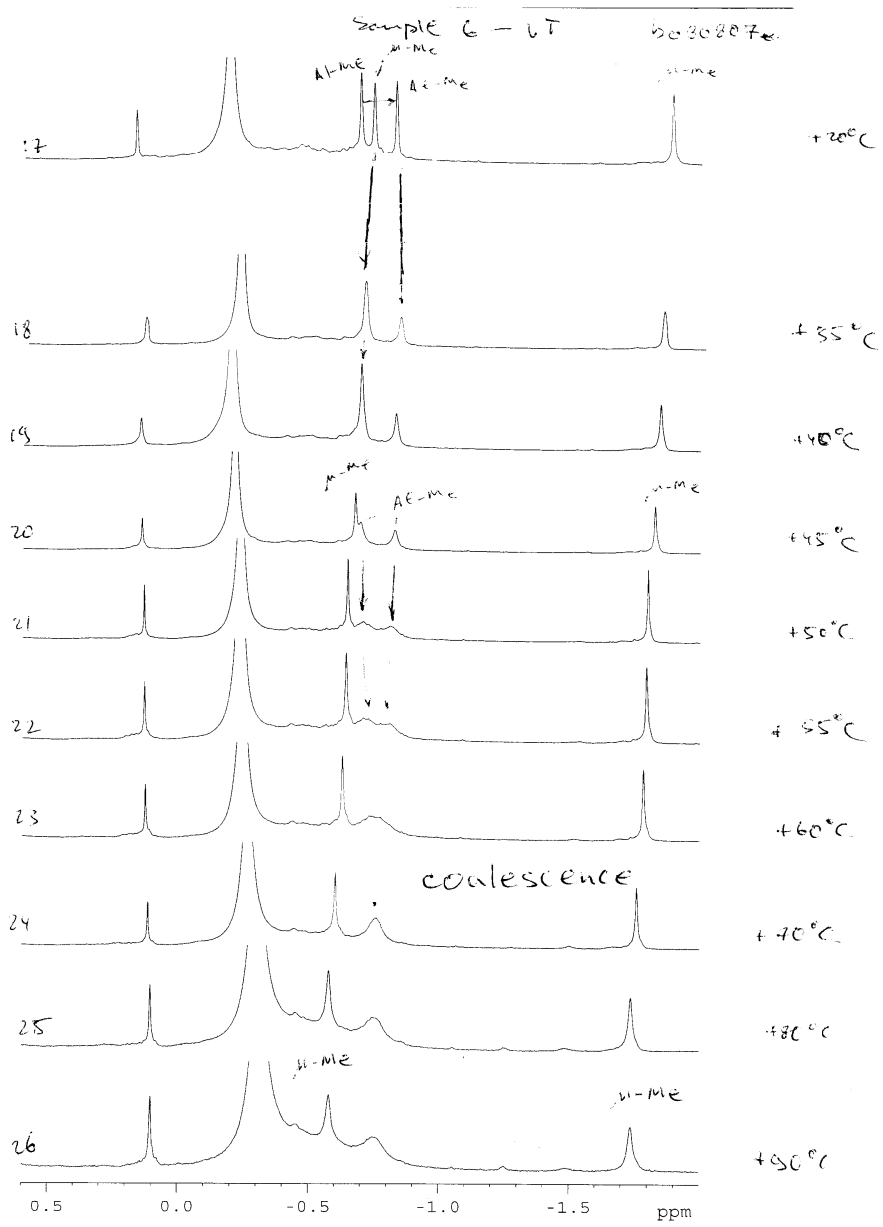


Figure S8. ^{1}H NMR spectra of the system **4** + $AlMe_3$ + $CPh_3B(C_6F_5)_4$, Hf:Al:B = 1:50:1.1, (oily phase + toluene-d_8/1,2-difluorobenzene) at differing temperatures. Signals of terminal $AlMe_3$ groups merge at +70 °C.

[$Ph_2C(Cp)(Flu)Hf(\mu\text{-}Cl)_2Hf(Flu)(Cp)SiPh_2$]·2[$B(C_6F_5)_4$]:

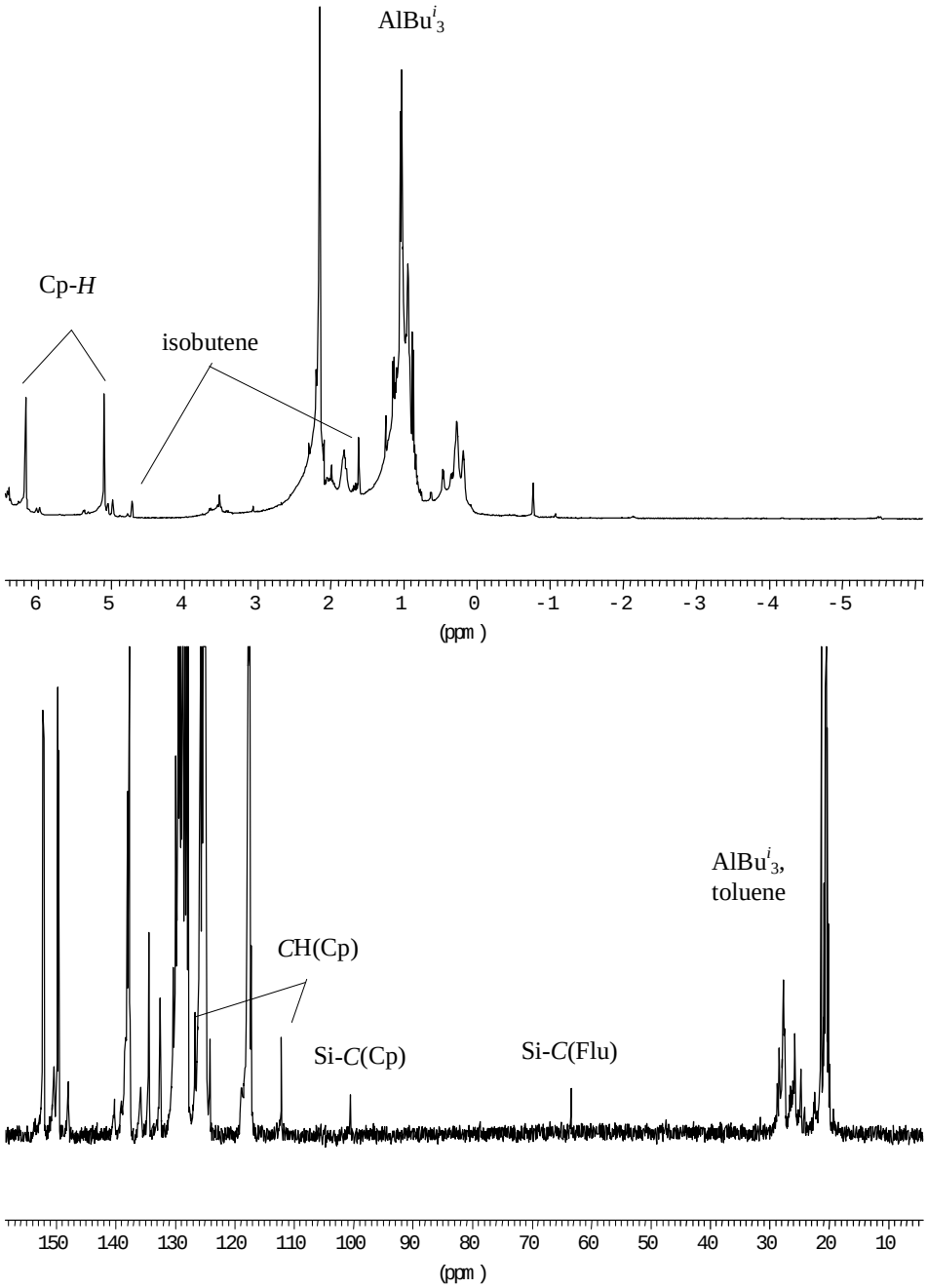


Figure S9. Upper trace: ^{1}H NMR spectrum (toluene-d_8/1,2-difluorobenzene, 2 °C) of the system **3** + Al(*i*-Bu)$_3$ + $CPh_3B(C_6F_5)_4$, Hf:Al:B = 1:25:1.1, 10 min stirring at 0 °C (oily phase + toluene-d_8/1,2-difluorobenzene).
Lower trace: $^{13}C\{^1H\}$ NMR spectrum of the same system (toluene-d_8/1,2-difluorobenzene, 2 °C).

[$Ph_2C(Cp)(Flu)Hf(\mu\text{-}Cl)_2Hf(Flu)(Cp)SiPh_2$]·2[$B(C_6F_5)_4$]:

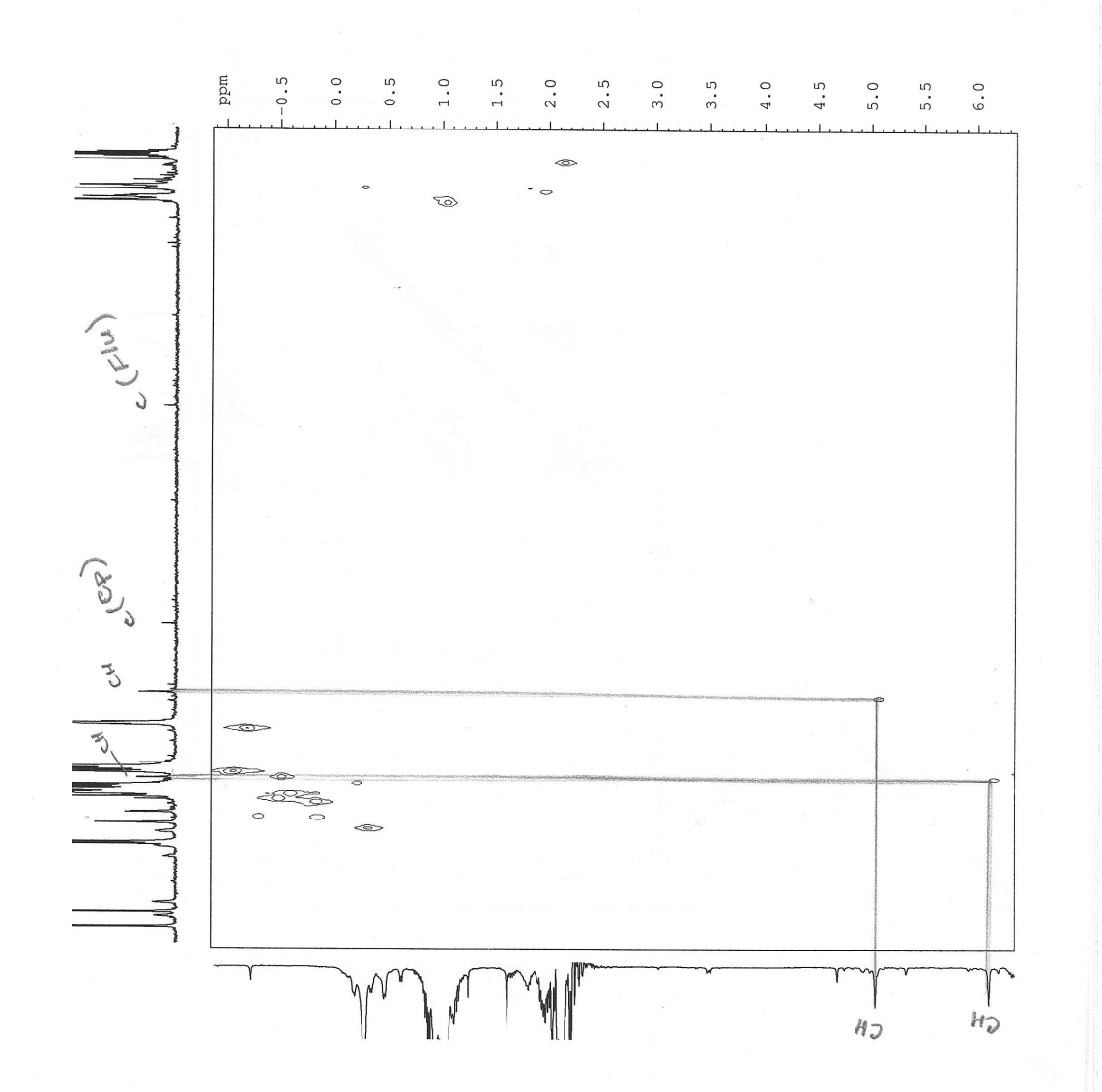


Figure S10. $^{1}H,^{13}C$-correlated NMR spectrum (toluene-d_8/1,2-difluorobenzene, 2 °C) of the system **2** + Al(*i*-Bu)$_3$ + $CPh_3B(C_6F_5)_4$, Hf:Al:B = 1:25:1.1, 10 min stirring at 0 °C (oily phase + toluene-d_8/1,2-difluorobenzene).

System **2** + Al(*i*-Bu)$_3$ + CPh$_3$B(C$_6$F$_5$)$_4$: species **a** and **b**:

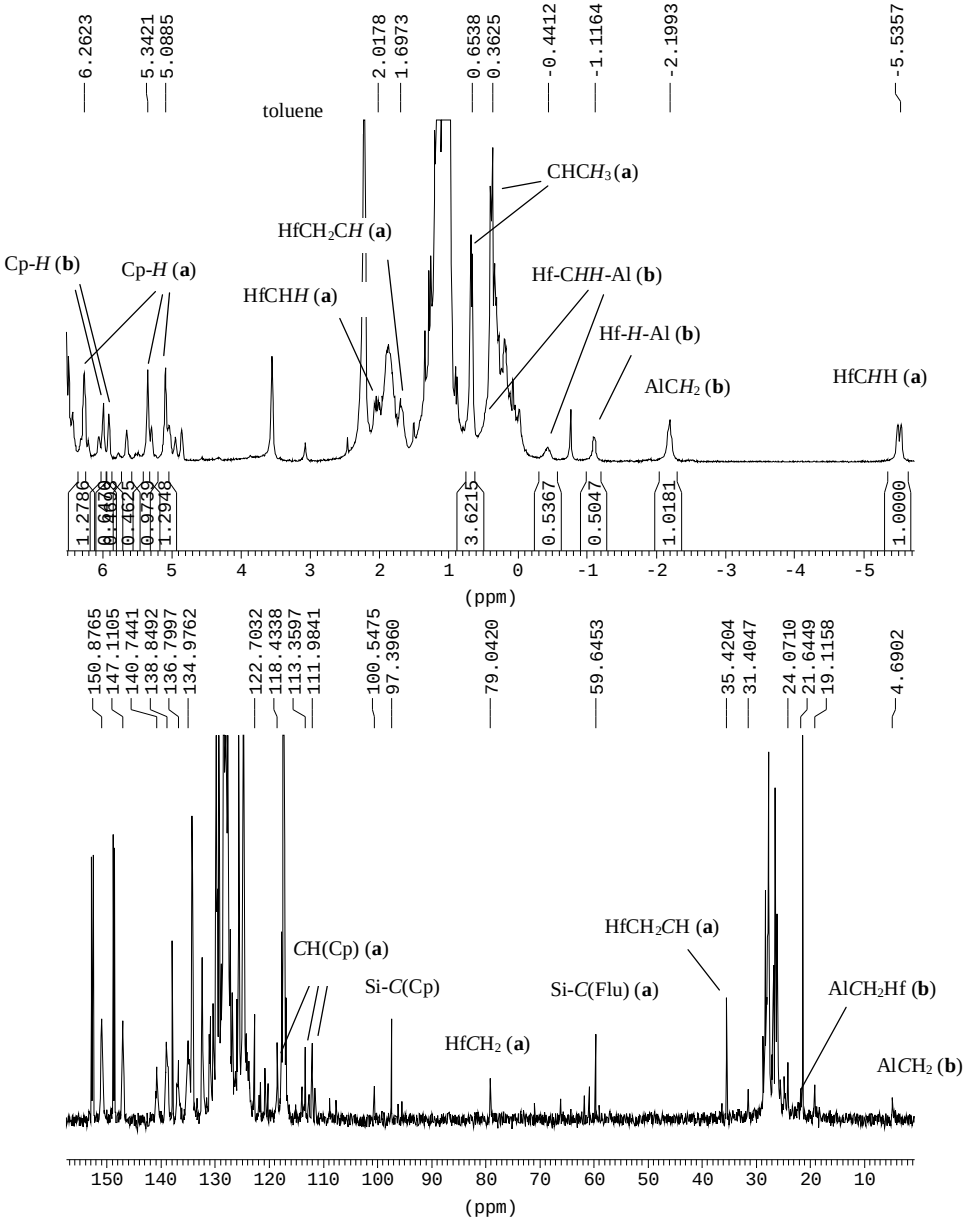


Figure S11. Upper trace: ^{1}H NMR spectrum (benzene-d$_6$/1,2-difluorobenzene, 2 °C) of the system **2** + Al(*i*-Bu)$_3$ + CPh$_3$B(C$_6$F$_5$)$_4$, Hf:Al:B = 1:25:1.1, 1h stirring at room temperature (oily phase washed with benzene-d$_6$ + benzene-d$_6$/1,2-difluorobenzene).
Lower trace: ^{13}C{^{1}H} NMR spectrum of the same system (benzene-d$_6$/1,2-difluorobenzene, 2 °C).

System **2** + Al(*i*-Bu)$_3$ + CPh$_3$B(C$_6$F$_5$)$_4$: species **a** and **b**:

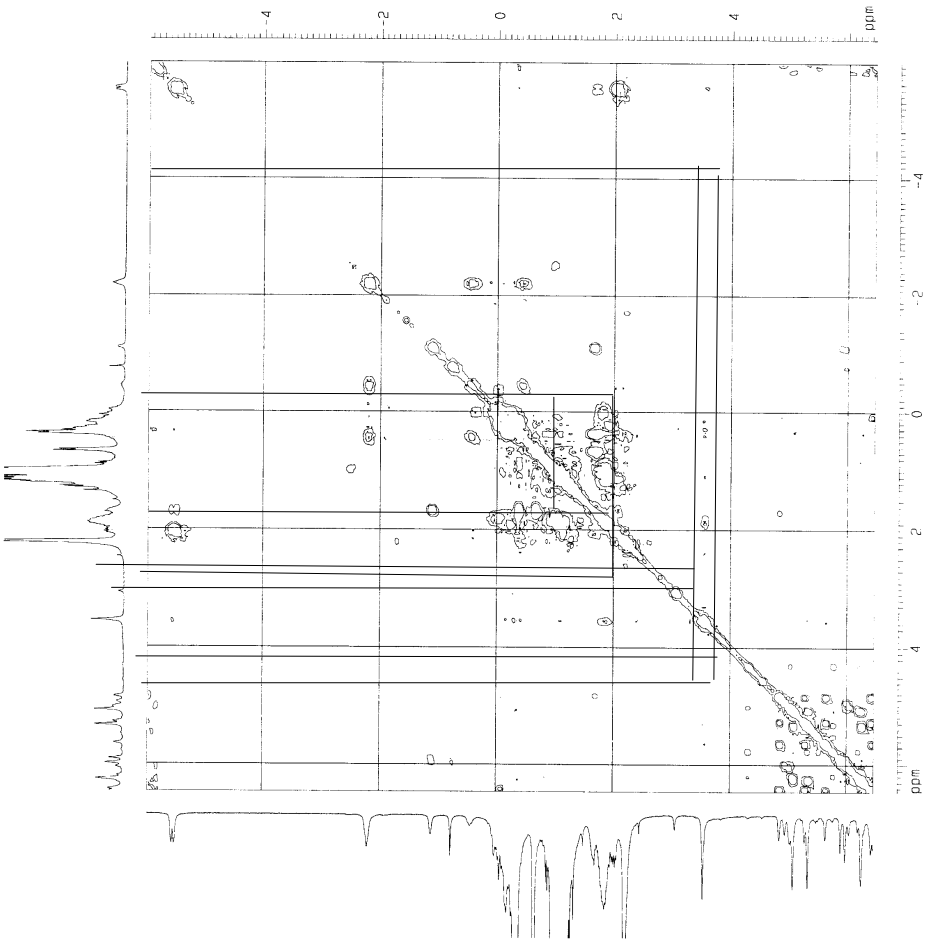


Figure S12. ^{1}H COSY NMR spectrum (benzene-d$_6$/1,2-difluorobenzene, 2 °C) of the system **2** + AlBu$^i_3$ + CPh$_3$B(C$_6$F$_5$)$_4$, Hf:Al:B = 1:25:1.1, 1h stirring at room temperature (oily phase washed with benzene-d$_6$ + benzene-d$_6$/1,2-difluorobenzene).

System **2** + Al(*i*-Bu)$_3$ + CPh$_3$B(C$_6$F$_5$)$_4$: species **a** and **b**:

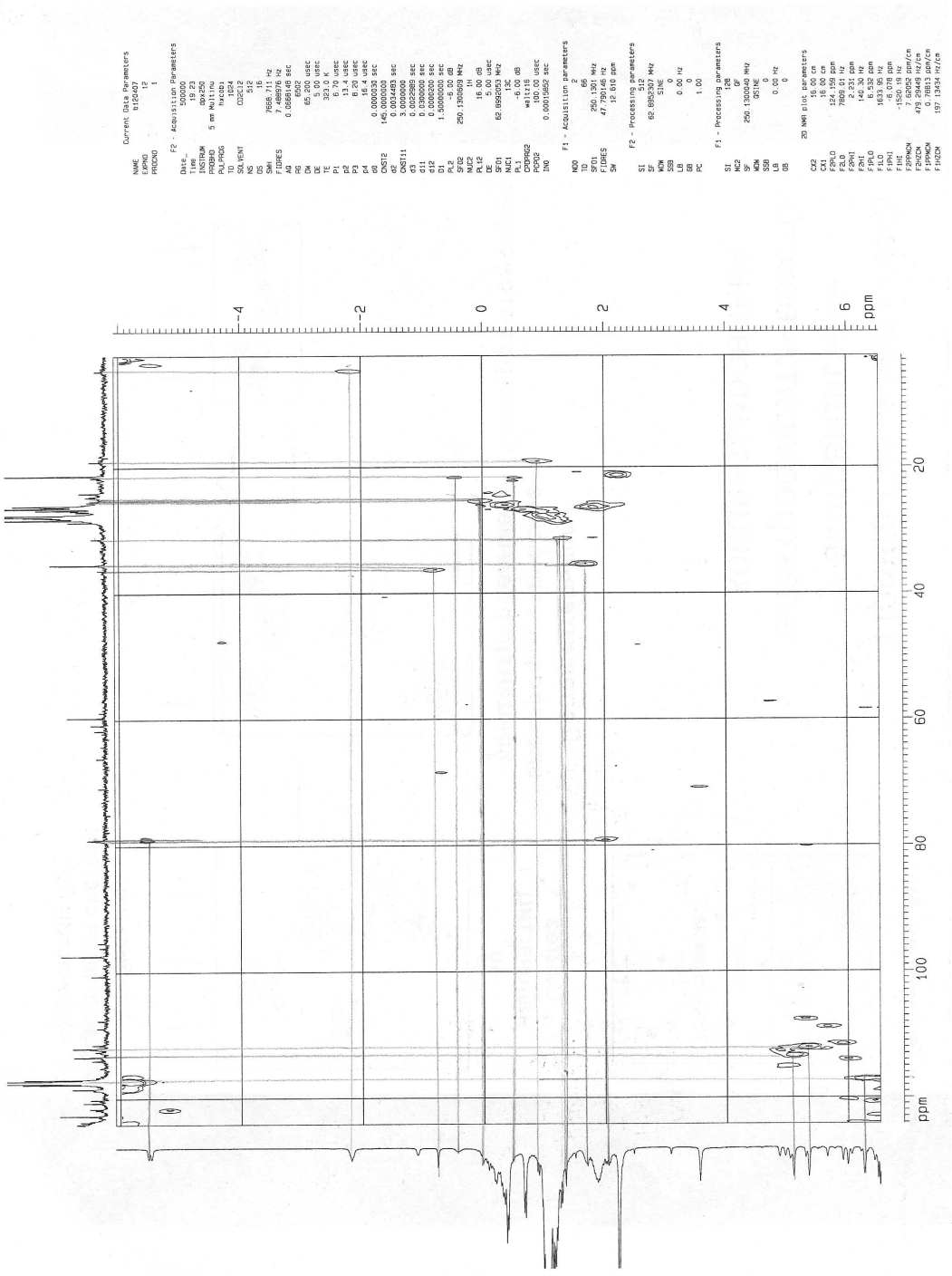


Figure S13. ^{1}H,^{13}C-correlated NMR spectrum (benzene-d$_6$/1,2-difluorobenzene, 2 °C) of the system **2** + Al(*i*-Bu)$_3$ + CPh$_3$B(C$_6$F$_5$)$_4$, Hf:Al:B = 1:25:1.1, 1h stirring at room temperature (oily phase washed with benzene-d$_6$ + benzene-d$_6$/1,2-difluorobenzene).

Species **14a** and **14b**:

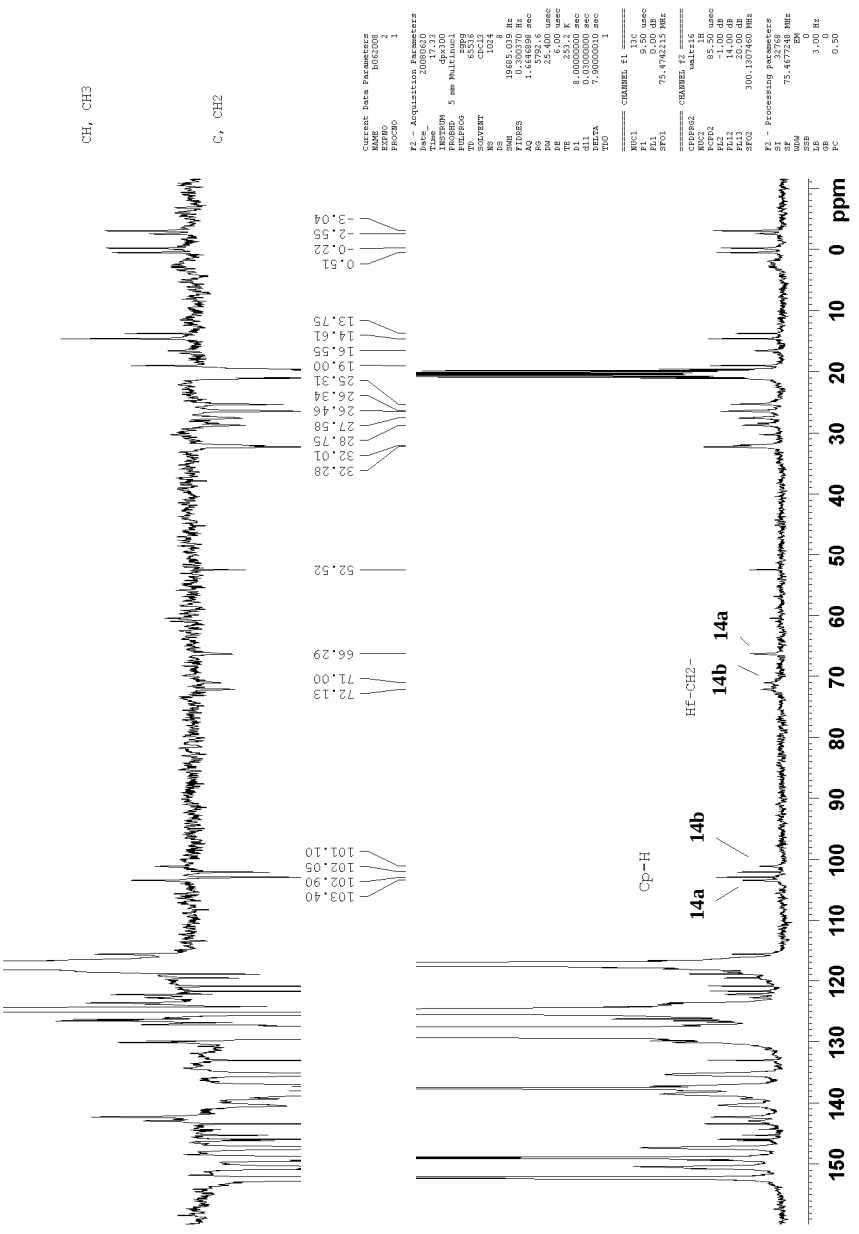


Figure S14. $^{13}C\{^{1}H\}$ J-modulated and $^{13}C\{^{1}H\}$ NMR spectra (toluene-d_8/1,2-difluorobenzene, -20 °C) of species **14a** (major) and **14b** (minor) formed in the system **13**/$CPh_3B(C_6F_5)_4$ (1:1.1).

Species **14a** and **14b**:

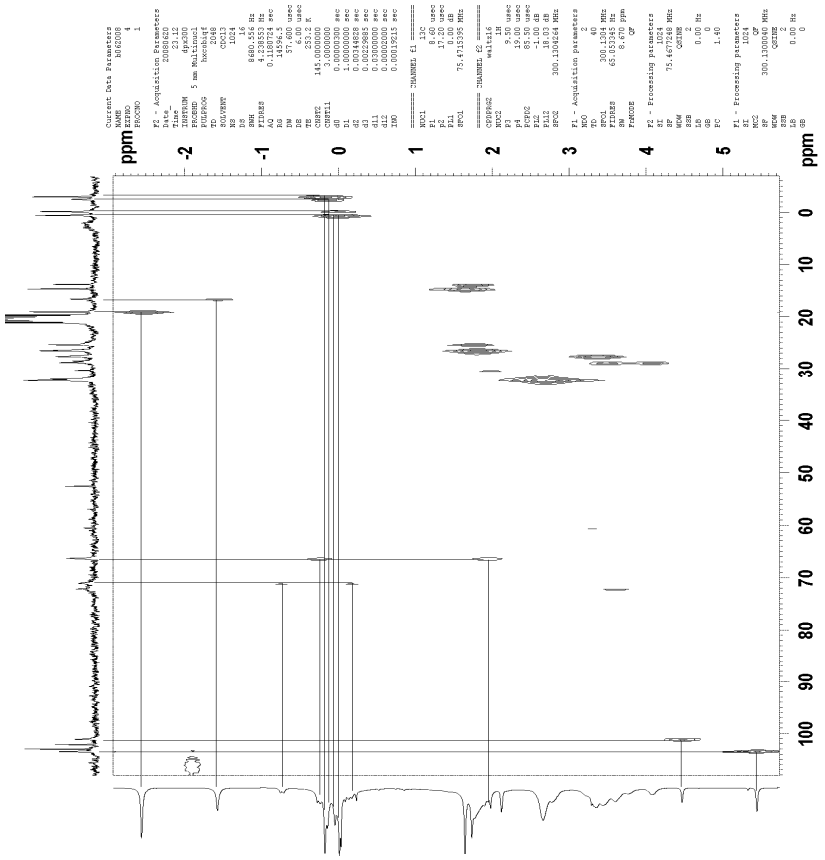


Figure S15. $^{13}C/^{1}H$ heteronuclear correlation NMR spectra (toluene-d_8/1,2-difluorobenzene, -20 °C) of species **14a** (major) and **14b** (minor) formed in the system **13**/$CPh_3B(C_6F_5)_4$ (1:1.1).

Species **14a** and **14b**:

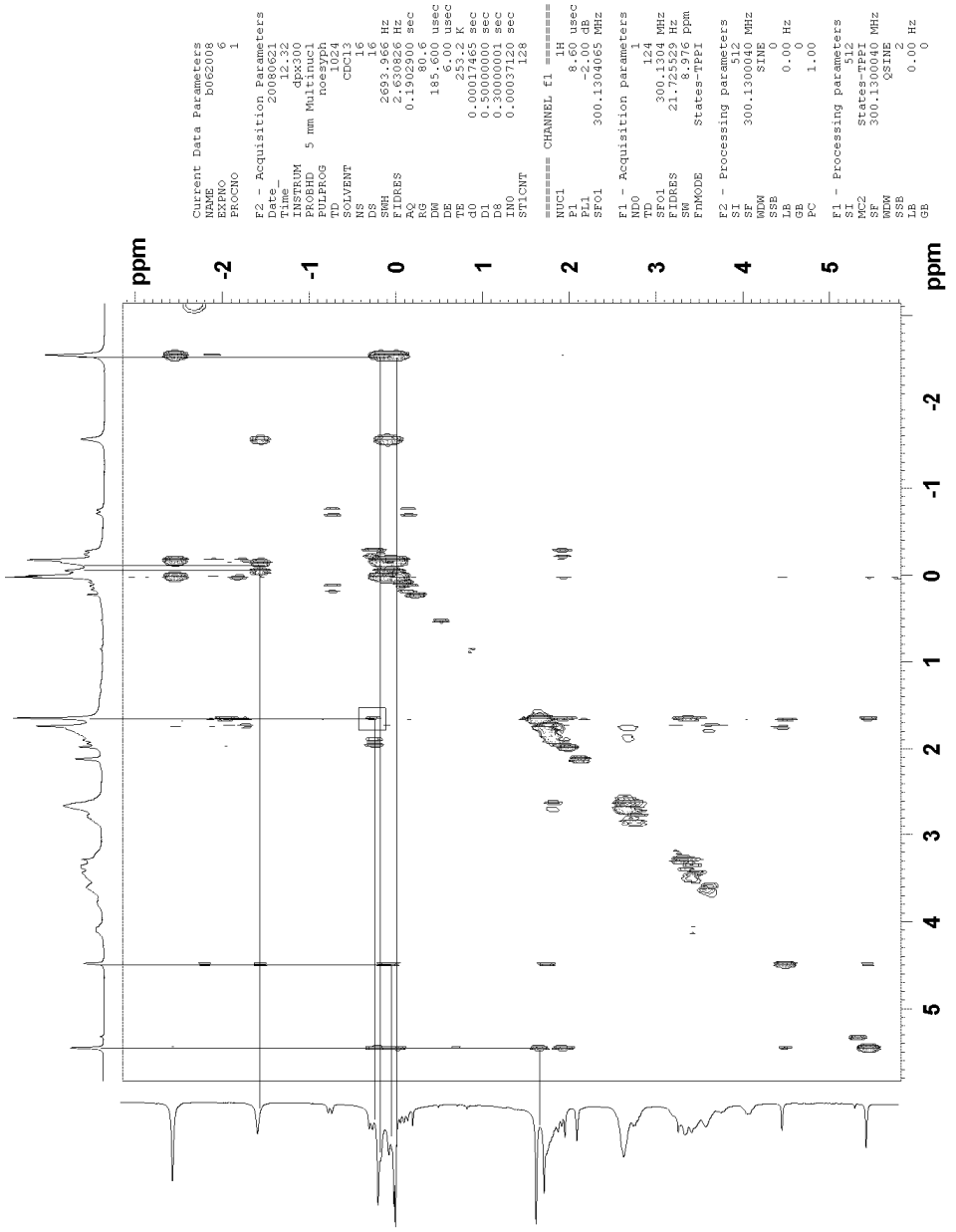


Figure S16. $^{1}H/^{1}H$ NOESY NMR spectra (toluene-d_8/1,2-difluorobenzene, -20 °C) of species **14a** (major) and **14b** (minor) formed in the system **13**/$CPh_3B(C_6F_5)_4$ (1:1.1). NOE correlation peak between the Hf-CH*H*-Si and Cp-CH_3 in the major isomer **14a** is marked with square box.

Species **14**:

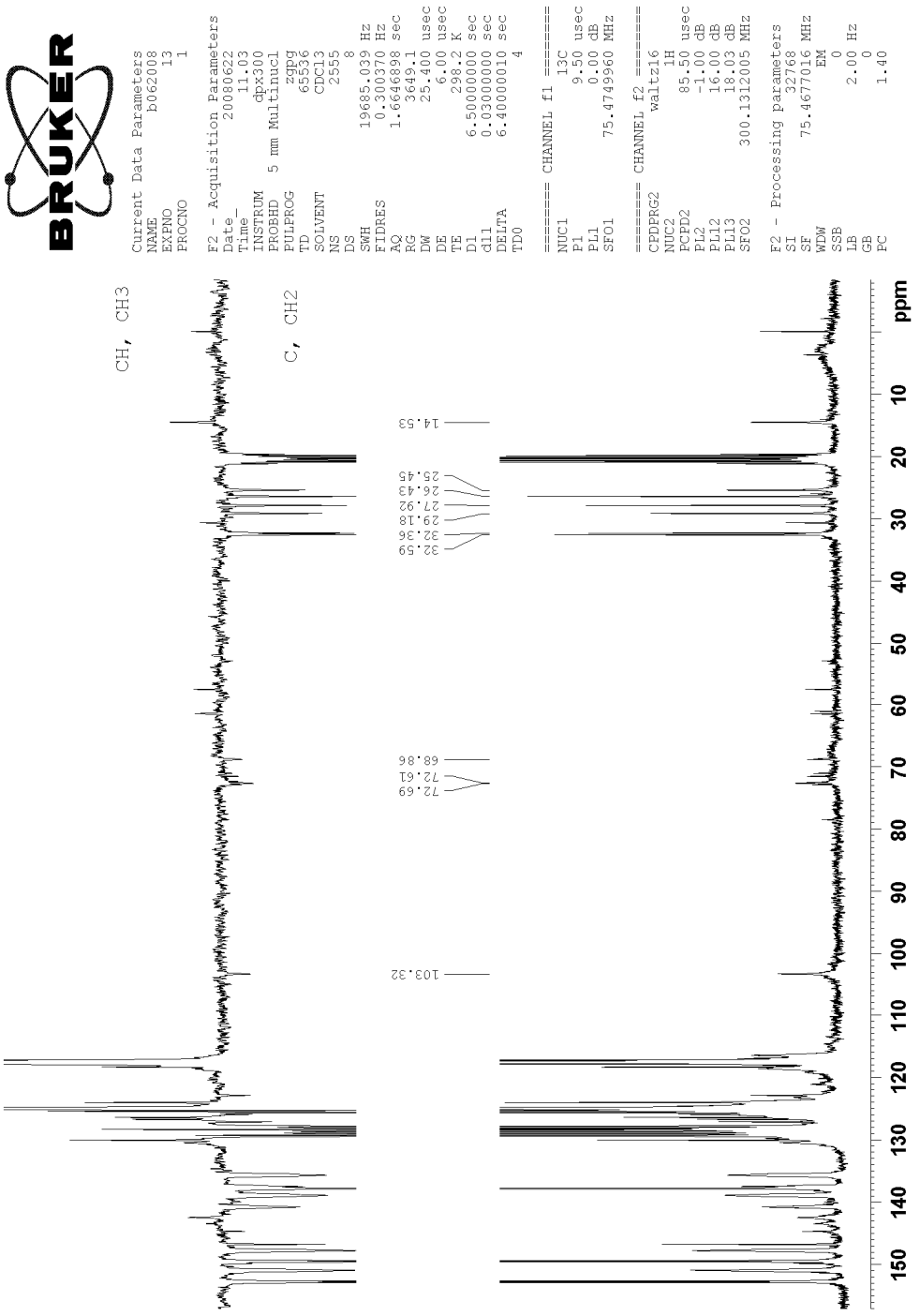


Figure S17. $^{13}C\{^{1}H\}$ J-modulated and $^{13}C\{^{1}H\}$ NMR spectra (toluene-d_8/1,2-difluorobenzene, +25 °C) of species **14** formed in the system **13**/$CPh_3B(C_6F_5)_4$ (1:1.1).

Crystal and structure refinement data for (chloro)(9-[2-(2-methyl-5,6,7-trihydroindacen-1-yl)ethyl]-fluorenyl)(trimethylsilylmethyl)hafnium

Identification code	2008src0396	
Elemental formula	C32 H35 Cl Hf Si	
Formula weight	661.6	
Crystal system	Monoclinic	
Space group	P $2_1/c$	
Unit cell dimensions	a = 17.2434(6) Å	α = 90°
	b = 10.0370(3) Å	β = 116.194(2)°
	c = 17.8692(5) Å	γ = 90°
Volume	2775.06(15) $Å^3$	
No. of formula units, Z	4	
Calculated density	1.584 Mg/m^3	
F(000)	1320	
Absorption coefficient	3.917 mm^{-1}	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal colour, shape	yellow plate	
Crystal size	0.07 × 0.04 × 0.015 mm	
Crystal mounting	on a glass fibre, in oil, fixed in cold N_2 stream	
On the diffractometer:		
θ range for data collection	3.0 to 25.0°	
Limiting indices	-19<=h<=20, -11<=k<=11, -21<=l<=21	
Completeness to theta = 25.0°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.943 and 0.643	
Reflections collected (not including absences)		21382
No. of unique reflections	4852 [R(int) for equivalents = 0.088]	
No. of 'observed' reflections (I > $2\sigma_I$)		3784
Structure determined by:	direct methods, in SHELXS	
Refinement:	Full-matrix least-squares on F^2 in SHELXL	
Data / restraints / parameters	4852 / 0 / 317	
Goodness-of-fit on F^2	1.137	
Final R indices ('observed' data)	R_1 = 0.054, wR_2 = 0.095	

Final R indices (all data) R_1 = 0.084, wR_2 = 0.104

Reflections weighted:

calc $w=1/[\sigma^2(F_o^2)+22.94P]$ where $P=(F_o^2+2F_c^2)/3$

Largest diff. peak and hole 1.27 and -1.07 e.$Å^{-3}$

Location of largest difference peak 0.96 Å from Hf1.

Table 1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor. E.s.ds are in parentheses.

	x	y	z	U(eq)
Hf(1)	3155.1(2)	7852.0(3)	552.7(2)	19.52(12)
Cl(1)	3511.8(14)	7549.3(19)	-599.7(13)	27.9(5)
C(1)	1922(5)	8983(7)	-56(4)	17.9(16)
Si(1)	1522.6(17)	9686(3)	-1117.5(15)	31.7(6)
C(11)	1039(7)	8330(11)	-1899(6)	51(3)
C(12)	2345(7)	10590(9)	-1345(6)	43(3)
C(13)	648(9)	10918(12)	-1274(7)	72(4)
C(21)	3229(6)	6100(7)	1519(5)	25.0(19)
C(22)	3477(6)	5408(7)	954(5)	23.4(19)
C(23)	4270(6)	4886(8)	1030(5)	25.8(19)
C(24)	4300(6)	4257(8)	361(5)	29(2)
C(25)	3547(6)	4136(8)	-405(5)	30(2)
C(26)	2776(6)	4606(8)	-507(5)	28(2)
C(27)	2715(5)	5275(7)	161(5)	19.6(17)
C(28)	2009(6)	5806(8)	265(5)	25.8(19)
C(29)	1119(6)	5853(8)	-277(6)	30(2)
C(30)	547(7)	6340(9)	1(6)	38(2)
C(31)	880(7)	6822(9)	837(7)	41(3)
C(32)	1710(7)	6802(8)	1373(6)	34(2)
C(33)	2316(6)	6283(7)	1101(5)	24.3(19)
C(41)	4310(6)	8343(8)	1961(5)	29(2)
C(42)	4663(6)	8630(9)	1404(6)	33(2)
C(43)	4218(6)	9732(8)	899(6)	32(2)
C(44)	3636(6)	10233(8)	1197(5)	25.6(19)
C(45)	3109(5)	11414(8)	992(5)	23.0(18)
C(46)	2607(5)	11623(8)	1387(5)	24.2(18)
C(47)	1992(6)	12725(8)	1281(5)	29(2)
C(48)	1375(6)	12093(9)	1591(5)	35(2)
C(49)	1951(6)	11139(8)	2288(5)	31(2)
C(50)	2599(6)	10672(8)	1996(5)	27(2)
C(51)	3127(6)	9579(9)	2234(5)	31(2)
C(52)	3668(6)	9338(8)	1838(5)	31(2)
C(101)	3799(7)	6327(9)	2443(5)	38(2)
C(102)	4575(7)	7220(9)	2590(5)	42(2)
C(421)	5405(6)	7937(10)	1339(7)	47(3)

Table 2. Molecular dimensions. Bond lengths are in Ångstroms, angles in degrees. E.s.ds are in parentheses.

Hf(1)-C(1)	2.224(8)	Hf(1)-C(22)	2.547(7)
Hf(1)-Cl(1)	2.4143(19)	Hf(1)-C(52)	2.547(8)
Hf(1)-C(21)	2.428(8)	Hf(1)-C(33)	2.605(8)
Hf(1)-C(41)	2.473(8)	Hf(1)-C(44)	2.623(8)
Hf(1)-C(42)	2.488(9)	Hf(1)-C(27)	2.699(7)
Hf(1)-C(43)	2.511(9)	Hf(1)-C(28)	2.737(8)
Hf(1)-CtF	2.304	Hf(1)-CtI	2.221
C(1)-Si(1)	1.849(7)	Si(1)-C(12)	1.873(10)
Si(1)-C(11)	1.862(10)	Si(1)-C(13)	1.873(11)
C(21)-C(33)	1.426(12)	C(41)-C(52)	1.433(12)
C(21)-C(22)	1.437(11)	C(41)-C(102)	1.514(12)
C(21)-C(101)	1.521(12)	C(42)-C(43)	1.420(12)
C(22)-C(23)	1.415(12)	C(42)-C(421)	1.505(13)
C(22)-C(27)	1.452(11)	C(43)-C(44)	1.420(12)
C(23)-C(24)	1.371(12)	C(44)-C(52)	1.437(12)
C(24)-C(25)	1.417(12)	C(44)-C(45)	1.438(11)
C(25)-C(26)	1.344(12)	C(45)-C(46)	1.353(11)
C(26)-C(27)	1.414(11)	C(46)-C(50)	1.453(11)
C(27)-C(28)	1.413(11)	C(46)-C(47)	1.485(12)
C(28)-C(29)	1.408(12)	C(47)-C(48)	1.537(12)
C(28)-C(33)	1.430(11)	C(48)-C(49)	1.537(12)
C(29)-C(30)	1.376(12)	C(49)-C(50)	1.501(12)
C(30)-C(31)	1.427(14)	C(50)-C(51)	1.368(12)
C(31)-C(32)	1.326(14)	C(51)-C(52)	1.419(13)
C(32)-C(33)	1.430(12)	C(101)-C(102)	1.533(14)
C(41)-C(42)	1.405(13)		
C(1)-Hf(1)-Cl(1)	101.27(19)	CtI-Hf(1)-Cl(1)	108.8
CtI-Hf(1)-CtF	128.4	CtF-Hf(1)-C(1)	104.5
CtI-Hf(1)-C(1)	105.5	CtF-Hf(1)-Cl(1)	105.3

Si(1)-C(1)-Hf(1)	122.6(4)	C(1)-Si(1)-C(13)	108.4(4)
C(1)-Si(1)-C(11)	109.3(4)	C(11)-Si(1)-C(13)	107.8(6)
C(1)-Si(1)-C(12)	115.6(4)	C(12)-Si(1)-C(13)	106.5(5)
C(11)-Si(1)-C(12)	108.8(5)		

C(33)-C(21)-C(22)	107.3(7)	C(43)-C(44)-C(45)	131.9(8)
C(33)-C(21)-C(101)	125.8(8)	C(52)-C(44)-C(45)	121.1(8)
C(22)-C(21)-C(101)	125.8(8)	C(46)-C(45)-C(44)	118.1(8)
C(23)-C(22)-C(21)	133.5(8)	C(45)-C(46)-C(50)	120.6(8)
C(23)-C(22)-C(27)	118.6(7)	C(45)-C(46)-C(47)	129.3(8)
C(21)-C(22)-C(27)	107.9(7)	C(50)-C(46)-C(47)	110.0(7)
C(24)-C(23)-C(22)	119.6(8)	C(46)-C(47)-C(48)	102.5(7)
C(23)-C(24)-C(25)	120.7(8)	C(49)-C(48)-C(47)	104.3(7)
C(26)-C(25)-C(24)	122.0(8)	C(50)-C(49)-C(48)	103.1(7)
C(25)-C(26)-C(27)	119.4(8)	C(51)-C(50)-C(46)	122.2(8)
C(28)-C(27)-C(26)	132.8(8)	C(51)-C(50)-C(49)	129.7(8)
C(28)-C(27)-C(22)	107.4(7)	C(46)-C(50)-C(49)	108.1(7)
C(26)-C(27)-C(22)	119.7(7)	C(50)-C(51)-C(52)	118.4(8)
C(29)-C(28)-C(27)	131.5(8)	C(51)-C(52)-C(41)	132.5(8)
C(29)-C(28)-C(33)	119.7(8)	C(51)-C(52)-C(44)	119.2(8)
C(27)-C(28)-C(33)	108.7(8)	C(41)-C(52)-C(44)	108.3(8)
C(30)-C(29)-C(28)	120.0(9)	C(21)-C(101)-C(102)	111.7(7)
C(29)-C(30)-C(31)	118.6(9)	C(41)-C(102)-C(101)	110.8(8)
C(32)-C(31)-C(30)	123.9(9)		
C(31)-C(32)-C(33)	118.6(9)		
C(21)-C(33)-C(28)	108.5(7)		
C(21)-C(33)-C(32)	132.2(8)		
C(28)-C(33)-C(32)	119.3(8)		
C(42)-C(41)-C(52)	107.2(8)		
C(42)-C(41)-C(102)	126.5(8)		
C(52)-C(41)-C(102)	126.3(8)		
C(41)-C(42)-C(43)	109.2(8)		
C(41)-C(42)-C(421)	127.5(9)		
C(43)-C(42)-C(421)	123.4(9)		
C(42)-C(43)-C(44)	108.1(8)		
C(43)-C(44)-C(52)	107.0(7)		

Table 3. Anisotropic displacement parameters ($Å^2 \times 10^3$) for the expression: $\exp -2\pi^2(h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12})$. E.s.ds are in parentheses.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Hf(1)	20.1(2)	17.4(2)	18.7(2)	-0.34(15)	6.38(13)	1.1(2)
Cl(1)	32.1(12)	26.8(12)	30.3(11)	0.7(8)	18.8(10)	1.4(9)
C(1)	18(4)	18(4)	16(4)	-5(3)	6(3)	-2(3)
Si(1)	29.5(15)	40.1(15)	23.6(13)	9.1(11)	10.0(11)	7.2(12)
C(11)	42(6)	78(8)	30(5)	-5(5)	13(5)	-20(6)
C(12)	57(7)	38(6)	34(5)	15(4)	20(5)	-2(5)
C(13)	83(10)	81(9)	50(7)	33(6)	27(7)	57(8)
C(21)	36(5)	14(4)	22(4)	3(3)	11(4)	6(4)
C(22)	31(5)	12(4)	19(4)	4(3)	4(4)	8(4)
C(23)	20(5)	18(4)	34(5)	5(4)	8(4)	0(4)
C(24)	30(5)	22(5)	42(5)	1(4)	21(4)	3(4)
C(25)	41(6)	29(5)	25(5)	-5(4)	18(4)	2(4)
C(26)	31(5)	32(5)	23(5)	0(4)	14(4)	-4(4)
C(27)	25(5)	12(4)	23(4)	-2(3)	12(4)	3(3)
C(28)	31(5)	17(4)	35(5)	4(4)	20(4)	-3(4)
C(29)	28(5)	22(5)	36(5)	6(4)	12(4)	-2(4)
C(30)	37(6)	33(5)	54(6)	9(5)	29(5)	-1(4)
C(31)	42(6)	35(6)	65(7)	14(5)	41(6)	15(4)
C(32)	50(7)	24(5)	41(6)	8(4)	33(5)	9(4)
C(33)	40(5)	11(4)	26(5)	4(3)	19(4)	0(4)
C(41)	27(5)	19(4)	26(5)	-9(4)	-1(4)	1(4)
C(42)	20(5)	24(5)	40(5)	-16(4)	0(4)	0(4)
C(43)	33(6)	20(5)	38(5)	-3(4)	11(4)	2(4)
C(44)	27(5)	15(4)	23(4)	-5(3)	1(4)	1(4)
C(45)	20(4)	14(4)	26(4)	-4(3)	2(4)	-8(3)
C(46)	25(5)	25(4)	21(4)	-5(3)	8(4)	-8(4)
C(47)	35(5)	15(4)	35(5)	-4(4)	13(4)	3(4)
C(48)	40(6)	31(5)	34(5)	-4(4)	15(4)	4(5)
C(49)	47(6)	27(5)	25(5)	-3(4)	20(4)	0(4)
C(50)	34(5)	24(5)	19(4)	-7(3)	8(4)	-4(4)
C(51)	38(6)	30(5)	20(5)	0(4)	7(4)	2(4)
C(52)	37(6)	18(4)	27(5)	-9(4)	6(4)	2(4)
C(101)	55(7)	25(5)	26(5)	2(4)	11(5)	4(5)
C(102)	48(6)	29(5)	26(5)	-8(4)	-5(4)	9(5)
C(421)	32(6)	28(5)	74(7)	-18(5)	15(5)	0(5)

Table 4. Torsion angle, in degrees. E.s.d is in parentheses.

C(21)-C(101)-C(102)-C(41)	40.1(10)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$). All hydrogen atoms were included in idealised positions with U(iso)'s set at 1.2 × U(eq) or, for the methyl groups, 1.5 × U(eq) of the parent carbon atom.

	x	y	z	U(iso)
H(1A)	1471	8401	-61	21
H(1B)	1965	9719	312	21
H(11A)	828	8694	-2451	77
H(11B)	569	7930	-1830	77
H(11C)	1470	7668	-1819	77
H(12A)	2078	10917	-1907	65
H(12B)	2806	9992	-1277	65
H(12C)	2573	11325	-966	65
H(13A)	431	11289	-1824	108
H(13B)	878	11617	-868	108
H(13C)	187	10478	-1209	108
H(23)	4768	4968	1529	31
H(24)	4820	3907	412	35
H(25)	3586	3719	-851	36
H(26)	2289	4492	-1012	33
H(29)	918	5555	-824	36
H(30)	-43	6354	-347	46
H(31)	491	7172	1016	49
H(32)	1895	7119	1914	40
H(43)	4295	10068	452	38
H(45)	3114	12017	599	28
H(47A)	1687	12991	701	35
H(47B)	2287	13492	1615	35
H(48A)	1123	12768	1805	42
H(48B)	914	11611	1145	42
H(49A)	2231	11599	2818	38
H(49B)	1618	10399	2343	38
H(51)	3132	9007	2646	37
H(10C)	4005	5476	2715	46

H(10D)	3459	6739	2692	46
H(10A)	4809	7587	3149	50
H(10B)	5022	6692	2543	50
H(42A)	5589	8453	994	71
H(42B)	5223	7071	1097	71
H(42C)	5876	7845	1885	71

*** Current Data Parameters ***
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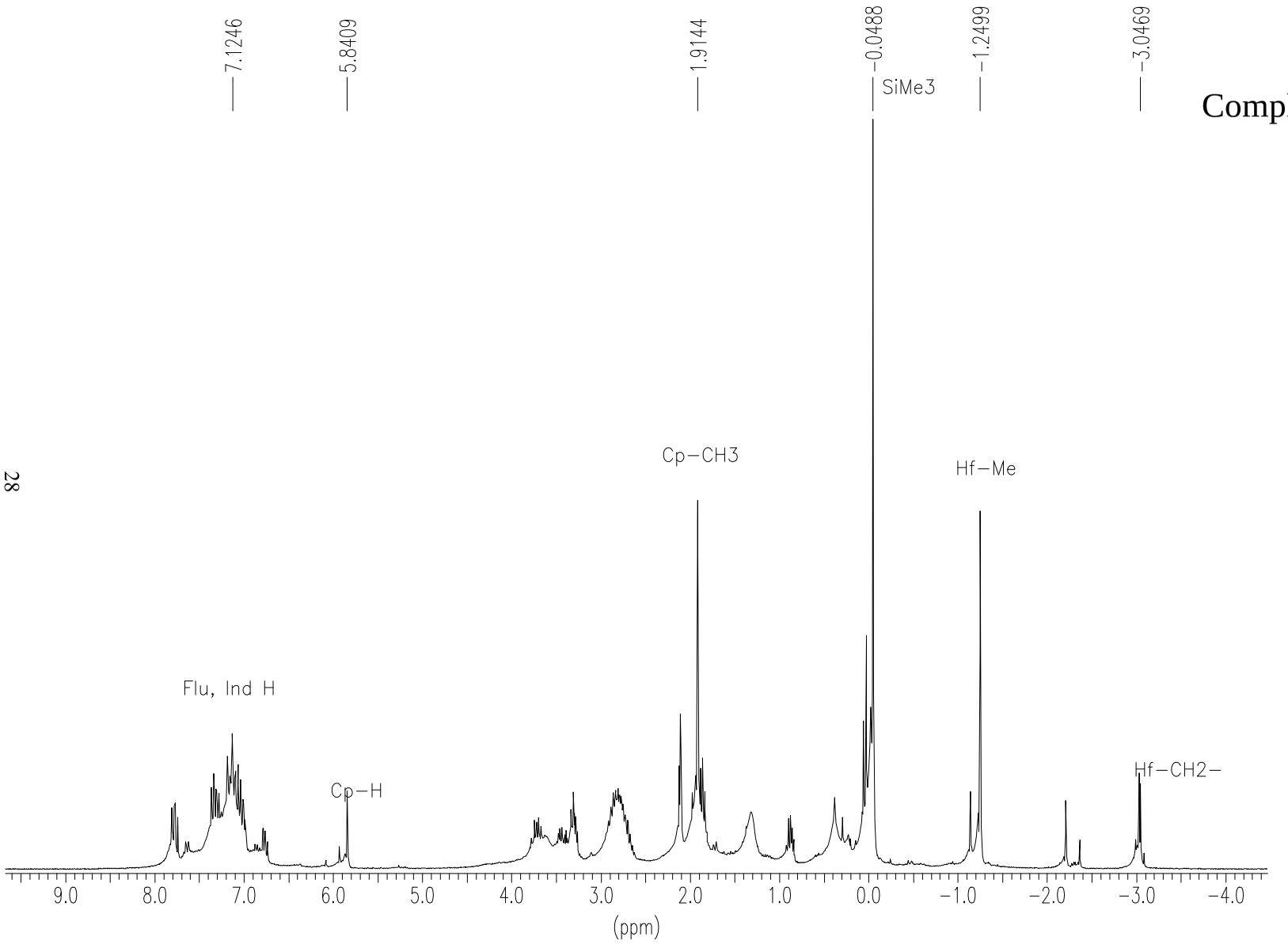
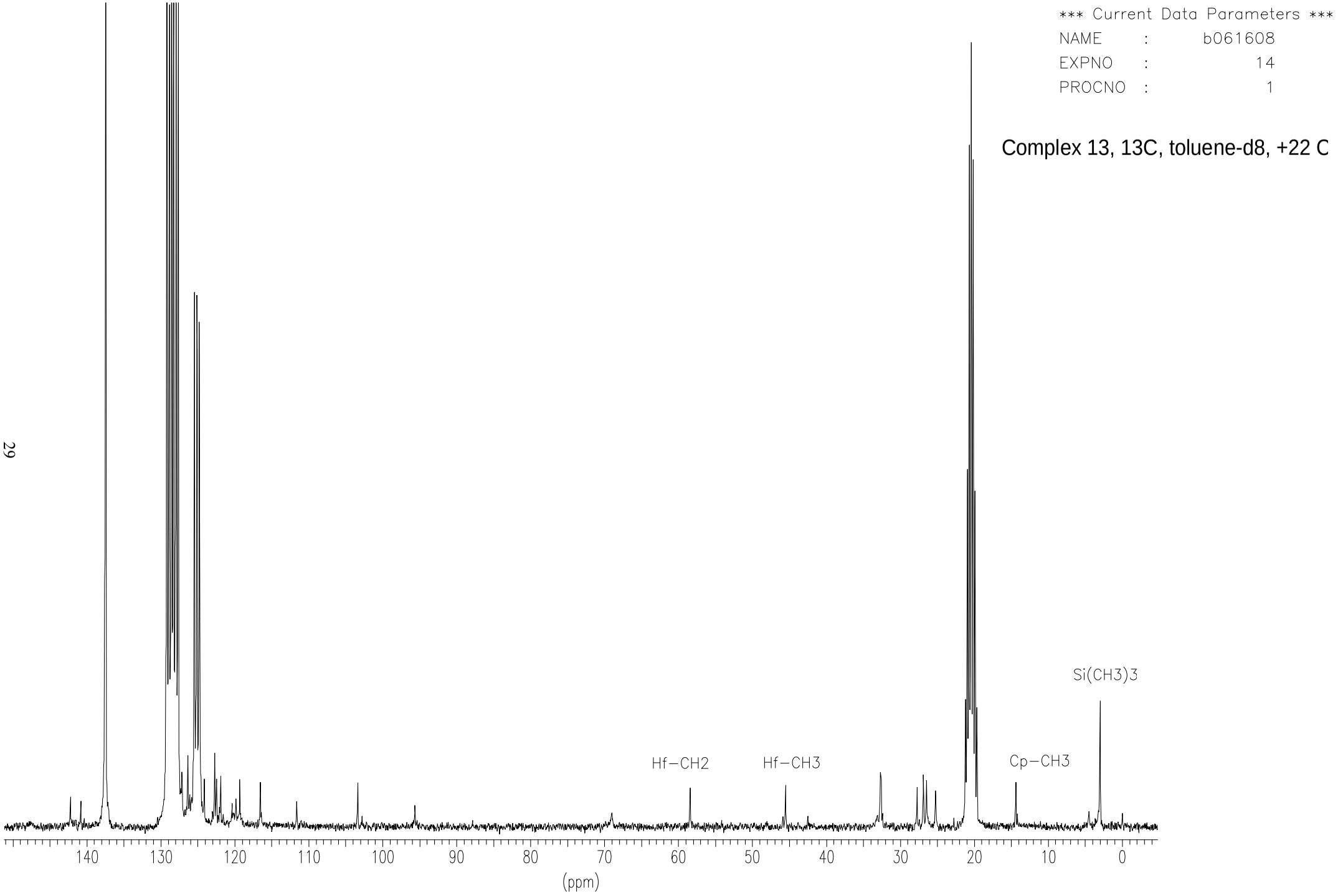
PROCNO : 1

Complex 13, 1H, toluene-d8, +22




*** Current Data Parameters ***
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Hf−CH3
Cp−CH3
Si(CH3)3
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)