Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supporting Information

to

Group 4 Metal Complexes Bearing the Aminoborane Motif: Origin of Tandem Ring-Opening Metathesis/Vinyl-Insertion Polymerization

M. Wang,[a] G. Xu,[a] D. Wang,[a] Y. Zou,[a] W. Frey[b] and M. R. Buchmeiser*[a,c]

[a] Lehrstuhl für Makromolekulare Stoffe und Faserchemie, Institut für Polymerchemie, Universität Stuttgart, Pfaffenwaldring 55, D-70569 Stuttgart, Germany, Fax: +49 (0) -711-685-64050; e-mail: michael.buchmeiser@ipoc.uni-stuttgart.de; [b] Institut für Organische Chemie, Universität Stuttgart, Pfaffenwaldring 55, D-70569 Stuttgart, Germany; [c] Institut für Textilchemie und Chemiefaser (ITCF) Denkendorf, Körschtalstr. 26, D-73770 Denkendorf, Germany

Compound **3** crystalizes in the orthorhombic system P_{bcn}, a = 2181.09(17), b = 1350.26(11), c = 1750.34(16) pm, $\alpha = \beta = \gamma = 90°$, Z = 8. In this ligand, the pyridine nitrogen is coordinated to the boryl group with an N-B distance of 165.5(3) pm (Figure S1).

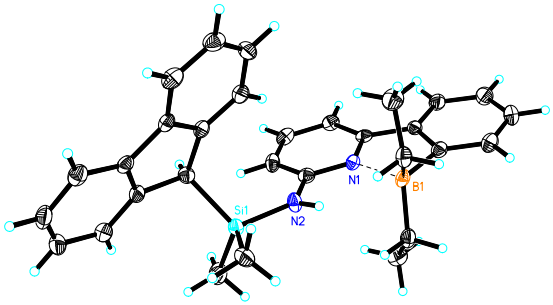


Figure S1. Single-crystal X-ray structure of compound **3**.

Compound **4** crystalizes in the monoclinic space group, P21/n with a = 1424.13(7), b = 1944.18(9), c = 1788.83(8) pm, $\alpha = \gamma = 90°$, β = 107.1°, Z = 4. In **4**, the fluorenyl ligand is coordinated to the lithium center in a η^1-manner and the amino nitrogen is bound to the same lithium atom, which is additionally coordinated by one THF molecule. Also some hydrogen-bonding to the ethyl group at the boron becomes visible, resulting in a distorted tetrahedral ligand sphere around Li. The counter cation to this anionic Li-complex is $Li(THF)_4^+$; consequently, the formula of 4 is $[(\eta^1\text{-}C_{13}H_8)Me_2Si(DbppN)\cdot Li(THF)\text{-}Li(THF)_4^+]$ (DbppN=6-(2-(diethylboryl)phenyl)pyridin-2-amido). Notably, as in **3**, the pyridine nitrogen in **4** is coordinated to the boryl group in the solid state, as evidenced by the N-B bond length of 162.8(2) pm (Figure S2).

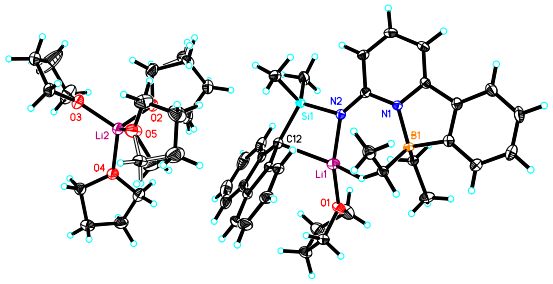


Figure S2. Single-crystal X-ray structure of compound **4**. Selected bond lengths [pm] and angles [°]: Li(1)-O(1) 191.9 (3), Li(1)-N(2) 195.9 (3), Li(1)-C(12) 239.4(3), Li(1)-C(13) 251.7(3), Li(1)-C(14) 273.8(3), N(1)-B(1) 162.8(2); O(1)-Li(1)-N(2) 157.77(19), O(1)-Li(1)-C(12) 107.60(14), N(2)-Li(1)-C(12) 80.45(11).

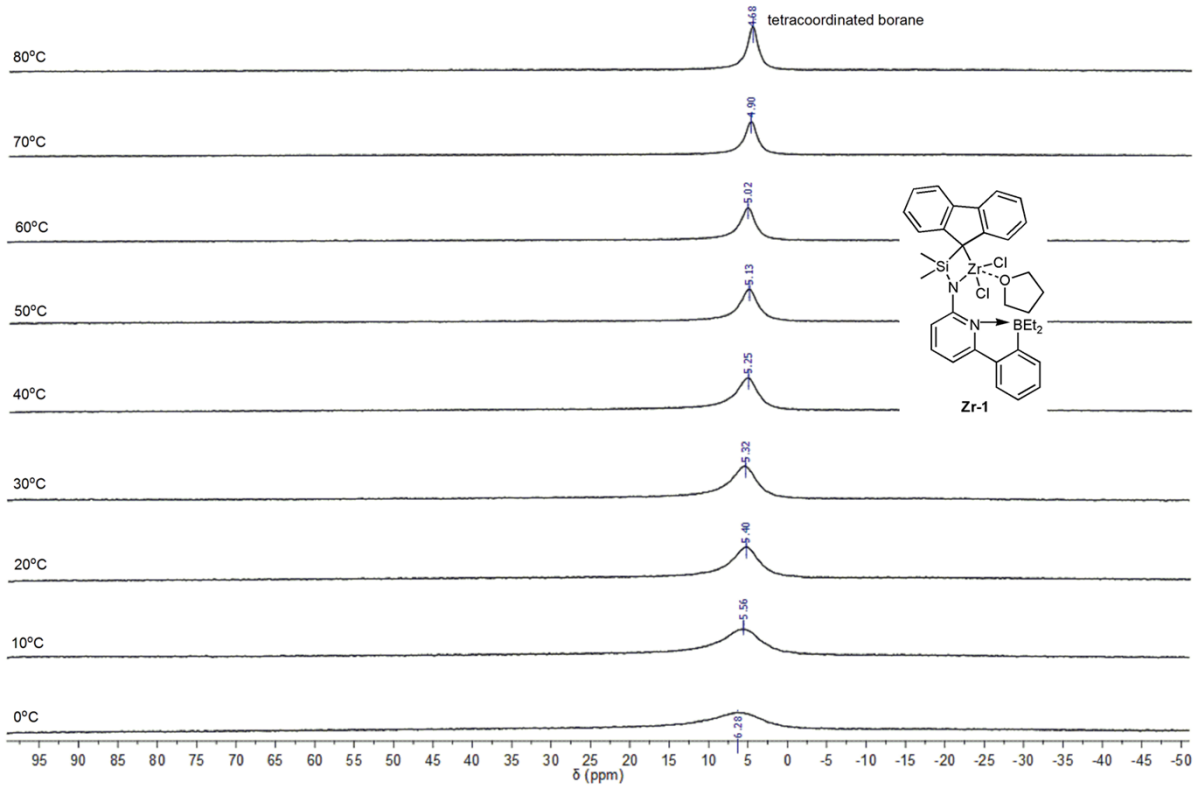


Figure S3. Variable-temperature ^{11}B NMR spectra of **Zr-1** in toluene-d_8 (0-80ºC).

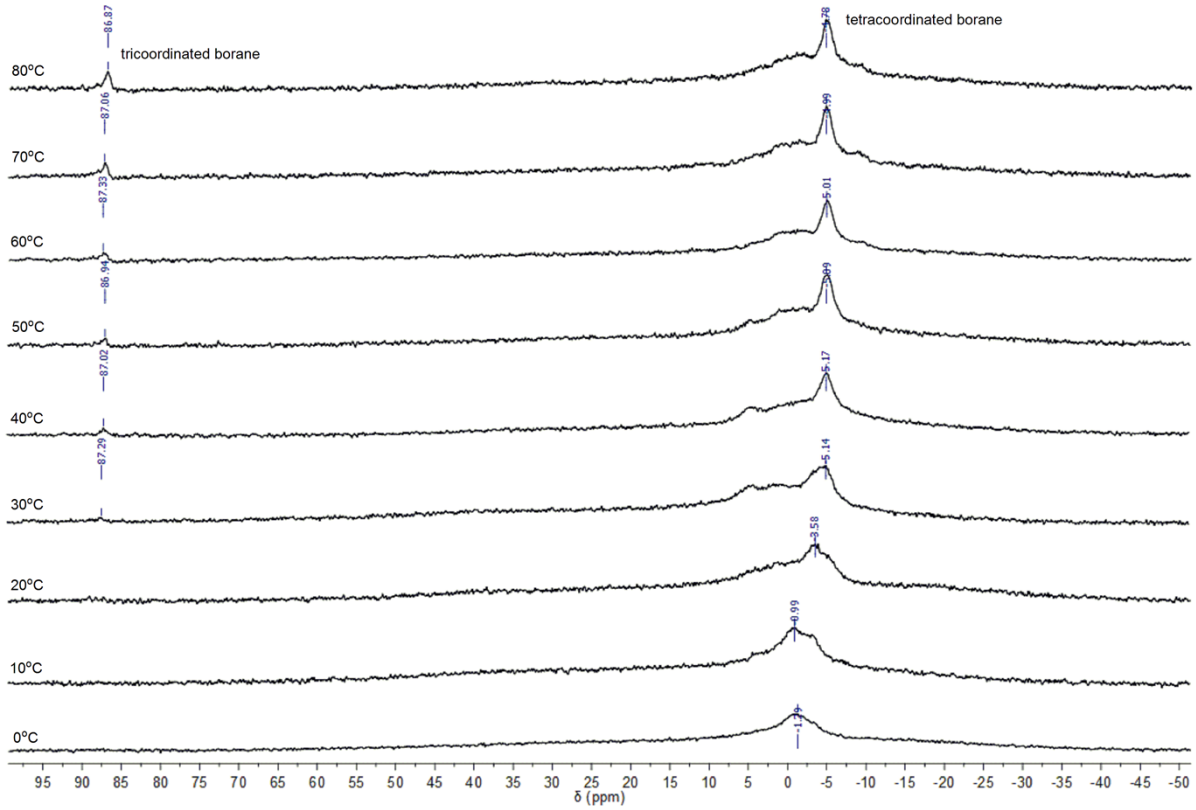


Figure S4. Variable-temperature ^{11}B NMR spectra of **Zr-1**/MAO in toluene-d_8 (0-80ºC).

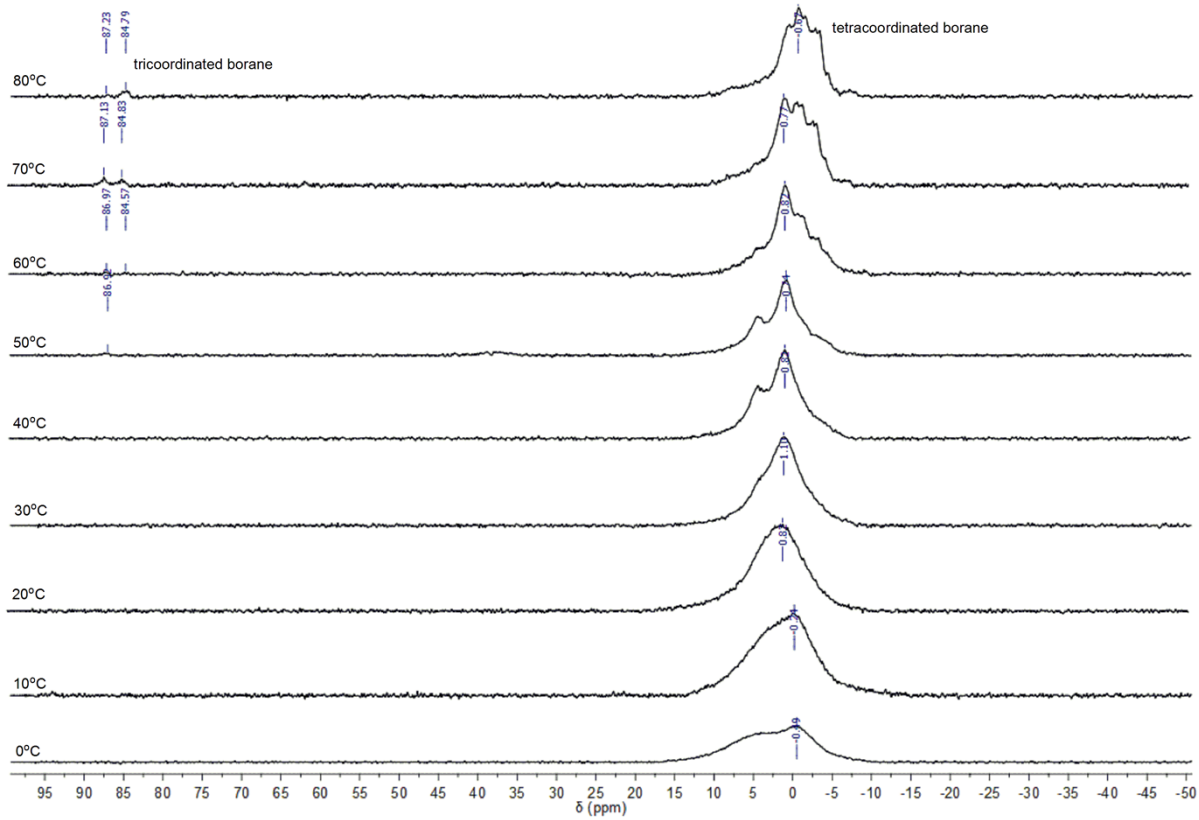


Figure S5. Variable-temperature ^{11}B NMR spectra of **Zr-1**/MAO/NBE in toluene-d_8 (0-80ºC).

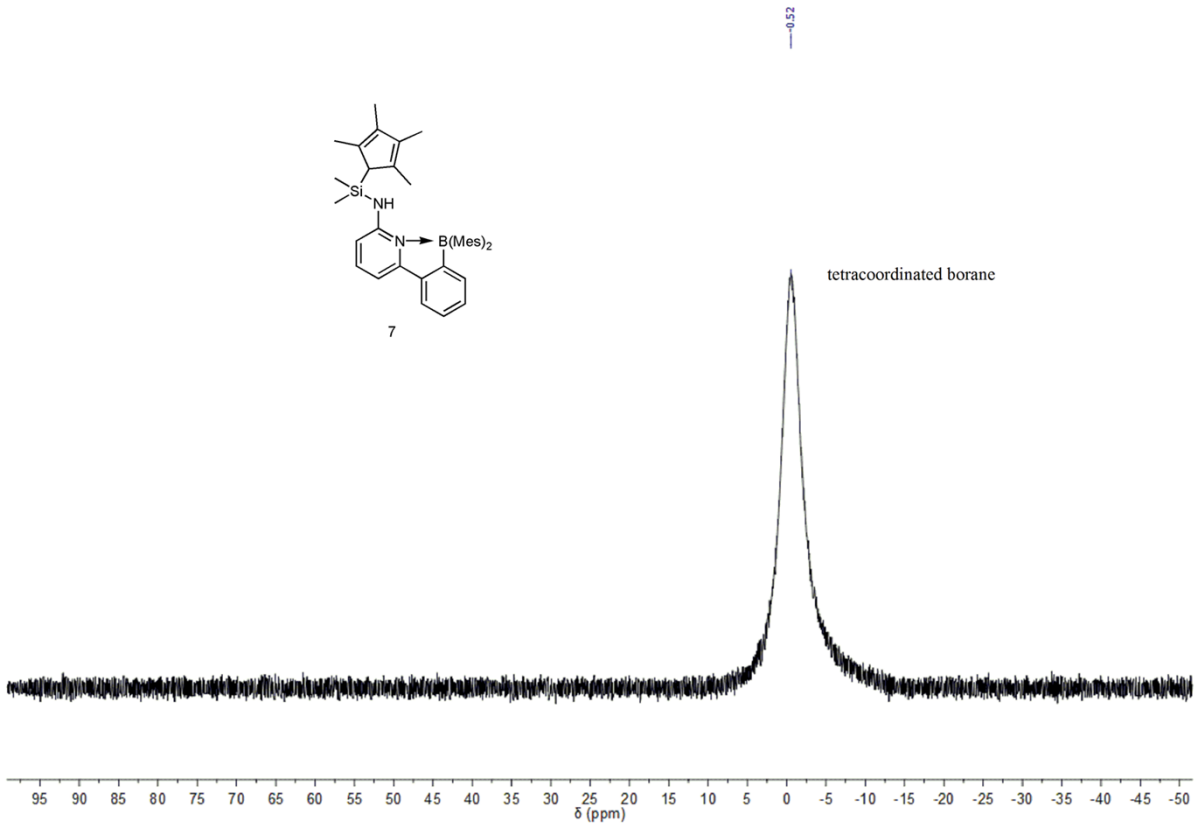


Figure S6. ^{11}B NMR of compound **7** in toluene-d_8.

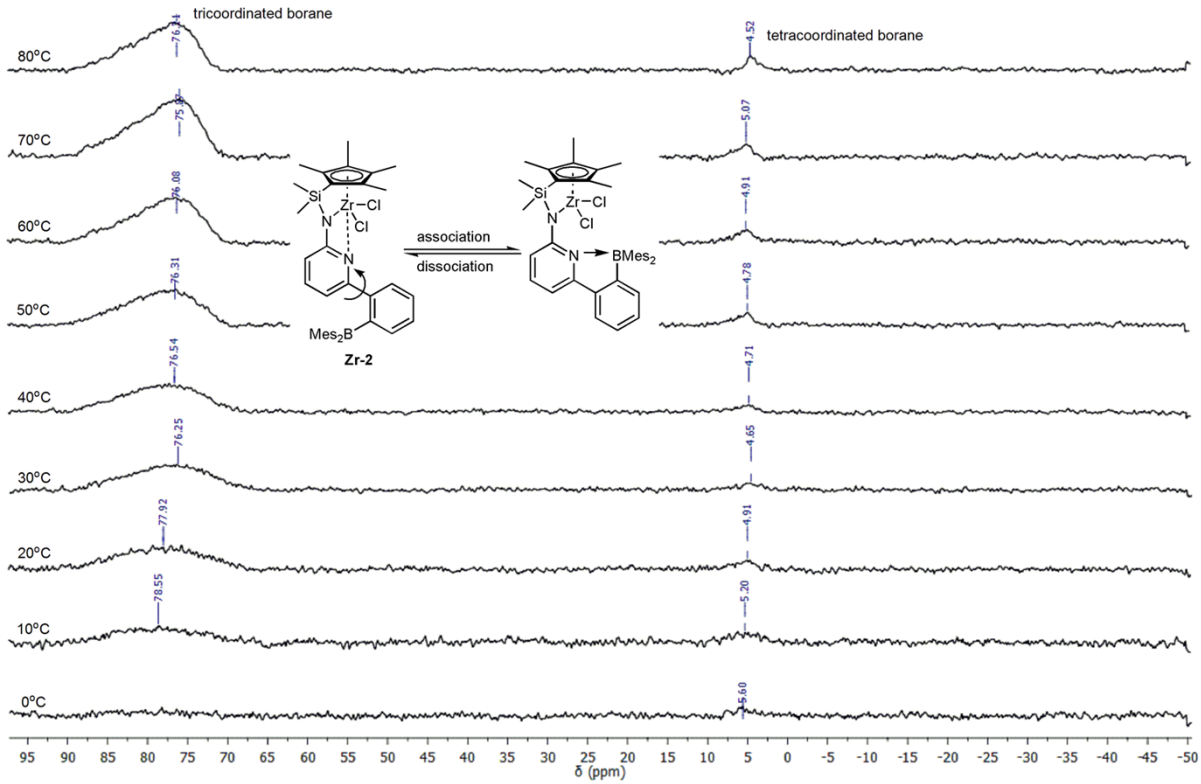


Figure S7. Variable-temperature ^{11}B NMR spectra of **Zr-2** in toluene-d_8 (0-80ºC).

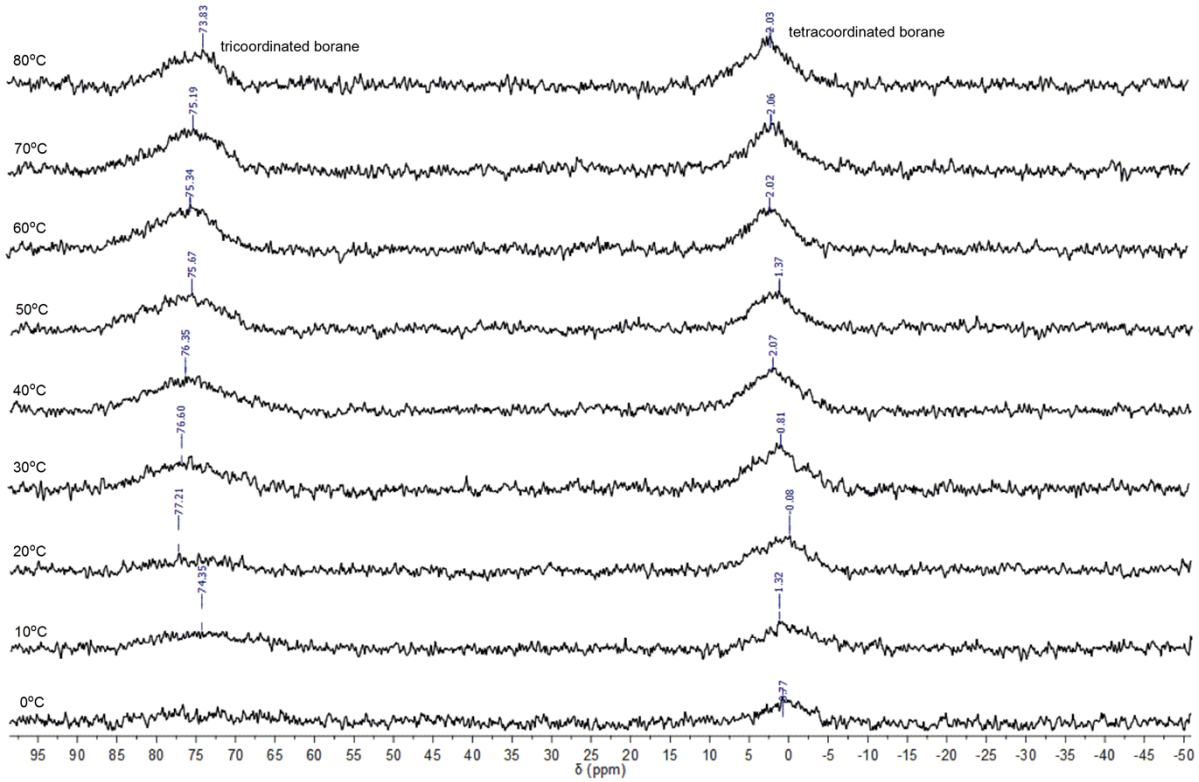


Figure S8. Variable-temperature ^{11}B NMR spectra of **Zr-2**/MAO in toluene-d_8 (0-80ºC).

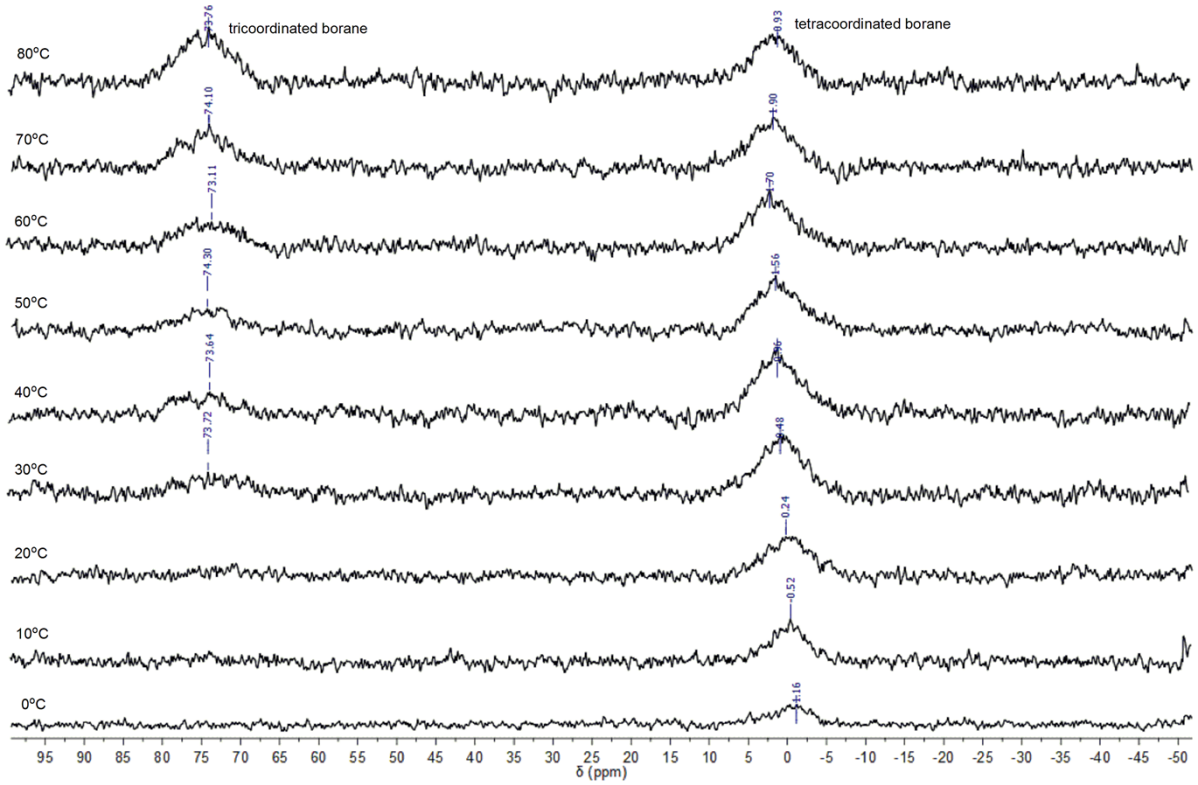


Figure S9. Variable-temperature ^{11}B NMR spectra of **Zr-2**/MAO/NBE in toluene-d_8 (0-80ºC).

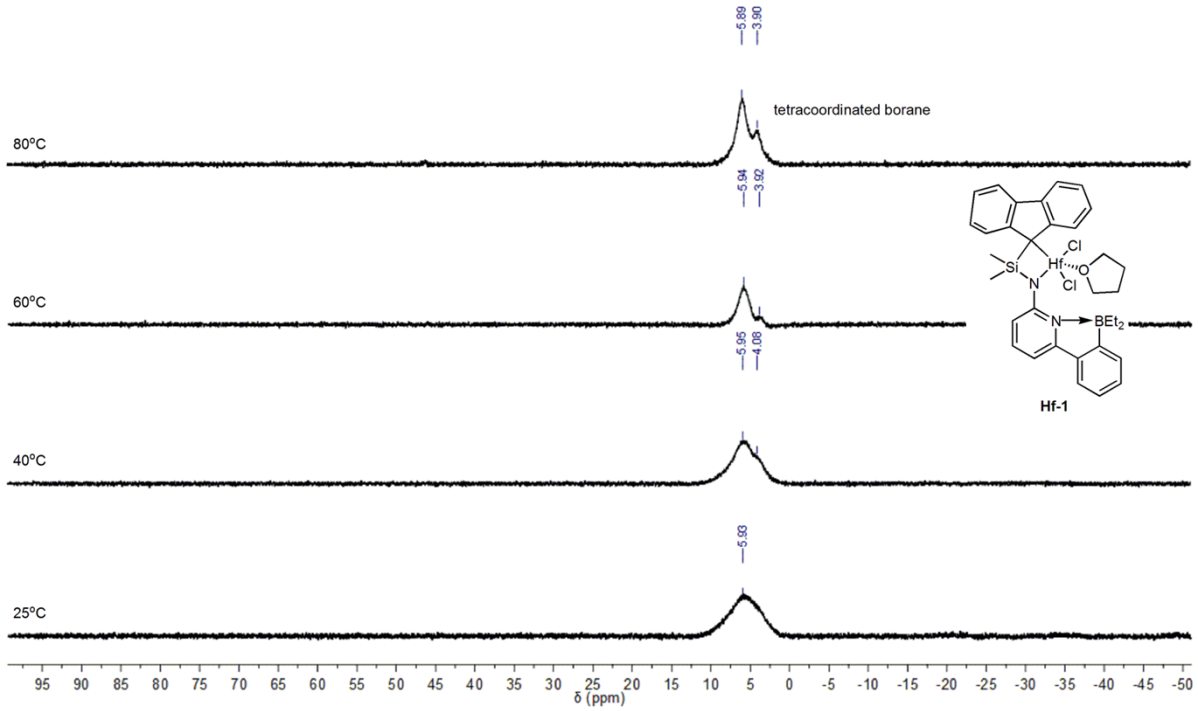


Figure S10. Variable-temperature ^{11}B NMR spectra of **Hf-1** in toluene-d_8 (25-80ºC).

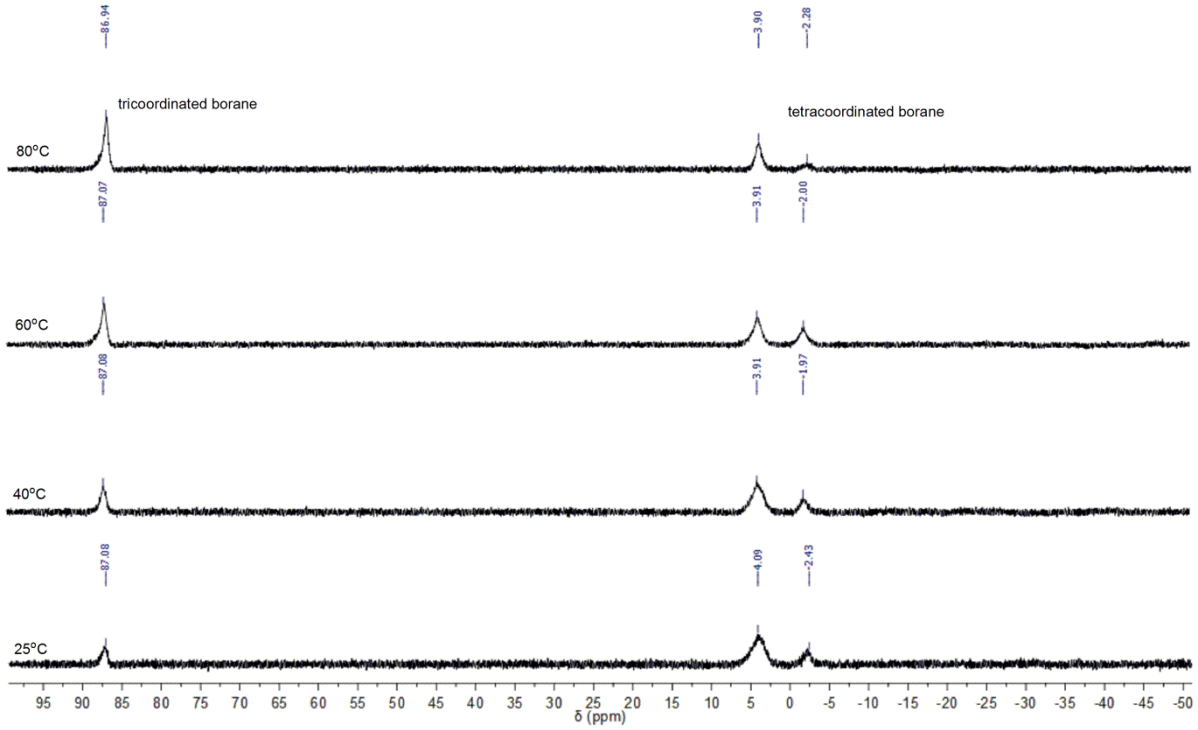


Figure S11. Variable-temperature ^{11}B NMR spectra of **Hf-1**/MAO in toluene-d_8 (25-80ºC).

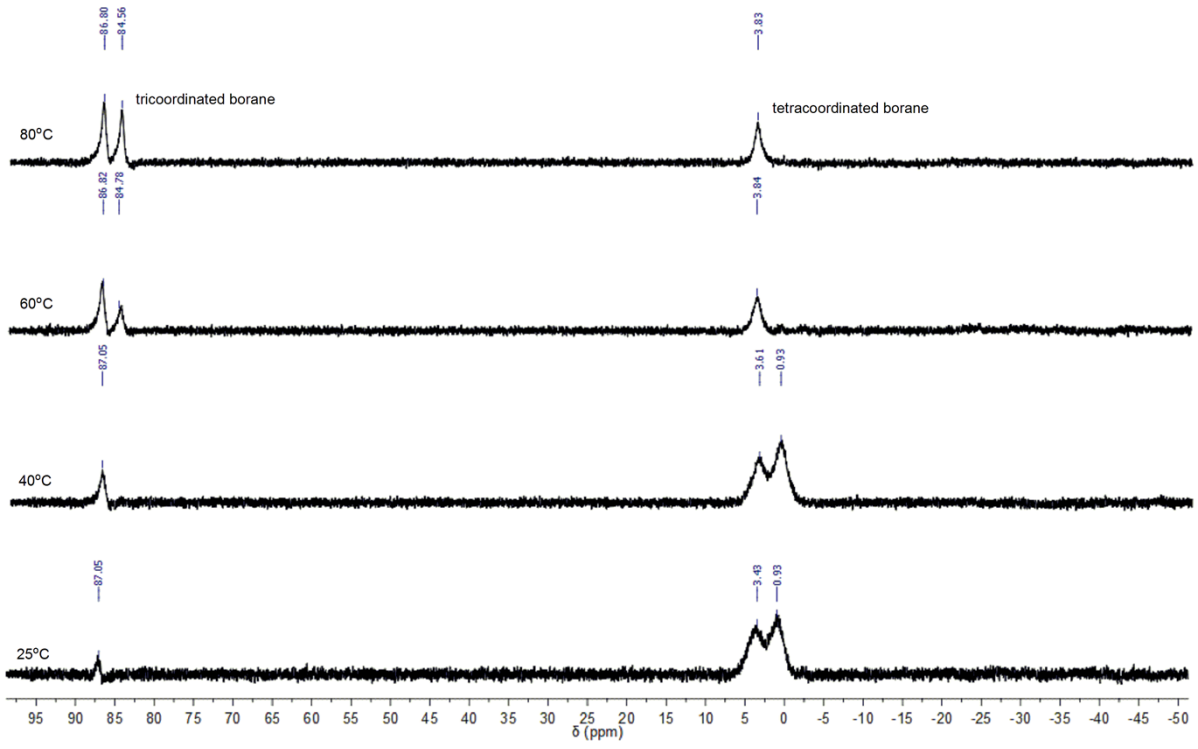


Figure S12. Variable-temperature ^{11}B NMR spectra of **Hf-1**/MAO/NBE in toluene-d_8 (25-80ºC).

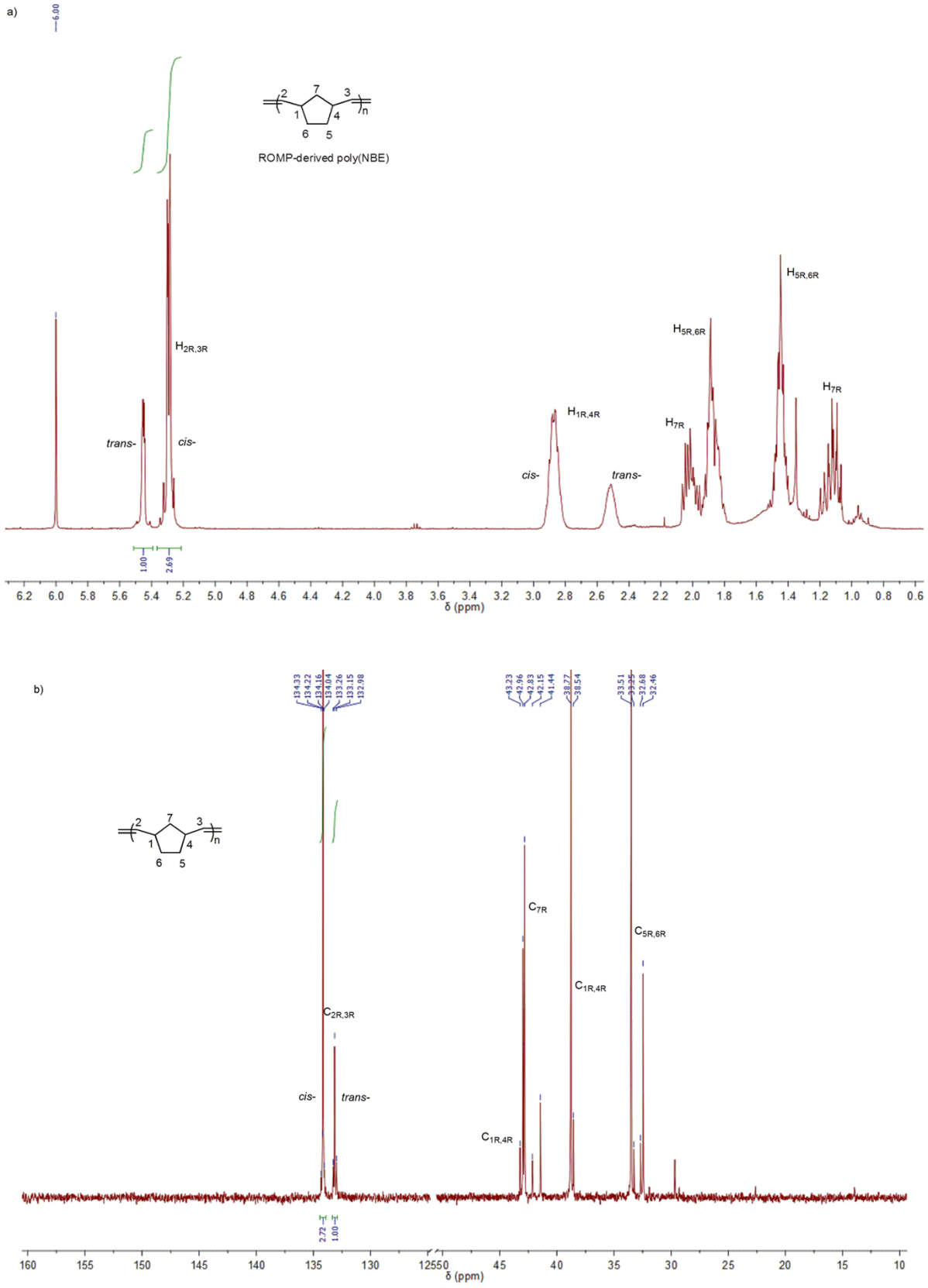


Figure S13. a) ^{1}H NMR and b) ^{13}C NMR spectra of poly(NBE)$_{ROMP}$ produced by **Zr-1**/MAO at 50ºC in 1,1,2,2-tetrachloroentane-d_2.

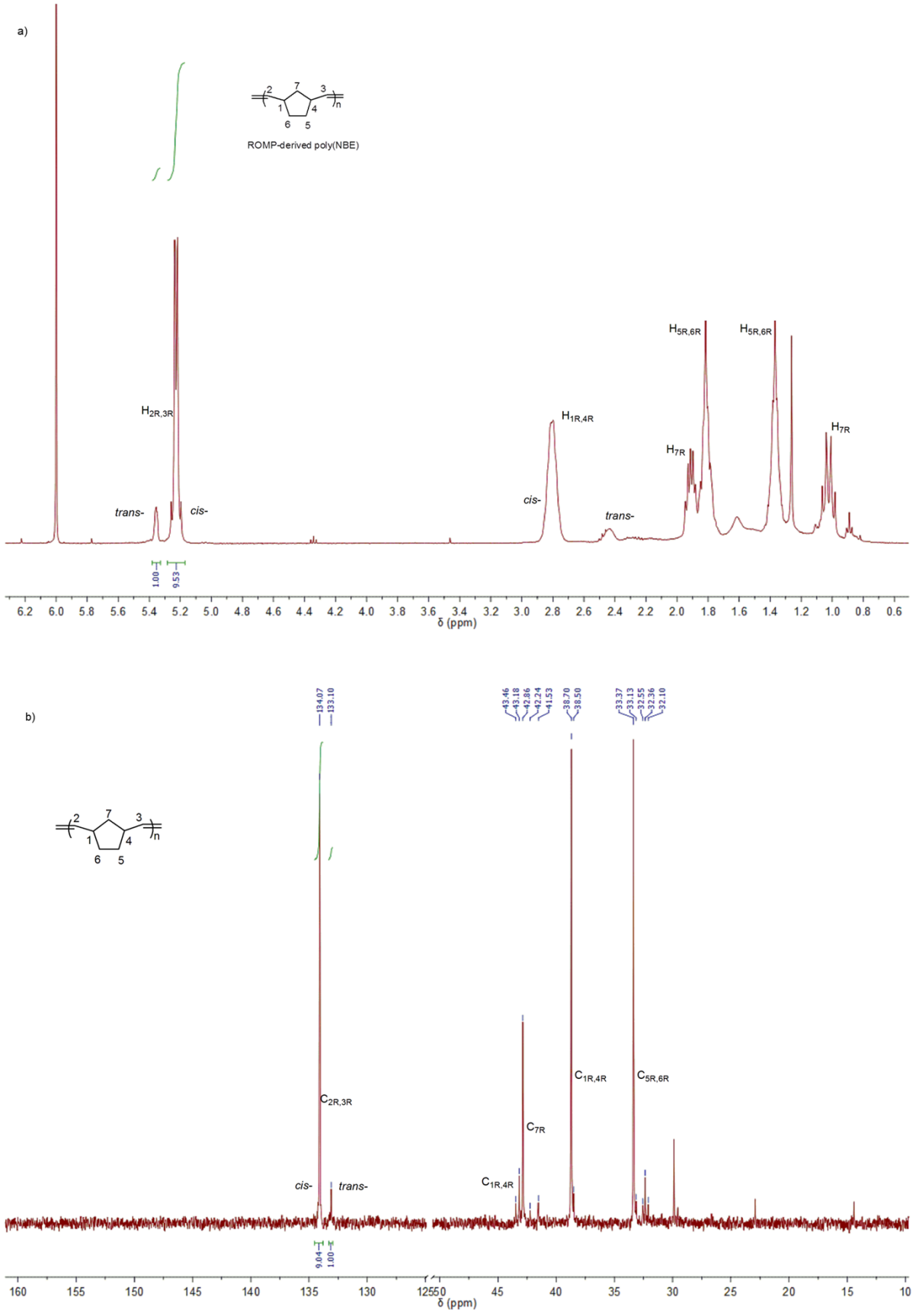


Figure S14. a) ^{1}H NMR and b) ^{13}C NMR spectra of poly(NBE)$_{ROMP}$ produced by **Zr-1**/MAO at 65ºC in 1,1,2,2-tetrachloroentane-d_2.

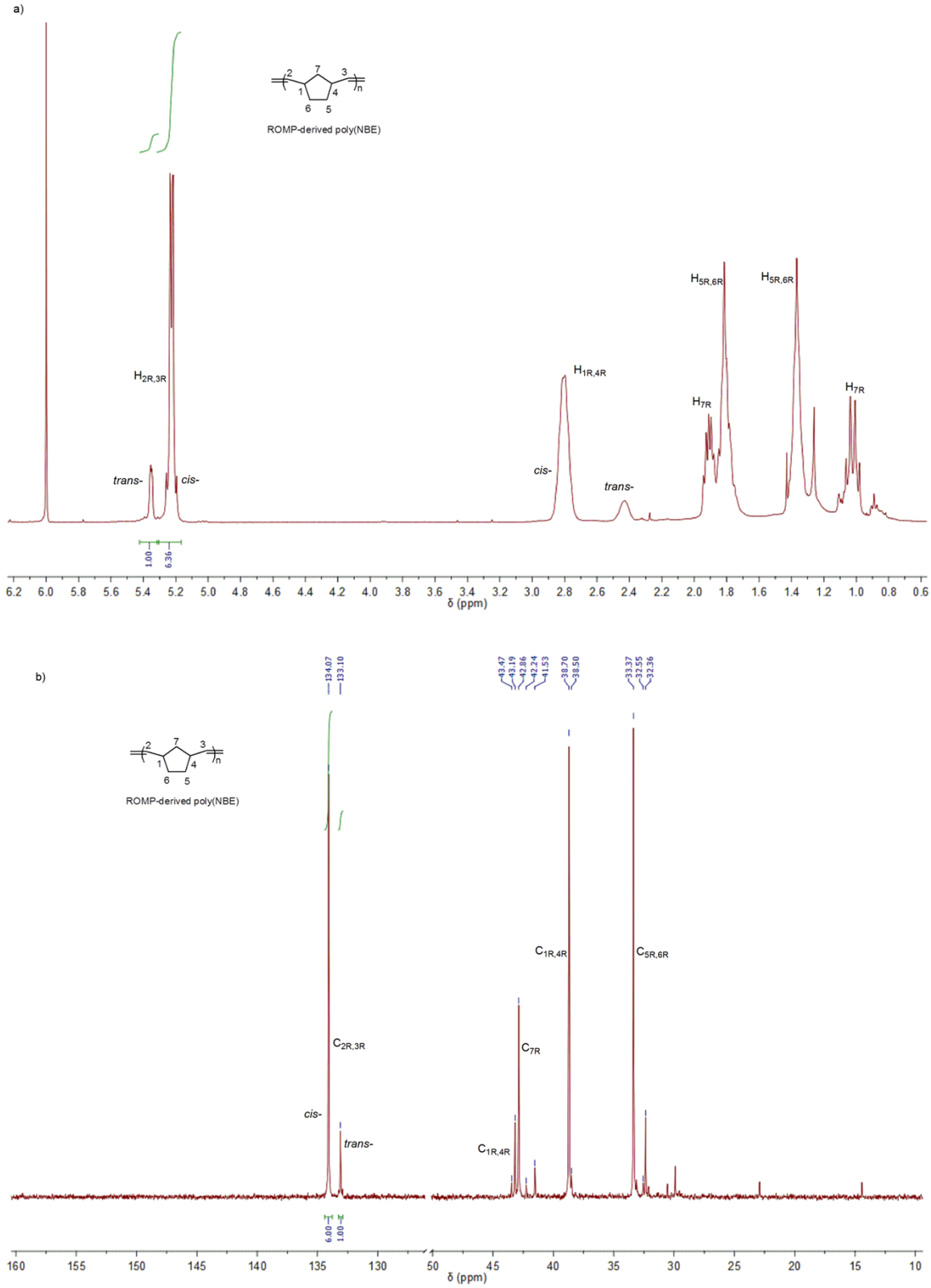


Figure S15. a) ^{1}H NMR and b) ^{13}C NMR spectra of poly(NBE)$_{ROMP}$ produced by **Zr-2**/MAO at 50ºC in 1,1,2,2-tetrachloroentane-d_2.

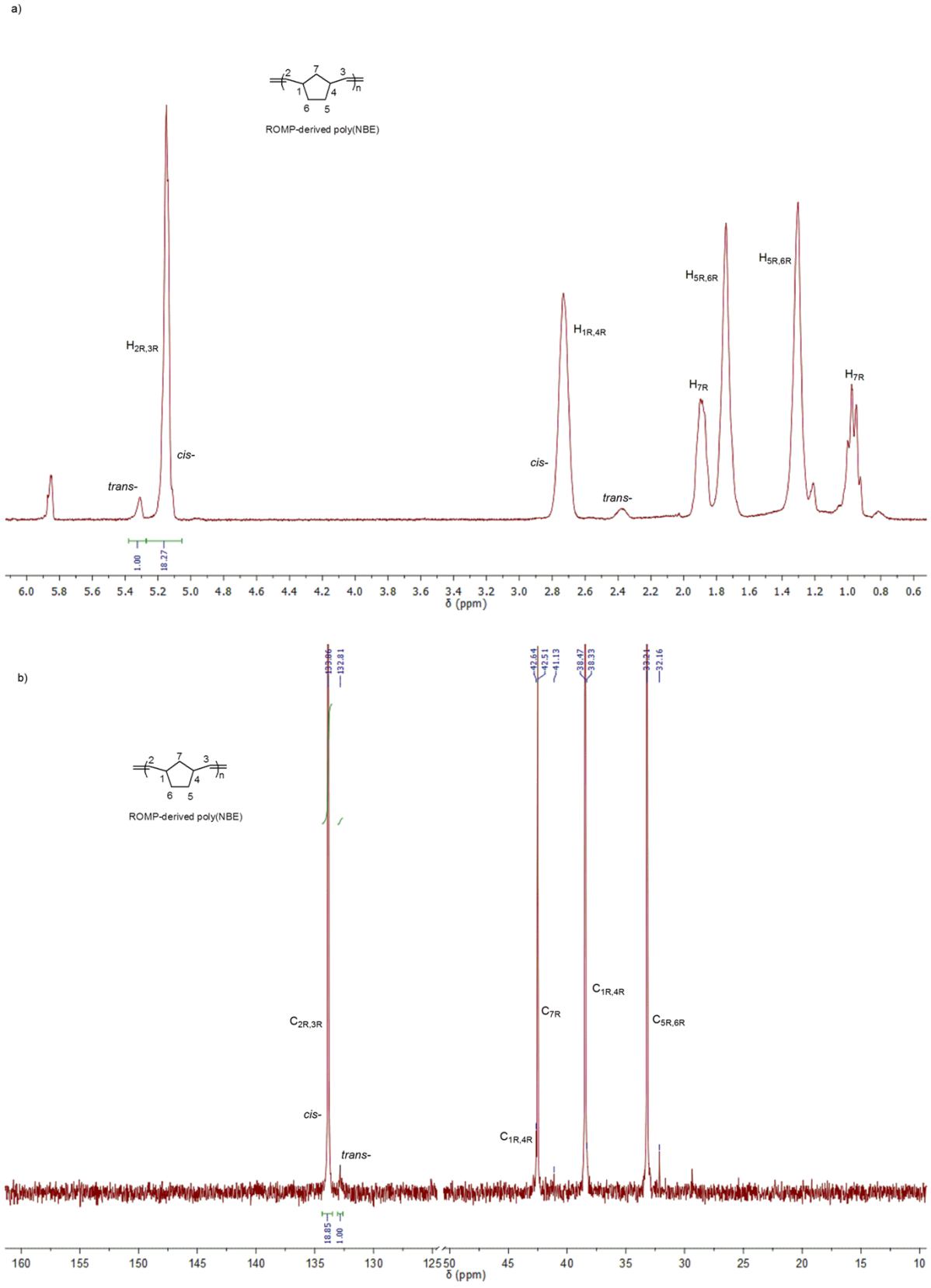


Figure S16. a) ^{1}H NMR and b) ^{13}C NMR spectra of poly(NBE)$_{ROMP}$ produced by **Zr-2**/MAO at 65ºC in 1,1,2,2-tetrachloroentane-d_2.

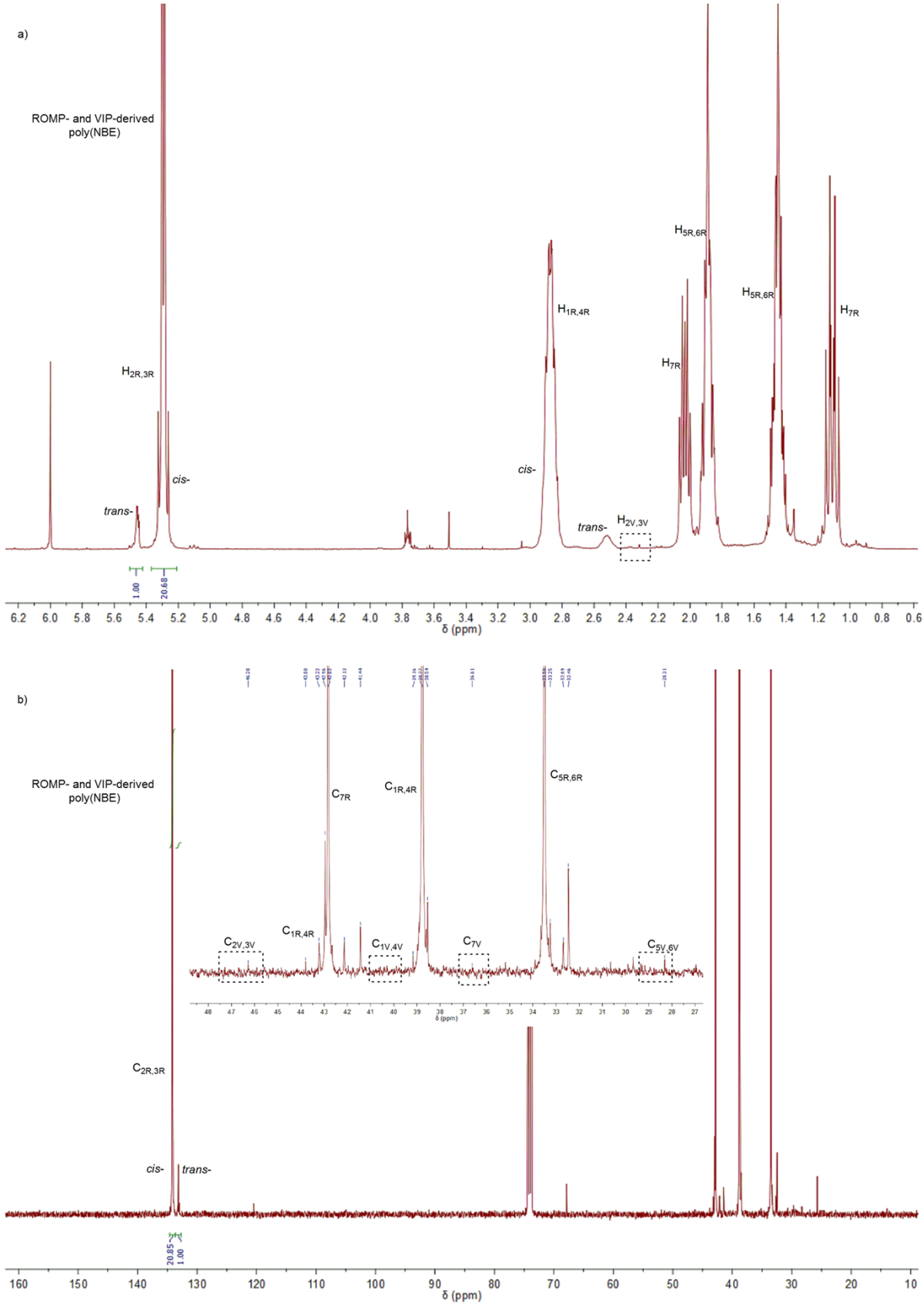


Figure S17. a) ^{1}H NMR and b) ^{13}C NMR spectra of poly(NBE)$_{VIP}$-*co*-poly(NBE)$_{ROMP}$ produced by **Hf-1**/MAO at 50ºC in 1,1,2,2-tetrachloroentane-d_2.

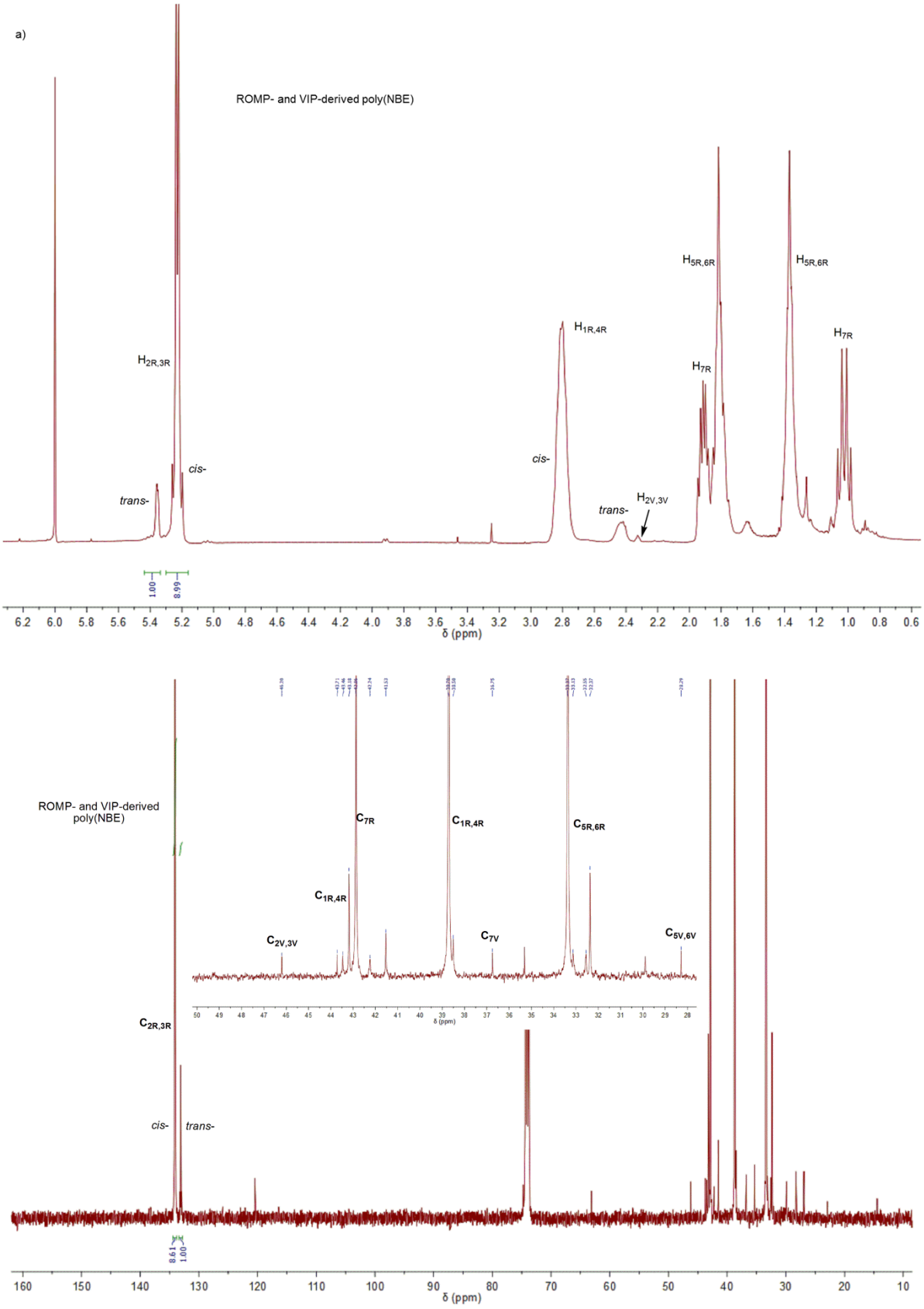


Figure S18. a) ^{1}H NMR and b) ^{13}C NMR spectra of poly(NBE)$_{VIP}$-*co*-poly(NBE)$_{ROMP}$ produced by **Hf-1**/MAO at 65ºC in 1,1,2,2-tetrachloroentane-d$_2$.

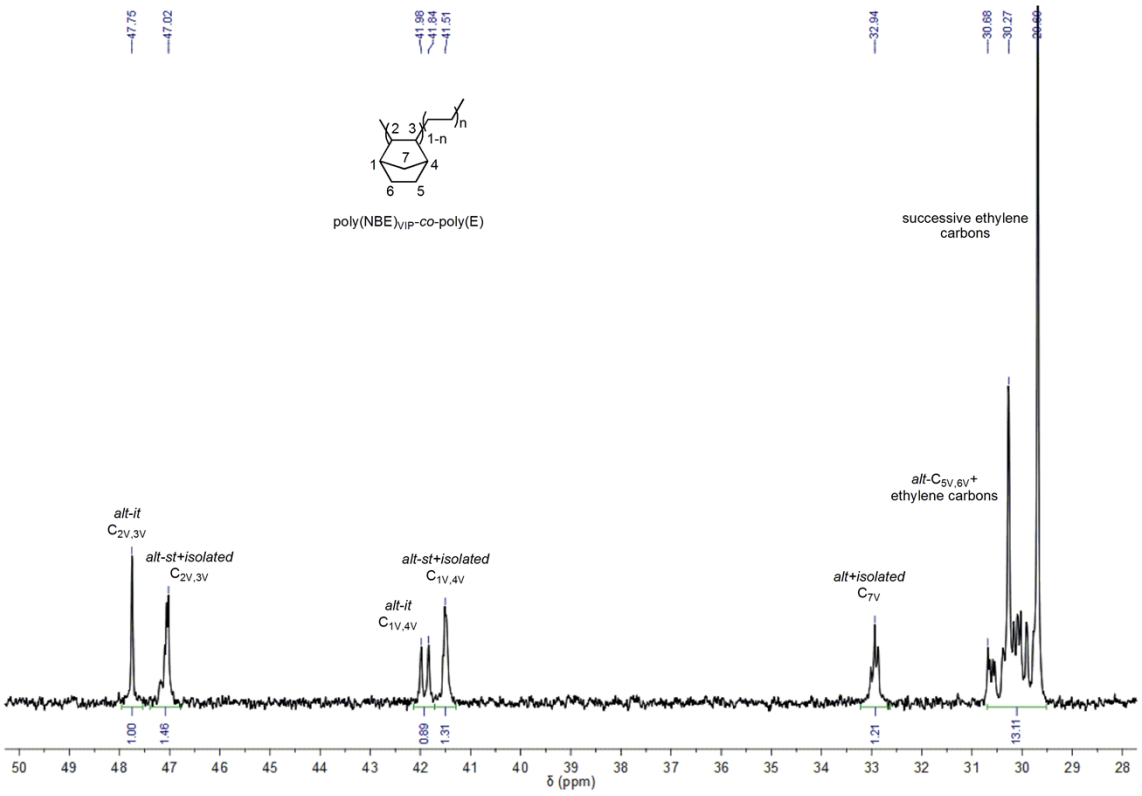


Figure S19. ^{13}C NMR spectrum of poly(E)-*co*-poly(NBE)$_{VIP}$ produced by **Hf-1**/MAO (Table 2, entry 9) in 1,1,2,2-tetrachloroethane-d_2.

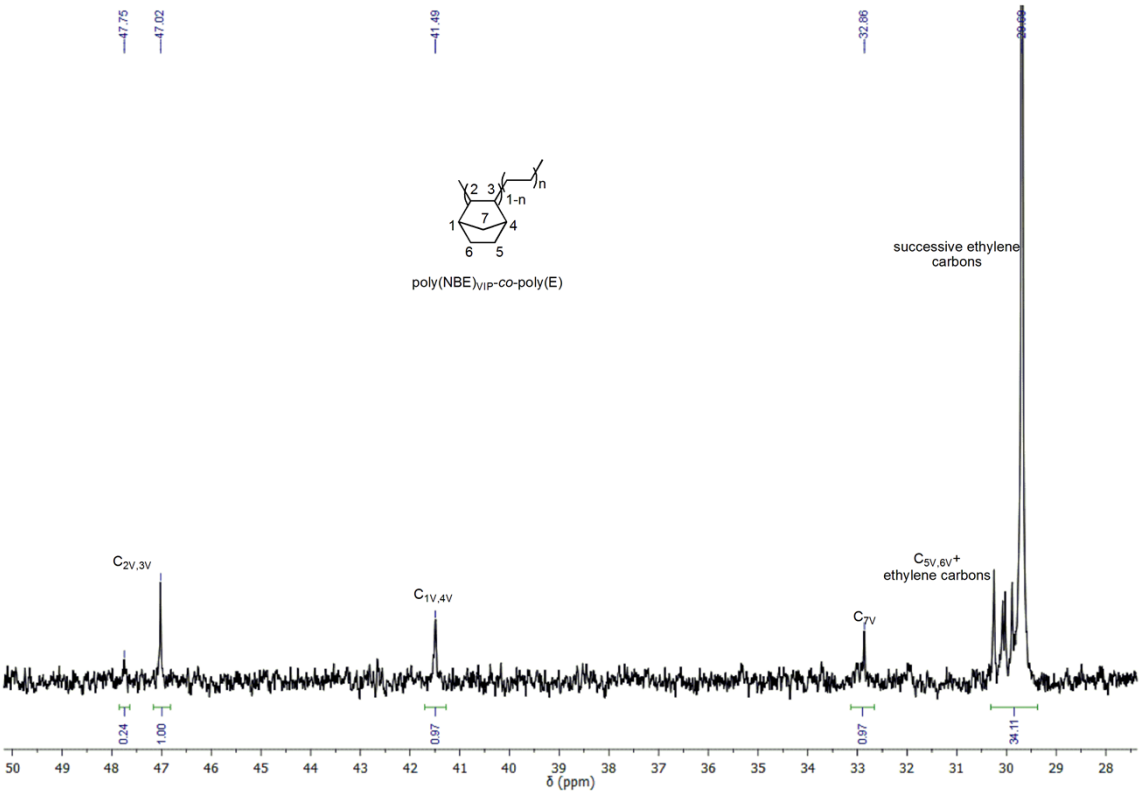


Figure S20. ^{13}C NMR spectrum of poly(E)-*co*-poly(NBE)$_{VIP}$ produced by **Zr-3**/MAO (Table 2, entry 10) in 1,1,2,2-tetrachloroethane-d_2.

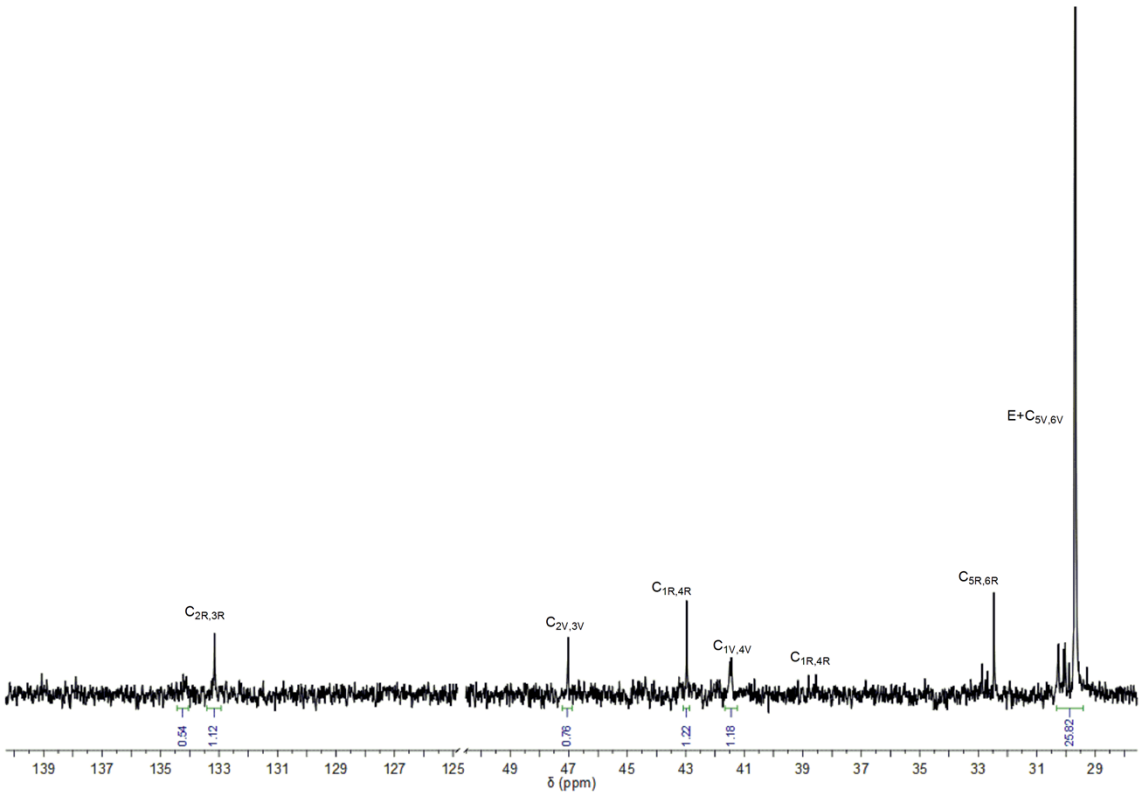


Figure S21. ^{13}C NMR spectrum of poly(E)-*co*-poly(NBE)$_{VIP}$-*co*-poly(NBE)$_{ROMP}$ produced by **Zr-2**/MAO (Table 2, entry 12) in 1,1,2,2-tetrachloroethane-d_2.

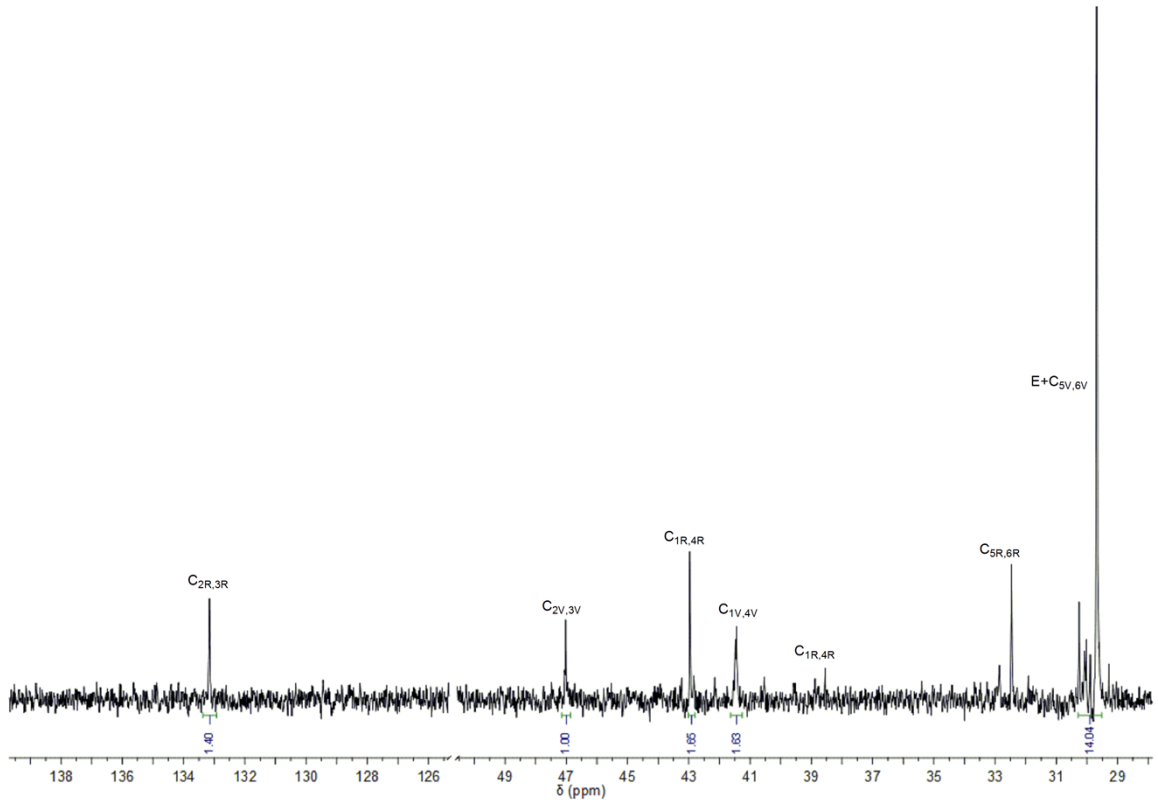


Figure S22. ^{13}C NMR spectrum of poly(E)-*co*-poly(NBE)$_{VIP}$-*co*-poly(NBE)$_{ROMP}$ produced by **Zr-2**/MAO (Table 2, entry 13) in 1,1,2,2-tetrachloroethane-d_2.

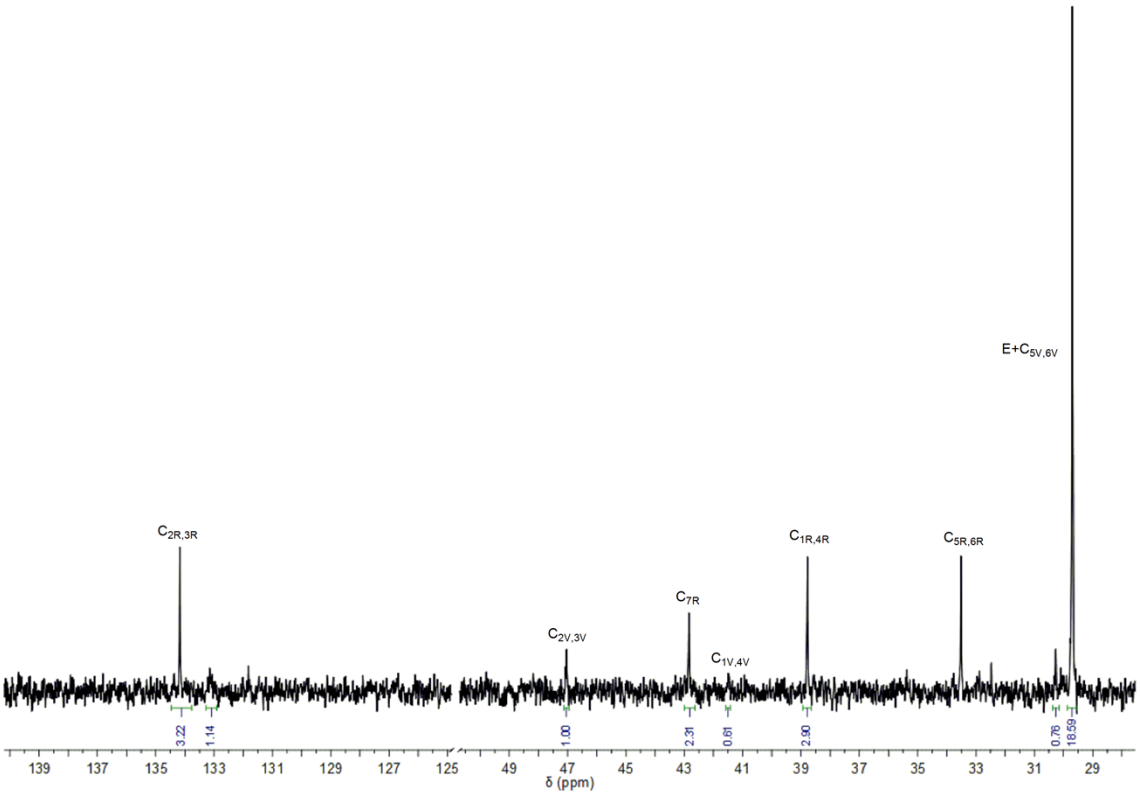


Figure S23. ^{13}C NMR spectrum of poly(E)-*co*-poly(NBE)$_{VIP}$-*co*-poly(NBE)$_{ROMP}$ produced by **Zr-2**/MAO (Table 2, entry 14) in 1,1,2,2-tetrachloroethane-d_2.

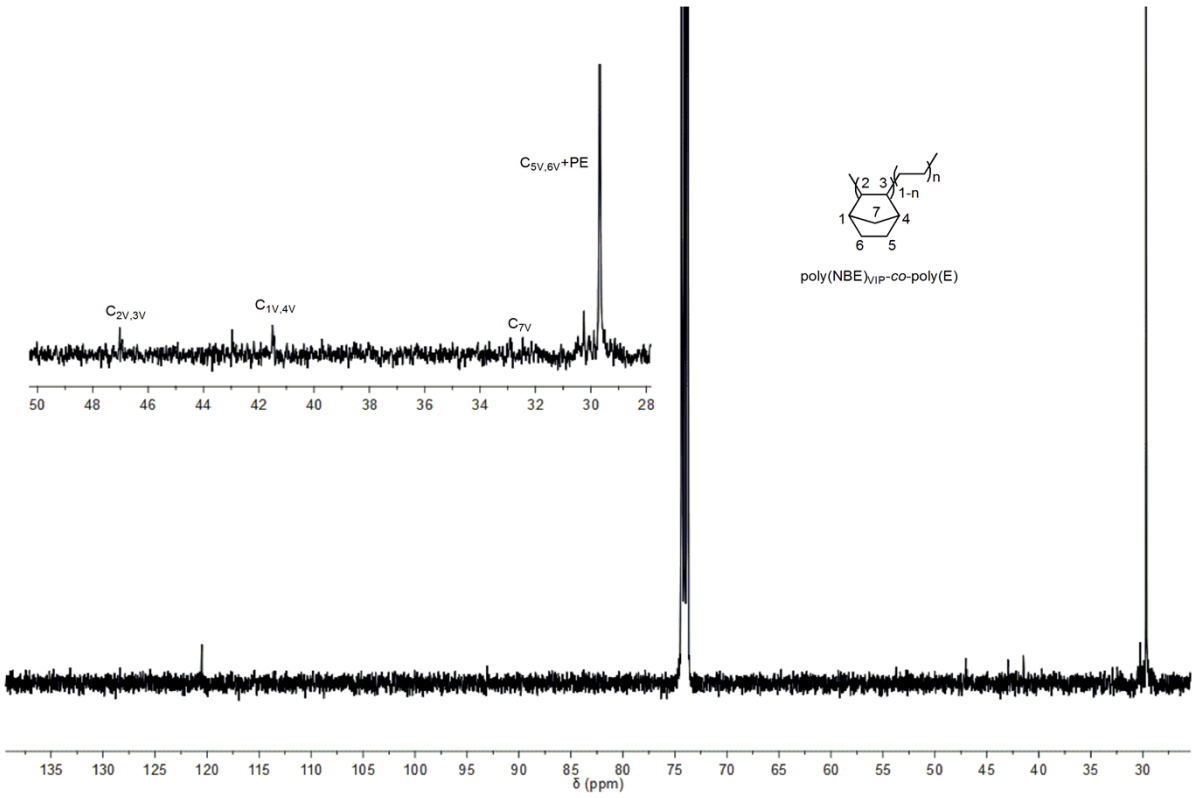


Figure S24. ^{13}C NMR spectrum of poly(E)-*co*-poly(NBE)$_{VIP}$ produced by **Zr-2**/MAO (Table 2, entry 16) in 1,1,2,2-tetrachloroethane-d_2.

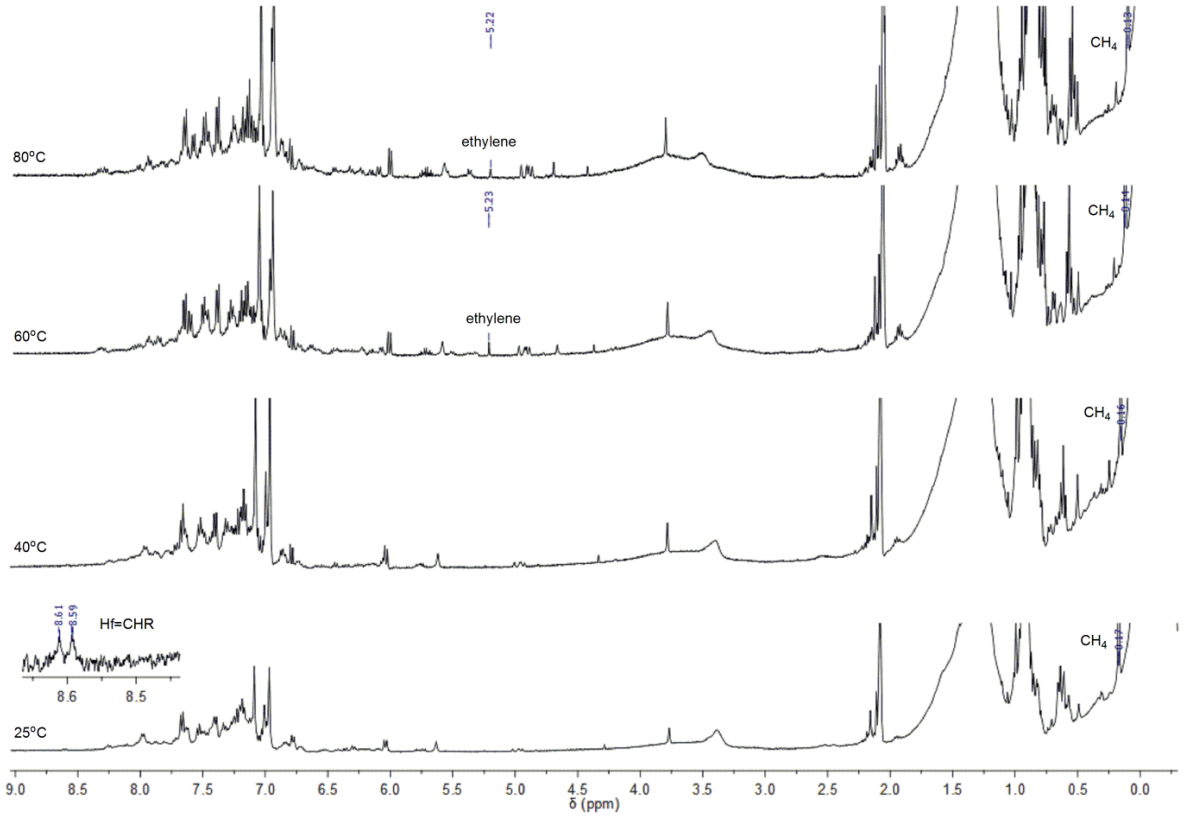
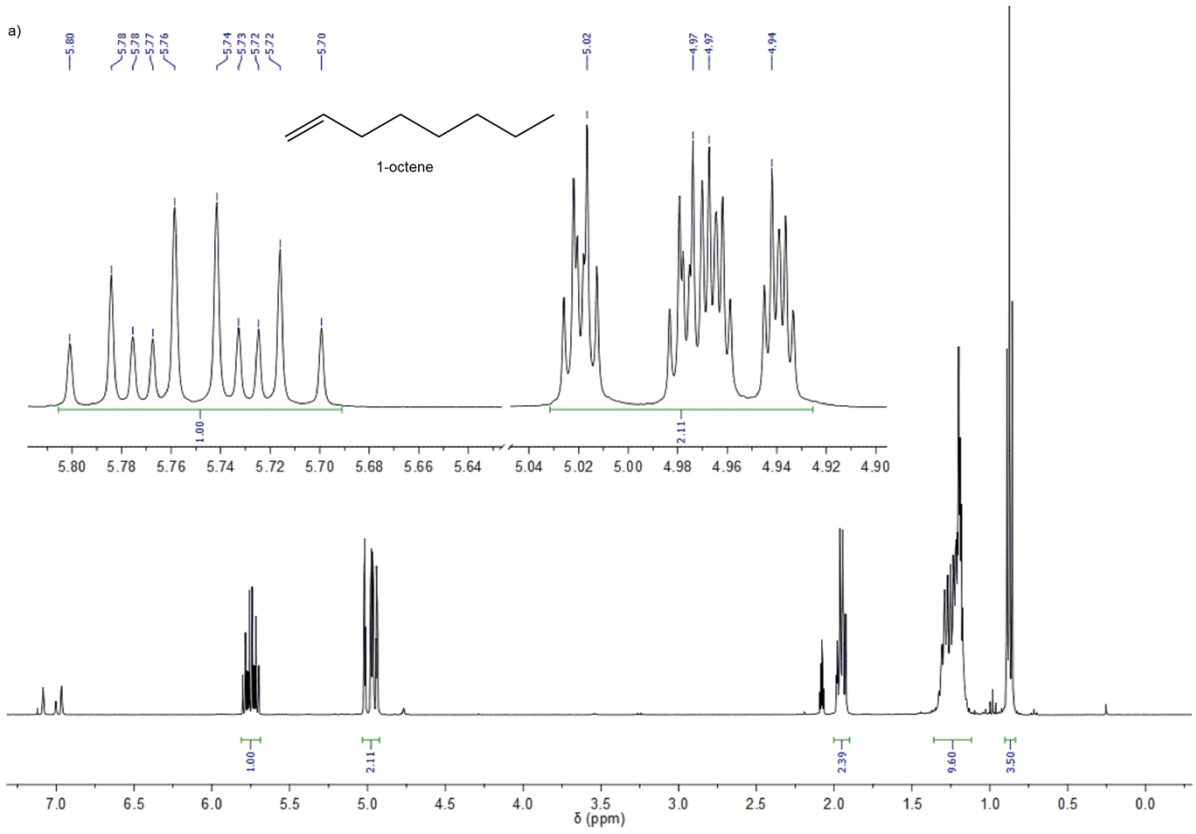


Figure S25. Variable-temperature ^{1}H NMR spectra of **Hf-1**/MAO in toluene-d_8 (25-80ºC).



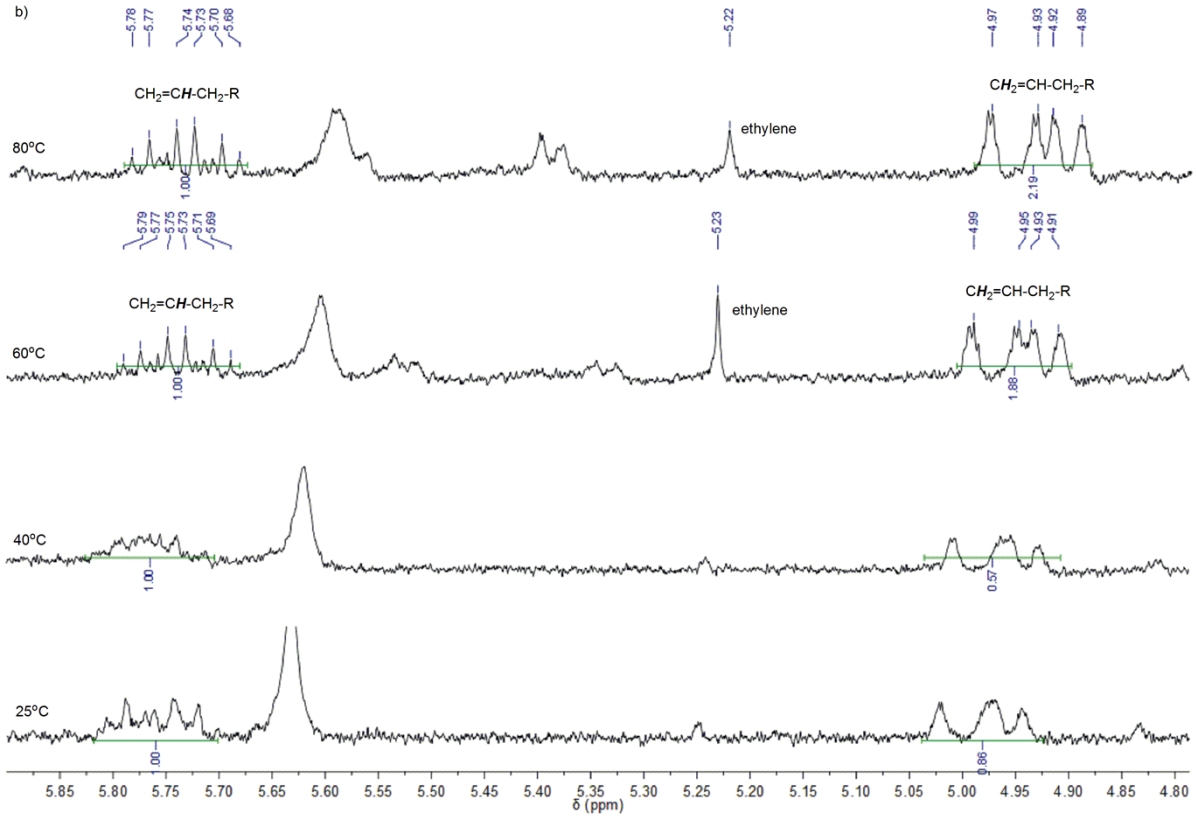


Figure S26. a) ^{1}H NMR spectrum of 1-octene in toluene-d_8 at 60ºC and b) Variable-temperature ^{1}H NMR spectra of **Hf-1**/MAO in toluene-d_8 (4.80-5.85 ppm, 25-80ºC).

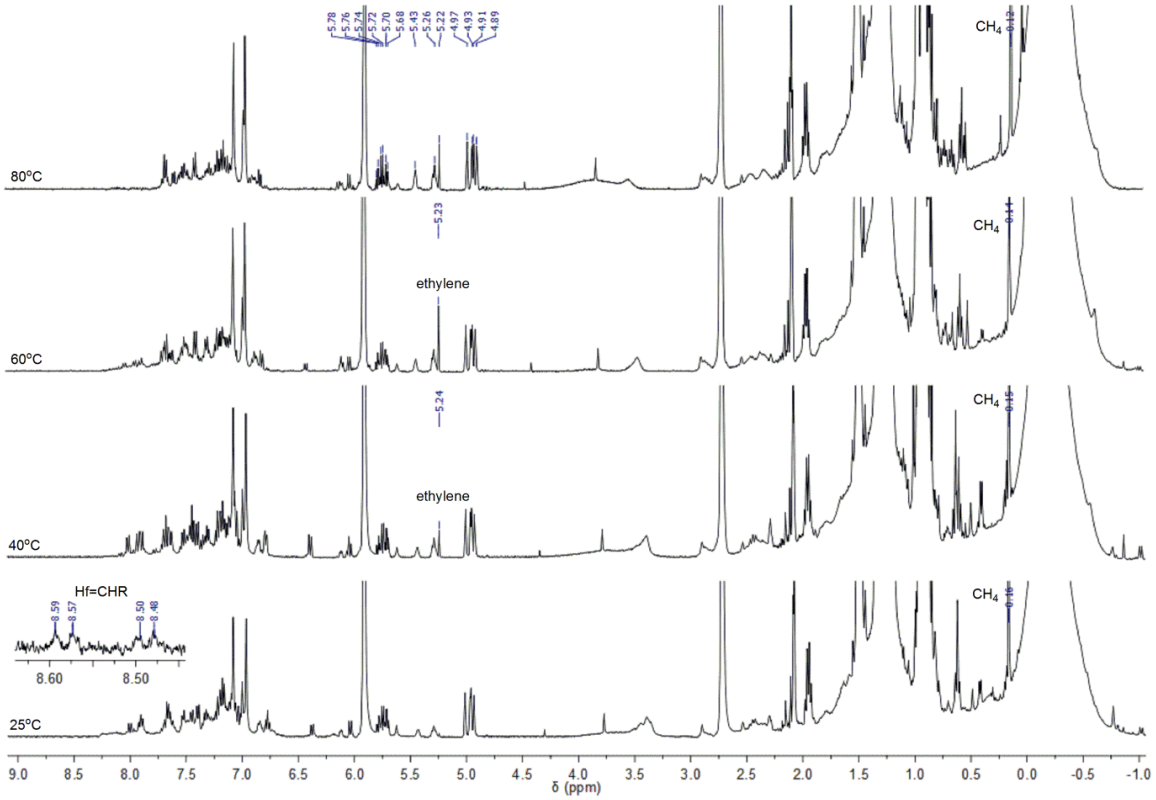


Figure S27. Variable-temperature ^{1}H NMR spectra of **Hf-1**/MAO/NBE in toluene-d_8 (25-80ºC).

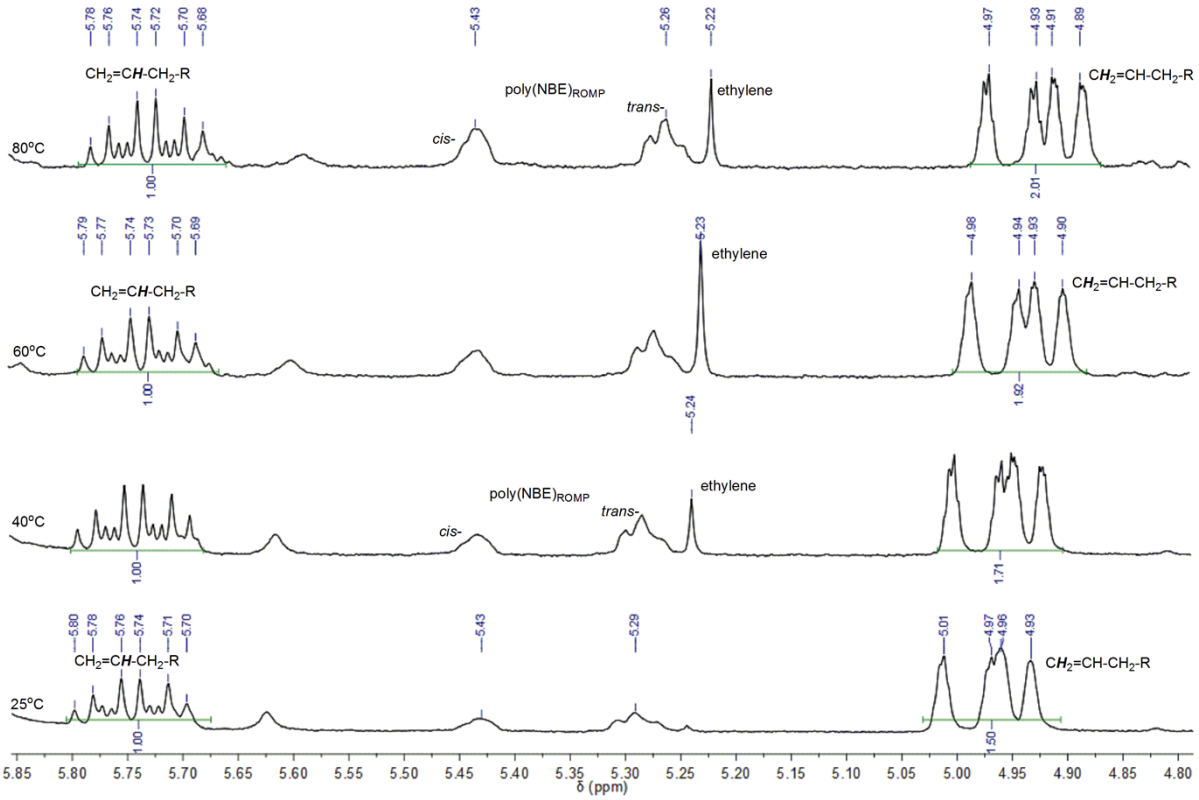


Figure S28. Variable-temperature ^{1}H NMR spectra of **Hf-1**/MAO/NBE in toluene-d_8 (4.80-5.85 ppm, 25-80ºC).

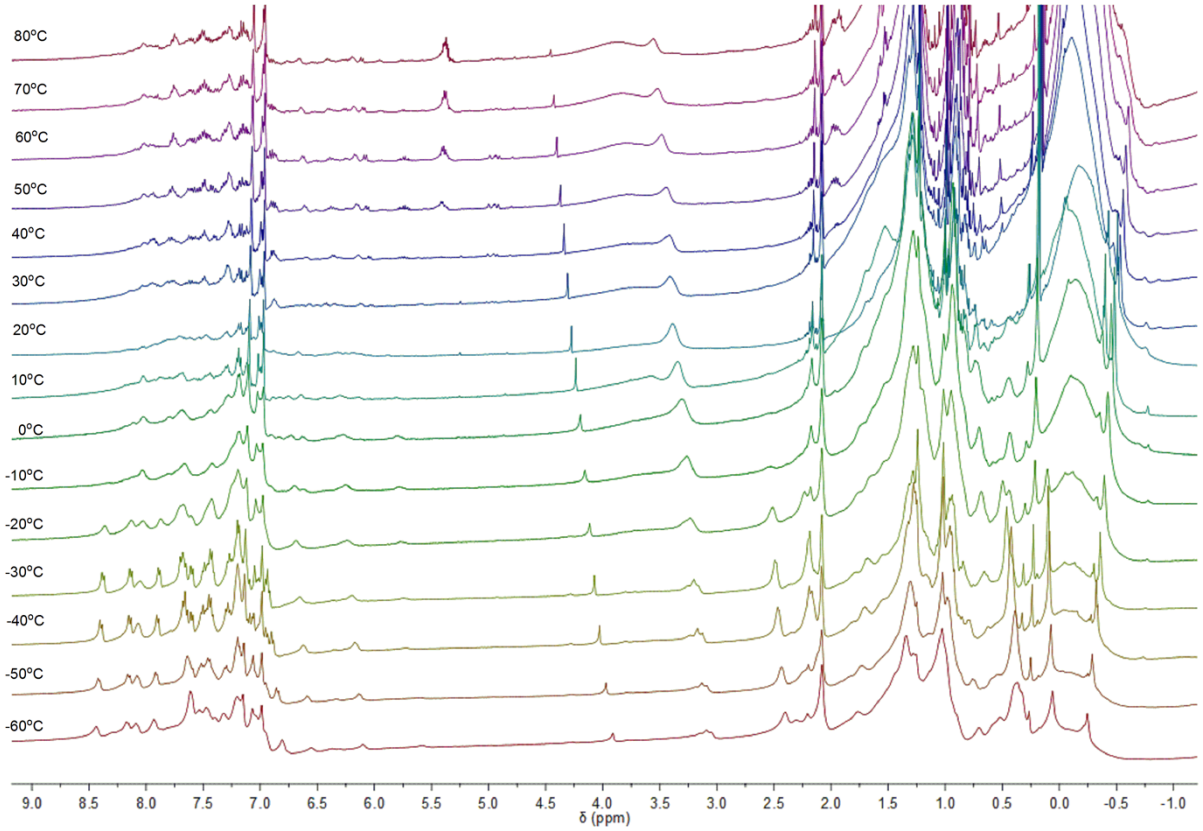


Figure S29. Variable-temperature ^{1}H NMR spectra of **Zr-1**/MAO in toluene-d_8 (-60-80ºC).

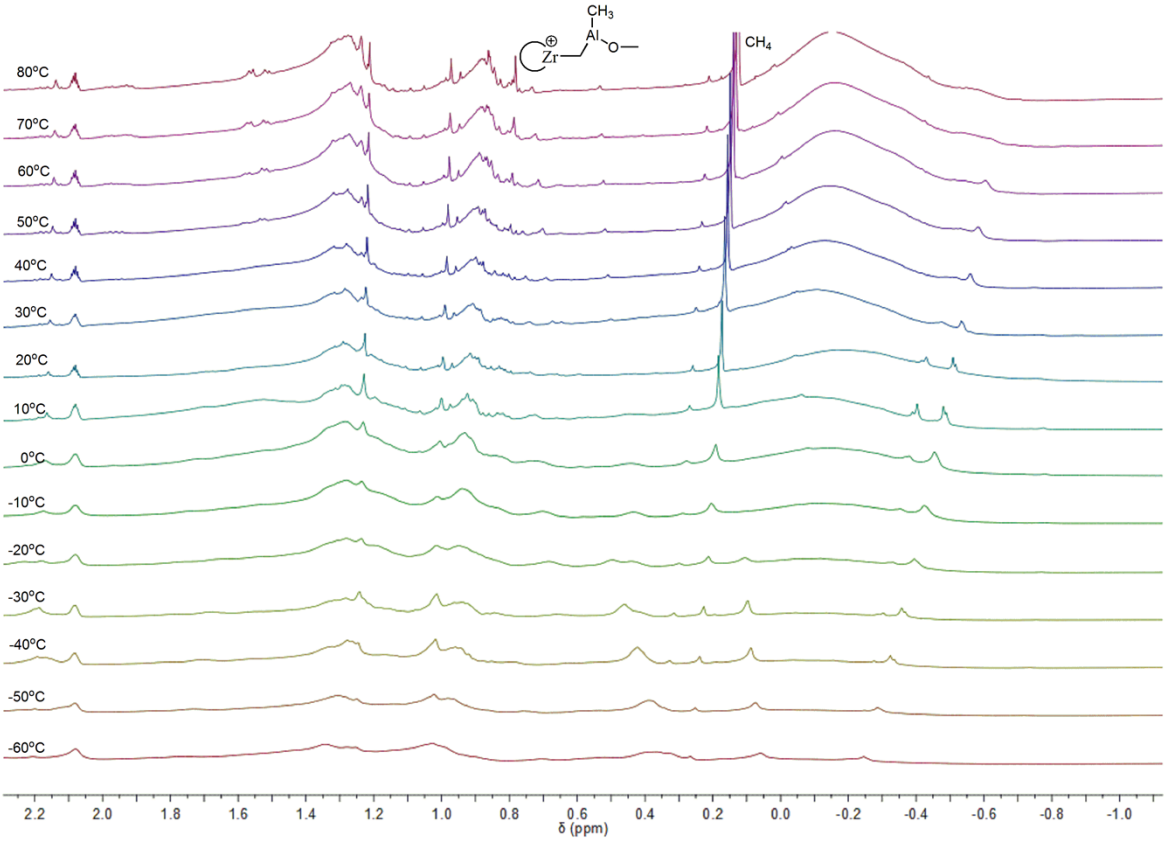


Figure S30. Variable-temperature ^{1}H NMR spectra of **Zr-1**/MAO in toluene-d_8 (-1.0-2.2 ppm, -60-80ºC).

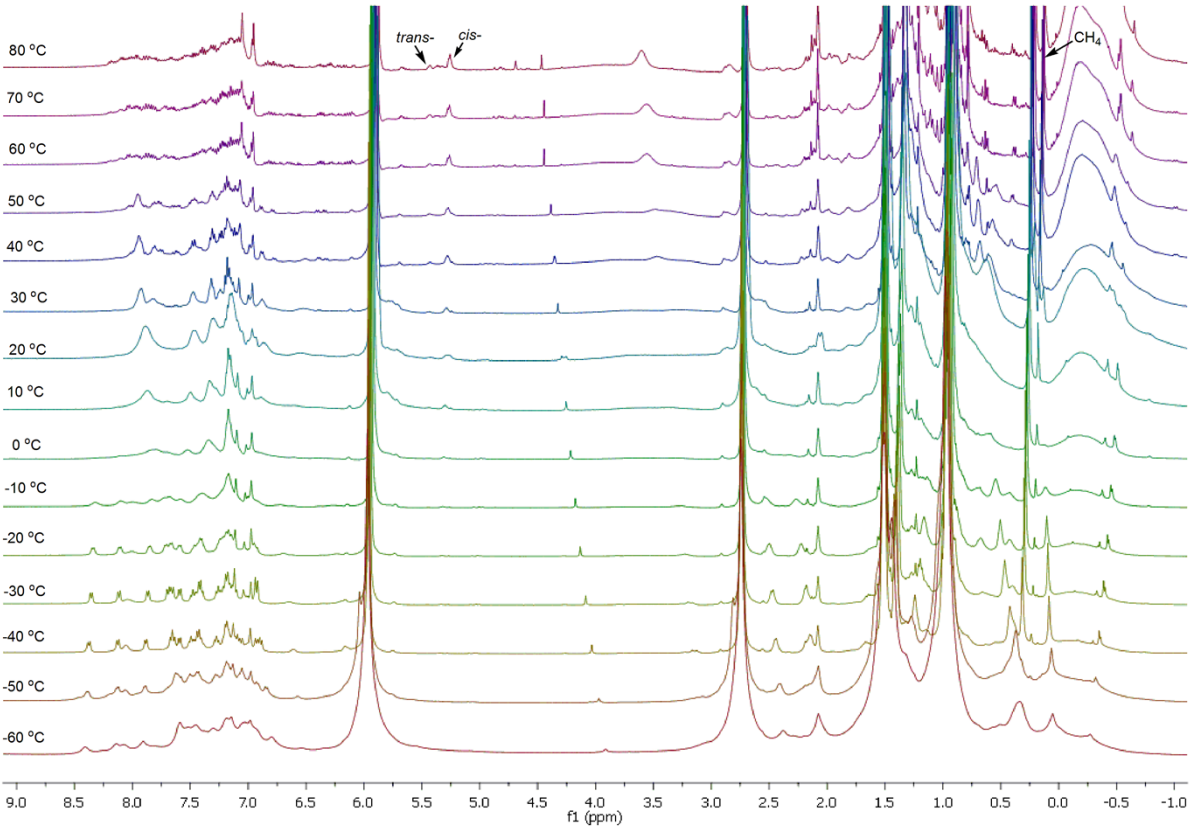


Figure S31. Variable-temperature ^{1}H NMR spectra of **Zr-1**/MAO/NBE in toluene-d_8 (-60-80ºC).

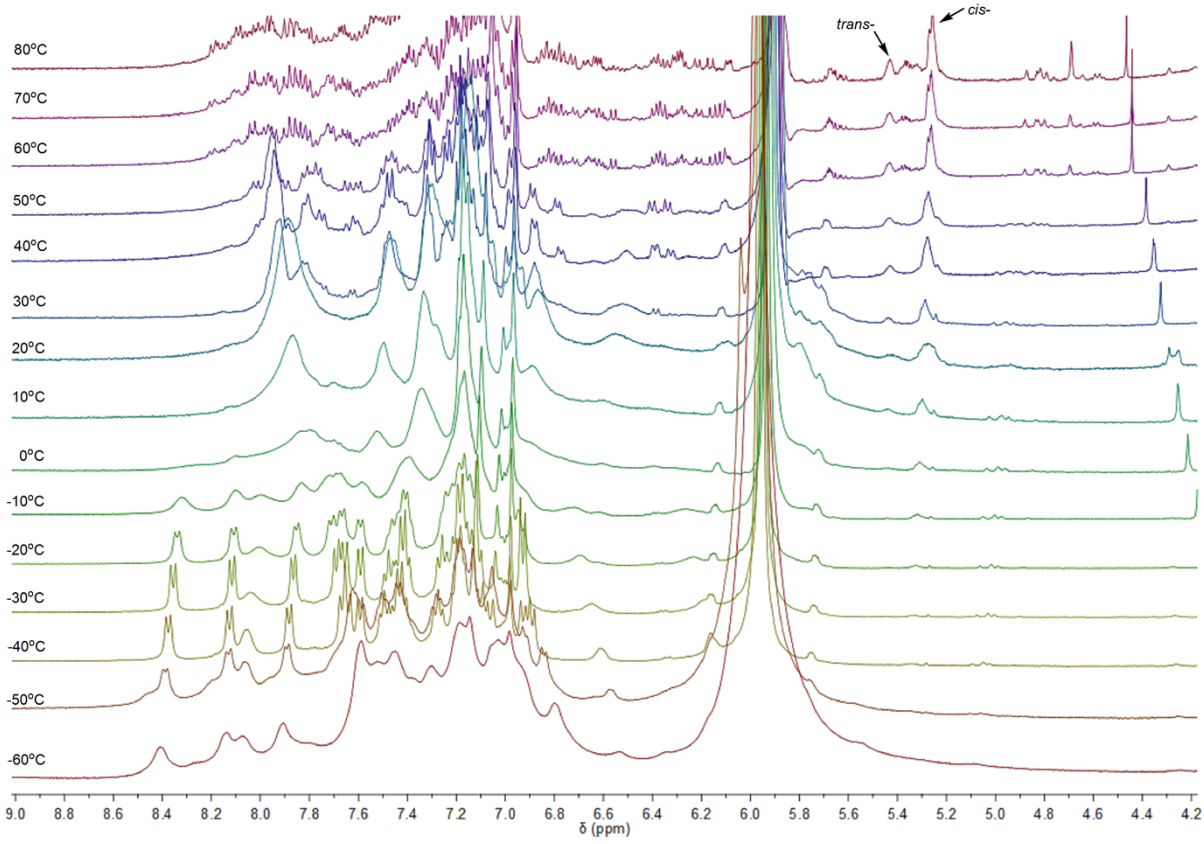


Figure S32. Variable-temperature ^{1}H NMR spectra of **Zr-1**/MAO/NBE in toluene-d_8 (4.2-9.0 ppm, -60-80ºC).

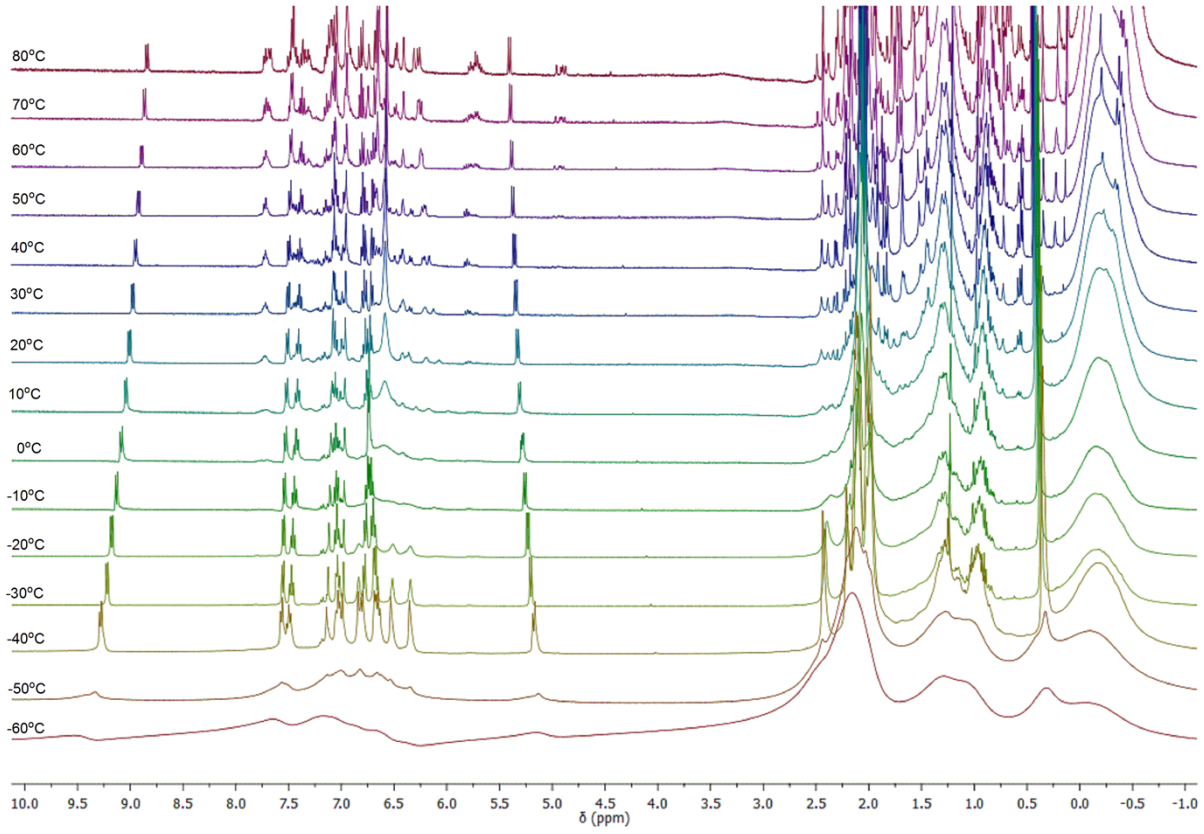


Figure S33. Variable-temperature ^{1}H NMR spectra of **Zr-2**/MAO in toluene-d_8 (-60-80ºC).

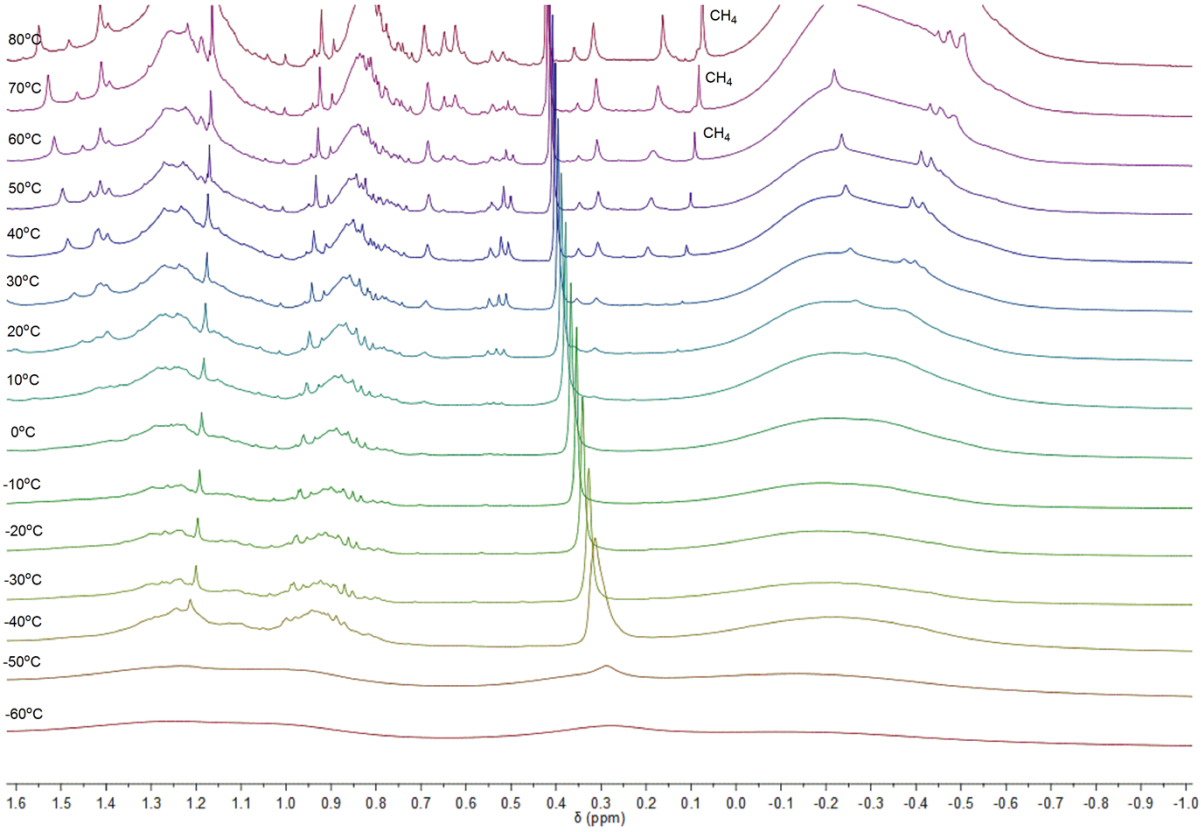


Figure S34. Variable-temperature ^{1}H NMR spectra of **Zr-2**/MAO in toluene-d_8 (-1.0-1.6 ppm, -60-80ºC).

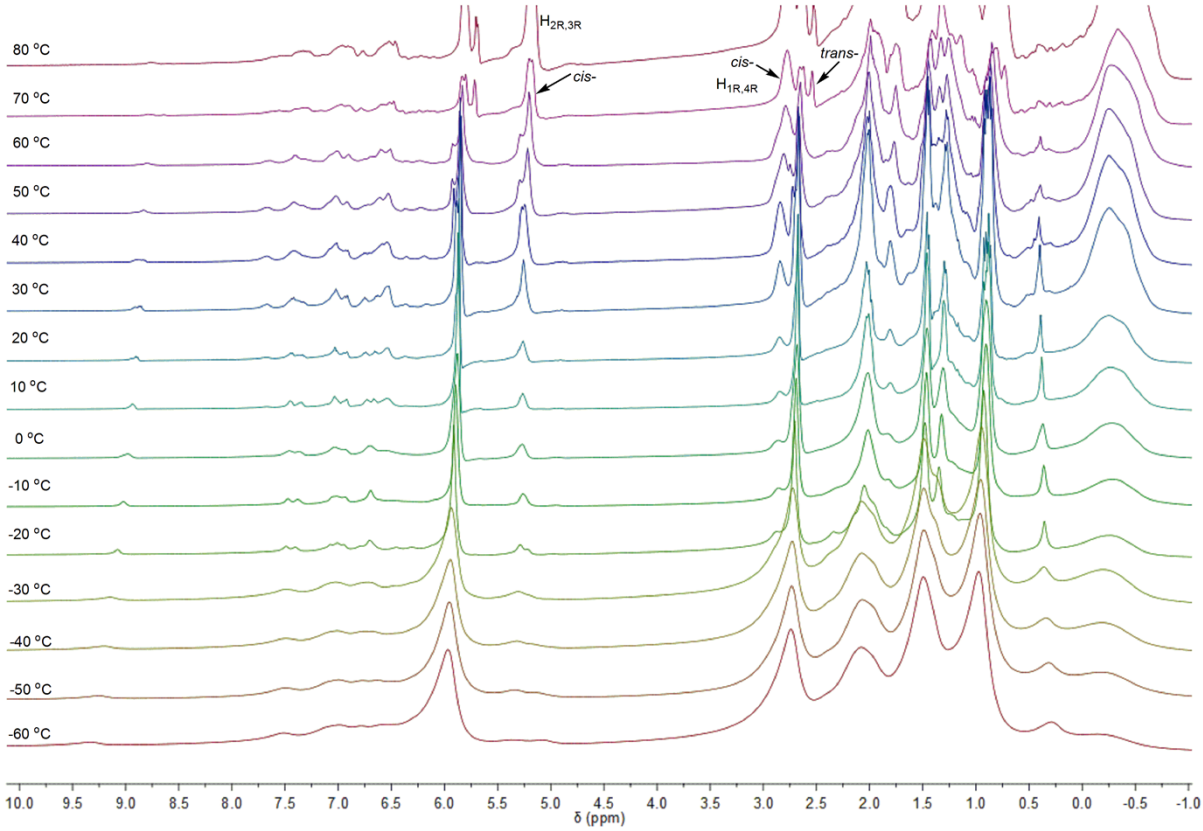


Figure S35. Variable-temperature ^{1}H NMR spectra of **Zr-2**/MAO/NBE in toluene-d_8 (-60-80ºC).

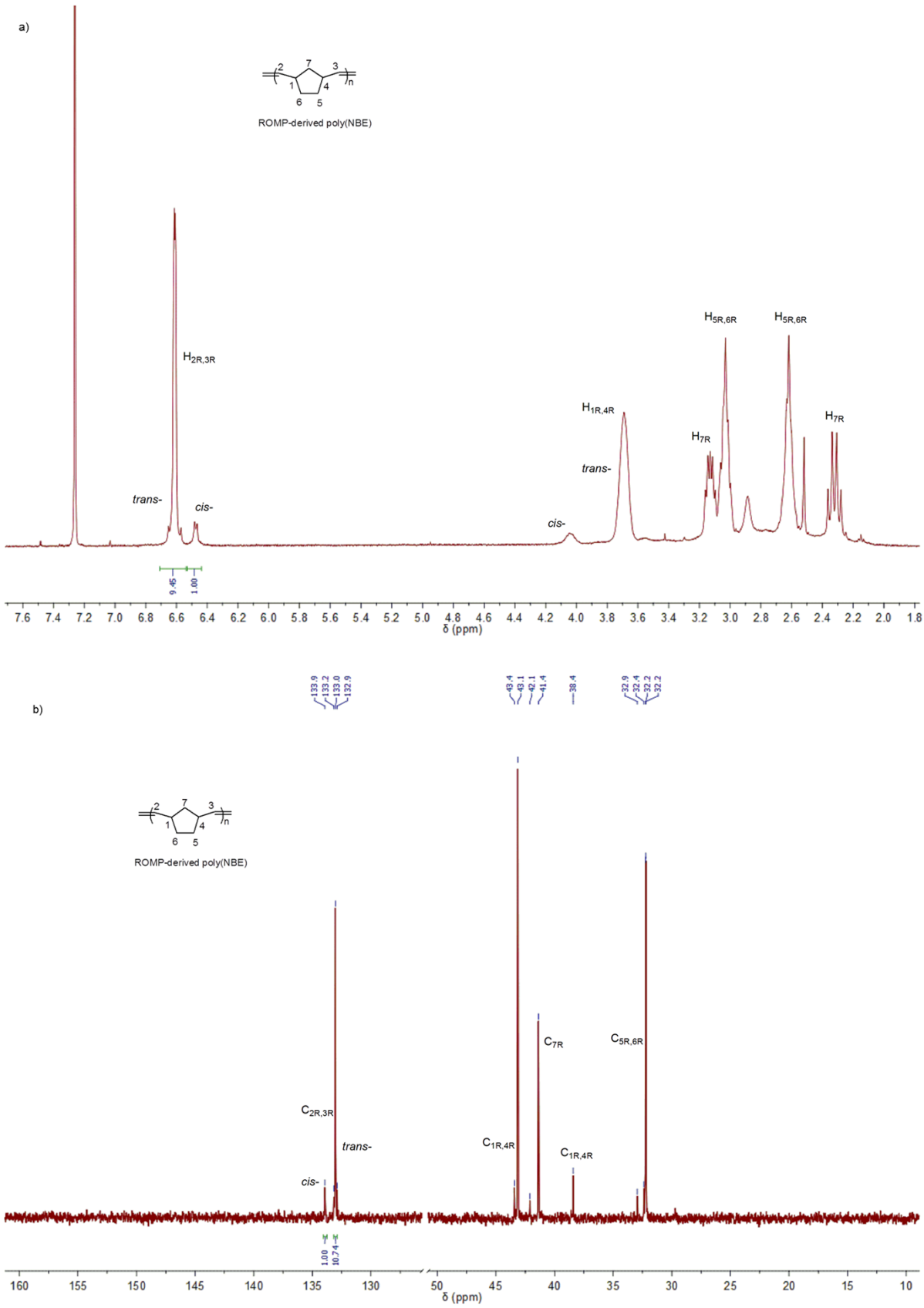


Figure S36. a) ^{1}H NMR and b) ^{13}C NMR spectra of poly(NBE)$_{ROMP}$ by **Zr-4**/MAO at 60ºC in $CDCl_3$.

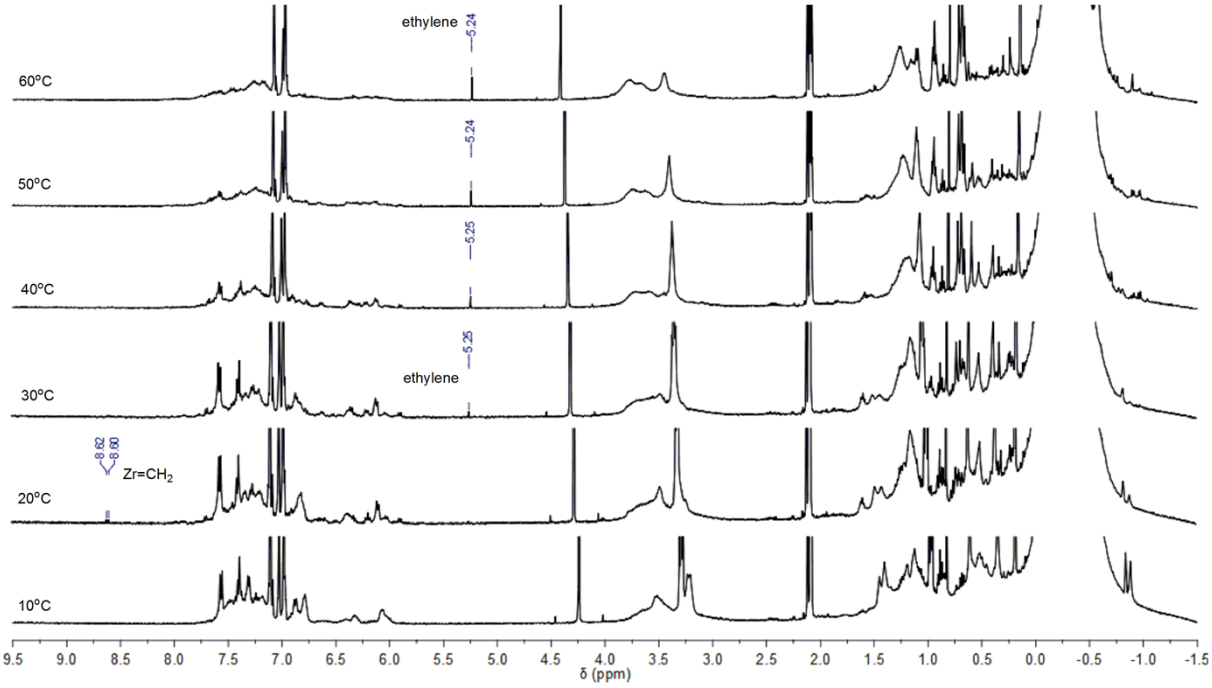


Figure S37. Variable-temperature ^{1}H NMR spectra of **Zr-4**/MAO in toluene-d_8 (10-60ºC).

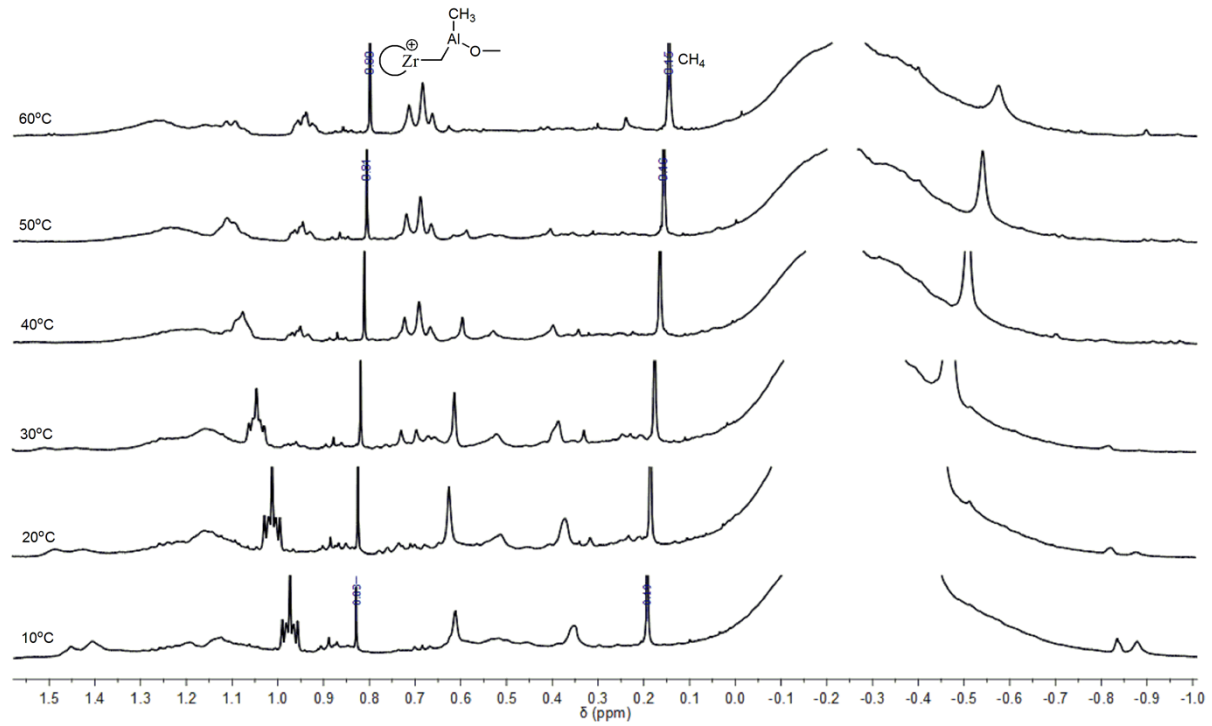


Figure S38. Variable-temperature ^{1}H NMR spectra of **Zr-4**/MAO in toluene-d_8 (-1.0-1.5 ppm, 10-60ºC).

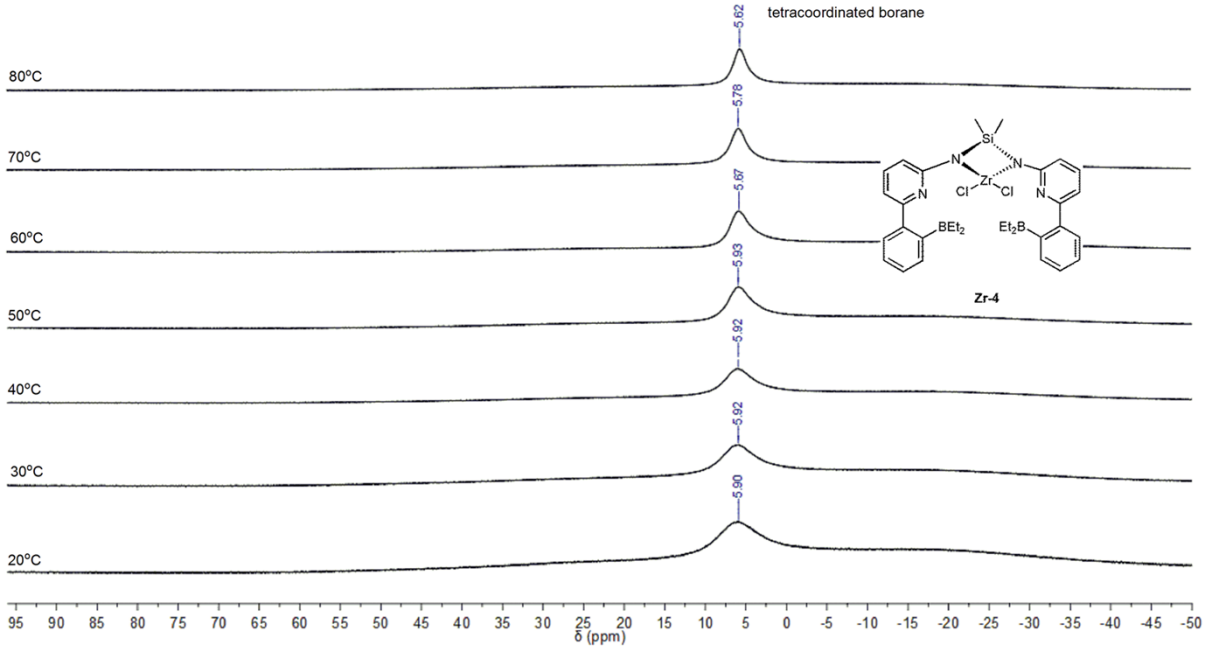


Figure S39. Variable-temperature ^{11}B NMR spectra of **Zr-4** in toluene-d_8 (20-80ºC).

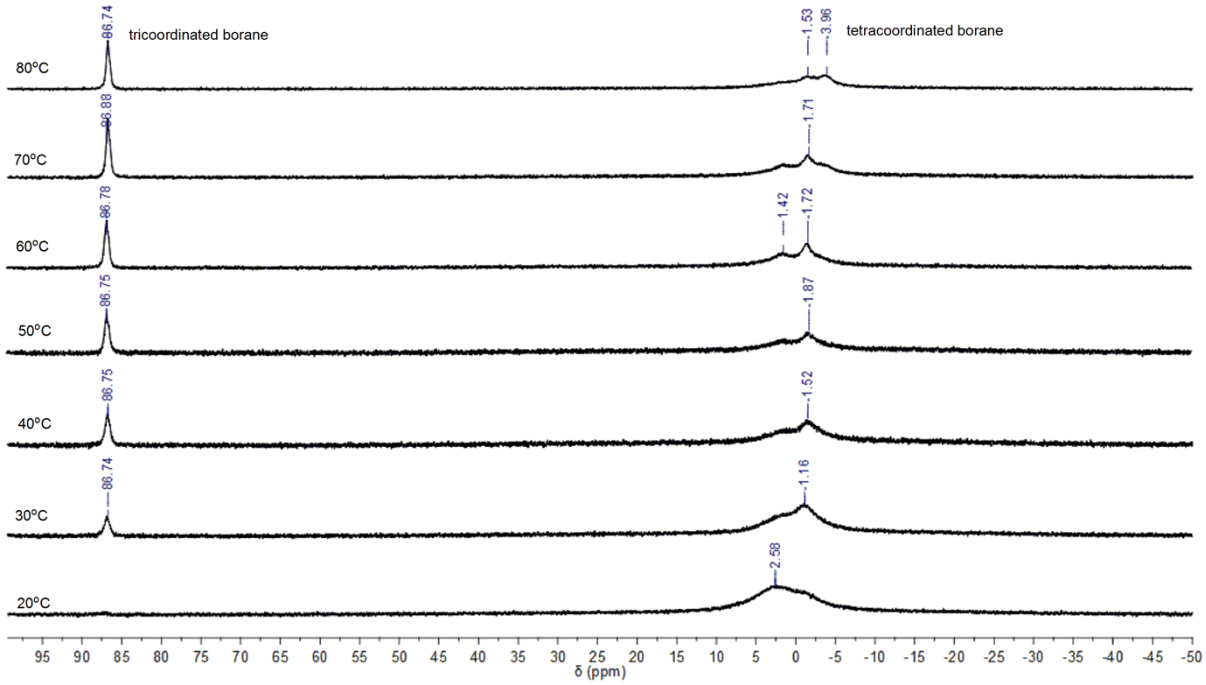


Figure S40. Variable-temperature ^{11}B NMR spectra of **Zr-4**/MAO in toluene-d_8 (20-80ºC).

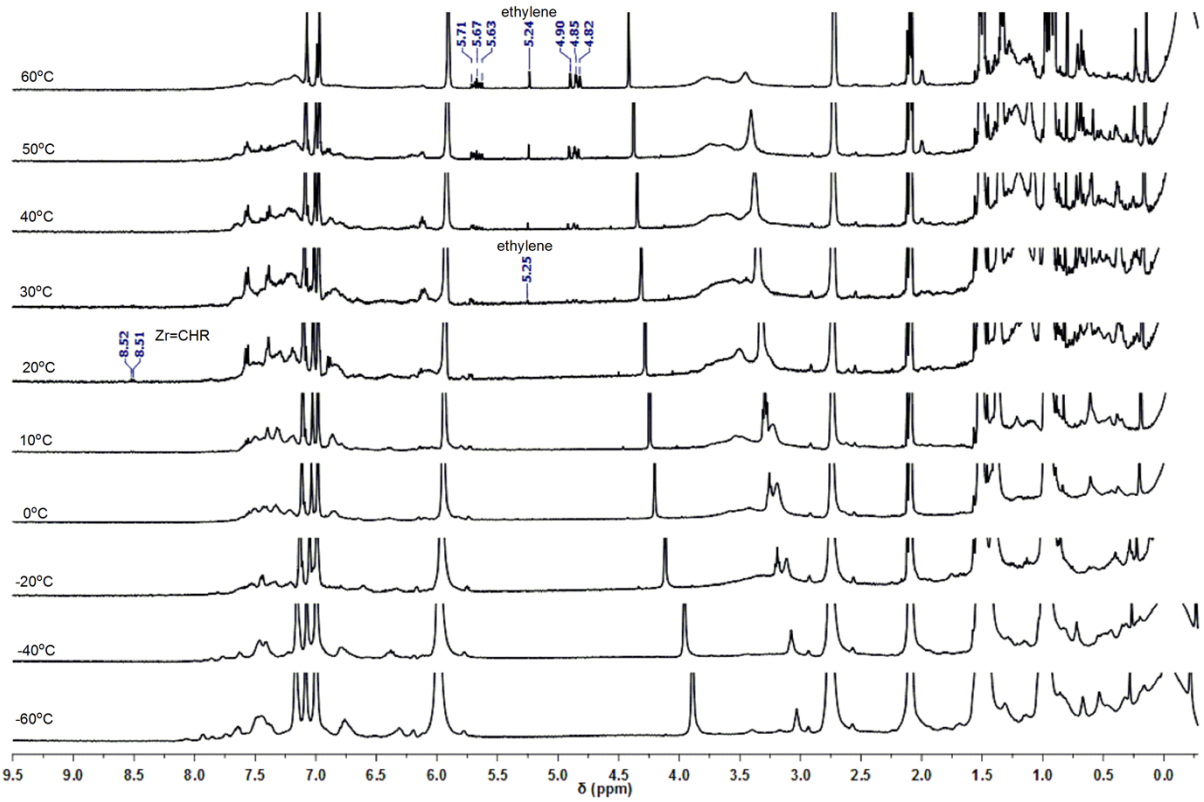


Figure S41. Variable-temperature ^{1}H NMR spectra of **Zr-4**/MAO/NBE in toluene-d_8 (-60-60ºC).

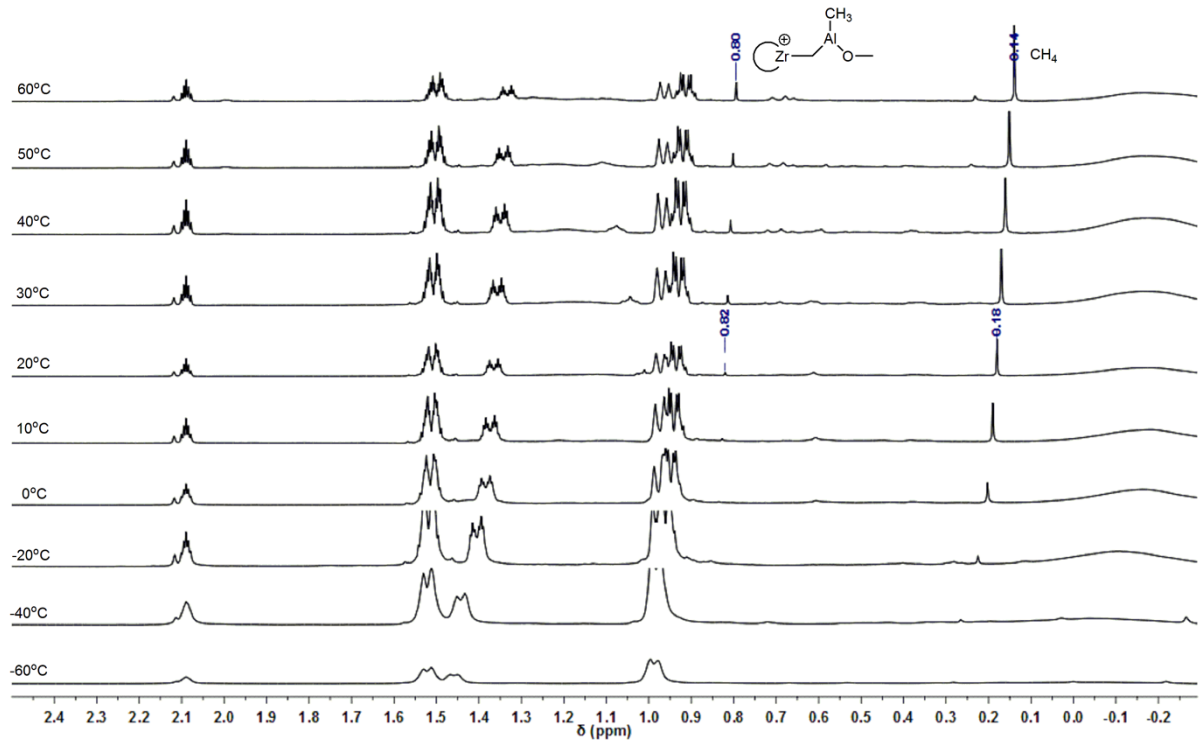


Figure S42. Variable-temperature ^{1}H NMR spectra of **Zr-4**/MAO/NBE in toluene-d_8 (-0.2-2.4 ppm, -60-60ºC).

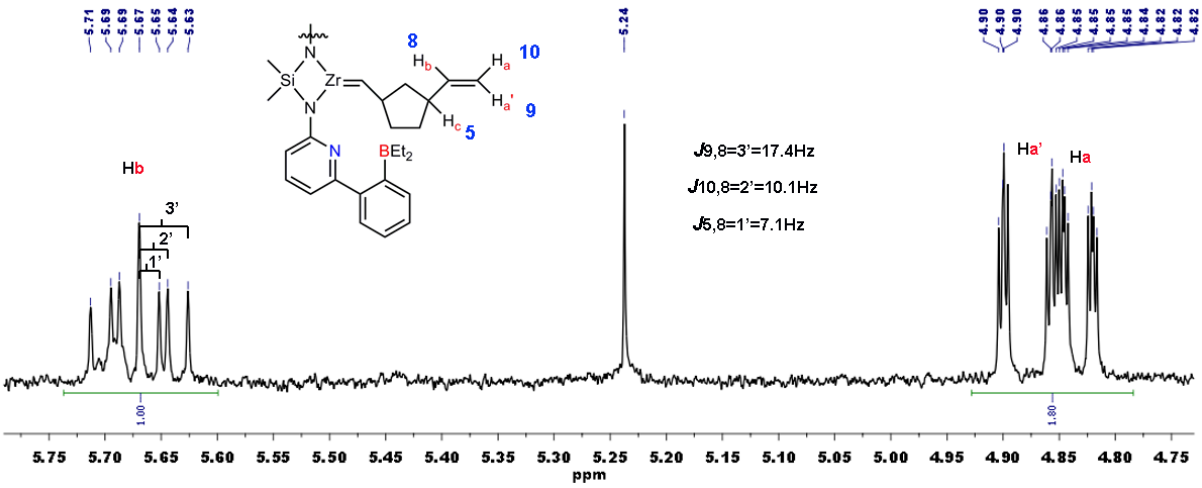


Figure S43. ^{1}H NMR spectrum of **Zr-4**/MAO/NBE in toluene-d_8(60°C, 4.75-5.75 ppm).

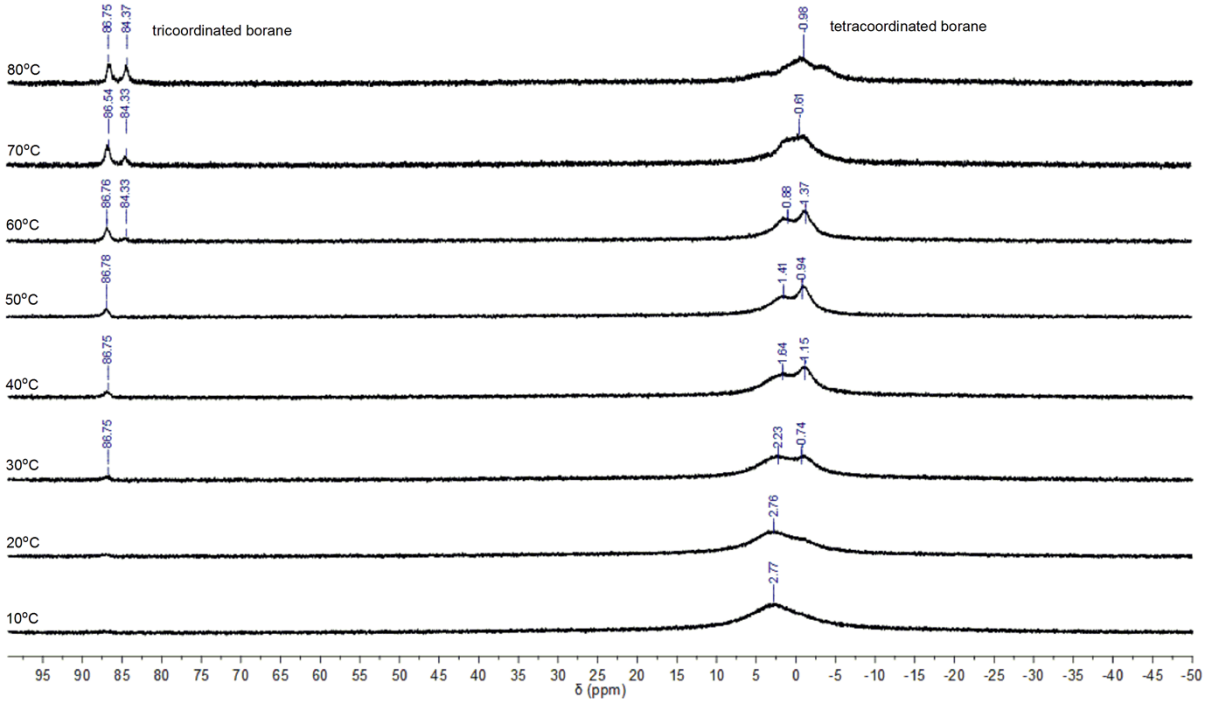


Figure S44. Variable-temperature ^{11}B NMR spectra of **Zr-4**/MAO/NBE in toluene-d_8 (10-80ºC).

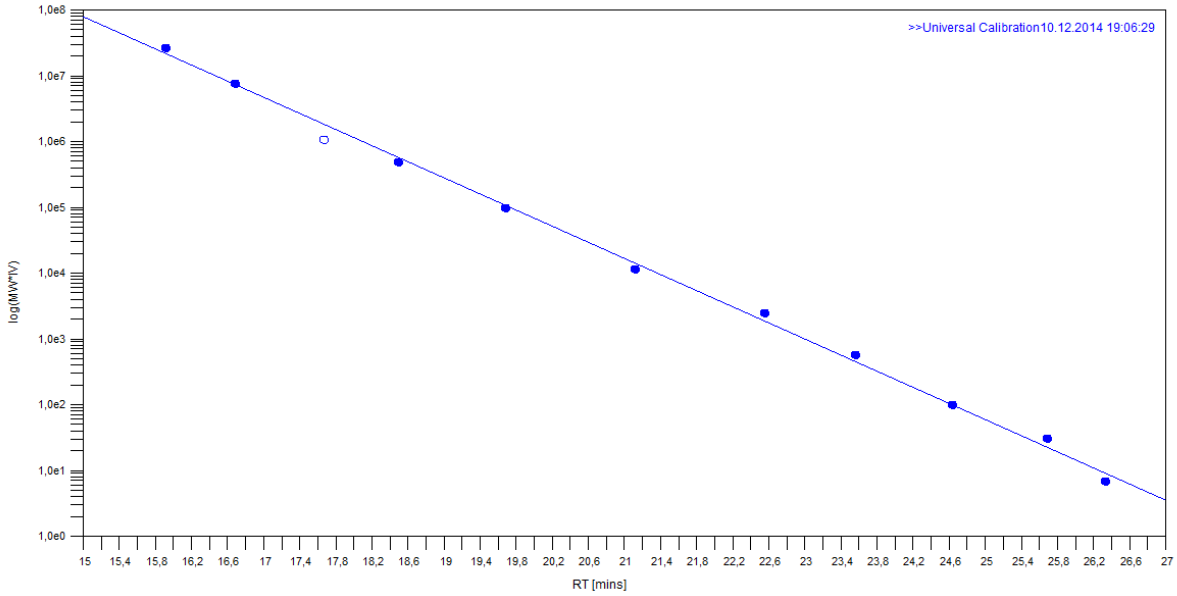


Figure S45. HT-GPC calibration curve with poly(stryrene) standards (162-6,035,000 g mol^{-1}).

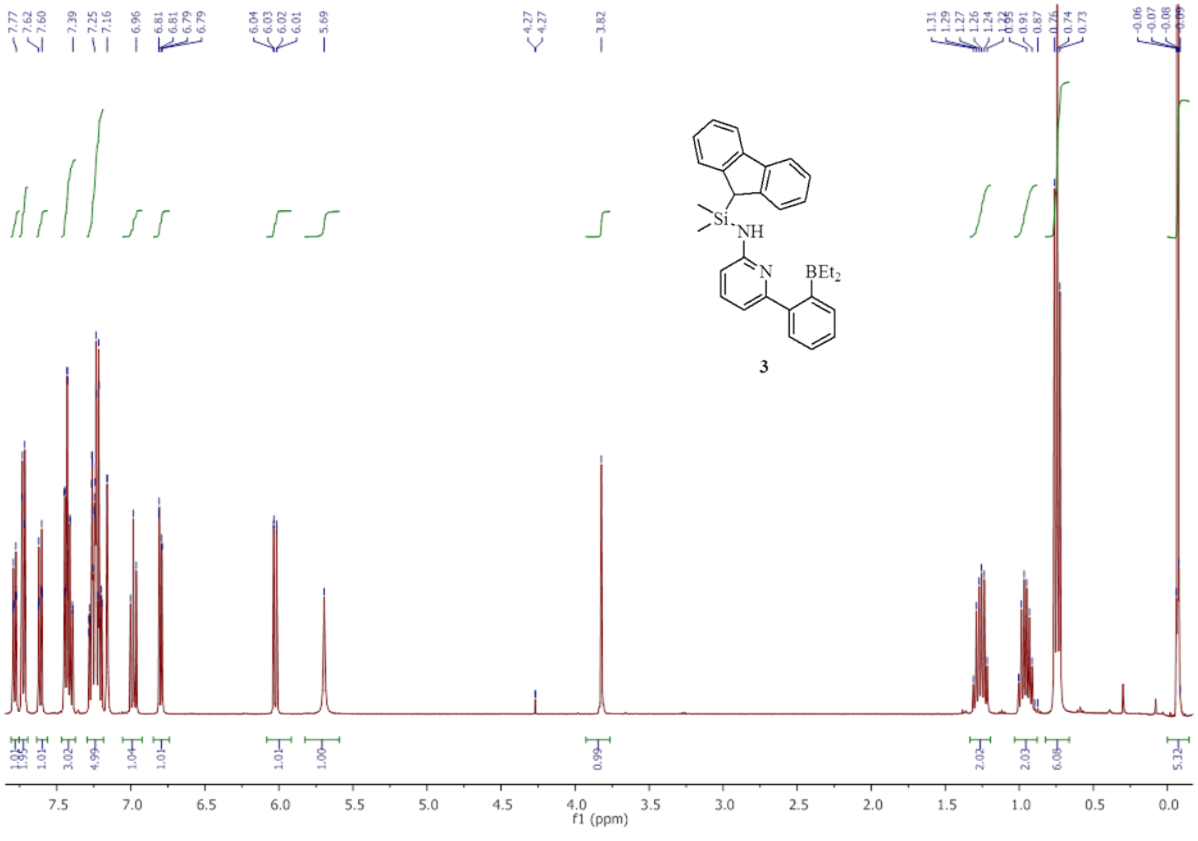


Figure S46. ^{1}H NMR of compound **3** in C_6D_6.

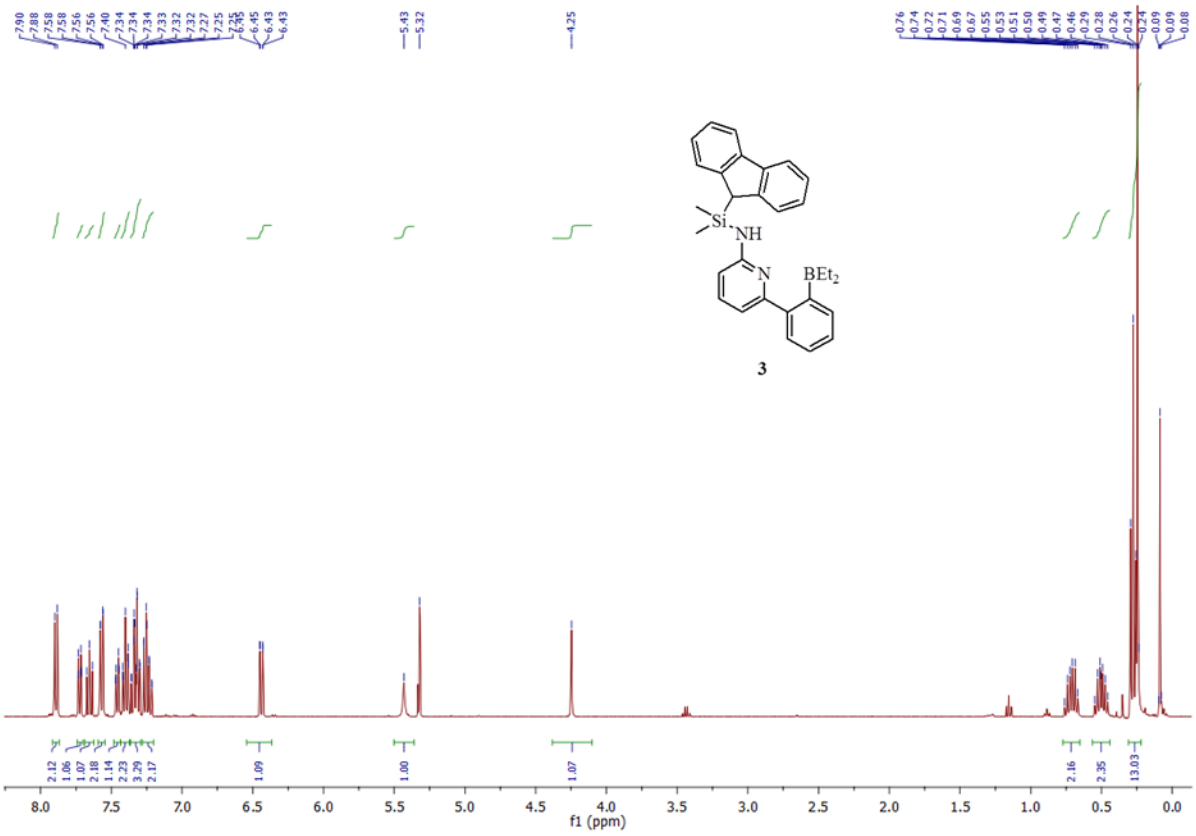


Figure S47. ^{1}H NMR of compound **3** in CD_2Cl_2.

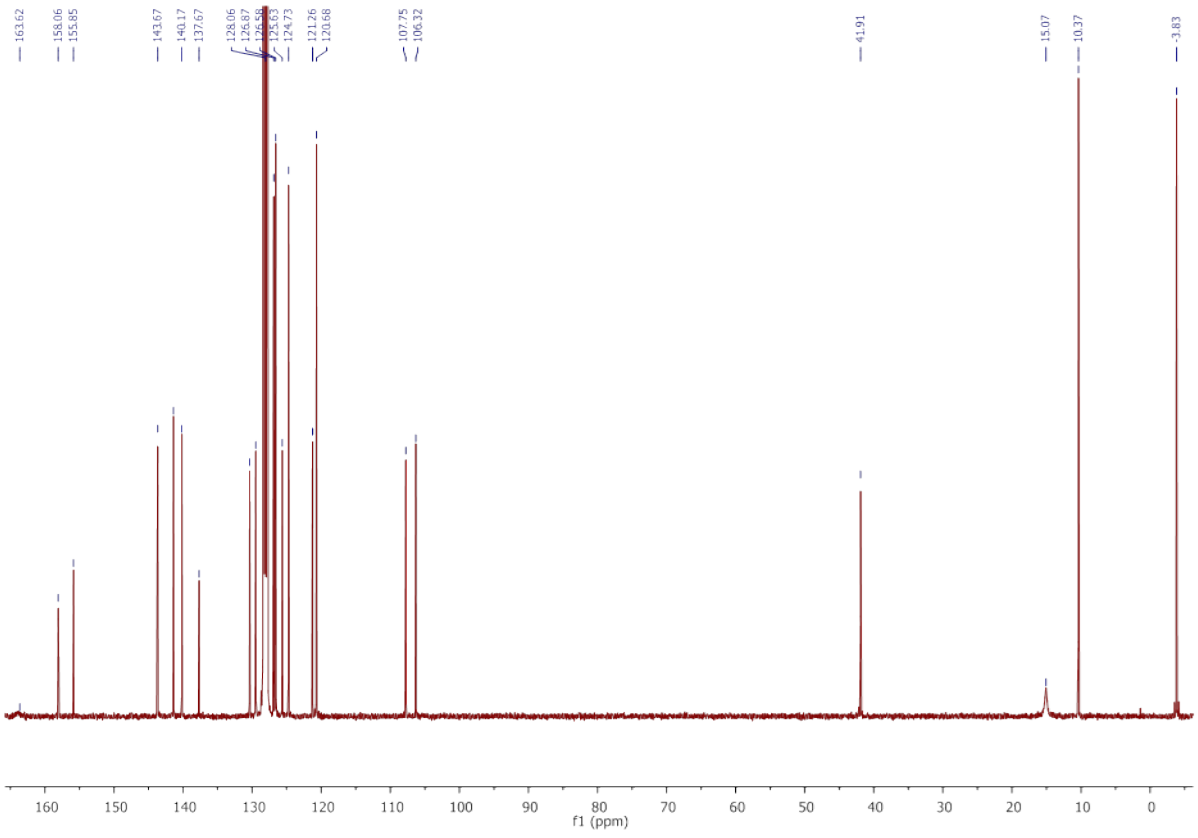


Figure S48. ^{13}C NMR of compound **3** in C_6D_6.

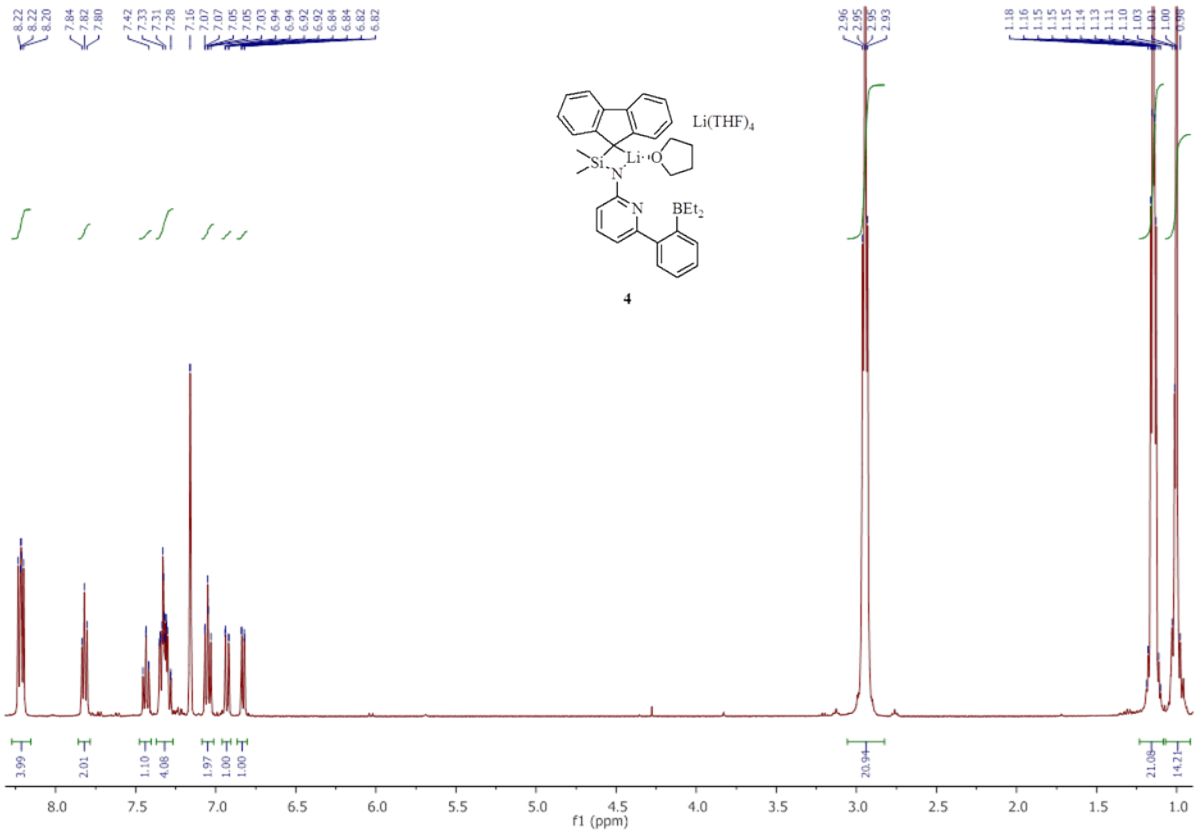


Figure S49. ^{1}H NMR of compound **4** in C_6D_6.

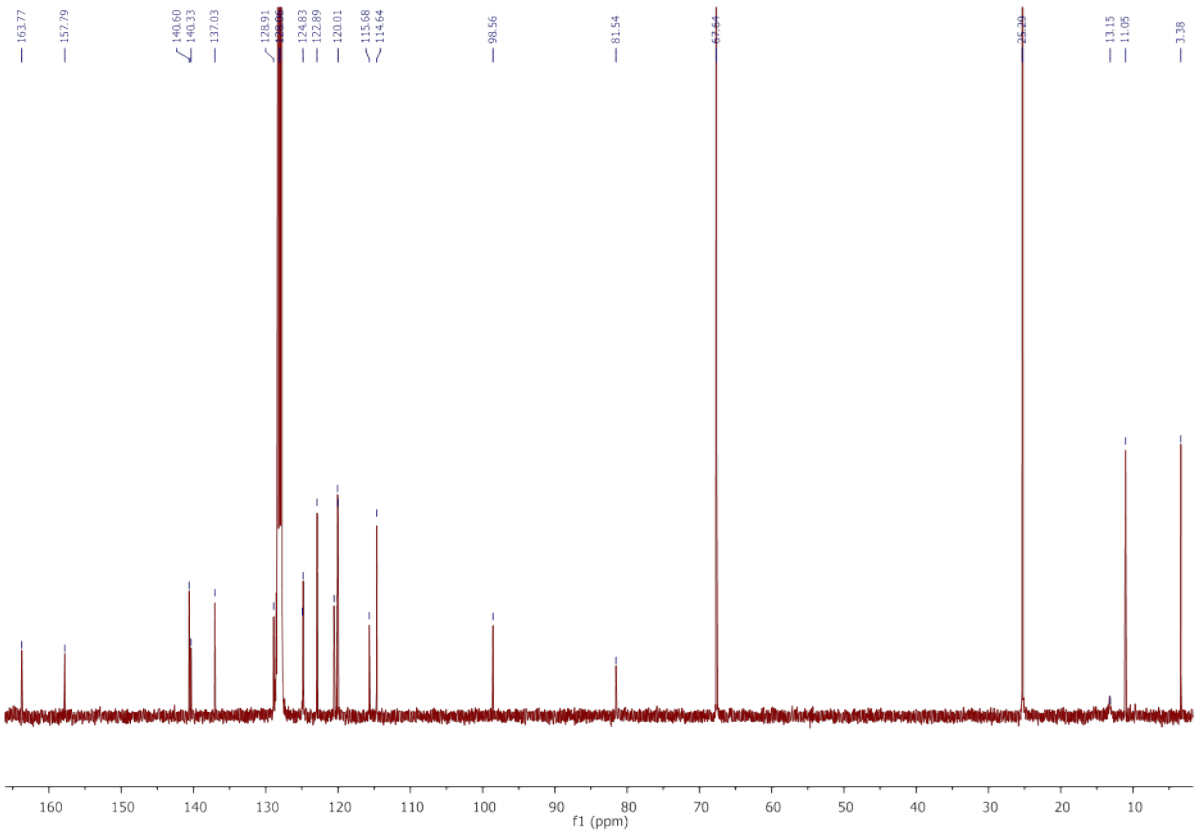


Figure S50. ^{13}C NMR of compound **4** in C_6D_6.

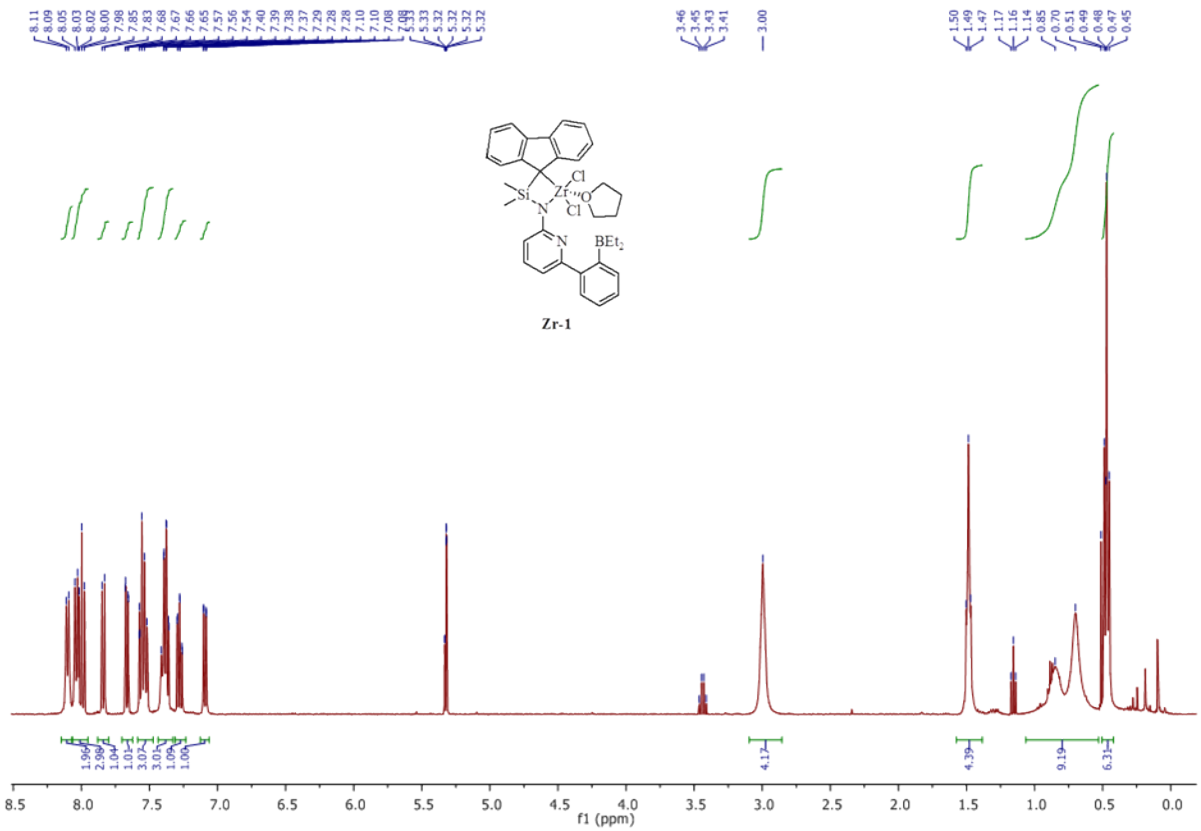


Figure S51. ^{1}H NMR of complex **Zr-1** in CD_2Cl_2.

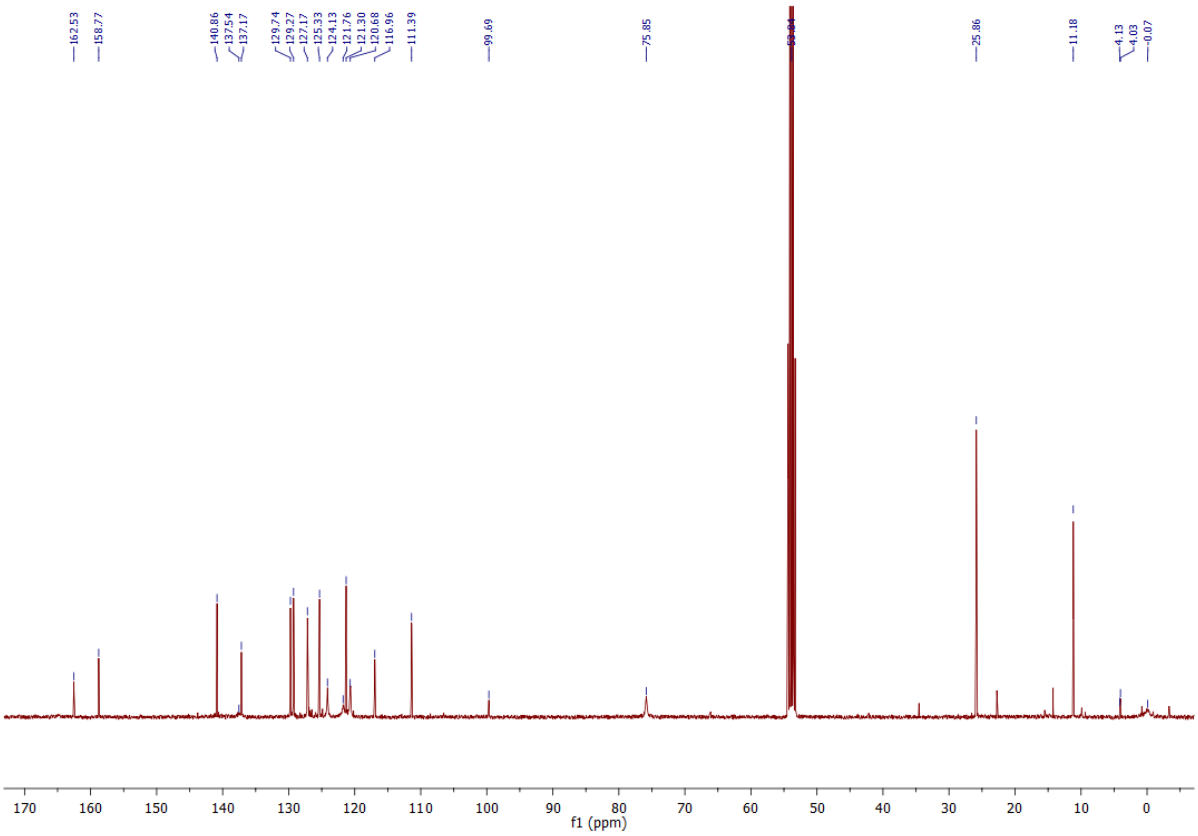


Figure S52. ^{13}C NMR of complex **Zr-1** in CD_2Cl_2.

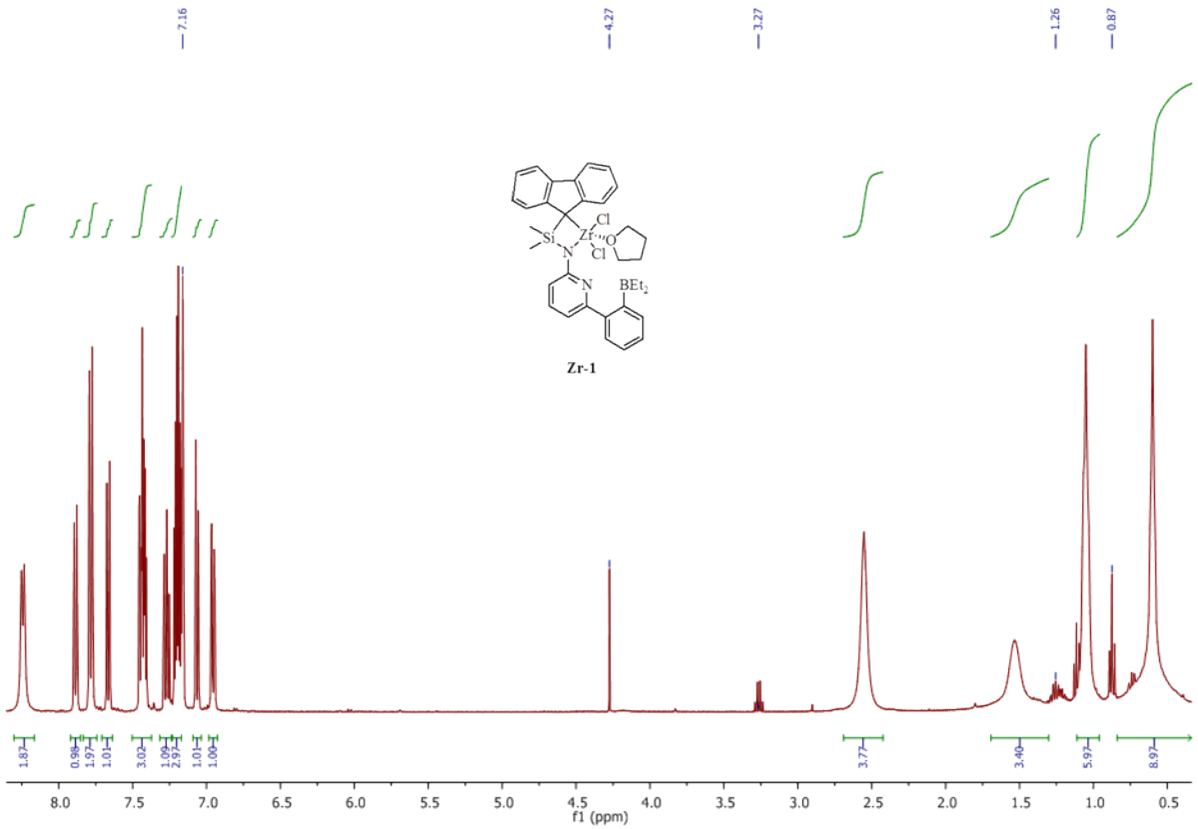


Figure S53. ^{1}H NMR of complex **Zr-1** in C_6D_6.

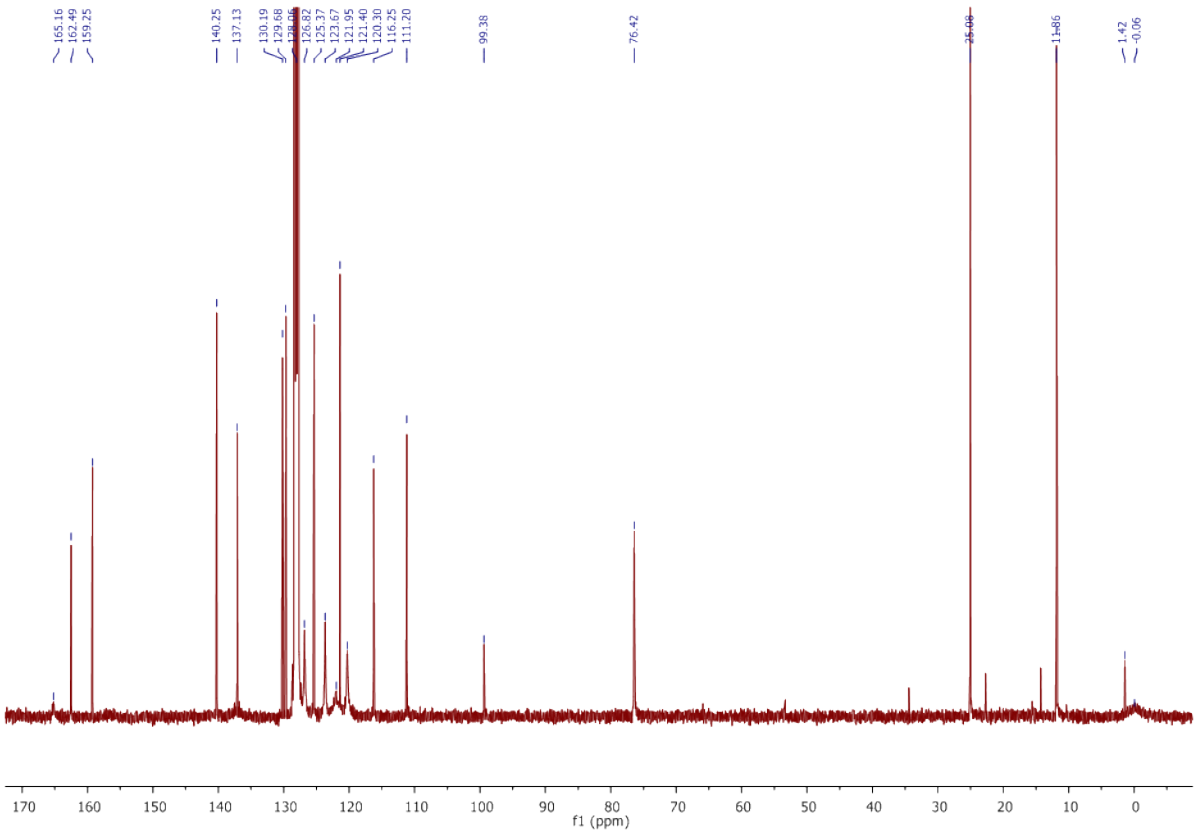


Figure S54. ^{13}C NMR of complex **Zr-1** in C_6D_6.

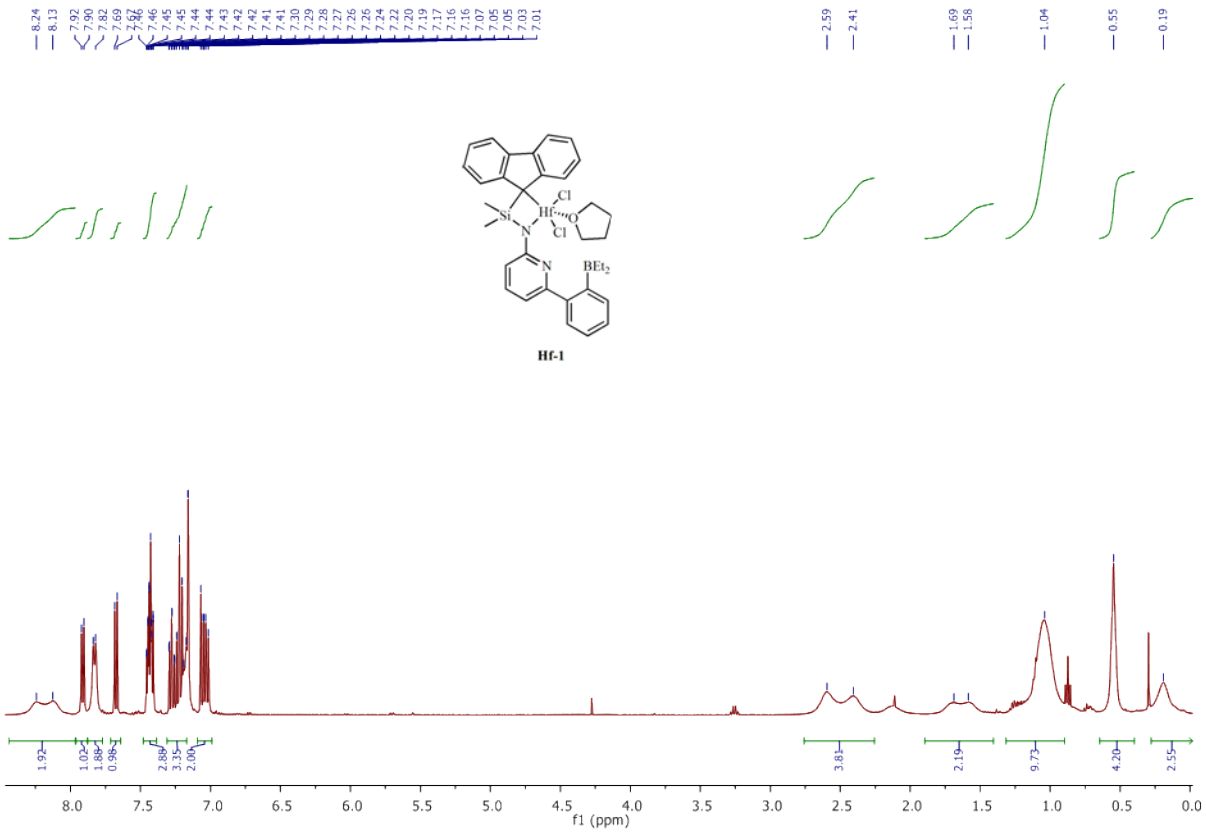


Figure S55. ^{1}H NMR of complex **Hf-1** in C_6D_6.

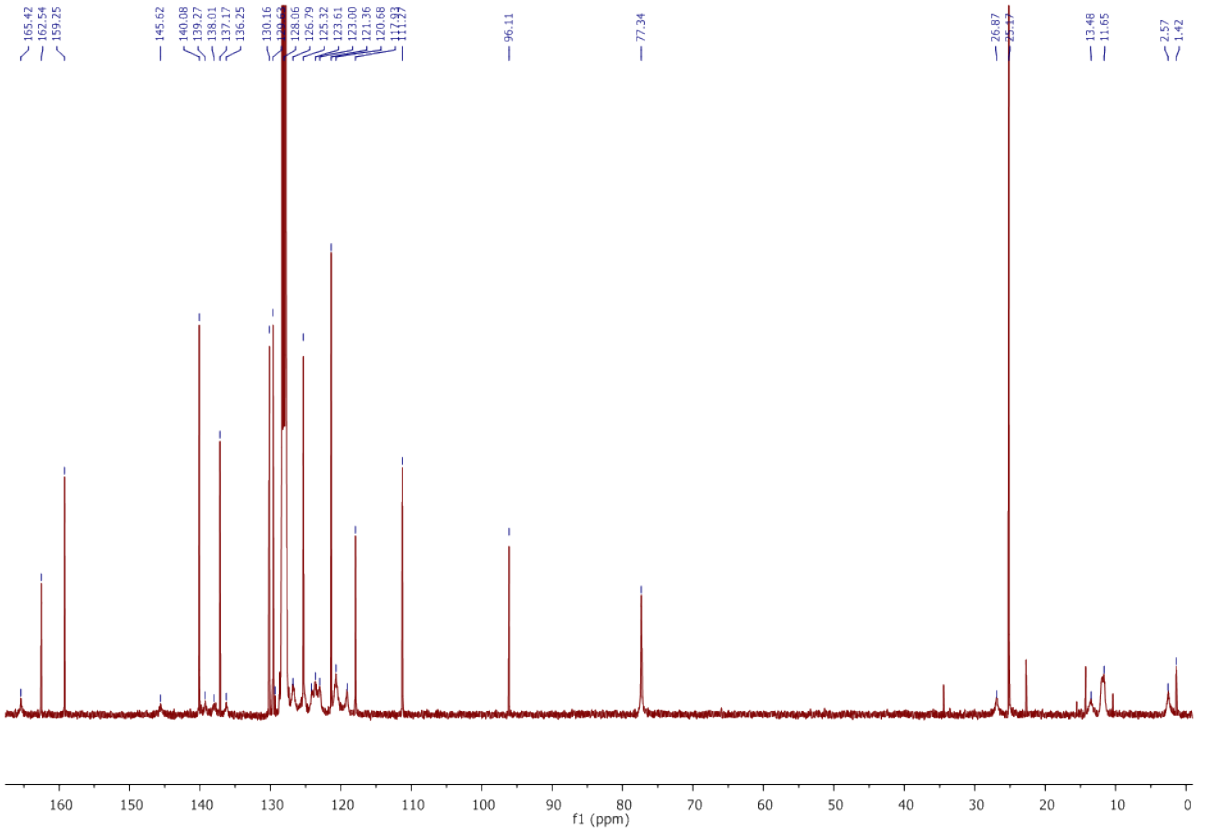


Figure S56. ^{13}C NMR of complex **Hf-1** in C_6D_6.

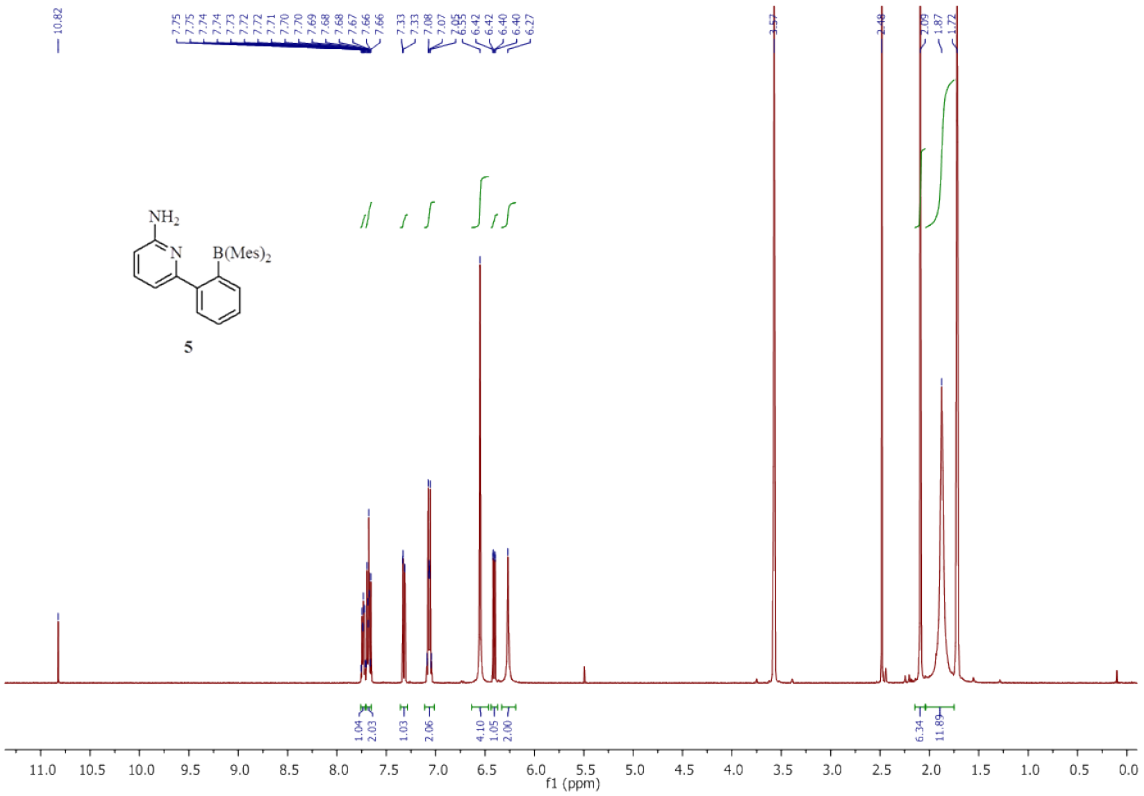


Figure S57. ^{1}H NMR of compound **5** in C_6D_6.

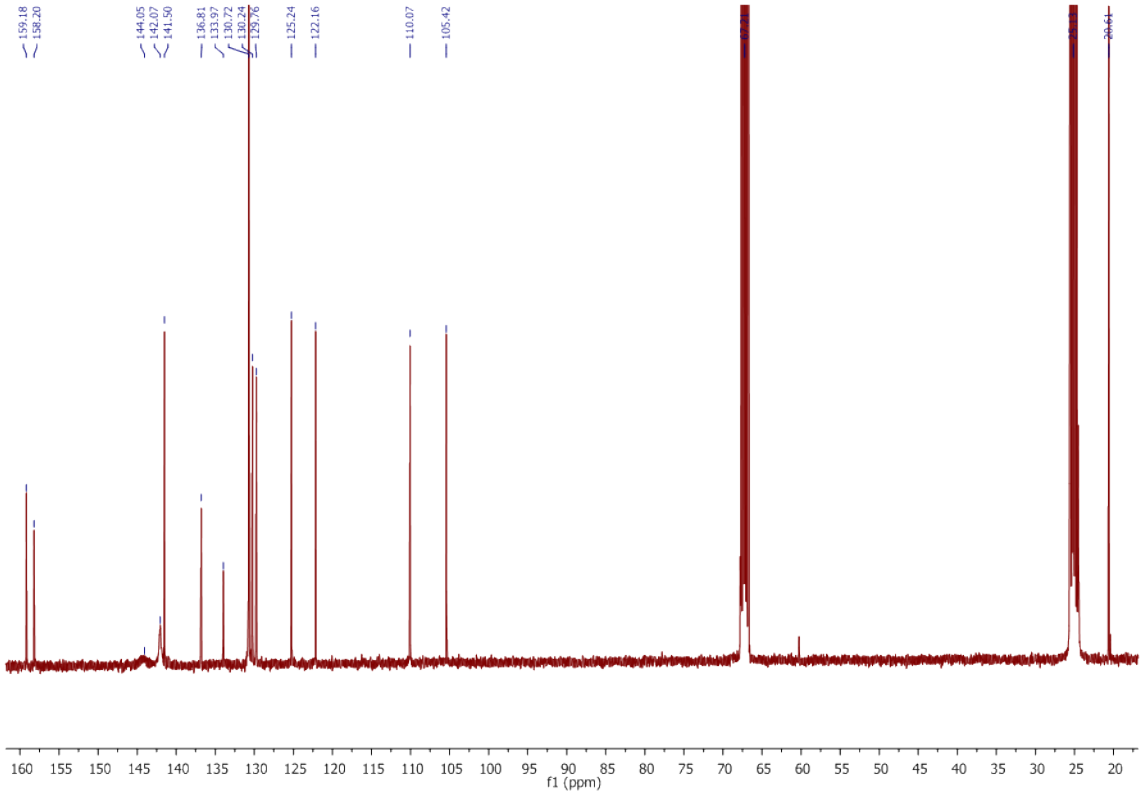


Figure S58. ^{13}C NMR of compound **5** in C_6D_6.

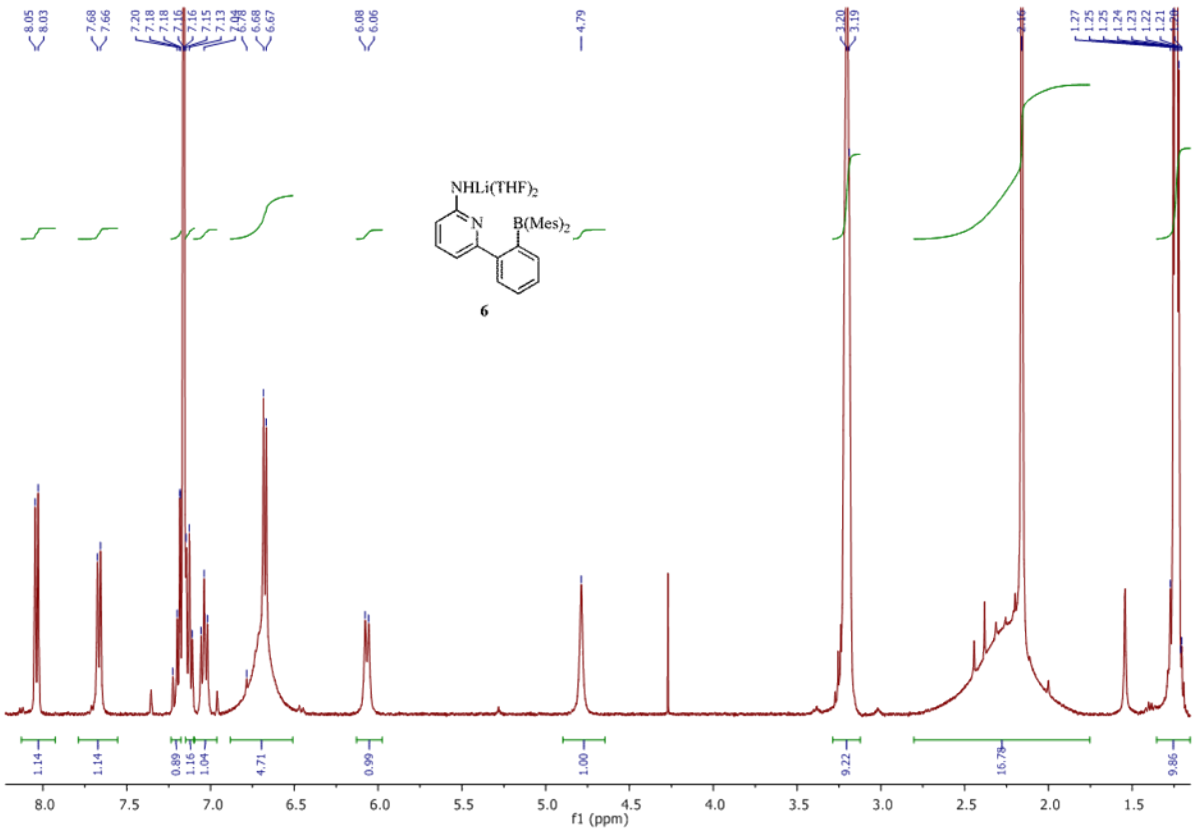


Figure S59. ^{1}H NMR of compound **6** in C_6D_6.

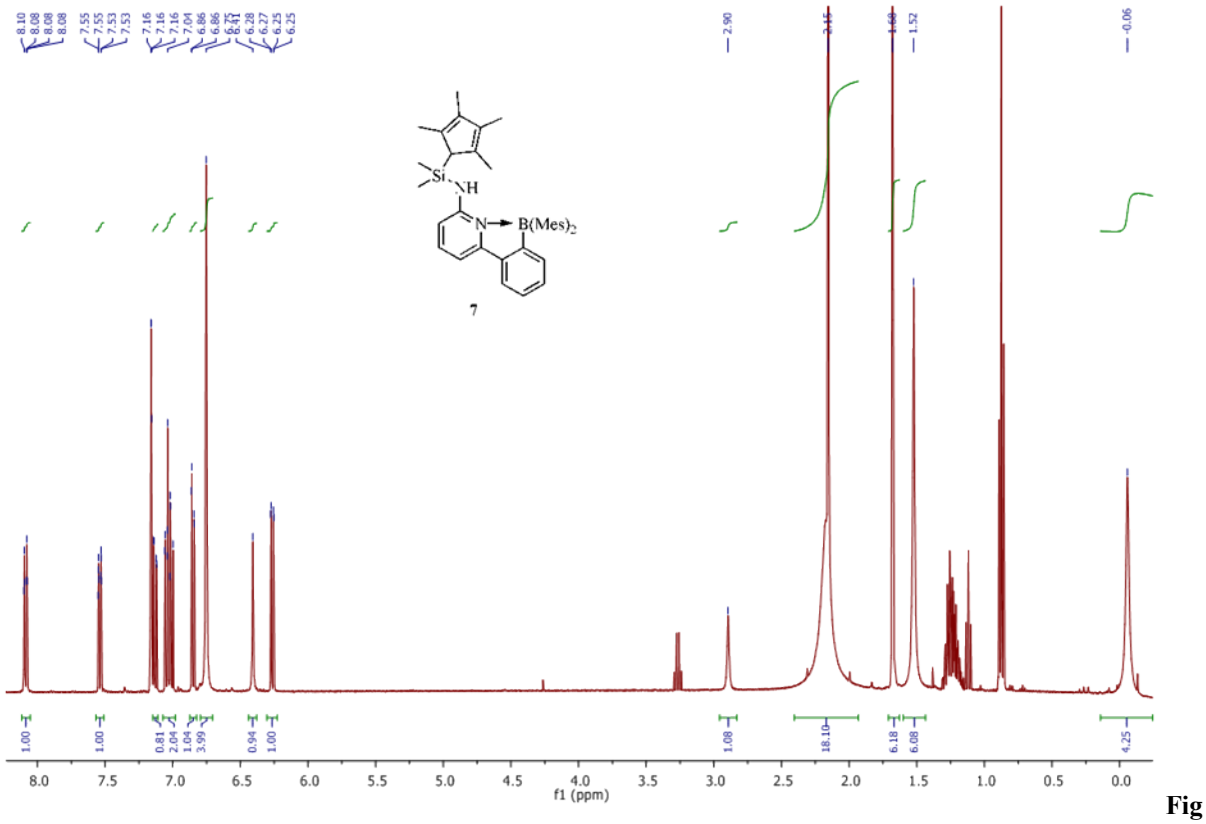


Figure S60. ^{1}H NMR of compound **7** in C_6D_6.

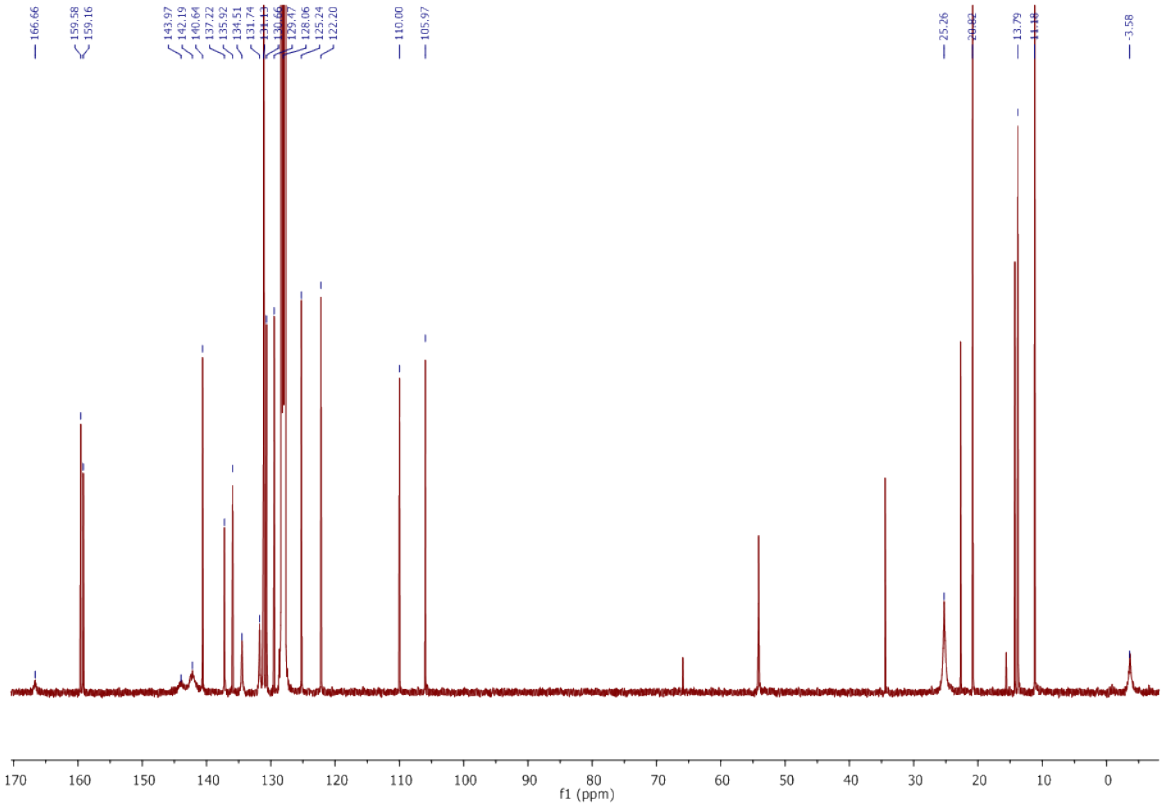


Figure S61. ^{13}C NMR of compound **7** in C_6D_6.

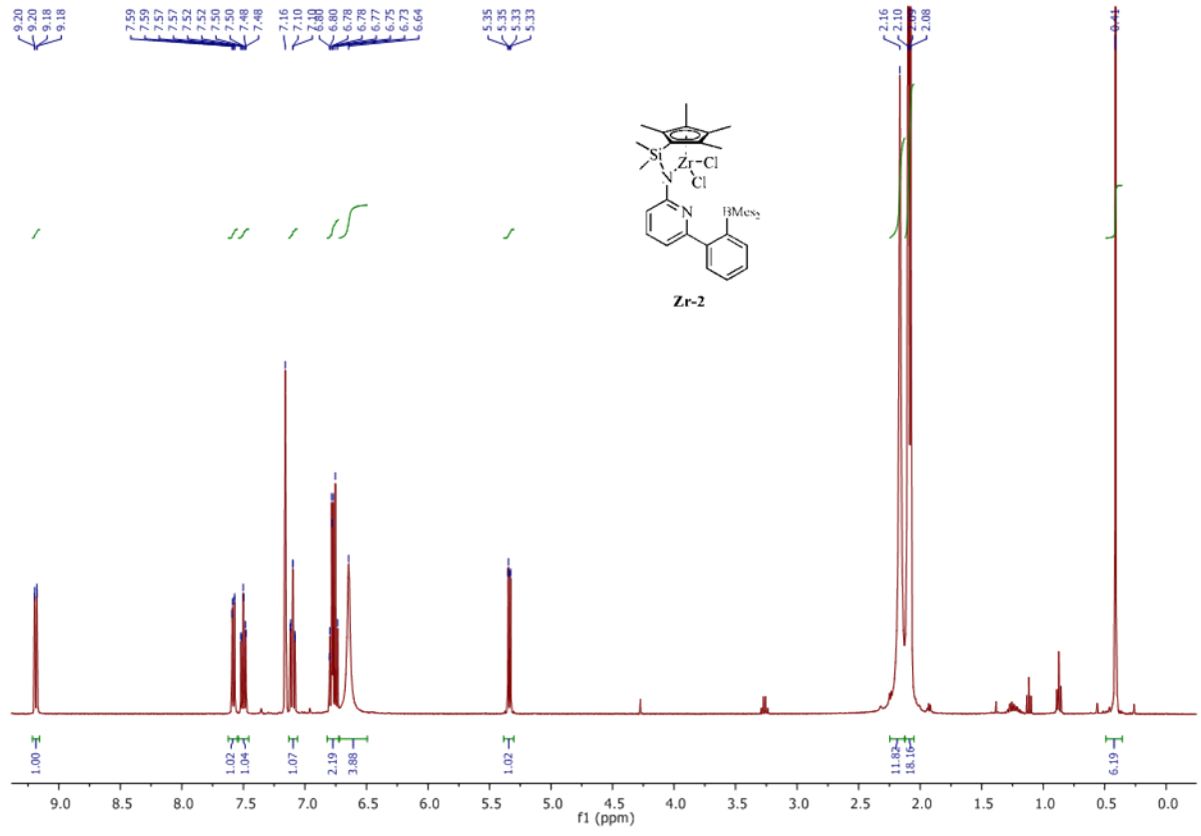


Figure S62. ^{1}H NMR of complex **Zr-2** in C_6D_6.

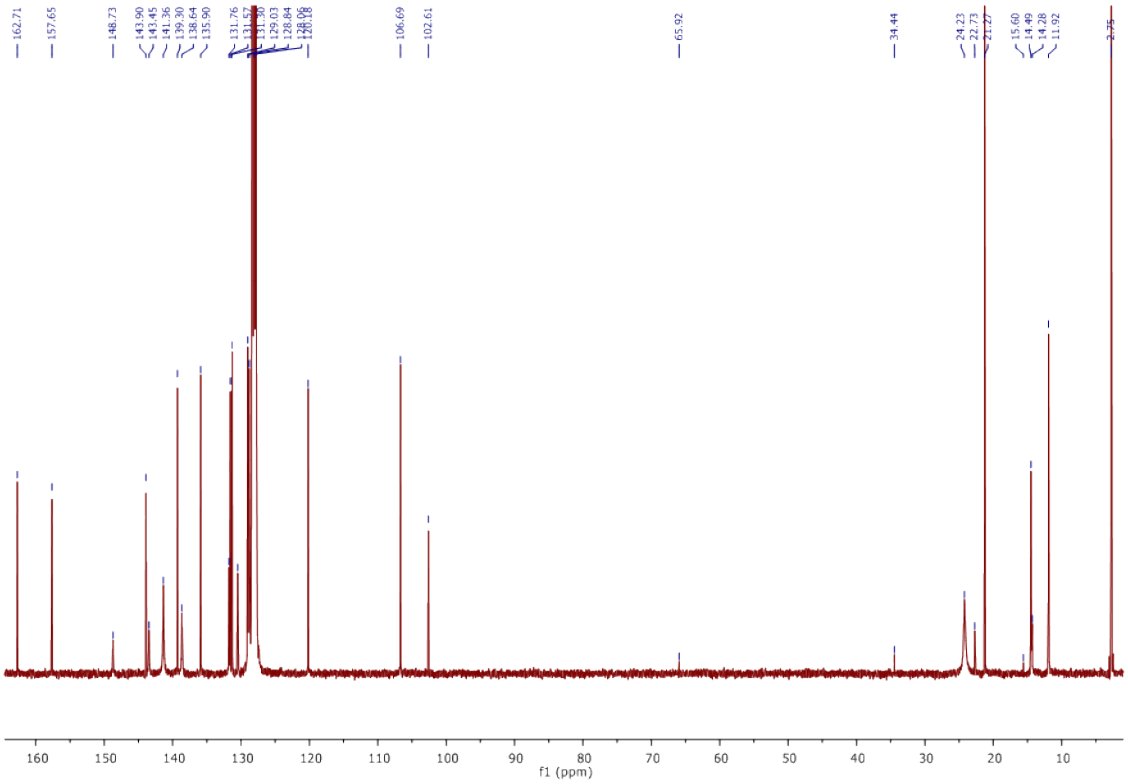


Figure S63. ^{13}C NMR of complex **Zr-2** in C_6D_6.

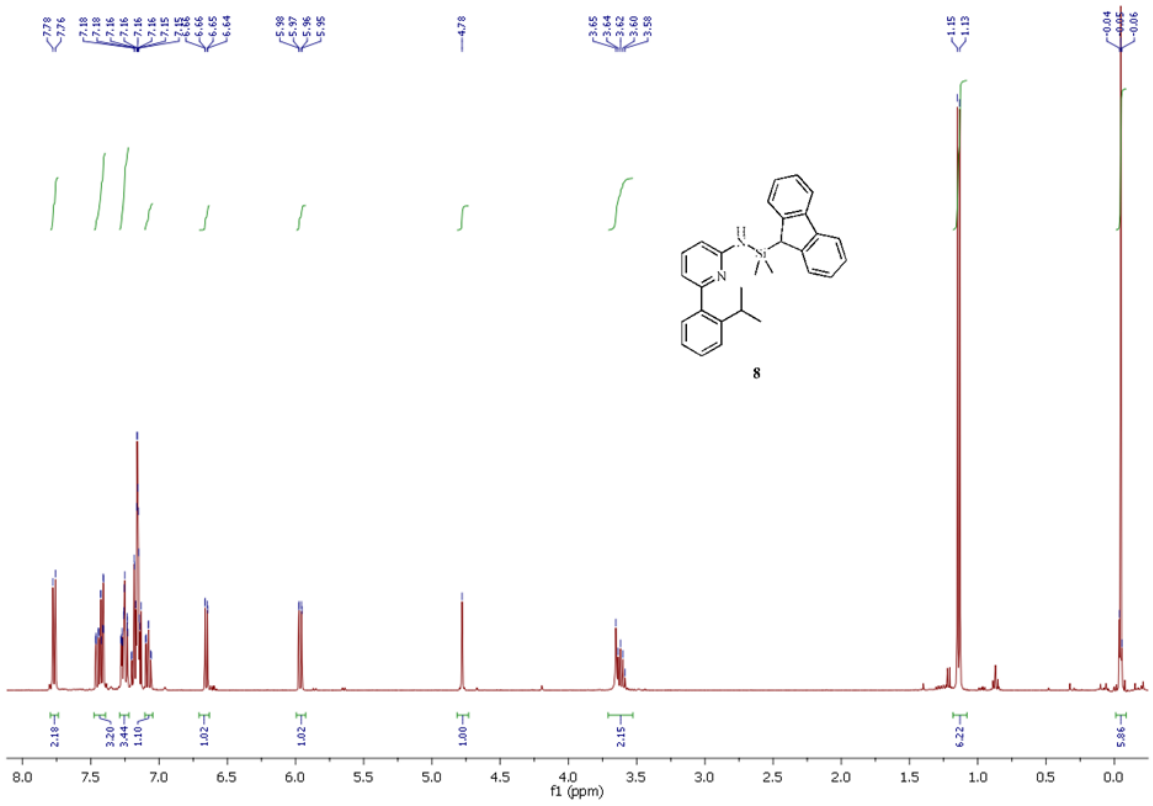


Figure S64. ^{1}H NMR of compound **8** in C_6D_6.

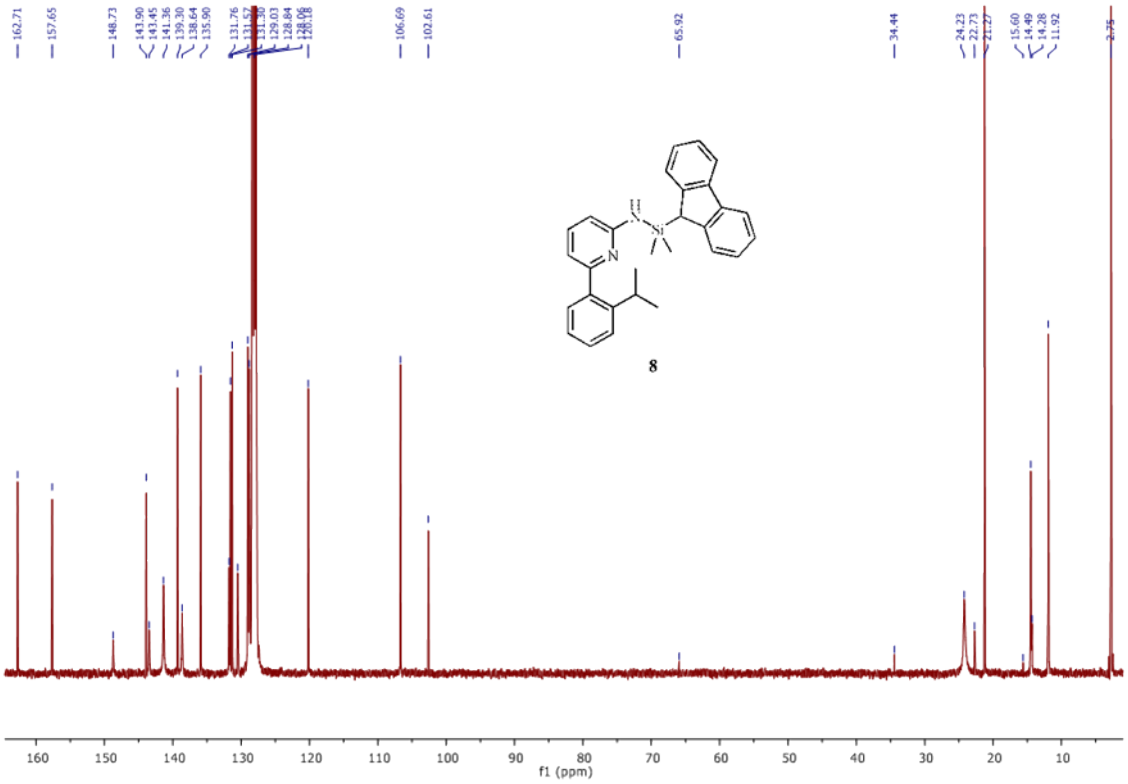


Figure S65. ^{13}C NMR of compound **8** in C_6D_6.

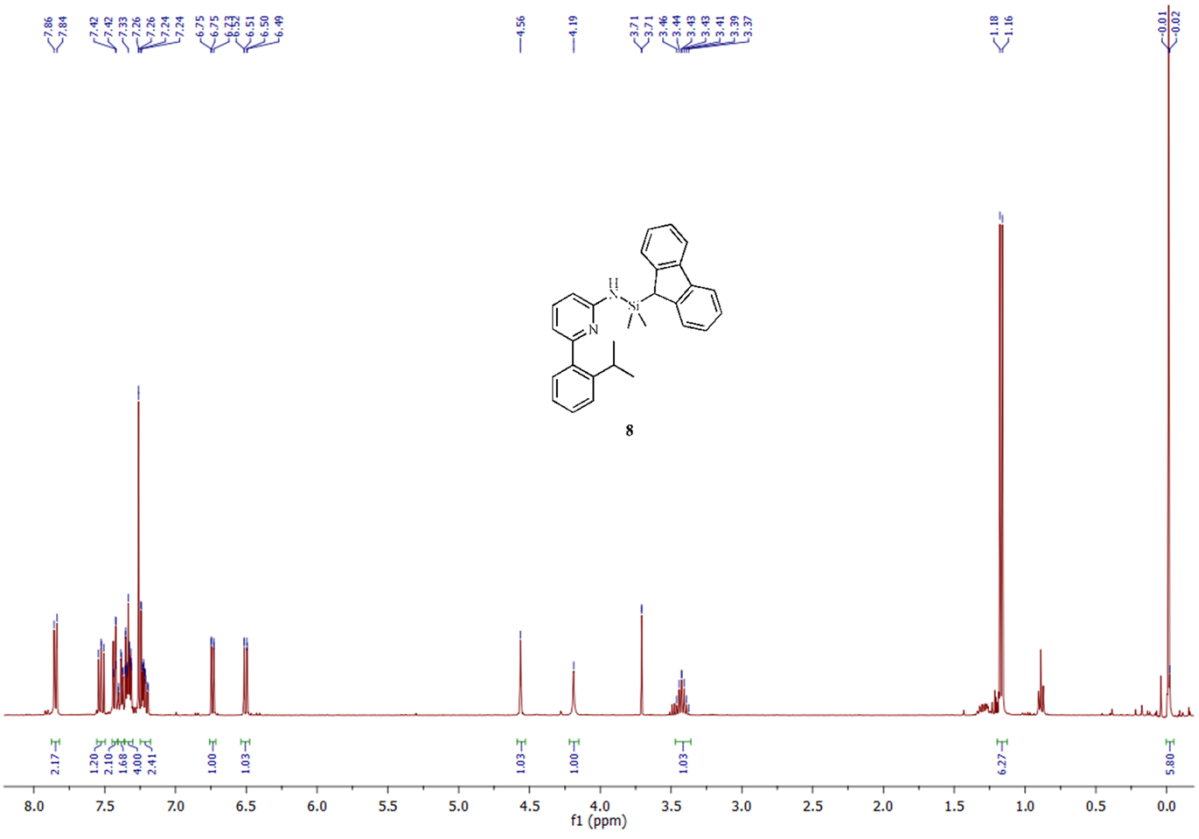


Figure S66. ^{1}H NMR of compound **8** in $CDCl_3$.

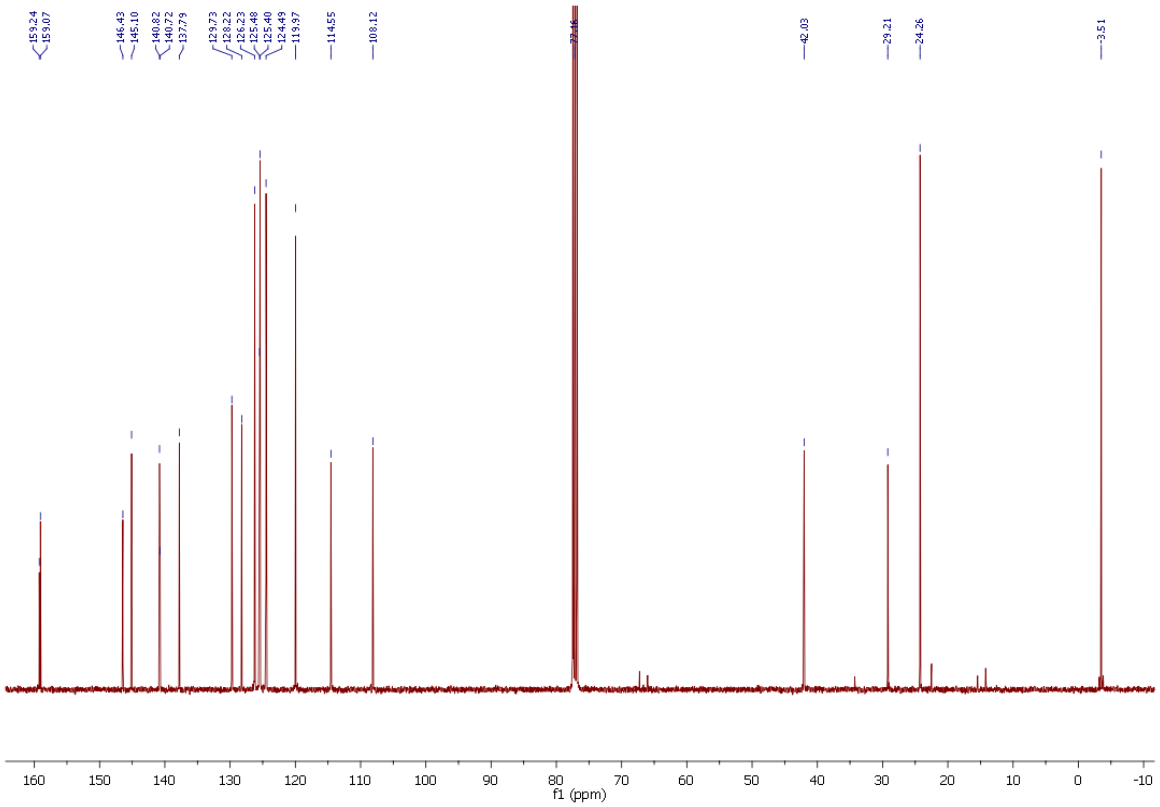


Figure S67. ^{13}C NMR of compound **8** in $CDCl_3$.

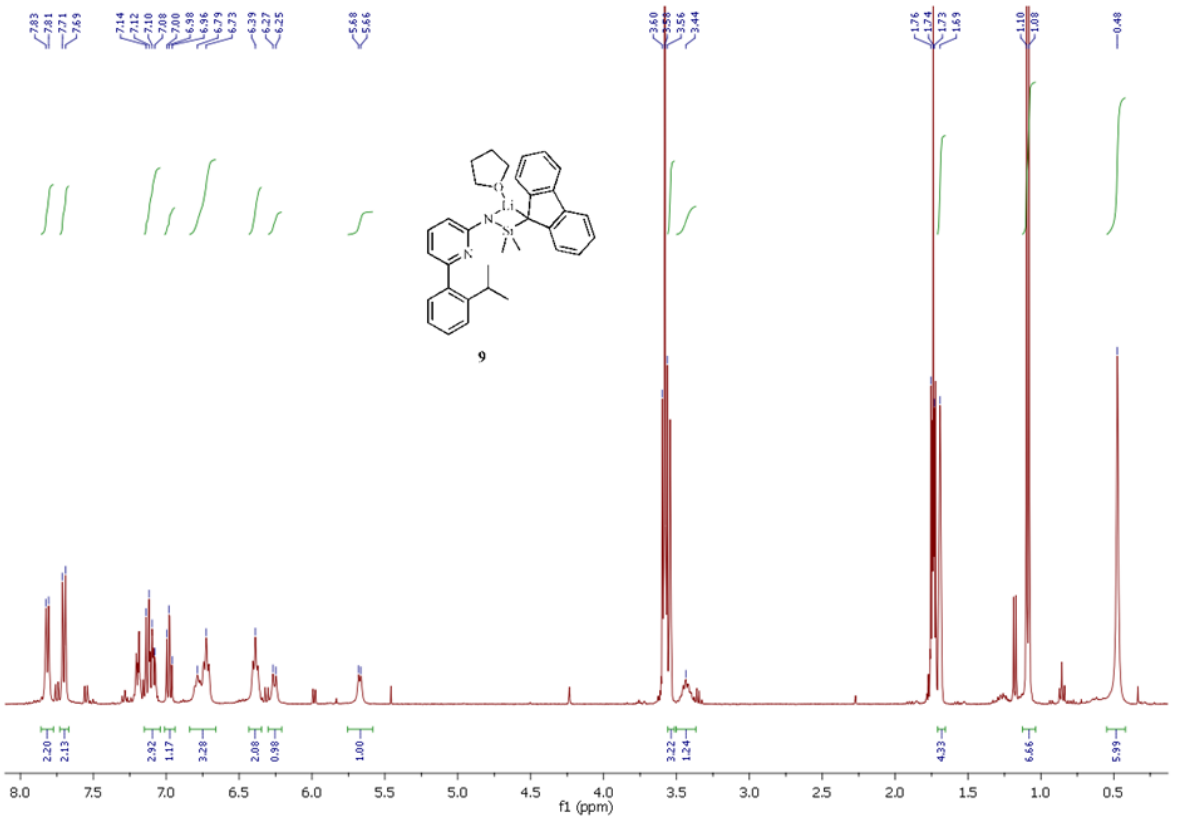


Figure 68. ^{1}H NMR of compound **9** in THF-d_8.

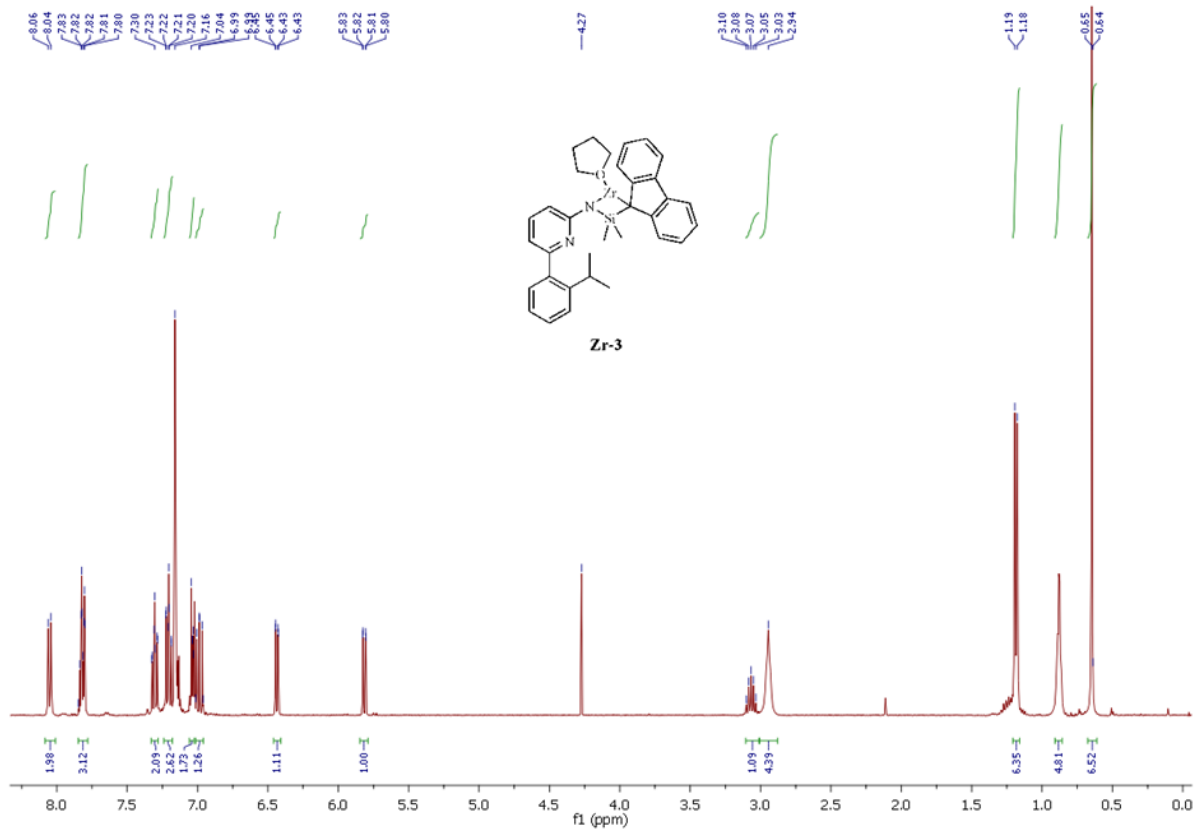


Figure 69. ^{1}H NMR of complex **Zr-3** in C_6D_6.

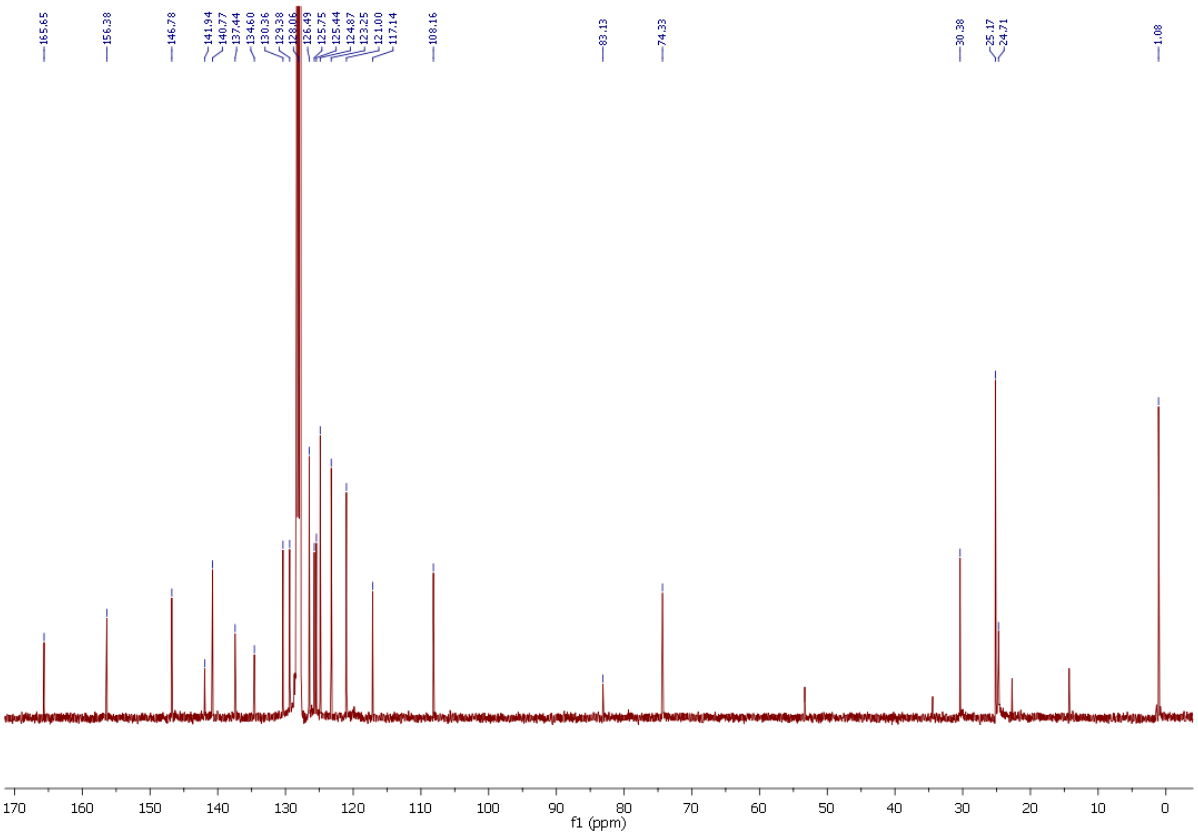


Figure 70. ^{13}C NMR of complex **Zr-3** in C_6D_6.

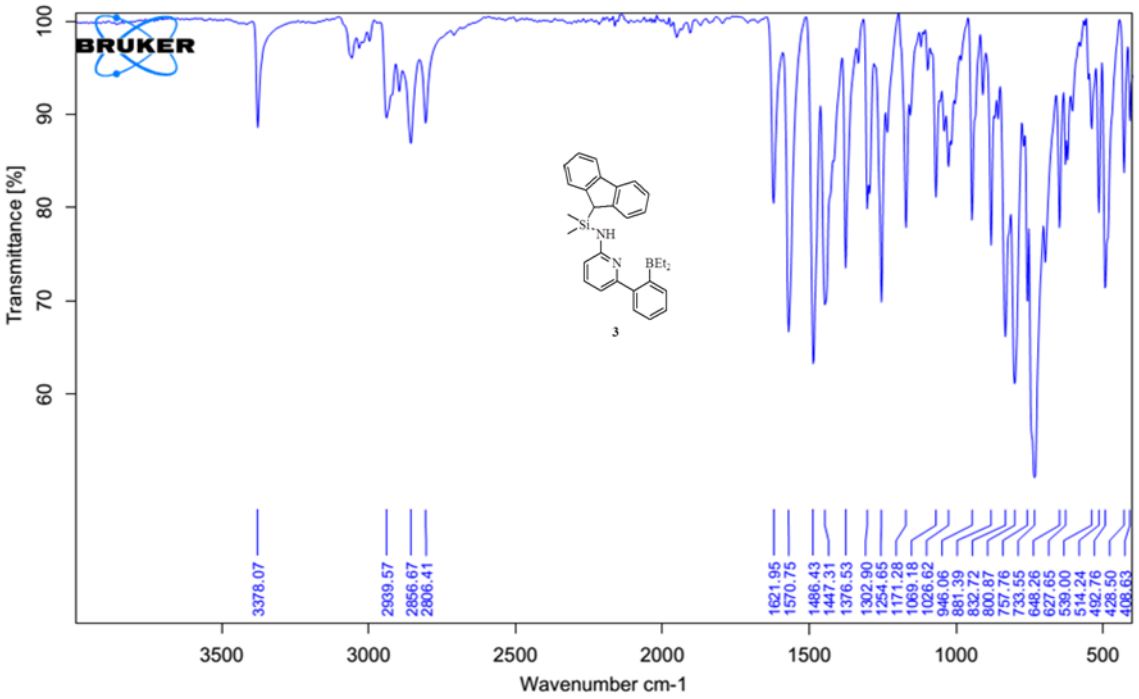


Figure S71. IR spectrum of compound **3**.

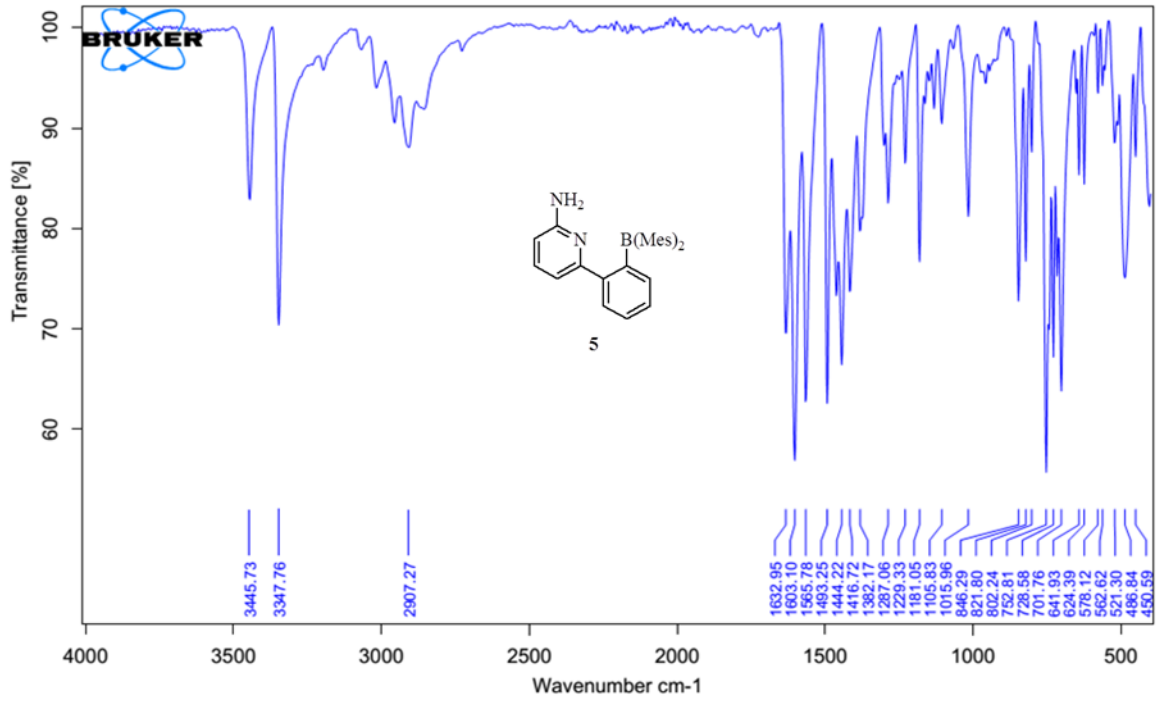


Figure S72. IR spectrum of compound **5**.

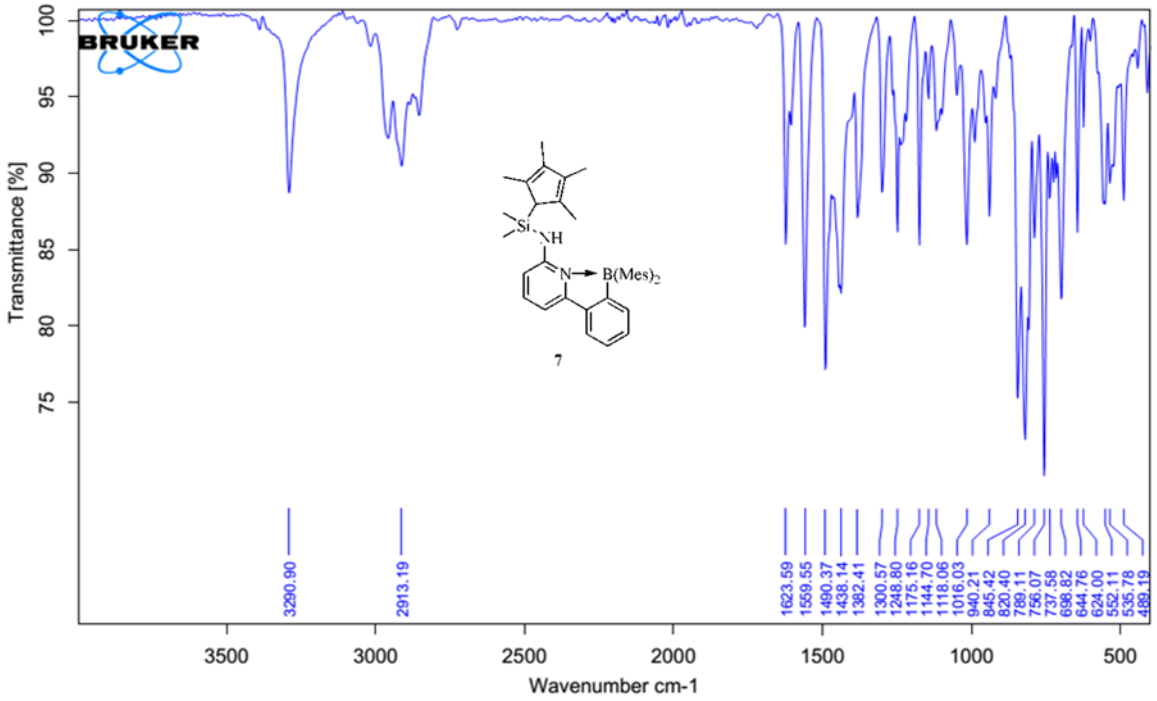


Figure S73. IR spectrum of compound **7**.

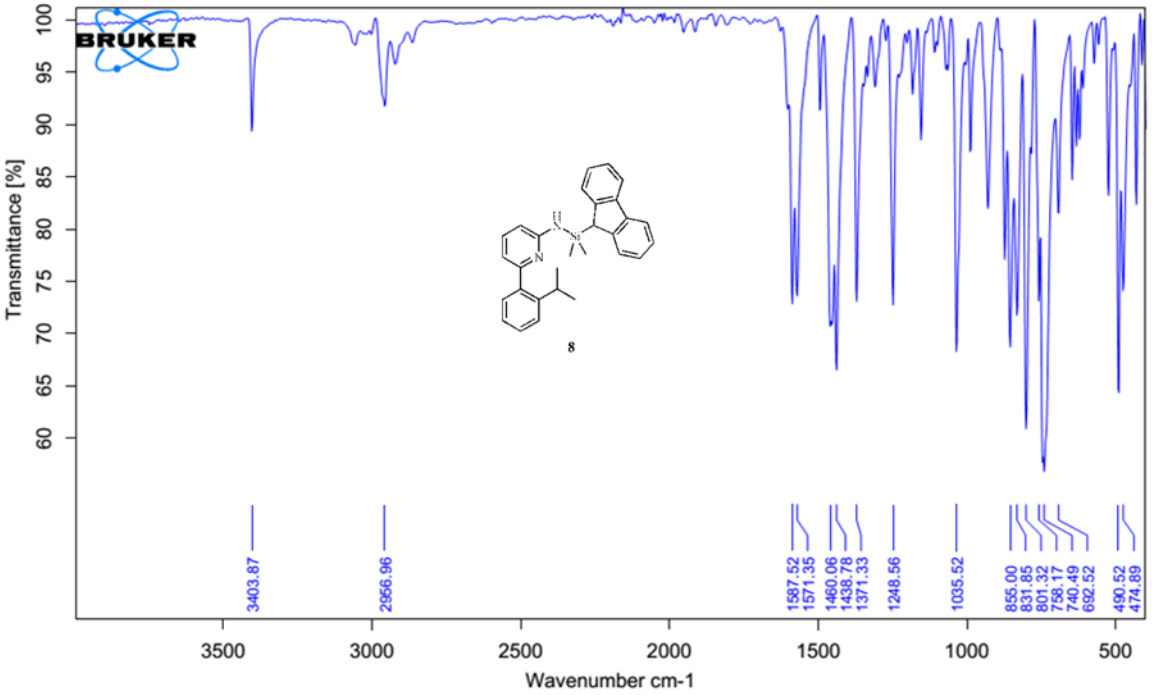


Figure S74. IR spectrum of compound **8**.

Table S1. Crystal data and structure refinement for **3**.

Empirical formula	C30 H33 B N2 Si
Formula weight	460.48
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, P b c n
Unit cell dimensions	a = 21.8109(17) Å α = 90 º.
	b = 13.5026(11) Å β = 90 º.
	c = 17.5034(16) Å γ = 90 º.
Volume	5154.8(7) $Å^3$
Z, Calculated density	8, 1.187 mg/m^3
Absorption coefficient	0.112 mm^{-1}
F(000)	1968
Crystal size	0.43 ×0.09 ×0.06 mm
Theta range for data collection	1.77 to 25.07 º.
Limiting indices	-25<=h<=24, -16<=k<=15, -19<=l<=20
Reflections collected / unique	17983 / 4564 [R(int) = 0.0865]
Completeness to theta = 25.07	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7452 and 0.6735
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4564 / 0 / 316
Goodness-of-fit on F^2	1.035
Final R indices [I>2σ(I)]	R1 = 0.0481, wR2 = 0.0802
R indices (all data)	R1 = 0.1145, wR2 = 0.0912
Extinction coefficient	0.00108(13)
Largest diff. peak and hole	0.293 and -0.273 $e.A^{-3}$

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($A^2 \times 10^3$) for **3**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Si(1)	6377(1)	8907(1)	1982(1)	21(1)
N(1)	6656(1)	6632(1)	3427(1)	17(1)
C(1)	6794(1)	7456(2)	3026(1)	20(1)
B(1)	6024(1)	5955(2)	3380(2)	20(1)

N(2)	6346(1)	7865(1)	2576(1)	21(1)
C(2)	7382(1)	7865(2)	3083(1)	22(1)
C(3)	7804(1)	7464(2)	3568(1)	23(1)
C(4)	7655(1)	6629(2)	3996(1)	21(1)
C(5)	7083(1)	6217(2)	3906(1)	19(1)
C(6)	6829(1)	5323(2)	4257(1)	18(1)
C(7)	6235(1)	5142(2)	3987(1)	21(1)
C(8)	5923(1)	4334(2)	4300(1)	25(1)
C(9)	6195(1)	3750(2)	4856(1)	30(1)
C(10)	6788(1)	3940(2)	5100(1)	30(1)
C(11)	7111(1)	4727(2)	4802(1)	26(1)
C(12)	6632(1)	10037(2)	2539(1)	20(1)
C(13)	6259(1)	10200(2)	3257(1)	19(1)
C(14)	6240(1)	9641(2)	3920(1)	22(1)
C(15)	5875(1)	9959(2)	4522(1)	25(1)
C(16)	5532(1)	10820(2)	4461(2)	28(1)
C(17)	5544(1)	11384(2)	3801(1)	26(1)
C(18)	5915(1)	11078(2)	3199(1)	19(1)
C(19)	6061(1)	11551(2)	2468(1)	20(1)
C(20)	5864(1)	12441(2)	2157(2)	26(1)
C(21)	6101(1)	12737(2)	1458(2)	32(1)
C(22)	6531(1)	12174(2)	1083(2)	32(1)
C(23)	6736(1)	11284(2)	1393(1)	27(1)
C(24)	6495(1)	10966(2)	2085(1)	21(1)
C(25)	5583(1)	9080(2)	1639(1)	30(1)
C(26)	6912(1)	8672(2)	1182(2)	38(1)
C(27)	5971(1)	5525(2)	2509(2)	24(1)
C(28)	6565(1)	5124(2)	2164(1)	32(1)
C(29)	5426(1)	6560(2)	3667(1)	25(1)
C(30)	5495(1)	7063(2)	4442(2)	32(1)

Table S3. Bond lengths [Å] and angles [º] for **3**.

Si(1)-N(2)	1.7498(19)
Si(1)-C(25)	1.847(2)
Si(1)-C(26)	1.851(2)
Si(1)-C(12)	1.894(2)

N(1)-C(1)	1.350(3)
N(1)-C(5)	1.373(3)
N(1)-B(1)	1.655(3)
C(1)-N(2)	1.371(3)
C(1)-C(2)	1.400(3)
B(1)-C(7)	1.596(3)
B(1)-C(29)	1.619(3)
B(1)-C(27)	1.636(4)
N(2)-H(2A)	0.88(2)
C(2)-C(3)	1.363(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.392(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.375(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.464(3)
C(6)-C(11)	1.392(3)
C(6)-C(7)	1.400(3)
C(7)-C(8)	1.397(3)
C(8)-C(9)	1.387(3)
C(8)-H(8)	0.9500
C(9)-C(10)	1.386(3)
C(9)-H(9)	0.9500
C(10)-C(11)	1.378(3)
C(10)-H(10)	0.9500
C(11)-H(11)	0.9500
C(12)-C(13)	1.513(3)
C(12)-C(24)	1.515(3)
C(12)-H(12)	1.0000
C(13)-C(14)	1.385(3)
C(13)-C(18)	1.407(3)
C(14)-C(15)	1.389(3)
C(14)-H(14)	0.9500
C(15)-C(16)	1.388(3)
C(15)-H(15)	0.9500
C(16)-C(17)	1.383(3)
C(16)-H(16)	0.9500
C(17)-C(18)	1.392(3)
C(17)-H(17)	0.9500

C(18)-C(19)	1.465(3)
C(19)-C(20)	1.387(3)
C(19)-C(24)	1.403(3)
C(20)-C(21)	1.387(3)
C(20)-H(20)	0.9500
C(21)-C(22)	1.375(3)
C(21)-H(21)	0.9500
C(22)-C(23)	1.392(3)
C(22)-H(22)	0.9500
C(23)-C(24)	1.389(3)
C(23)-H(23)	0.9500
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-C(28)	1.530(3)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-C(30)	1.523(3)
C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800

N(2)-Si(1)-C(25)	105.00(10)
N(2)-Si(1)-C(26)	109.61(11)
C(25)-Si(1)-C(26)	111.53(12)
N(2)-Si(1)-C(12)	110.72(10)
C(25)-Si(1)-C(12)	109.93(11)
C(26)-Si(1)-C(12)	109.96(11)
C(1)-N(1)-C(5)	120.16(19)
C(1)-N(1)-B(1)	127.94(19)
C(5)-N(1)-B(1)	111.74(18)

N(1)-C(1)-N(2)	118.2(2)
N(1)-C(1)-C(2)	119.5(2)
N(2)-C(1)-C(2)	122.4(2)
C(7)-B(1)-C(29)	111.9(2)
C(7)-B(1)-C(27)	113.4(2)
C(29)-B(1)-C(27)	114.3(2)
C(7)-B(1)-N(1)	96.14(17)
C(29)-B(1)-N(1)	112.17(19)
C(27)-B(1)-N(1)	107.53(18)
C(1)-N(2)-Si(1)	129.58(17)
C(1)-N(2)-H(2A)	115.6(15)
Si(1)-N(2)-H(2A)	114.5(15)
C(3)-C(2)-C(1)	120.4(2)
C(3)-C(2)-H(2)	119.8
C(1)-C(2)-H(2)	119.8
C(2)-C(3)-C(4)	120.0(2)
C(2)-C(3)-H(3)	120.0
C(4)-C(3)-H(3)	120.0
C(5)-C(4)-C(3)	118.5(2)
C(5)-C(4)-H(4)	120.7
C(3)-C(4)-H(4)	120.7
N(1)-C(5)-C(4)	121.4(2)
N(1)-C(5)-C(6)	109.57(19)
C(4)-C(5)-C(6)	129.1(2)
C(11)-C(6)-C(7)	122.7(2)
C(11)-C(6)-C(5)	126.6(2)
C(7)-C(6)-C(5)	110.7(2)
C(8)-C(7)-C(6)	117.0(2)
C(8)-C(7)-B(1)	131.1(2)
C(6)-C(7)-B(1)	111.77(19)
C(9)-C(8)-C(7)	120.7(2)
C(9)-C(8)-H(8)	119.6
C(7)-C(8)-H(8)	119.6
C(10)-C(9)-C(8)	120.7(2)
C(10)-C(9)-H(9)	119.7
C(8)-C(9)-H(9)	119.7
C(11)-C(10)-C(9)	120.3(2)
C(11)-C(10)-H(10)	119.9
C(9)-C(10)-H(10)	119.9

C(10)-C(11)-C(6)	118.6(2)
C(10)-C(11)-H(11)	120.7
C(6)-C(11)-H(11)	120.7
C(13)-C(12)-C(24)	102.04(17)
C(13)-C(12)-Si(1)	112.70(15)
C(24)-C(12)-Si(1)	109.88(16)
C(13)-C(12)-H(12)	110.6
C(24)-C(12)-H(12)	110.6
Si(1)-C(12)-H(12)	110.6
C(14)-C(13)-C(18)	120.2(2)
C(14)-C(13)-C(12)	129.3(2)
C(18)-C(13)-C(12)	110.4(2)
C(13)-C(14)-C(15)	119.0(2)
C(13)-C(14)-H(14)	120.5
C(15)-C(14)-H(14)	120.5
C(16)-C(15)-C(14)	120.7(2)
C(16)-C(15)-H(15)	119.7
C(14)-C(15)-H(15)	119.7
C(17)-C(16)-C(15)	121.0(2)
C(17)-C(16)-H(16)	119.5
C(15)-C(16)-H(16)	119.5
C(16)-C(17)-C(18)	118.7(2)
C(16)-C(17)-H(17)	120.6
C(18)-C(17)-H(17)	120.6
C(17)-C(18)-C(13)	120.4(2)
C(17)-C(18)-C(19)	131.2(2)
C(13)-C(18)-C(19)	108.3(2)
C(20)-C(19)-C(24)	120.5(2)
C(20)-C(19)-C(18)	130.8(2)
C(24)-C(19)-C(18)	108.6(2)
C(21)-C(20)-C(19)	118.8(2)
C(21)-C(20)-H(20)	120.6
C(19)-C(20)-H(20)	120.6
C(22)-C(21)-C(20)	121.1(2)
C(22)-C(21)-H(21)	119.5
C(20)-C(21)-H(21)	119.5
C(21)-C(22)-C(23)	120.6(3)
C(21)-C(22)-H(22)	119.7
C(23)-C(22)-H(22)	119.7

C(24)-C(23)-C(22)	119.1(2)
C(24)-C(23)-H(23)	120.5
C(22)-C(23)-H(23)	120.5
C(23)-C(24)-C(19)	119.9(2)
C(23)-C(24)-C(12)	129.7(2)
C(19)-C(24)-C(12)	110.4(2)
Si(1)-C(25)-H(25A)	109.5
Si(1)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
Si(1)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
Si(1)-C(26)-H(26A)	109.5
Si(1)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
Si(1)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(28)-C(27)-B(1)	115.74(19)
C(28)-C(27)-H(27A)	108.3
B(1)-C(27)-H(27A)	108.3
C(28)-C(27)-H(27B)	108.3
B(1)-C(27)-H(27B)	108.3
H(27A)-C(27)-H(27B)	107.4
C(27)-C(28)-H(28A)	109.5
C(27)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(27)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(30)-C(29)-B(1)	114.9(2)
C(30)-C(29)-H(29A)	108.5
B(1)-C(29)-H(29A)	108.5
C(30)-C(29)-H(29B)	108.5
B(1)-C(29)-H(29B)	108.5
H(29A)-C(29)-H(29B)	107.5
C(29)-C(30)-H(30A)	109.5
C(29)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5

C(29)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5

Table S4. Anisotropic displacement parameters ($A^2 \times 10^3$) for **3**. The anisotropic displacement factor exponent takes the form: $-2\,pi^2\,[\,h^2\,a^{*2}\,U11 + ... + 2\,h\,k\,a^*\,b^*\,U12\,]$

	U11	U22	U33	U23	U13	U12
Si(1)	26(1)	17(1)	20(1)	1(1)	1(1)	0(1)
N(1)	18(1)	14(1)	20(1)	-1(1)	0(1)	0(1)
C(1)	21(1)	19(1)	19(1)	-3(1)	1(1)	2(1)
B(1)	15(1)	19(2)	25(2)	0(1)	-3(1)	-5(1)
N(2)	18(1)	19(1)	26(1)	7(1)	-3(1)	-2(1)
C(2)	20(1)	18(1)	29(2)	0(1)	6(1)	-2(1)
C(3)	15(1)	23(1)	31(2)	-7(1)	-1(1)	2(1)
C(4)	19(1)	22(1)	23(2)	-1(1)	-4(1)	3(1)
C(5)	22(1)	18(1)	16(1)	-4(1)	-2(1)	3(1)
C(6)	21(1)	16(1)	17(1)	0(1)	0(1)	1(1)
C(7)	21(1)	19(1)	22(1)	-3(1)	1(1)	1(1)
C(8)	20(1)	24(2)	32(2)	-2(1)	-2(1)	-2(1)
C(9)	35(2)	23(2)	31(2)	5(1)	2(1)	-6(1)
C(10)	40(2)	25(2)	26(2)	7(1)	-11(1)	-3(1)
C(11)	32(2)	24(2)	23(2)	2(1)	-8(1)	-4(1)
C(12)	19(1)	20(1)	20(1)	0(1)	3(1)	1(1)
C(13)	16(1)	17(1)	23(1)	-2(1)	-1(1)	-2(1)
C(14)	20(1)	20(1)	26(2)	-1(1)	-1(1)	-2(1)
C(15)	28(1)	28(2)	20(1)	3(1)	2(1)	-3(1)
C(16)	25(1)	31(2)	27(2)	-8(1)	4(1)	-2(1)
C(17)	21(1)	24(2)	32(2)	-7(1)	-1(1)	3(1)
C(18)	18(1)	16(1)	24(2)	-2(1)	-4(1)	-2(1)
C(19)	19(1)	17(1)	23(2)	-3(1)	-6(1)	-3(1)
C(20)	24(1)	22(1)	32(2)	-1(1)	-9(1)	0(1)
C(21)	39(2)	17(1)	39(2)	5(1)	-15(2)	-4(1)
C(22)	41(2)	25(2)	29(2)	6(1)	-5(1)	-11(1)
C(23)	30(1)	24(2)	26(2)	0(1)	-1(1)	-5(1)

C(24)	22(1)	18(1)	22(2)	1(1)	-2(1)	-5(1)
C(25)	37(2)	32(2)	23(2)	7(1)	-5(1)	-4(1)
C(26)	54(2)	23(2)	37(2)	-5(1)	14(2)	-3(1)
C(27)	25(1)	19(1)	29(2)	5(1)	-6(1)	-4(1)
C(28)	35(2)	30(2)	30(2)	-4(1)	0(1)	-1(1)
C(29)	21(1)	23(1)	30(2)	3(1)	1(1)	-4(1)
C(30)	29(2)	31(2)	37(2)	-6(1)	6(1)	1(1)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($A^2 \times 10^3$) for **3**.

	x	y	z	U(eq)
H(2A)	5978(10)	7605(16)	2625(14)	24(7)
H(2)	7488	8424	2781	27
H(3)	8198	7755	3613	27
H(4)	7943	6351	4342	26
H(8)	5520	4184	4130	30
H(9)	5973	3213	5072	36
H(10)	6973	3526	5473	36
H(11)	7519	4861	4965	31
H(12)	7079	9995	2662	24
H(14)	6473	9049	3962	26
H(15)	5861	9582	4980	30
H(16)	5285	11026	4879	33
H(17)	5303	11968	3760	31
H(20)	5573	12840	2418	31
H(21)	5963	13338	1234	38
H(22)	6690	12394	607	38
H(23)	7037	10900	1136	32
H(25A)	5431	8456	1425	46
H(25B)	5577	9593	1243	46
H(25C)	5321	9283	2066	46
H(26A)	7333	8651	1377	56
H(26B)	6875	9203	804	56
H(26C)	6812	8036	943	56
H(27A)	5662	4988	2505	29

H(27B)	5816	6062	2175	29
H(28A)	6867	5659	2129	48
H(28B)	6482	4862	1652	48
H(28C)	6726	4593	2489	48
H(29A)	5326	7071	3282	30
H(29B)	5075	6096	3693	30
H(30A)	5621	6573	4823	48
H(30B)	5101	7355	4593	48
H(30C)	5806	7585	4407	48

Table S6. Torsion angles [°] for **3**.

C(5)-N(1)-C(1)-N(2)	-177.7(2)
B(1)-N(1)-C(1)-N(2)	7.3(3)
C(5)-N(1)-C(1)-C(2)	2.2(3)
B(1)-N(1)-C(1)-C(2)	-172.8(2)
C(1)-N(1)-B(1)-C(7)	178.2(2)
C(5)-N(1)-B(1)-C(7)	2.8(2)
C(1)-N(1)-B(1)-C(29)	-65.2(3)
C(5)-N(1)-B(1)-C(29)	119.5(2)
C(1)-N(1)-B(1)-C(27)	61.3(3)
C(5)-N(1)-B(1)-C(27)	-114.1(2)
N(1)-C(1)-N(2)-Si(1)	-179.03(16)
C(2)-C(1)-N(2)-Si(1)	1.1(3)
C(25)-Si(1)-N(2)-C(1)	-174.3(2)
C(26)-Si(1)-N(2)-C(1)	65.8(2)
C(12)-Si(1)-N(2)-C(1)	-55.7(2)
N(1)-C(1)-C(2)-C(3)	-3.3(3)
N(2)-C(1)-C(2)-C(3)	176.5(2)
C(1)-C(2)-C(3)-C(4)	1.6(4)
C(2)-C(3)-C(4)-C(5)	1.1(3)
C(1)-N(1)-C(5)-C(4)	0.6(3)
B(1)-N(1)-C(5)-C(4)	176.4(2)
C(1)-N(1)-C(5)-C(6)	-178.65(19)
B(1)-N(1)-C(5)-C(6)	-2.9(3)
C(3)-C(4)-C(5)-N(1)	-2.3(3)
C(3)-C(4)-C(5)-C(6)	176.8(2)

N(1)-C(5)-C(6)-C(11)	-176.7(2)
C(4)-C(5)-C(6)-C(11)	4.1(4)
N(1)-C(5)-C(6)-C(7)	1.6(3)
C(4)-C(5)-C(6)-C(7)	-177.6(2)
C(11)-C(6)-C(7)-C(8)	1.2(3)
C(5)-C(6)-C(7)-C(8)	-177.2(2)
C(11)-C(6)-C(7)-B(1)	178.8(2)
C(5)-C(6)-C(7)-B(1)	0.4(3)
C(29)-B(1)-C(7)-C(8)	58.4(3)
C(27)-B(1)-C(7)-C(8)	-72.5(3)
N(1)-B(1)-C(7)-C(8)	175.3(2)
C(29)-B(1)-C(7)-C(6)	-118.7(2)
C(27)-B(1)-C(7)-C(6)	110.3(2)
N(1)-B(1)-C(7)-C(6)	-1.8(2)
C(6)-C(7)-C(8)-C(9)	0.3(3)
B(1)-C(7)-C(8)-C(9)	-176.7(2)
C(7)-C(8)-C(9)-C(10)	-1.6(4)
C(8)-C(9)-C(10)-C(11)	1.3(4)
C(9)-C(10)-C(11)-C(6)	0.2(4)
C(7)-C(6)-C(11)-C(10)	-1.5(4)
C(5)-C(6)-C(11)-C(10)	176.6(2)
N(2)-Si(1)-C(12)-C(13)	-51.79(18)
C(25)-Si(1)-C(12)-C(13)	63.77(19)
C(26)-Si(1)-C(12)-C(13)	-173.07(16)
N(2)-Si(1)-C(12)-C(24)	-164.85(14)
C(25)-Si(1)-C(12)-C(24)	-49.29(18)
C(26)-Si(1)-C(12)-C(24)	73.87(18)
C(24)-C(12)-C(13)-C(14)	-173.7(2)
Si(1)-C(12)-C(13)-C(14)	68.5(3)
C(24)-C(12)-C(13)-C(18)	3.9(2)
Si(1)-C(12)-C(13)-C(18)	-113.87(18)
C(18)-C(13)-C(14)-C(15)	0.2(3)
C(12)-C(13)-C(14)-C(15)	177.6(2)
C(13)-C(14)-C(15)-C(16)	0.3(3)
C(14)-C(15)-C(16)-C(17)	0.0(3)
C(15)-C(16)-C(17)-C(18)	-0.9(3)
C(16)-C(17)-C(18)-C(13)	1.4(3)
C(16)-C(17)-C(18)-C(19)	-174.3(2)
C(14)-C(13)-C(18)-C(17)	-1.1(3)

C(12)-C(13)-C(18)-C(17)	-179.0(2)
C(14)-C(13)-C(18)-C(19)	175.5(2)
C(12)-C(13)-C(18)-C(19)	-2.4(2)
C(17)-C(18)-C(19)-C(20)	-1.0(4)
C(13)-C(18)-C(19)-C(20)	-177.1(2)
C(17)-C(18)-C(19)-C(24)	175.8(2)
C(13)-C(18)-C(19)-C(24)	-0.3(2)
C(24)-C(19)-C(20)-C(21)	0.5(3)
C(18)-C(19)-C(20)-C(21)	177.0(2)
C(19)-C(20)-C(21)-C(22)	-1.3(4)
C(20)-C(21)-C(22)-C(23)	0.6(4)
C(21)-C(22)-C(23)-C(24)	0.7(4)
C(22)-C(23)-C(24)-C(19)	-1.4(3)
C(22)-C(23)-C(24)-C(12)	179.5(2)
C(20)-C(19)-C(24)-C(23)	0.8(3)
C(18)-C(19)-C(24)-C(23)	-176.4(2)
C(20)-C(19)-C(24)-C(12)	-179.9(2)
C(18)-C(19)-C(24)-C(12)	2.9(2)
C(13)-C(12)-C(24)-C(23)	175.1(2)
Si(1)-C(12)-C(24)-C(23)	-65.1(3)
C(13)-C(12)-C(24)-C(19)	-4.1(2)
Si(1)-C(12)-C(24)-C(19)	115.67(18)
C(7)-B(1)-C(27)-C(28)	-61.3(3)
C(29)-B(1)-C(27)-C(28)	168.9(2)
N(1)-B(1)-C(27)-C(28)	43.7(3)
C(7)-B(1)-C(29)-C(30)	56.0(3)
C(27)-B(1)-C(29)-C(30)	-173.5(2)
N(1)-B(1)-C(29)-C(30)	-50.8(3)

Table S7. Crystal data and structure refinement for **4**.

Empirical formula	C50H71BLi2N2O5Si
Formula weight	832.87
Temperature	110(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P 21/n
Unit cell dimensions	a = 14.2413(7) Å α = 90 º.
	b = 19.4418(9) Å β = 107.095(2) º.

	c = 17.8883(8) Å γ = 90 º.
Volume	4734.0(4) Å ^{3}
Z, Calculated density	4, 1.169 mg/m^3
Absorption coefficient	0.097 mm^{-1}
F(000)	1800
Crystal size	0.36 × 0.27 × 0.21 mm
Theta range for data collection	1.59 to 28.35 º.
Limiting indices	-12<=h<=12, -17<=k<=17, -23<=l<=23
Reflections collected / unique	43094 / 11732 [R(int) = 0.0476]
Completeness to theta = 30.66	99.1 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7457 and 0.7175
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11732 / 0 / 572
Goodness-of-fit on F^2	1.058
Final R indices [I>2σ(I)]	R1 = 0.0513, wR2 = 0.1163
R indices (all data)	R1 = 0.0916, wR2 = 0.1279
Extinction coefficient	0.0064(4)
Largest diff. peak and hole	0.351 and -0.441e.A^{-3}

Table S8. Atomic coordinates (×10^4) and equivalent isotropic displacement parameters (A^2 × 10^3) for **4**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Si(1)	8949(1)	1987(1)	1541(1)	16(1)
N(1)	11353(1)	3148(1)	1900(1)	14(1)
C(1)	10505(1)	2791(1)	1518(1)	15(1)
B(1)	11916(1)	3141(1)	2835(1)	16(1)
Li(1)	10230(2)	2134(2)	3006(2)	26(1)
N(2)	10050(1)	2423(1)	1924(1)	16(1)
C(2)	10193(1)	2858(1)	677(1)	19(1)
C(3)	10714(1)	3219(1)	284(1)	20(1)
C(4)	11576(1)	3561(1)	694(1)	19(1)
C(5)	11860(1)	3518(1)	1496(1)	15(1)
C(6)	12713(1)	3854(1)	2043(1)	17(1)
C(7)	13385(1)	4285(1)	1851(1)	22(1)

C(8)	14131(1)	4572(1)	2450(1)	28(1)
C(9)	14190(1)	4427(1)	3224(1)	26(1)
C(10)	13515(1)	3994(1)	3406(1)	21(1)
C(11)	12760(1)	3690(1)	2813(1)	16(1)
C(12)	8653(1)	1634(1)	2397(1)	19(1)
C(13)	8456(1)	2071(1)	2982(1)	19(1)
C(14)	8571(1)	2787(1)	3112(1)	22(1)
C(15)	8373(1)	3081(1)	3752(1)	28(1)
C(16)	8045(1)	2684(1)	4278(1)	34(1)
C(17)	7907(1)	1986(1)	4159(1)	33(1)
C(18)	8107(1)	1671(1)	3524(1)	24(1)
C(19)	8066(1)	971(1)	3270(1)	25(1)
C(20)	7770(1)	369(1)	3567(1)	35(1)
C(21)	7789(1)	-247(1)	3202(1)	42(1)
C(22)	8115(1)	-278(1)	2535(1)	38(1)
C(23)	8425(1)	304(1)	2233(1)	28(1)
C(24)	8407(1)	951(1)	2588(1)	22(1)
C(25)	7946(1)	2595(1)	1014(1)	24(1)
C(26)	9050(1)	1291(1)	841(1)	26(1)
C(27)	11243(1)	3423(1)	3368(1)	17(1)
C(28)	10574(1)	4025(1)	3014(1)	24(1)
C(29)	12396(1)	2382(1)	3056(1)	18(1)
C(30)	13034(1)	2324(1)	3906(1)	26(1)
O(1)	10798(1)	1652(1)	3969(1)	22(1)
C(31)	11256(2)	991(1)	4031(1)	32(1)
C(32)	10641(2)	535(1)	4379(1)	32(1)
C(33)	10293(1)	1019(1)	4919(1)	27(1)
C(34)	10519(1)	1741(1)	4674(1)	23(1)
Li(2)	4111(2)	1220(2)	1818(2)	29(1)
O(2)	4929(1)	835(1)	1237(1)	35(1)
C(35)	4663(1)	892(2)	424(1)	51(1)
C(36)	5589(5)	1329(3)	327(4)	30(1)
C(36A)	5499(5)	1003(3)	173(4)	45(2)
C(37)	6387(1)	857(1)	863(1)	33(1)
C(38)	5991(1)	809(2)	1542(1)	60(1)
O(3)	2804(1)	1111(1)	1130(1)	27(1)
C(39)	1966(1)	1560(1)	913(1)	28(1)
C(40)	1332(1)	1298(1)	123(1)	29(1)
C(41)	1706(2)	594(1)	63(2)	82(1)

C(42)	2461(2)	448(1)	821(1)	44(1)
O(4)	4283(1)	757(1)	2792(1)	28(1)
C(43)	3476(1)	569(1)	3084(1)	22(1)
C(44)	3948(1)	369(1)	3931(1)	26(1)
C(45)	4899(1)	36(1)	3895(1)	30(1)
C(46)	5186(1)	469(1)	3296(1)	30(1)
O(5)	4509(1)	2156(1)	2024(1)	37(1)
C(47)	5256(4)	2266(3)	2796(3)	43(1)
C(47A)	4867(3)	2543(2)	2749(2)	24(1)
C(48)	5712(2)	2919(1)	2705(1)	50(1)
C(49)	5500(2)	3062(1)	1842(1)	43(1)
C(50)	4569(2)	2664(1)	1471(1)	34(1)

Table S9. Bond lengths [Å] and angles [º] for **4**.

Si(1)-N(2)	1.7357(13)
Si(1)-C(12)	1.8361(17)
Si(1)-C(26)	1.8779(18)
Si(1)-C(25)	1.8796(17)
Si(1)-Li(1)	2.732(3)
N(1)-C(5)	1.368(2)
N(1)-C(1)	1.3856(19)
N(1)-B(1)	1.628(2)
C(1)-N(2)	1.318(2)
C(1)-C(2)	1.444(2)
B(1)-C(11)	1.615(2)
B(1)-C(29)	1.626(2)
B(1)-C(27)	1.632(2)
Li(1)-O(1)	1.919(3)
Li(1)-N(2)	1.959(3)
Li(1)-C(12)	2.394(3)
Li(1)-C(13)	2.517(3)
Li(1)-C(14)	2.738(3)
C(2)-C(3)	1.358(2)
C(2)-H(2)	0.9500
C(3)-C(4)	1.400(2)
C(3)-H(3)	0.9500

C(4)-C(5)	1.373(2)
C(4)-H(4)	0.9500
C(5)-C(6)	1.470(2)
C(6)-C(7)	1.388(2)
C(6)-C(11)	1.398(2)
C(7)-C(8)	1.385(2)
C(7)-H(7)	0.9500
C(8)-C(9)	1.391(3)
C(8)-H(8)	0.9500
C(9)-C(10)	1.386(2)
C(9)-H(9)	0.9500
C(10)-C(11)	1.400(2)
C(10)-H(10)	0.9500
C(12)-C(13)	1.439(2)
C(12)-C(24)	1.440(2)
C(13)-C(14)	1.413(2)
C(13)-C(18)	1.440(2)
C(14)-C(15)	1.380(2)
C(14)-H(14)	0.9500
C(15)-C(16)	1.399(3)
C(15)-H(15)	0.9500
C(16)-C(17)	1.379(3)
C(16)-H(16)	0.9500
C(17)-C(18)	1.392(3)
C(17)-H(17)	0.9500
C(18)-C(19)	1.431(3)
C(19)-C(20)	1.400(3)
C(19)-C(24)	1.441(2)
C(20)-C(21)	1.367(3)
C(20)-H(20)	0.9500
C(21)-C(22)	1.403(3)
C(21)-H(21)	0.9500
C(22)-C(23)	1.382(3)
C(22)-H(22)	0.9500
C(23)-C(24)	1.412(3)
C(23)-H(23)	0.9500
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800

C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-C(28)	1.525(2)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-C(30)	1.530(2)
C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
O(1)-C(31)	1.431(2)
O(1)-C(34)	1.438(2)
C(31)-C(32)	1.502(3)
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(32)-C(33)	1.531(3)
C(32)-H(32A)	0.9900
C(32)-H(32B)	0.9900
C(33)-C(34)	1.532(2)
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(34)-H(34A)	0.9900
C(34)-H(34B)	0.9900
Li(2)-O(5)	1.909(4)
Li(2)-O(4)	1.913(3)
Li(2)-O(3)	1.917(3)
Li(2)-O(2)	1.926(4)
O(2)-C(35)	1.396(2)
O(2)-C(38)	1.449(2)
C(35)-C(36A)	1.408(8)
C(35)-C(36)	1.620(7)
C(35)-H(35A)	0.9900
C(35)-H(35B)	0.9900
C(36)-C(37)	1.552(7)

C(36)-H(36A)	0.9900
C(36)-H(36B)	0.9900
C(36A)-C(37)	1.512(7)
C(36A)-H(36C)	0.9900
C(36A)-H(36D)	0.9900
C(37)-C(38)	1.485(3)
C(37)-H(37A)	0.9900
C(37)-H(37B)	0.9900
C(38)-H(38A)	0.9900
C(38)-H(38B)	0.9900
O(3)-C(42)	1.430(2)
O(3)-C(39)	1.438(2)
C(39)-C(40)	1.523(2)
C(39)-H(39A)	0.9900
C(39)-H(39B)	0.9900
C(40)-C(41)	1.485(3)
C(40)-H(40A)	0.9900
C(40)-H(40B)	0.9900
C(41)-C(42)	1.489(3)
C(41)-H(41A)	0.9900
C(41)-H(41B)	0.9900
C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900
O(4)-C(43)	1.441(2)
O(4)-C(46)	1.448(2)
C(43)-C(44)	1.516(2)
C(43)-H(43A)	0.9900
C(43)-H(43B)	0.9900
C(44)-C(45)	1.520(3)
C(44)-H(44A)	0.9900
C(44)-H(44B)	0.9900
C(45)-C(46)	1.511(3)
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900
C(46)-H(46A)	0.9900
C(46)-H(46B)	0.9900
O(5)-C(50)	1.417(2)
O(5)-C(47A)	1.456(4)
O(5)-C(47)	1.491(5)

C(47)-C(48)	1.457(6)
C(47)-H(47A)	0.9900
C(47)-H(47B)	0.9900
C(47A)-C(48)	1.429(5)
C(47A)-H(47C)	0.9900
C(47A)-H(47D)	0.9900
C(48)-C(49)	1.510(3)
C(48)-H(48A)	0.9900
C(48)-H(48B)	0.9900
C(49)-C(50)	1.509(3)
C(49)-H(49A)	0.9900
C(49)-H(49B)	0.9900
C(50)-H(50A)	0.9900
C(50)-H(50B)	0.9900

N(2)-Si(1)-C(12)	104.81(7)
N(2)-Si(1)-C(26)	112.15(7)
C(12)-Si(1)-C(26)	111.59(8)
N(2)-Si(1)-C(25)	110.87(8)
C(12)-Si(1)-C(25)	109.01(8)
C(26)-Si(1)-C(25)	108.36(8)
N(2)-Si(1)-Li(1)	45.57(8)
C(12)-Si(1)-Li(1)	59.43(8)
C(26)-Si(1)-Li(1)	123.65(9)
C(25)-Si(1)-Li(1)	127.57(9)
C(5)-N(1)-C(1)	121.41(13)
C(5)-N(1)-B(1)	111.74(12)
C(1)-N(1)-B(1)	126.68(13)
N(2)-C(1)-N(1)	119.94(13)
N(2)-C(1)-C(2)	124.87(14)
N(1)-C(1)-C(2)	115.19(14)
C(11)-B(1)-C(29)	110.07(13)
C(11)-B(1)-N(1)	96.63(12)
C(29)-B(1)-N(1)	107.52(12)
C(11)-B(1)-C(27)	111.15(13)
C(29)-B(1)-C(27)	116.12(13)
N(1)-B(1)-C(27)	113.60(12)
O(1)-Li(1)-N(2)	157.77(19)
O(1)-Li(1)-C(12)	107.60(14)

N(2)-Li(1)-C(12)	80.45(11)
O(1)-Li(1)-C(13)	98.49(13)
N(2)-Li(1)-C(13)	99.12(12)
C(12)-Li(1)-C(13)	33.97(7)
O(1)-Li(1)-Si(1)	142.85(15)
N(2)-Li(1)-Si(1)	39.25(6)
C(12)-Li(1)-Si(1)	41.32(6)
C(13)-Li(1)-Si(1)	66.13(8)
O(1)-Li(1)-C(14)	107.97(14)
N(2)-Li(1)-C(14)	94.07(12)
C(12)-Li(1)-C(14)	60.47(9)
C(13)-Li(1)-C(14)	30.83(6)
Si(1)-Li(1)-C(14)	76.64(8)
C(1)-N(2)-Si(1)	125.58(11)
C(1)-N(2)-Li(1)	139.23(14)
Si(1)-N(2)-Li(1)	95.18(11)
C(3)-C(2)-C(1)	122.61(15)
C(3)-C(2)-H(2)	118.7
C(1)-C(2)-H(2)	118.7
C(2)-C(3)-C(4)	120.12(15)
C(2)-C(3)-H(3)	119.9
C(4)-C(3)-H(3)	119.9
C(5)-C(4)-C(3)	117.56(15)
C(5)-C(4)-H(4)	121.2
C(3)-C(4)-H(4)	121.2
N(1)-C(5)-C(4)	123.05(14)
N(1)-C(5)-C(6)	110.07(13)
C(4)-C(5)-C(6)	126.88(15)
C(7)-C(6)-C(11)	123.06(15)
C(7)-C(6)-C(5)	126.76(15)
C(11)-C(6)-C(5)	110.18(14)
C(8)-C(7)-C(6)	118.67(16)
C(8)-C(7)-H(7)	120.7
C(6)-C(7)-H(7)	120.7
C(7)-C(8)-C(9)	119.73(16)
C(7)-C(8)-H(8)	120.1
C(9)-C(8)-H(8)	120.1
C(10)-C(9)-C(8)	120.93(16)
C(10)-C(9)-H(9)	119.5

C(8)-C(9)-H(9)	119.5
C(9)-C(10)-C(11)	120.68(16)
C(9)-C(10)-H(10)	119.7
C(11)-C(10)-H(10)	119.7
C(6)-C(11)-C(10)	116.91(15)
C(6)-C(11)-B(1)	110.79(13)
C(10)-C(11)-B(1)	132.26(15)
C(13)-C(12)-C(24)	104.96(14)
C(13)-C(12)-Si(1)	121.86(13)
C(24)-C(12)-Si(1)	132.41(13)
C(13)-C(12)-Li(1)	77.71(12)
C(24)-C(12)-Li(1)	121.79(13)
Si(1)-C(12)-Li(1)	79.25(9)
C(14)-C(13)-C(12)	131.56(15)
C(14)-C(13)-C(18)	117.88(15)
C(12)-C(13)-C(18)	110.53(15)
C(14)-C(13)-Li(1)	83.24(12)
C(12)-C(13)-Li(1)	68.33(11)
C(18)-C(13)-Li(1)	123.88(12)
C(15)-C(14)-C(13)	120.13(17)
C(15)-C(14)-Li(1)	129.84(13)
C(13)-C(14)-Li(1)	65.93(11)
C(15)-C(14)-H(14)	119.9
C(13)-C(14)-H(14)	119.9
Li(1)-C(14)-H(14)	76.5
C(14)-C(15)-C(16)	121.28(19)
C(14)-C(15)-H(15)	119.4
C(16)-C(15)-H(15)	119.4
C(17)-C(16)-C(15)	120.05(17)
C(17)-C(16)-H(16)	120.0
C(15)-C(16)-H(16)	120.0
C(16)-C(17)-C(18)	120.22(18)
C(16)-C(17)-H(17)	119.9
C(18)-C(17)-H(17)	119.9
C(17)-C(18)-C(19)	132.66(17)
C(17)-C(18)-C(13)	120.42(18)
C(19)-C(18)-C(13)	106.89(15)
C(20)-C(19)-C(18)	131.63(18)
C(20)-C(19)-C(24)	120.81(19)

C(18)-C(19)-C(24)	107.56(15)
C(21)-C(20)-C(19)	120.1(2)
C(21)-C(20)-H(20)	120.0
C(19)-C(20)-H(20)	120.0
C(20)-C(21)-C(22)	120.12(19)
C(20)-C(21)-H(21)	119.9
C(22)-C(21)-H(21)	119.9
C(23)-C(22)-C(21)	121.3(2)
C(23)-C(22)-H(22)	119.3
C(21)-C(22)-H(22)	119.3
C(22)-C(23)-C(24)	120.3(2)
C(22)-C(23)-H(23)	119.9
C(24)-C(23)-H(23)	119.9
C(23)-C(24)-C(12)	132.56(17)
C(23)-C(24)-C(19)	117.39(17)
C(12)-C(24)-C(19)	110.04(16)
Si(1)-C(25)-H(25A)	109.5
Si(1)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
Si(1)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
Si(1)-C(26)-H(26A)	109.5
Si(1)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
Si(1)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(28)-C(27)-B(1)	114.74(13)
C(28)-C(27)-H(27A)	108.6
B(1)-C(27)-H(27A)	108.6
C(28)-C(27)-H(27B)	108.6
B(1)-C(27)-H(27B)	108.6
H(27A)-C(27)-H(27B)	107.6
C(27)-C(28)-H(28A)	109.5
C(27)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(27)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5

H(28B)-C(28)-H(28C) 109.5
C(30)-C(29)-B(1) 113.06(13)
C(30)-C(29)-H(29A) 109.0
B(1)-C(29)-H(29A) 109.0
C(30)-C(29)-H(29B) 109.0
B(1)-C(29)-H(29B) 109.0
H(29A)-C(29)-H(29B) 107.8
C(29)-C(30)-H(30A) 109.5
C(29)-C(30)-H(30B) 109.5
H(30A)-C(30)-H(30B) 109.5
C(29)-C(30)-H(30C) 109.5
H(30A)-C(30)-H(30C) 109.5
H(30B)-C(30)-H(30C) 109.5
C(31)-O(1)-C(34) 106.02(13)
C(31)-O(1)-Li(1) 124.78(14)
C(34)-O(1)-Li(1) 125.21(14)
O(1)-C(31)-C(32) 104.74(15)
O(1)-C(31)-H(31A) 110.8
C(32)-C(31)-H(31A) 110.8
O(1)-C(31)-H(31B) 110.8
C(32)-C(31)-H(31B) 110.8
H(31A)-C(31)-H(31B) 108.9
C(31)-C(32)-C(33) 103.58(15)
C(31)-C(32)-H(32A) 111.0
C(33)-C(32)-H(32A) 111.0
C(31)-C(32)-H(32B) 111.0
C(33)-C(32)-H(32B) 111.0
H(32A)-C(32)-H(32B) 109.0
C(32)-C(33)-C(34) 104.35(14)
C(32)-C(33)-H(33A) 110.9
C(34)-C(33)-H(33A) 110.9
C(32)-C(33)-H(33B) 110.9
C(34)-C(33)-H(33B) 110.9
H(33A)-C(33)-H(33B) 108.9
O(1)-C(34)-C(33) 106.05(14)
O(1)-C(34)-H(34A) 110.5
C(33)-C(34)-H(34A) 110.5
O(1)-C(34)-H(34B) 110.5
C(33)-C(34)-H(34B) 110.5

H(34A)-C(34)-H(34B)	108.7
O(5)-Li(2)-O(4)	108.72(16)
O(5)-Li(2)-O(3)	113.99(17)
O(4)-Li(2)-O(3)	111.85(16)
O(5)-Li(2)-O(2)	106.40(16)
O(4)-Li(2)-O(2)	111.89(17)
O(3)-Li(2)-O(2)	103.82(16)
C(35)-O(2)-C(38)	109.21(15)
C(35)-O(2)-Li(2)	120.55(14)
C(38)-O(2)-Li(2)	122.69(16)
O(2)-C(35)-C(36A)	110.4(3)
O(2)-C(35)-C(36)	99.9(3)
C(36A)-C(35)-C(36)	25.0(3)
O(2)-C(35)-H(35A)	111.8
C(36A)-C(35)-H(35A)	123.8
C(36)-C(35)-H(35A)	111.8
O(2)-C(35)-H(35B)	111.8
C(36A)-C(35)-H(35B)	86.8
C(36)-C(35)-H(35B)	111.8
H(35A)-C(35)-H(35B)	109.5
C(37)-C(36)-C(35)	95.5(3)
C(37)-C(36)-H(36A)	112.6
C(35)-C(36)-H(36A)	112.6
C(37)-C(36)-H(36B)	112.6
C(35)-C(36)-H(36B)	112.6
H(36A)-C(36)-H(36B)	110.1
C(35)-C(36A)-C(37)	107.0(5)
C(35)-C(36A)-H(36C)	110.3
C(37)-C(36A)-H(36C)	110.3
C(35)-C(36A)-H(36D)	110.3
C(37)-C(36A)-H(36D)	110.3
H(36C)-C(36A)-H(36D)	108.6
C(38)-C(37)-C(36A)	104.6(3)
C(38)-C(37)-C(36)	99.0(3)
C(36A)-C(37)-C(36)	25.9(3)
C(38)-C(37)-H(37A)	112.0
C(36A)-C(37)-H(37A)	86.7
C(36)-C(37)-H(37A)	112.0
C(38)-C(37)-H(37B)	112.0

C(36A)-C(37)-H(37B) 129.2
C(36)-C(37)-H(37B) 112.0
H(37A)-C(37)-H(37B) 109.6
O(2)-C(38)-C(37) 107.16(16)
O(2)-C(38)-H(38A) 110.3
C(37)-C(38)-H(38A) 110.3
O(2)-C(38)-H(38B) 110.3
C(37)-C(38)-H(38B) 110.3
H(38A)-C(38)-H(38B) 108.5
C(42)-O(3)-C(39) 106.31(13)
C(42)-O(3)-Li(2) 120.33(15)
C(39)-O(3)-Li(2) 132.72(15)
O(3)-C(39)-C(40) 105.42(14)
O(3)-C(39)-H(39A) 110.7
C(40)-C(39)-H(39A) 110.7
O(3)-C(39)-H(39B) 110.7
C(40)-C(39)-H(39B) 110.7
H(39A)-C(39)-H(39B) 108.8
C(41)-C(40)-C(39) 104.39(16)
C(41)-C(40)-H(40A) 110.9
C(39)-C(40)-H(40A) 110.9
C(41)-C(40)-H(40B) 110.9
C(39)-C(40)-H(40B) 110.9
H(40A)-C(40)-H(40B) 108.9
C(40)-C(41)-C(42) 106.72(18)
C(40)-C(41)-H(41A) 110.4
C(42)-C(41)-H(41A) 110.4
C(40)-C(41)-H(41B) 110.4
C(42)-C(41)-H(41B) 110.4
H(41A)-C(41)-H(41B) 108.6
O(3)-C(42)-C(41) 104.76(17)
O(3)-C(42)-H(42A) 110.8
C(41)-C(42)-H(42A) 110.8
O(3)-C(42)-H(42B) 110.8
C(41)-C(42)-H(42B) 110.8
H(42A)-C(42)-H(42B) 108.9
C(43)-O(4)-C(46) 109.47(12)
C(43)-O(4)-Li(2) 123.18(13)
C(46)-O(4)-Li(2) 126.93(14)

O(4)-C(43)-C(44) 105.12(13)
O(4)-C(43)-H(43A) 110.7
C(44)-C(43)-H(43A) 110.7
O(4)-C(43)-H(43B) 110.7
C(44)-C(43)-H(43B) 110.7
H(43A)-C(43)-H(43B) 108.8
C(43)-C(44)-C(45) 101.85(14)
C(43)-C(44)-H(44A) 111.4
C(45)-C(44)-H(44A) 111.4
C(43)-C(44)-H(44B) 111.4
C(45)-C(44)-H(44B) 111.4
H(44A)-C(44)-H(44B) 109.3
C(46)-C(45)-C(44) 102.84(15)
C(46)-C(45)-H(45A) 111.2
C(44)-C(45)-H(45A) 111.2
C(46)-C(45)-H(45B) 111.2
C(44)-C(45)-H(45B) 111.2
H(45A)-C(45)-H(45B) 109.1
O(4)-C(46)-C(45) 106.32(14)
O(4)-C(46)-H(46A) 110.5
C(45)-C(46)-H(46A) 110.5
O(4)-C(46)-H(46B) 110.5
C(45)-C(46)-H(46B) 110.5
H(46A)-C(46)-H(46B) 108.7
C(50)-O(5)-C(47A) 100.6(2)
C(50)-O(5)-C(47) 112.0(2)
C(47A)-O(5)-C(47) 29.8(2)
C(50)-O(5)-Li(2) 127.22(15)
C(47A)-O(5)-Li(2) 132.1(2)
C(47)-O(5)-Li(2) 113.9(2)
C(48)-C(47)-O(5) 104.0(3)
C(48)-C(47)-H(47A) 111.0
O(5)-C(47)-H(47A) 111.0
C(48)-C(47)-H(47B) 111.0
O(5)-C(47)-H(47B) 111.0
H(47A)-C(47)-H(47B) 109.0
C(48)-C(47A)-O(5) 107.2(3)
C(48)-C(47A)-H(47C) 110.3
O(5)-C(47A)-H(47C) 110.3

C(48)-C(47A)-H(47D)	110.3
O(5)-C(47A)-H(47D)	110.3
H(47C)-C(47A)-H(47D)	108.5
C(47A)-C(48)-C(47)	30.5(2)
C(47A)-C(48)-C(49)	103.4(2)
C(47)-C(48)-C(49)	108.2(3)
C(47A)-C(48)-H(48A)	136.5
C(47)-C(48)-H(48A)	110.1
C(49)-C(48)-H(48A)	110.1
C(47A)-C(48)-H(48B)	84.5
C(47)-C(48)-H(48B)	110.1
C(49)-C(48)-H(48B)	110.1
H(48A)-C(48)-H(48B)	108.4
C(50)-C(49)-C(48)	103.91(17)
C(50)-C(49)-H(49A)	111.0
C(48)-C(49)-H(49A)	111.0
C(50)-C(49)-H(49B)	111.0
C(48)-C(49)-H(49B)	111.0
H(49A)-C(49)-H(49B)	109.0
O(5)-C(50)-C(49)	106.05(15)
O(5)-C(50)-H(50A)	110.5
C(49)-C(50)-H(50A)	110.5
O(5)-C(50)-H(50B)	110.5
C(49)-C(50)-H(50B)	110.5
H(50A)-C(50)-H(50B)	108.7

Table S10. Anisotropic displacement parameters ($A^2 \times 10^3$) for **4**. The anisotropic displacement factor exponent takes the form: $-2\,pi^2\,[\,h^2\,a^{*2}\,U11 + ... + 2\,h\,k\,a^*\,b^*\,U12\,]$

	U11	U22	U33	U23	U13	U12
Si(1)	13(1)	22(1)	14(1)	-3(1)	4(1)	-2(1)
N(1)	14(1)	16(1)	12(1)	-1(1)	4(1)	0(1)
C(1)	15(1)	17(1)	14(1)	-2(1)	4(1)	2(1)
B(1)	16(1)	20(1)	11(1)	-1(1)	3(1)	-1(1)
Li(1)	24(2)	32(2)	19(1)	5(1)	4(1)	0(1)

N(2)	15(1)	18(1)	15(1)	-1(1)	4(1)	-3(1)
C(2)	19(1)	24(1)	13(1)	-1(1)	3(1)	0(1)
C(3)	25(1)	23(1)	13(1)	1(1)	5(1)	3(1)
C(4)	23(1)	20(1)	16(1)	3(1)	10(1)	1(1)
C(5)	16(1)	14(1)	17(1)	0(1)	8(1)	2(1)
C(6)	15(1)	16(1)	20(1)	-1(1)	7(1)	3(1)
C(7)	20(1)	23(1)	25(1)	4(1)	10(1)	1(1)
C(8)	17(1)	29(1)	38(1)	5(1)	11(1)	-5(1)
C(9)	18(1)	25(1)	31(1)	-4(1)	1(1)	-4(1)
C(10)	19(1)	21(1)	20(1)	-1(1)	3(1)	0(1)
C(11)	16(1)	14(1)	19(1)	-1(1)	6(1)	3(1)
C(12)	14(1)	23(1)	18(1)	-1(1)	4(1)	-1(1)
C(13)	13(1)	29(1)	14(1)	2(1)	3(1)	0(1)
C(14)	18(1)	31(1)	16(1)	-1(1)	5(1)	2(1)
C(15)	24(1)	38(1)	20(1)	-5(1)	5(1)	8(1)
C(16)	29(1)	55(1)	20(1)	-1(1)	10(1)	14(1)
C(17)	20(1)	61(2)	20(1)	14(1)	9(1)	8(1)
C(18)	13(1)	39(1)	18(1)	10(1)	3(1)	1(1)
C(19)	12(1)	35(1)	26(1)	14(1)	1(1)	0(1)
C(20)	19(1)	44(1)	39(1)	23(1)	2(1)	-2(1)
C(21)	22(1)	36(1)	60(1)	28(1)	0(1)	-3(1)
C(22)	22(1)	22(1)	59(1)	8(1)	-5(1)	1(1)
C(23)	16(1)	24(1)	38(1)	2(1)	0(1)	1(1)
C(24)	9(1)	26(1)	27(1)	5(1)	-1(1)	0(1)
C(25)	20(1)	35(1)	18(1)	1(1)	5(1)	3(1)
C(26)	24(1)	30(1)	28(1)	-11(1)	12(1)	-8(1)
C(27)	19(1)	18(1)	14(1)	-2(1)	6(1)	-2(1)
C(28)	24(1)	25(1)	25(1)	-2(1)	11(1)	1(1)
C(29)	18(1)	19(1)	15(1)	0(1)	4(1)	0(1)
C(30)	31(1)	24(1)	18(1)	3(1)	1(1)	4(1)
O(1)	28(1)	21(1)	20(1)	6(1)	11(1)	4(1)
C(31)	40(1)	23(1)	41(1)	6(1)	21(1)	7(1)
C(32)	38(1)	27(1)	33(1)	7(1)	14(1)	0(1)
C(33)	28(1)	31(1)	22(1)	9(1)	9(1)	1(1)
C(34)	22(1)	30(1)	17(1)	-1(1)	6(1)	-2(1)
Li(2)	20(1)	43(2)	23(2)	7(1)	4(1)	-6(1)
O(2)	18(1)	58(1)	29(1)	18(1)	8(1)	8(1)
C(35)	21(1)	106(2)	23(1)	-17(1)	3(1)	7(1)
C(36)	26(2)	46(4)	22(3)	10(3)	12(2)	3(3)

C(36A)	37(3)	66(5)	35(4)	16(3)	14(3)	11(4)
C(37)	19(1)	47(1)	32(1)	-2(1)	9(1)	-3(1)
C(38)	19(1)	121(2)	39(1)	24(1)	8(1)	17(1)
O(3)	19(1)	29(1)	29(1)	-2(1)	2(1)	-1(1)
C(39)	20(1)	37(1)	27(1)	-3(1)	8(1)	4(1)
C(40)	20(1)	39(1)	27(1)	0(1)	6(1)	-1(1)
C(41)	79(2)	48(2)	77(2)	-31(2)	-43(2)	23(2)
C(42)	33(1)	24(1)	62(2)	7(1)	-5(1)	-8(1)
O(4)	21(1)	39(1)	23(1)	11(1)	4(1)	-3(1)
C(43)	22(1)	23(1)	24(1)	2(1)	7(1)	-1(1)
C(44)	34(1)	23(1)	22(1)	2(1)	10(1)	3(1)
C(45)	32(1)	34(1)	23(1)	5(1)	6(1)	6(1)
C(46)	21(1)	37(1)	28(1)	2(1)	3(1)	-1(1)
O(5)	44(1)	41(1)	25(1)	-2(1)	8(1)	-22(1)
C(47)	49(3)	39(3)	29(2)	10(2)	-10(2)	-9(2)
C(47A)	32(2)	24(3)	18(2)	0(2)	8(2)	-2(2)
C(48)	50(1)	57(2)	35(1)	7(1)	0(1)	-21(1)
C(49)	53(1)	40(1)	40(1)	-3(1)	20(1)	-15(1)
C(50)	47(1)	24(1)	28(1)	1(1)	4(1)	1(1)

Table S11. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($A^2 \times 10^3$) for **4**.

	x	y	z	U(eq)
H(2)	9600	2641	388	23
H(3)	10492	3239	-271	24
H(4)	11952	3813	428	22
H(7)	13334	4381	1320	26
H(8)	14600	4867	2332	33
H(9)	14699	4627	3633	31
H(10)	13565	3904	3938	25
H(14)	8785	3067	2759	26
H(15)	8461	3562	3837	33
H(16)	7918	2896	4717	41
H(17)	7673	1719	4512	39

H(20)	7555	388	4021	43
H(21)	7581	-654	3401	50
H(22)	8123	-709	2286	46
H(23)	8651	269	1785	33
H(25A)	7745	2874	1397	37
H(25B)	7382	2331	699	37
H(25C)	8189	2896	673	37
H(26A)	9174	1498	379	39
H(26B)	8436	1029	680	39
H(26C)	9594	983	1097	39
H(27A)	10832	3039	3458	21
H(27B)	11683	3565	3883	21
H(28A)	10969	4402	2901	36
H(28B)	10234	4183	3386	36
H(28C)	10090	3877	2529	36
H(29A)	11861	2037	2960	21
H(29B)	12801	2271	2707	21
H(30A)	13590	2643	3997	38
H(30B)	13281	1853	4011	38
H(30C)	12641	2441	4255	38
H(31A)	11941	1011	4375	39
H(31B)	11257	820	3510	39
H(32A)	11037	152	4678	38
H(32B)	10077	342	3967	38
H(33A)	10653	930	5474	32
H(33B)	9580	963	4844	32
H(34A)	9933	2040	4576	27
H(34B)	11062	1953	5088	27
H(35A)	4037	1145	216	61
H(35B)	4611	437	168	61
H(36A)	5617	1337	-219	36
H(36B)	5610	1803	532	36
H(36C)	5514	1485	-4	55
H(36D)	5491	693	-268	55
H(37A)	6415	402	622	39
H(37B)	7045	1074	1006	39
H(38A)	6200	373	1828	71
H(38B)	6234	1197	1906	71
H(39A)	2172	2041	870	33

H(39B)	1600	1541	1305	33
H(40A)	630	1287	104	34
H(40B)	1407	1594	-306	34
H(41A)	2000	568	-373	99
H(41B)	1164	255	-32	99
H(42A)	2169	196	1179	52
H(42B)	3005	171	738	52
H(43A)	3105	178	2784	27
H(43B)	3023	962	3047	27
H(44A)	3533	40	4114	31
H(44B)	4076	777	4277	31
H(45A)	5408	55	4409	36
H(45B)	4793	-450	3724	36
H(46A)	5641	841	3556	36
H(46B)	5514	183	2989	36
H(47A)	4941	2292	3221	52
H(47B)	5746	1889	2914	52
H(47C)	4354	2863	2810	29
H(47D)	5045	2226	3202	29
H(48A)	6430	2895	2957	60
H(48B)	5442	3292	2957	60
H(49A)	5401	3560	1731	52
H(49B)	6044	2898	1648	52
H(50A)	3991	2972	1356	41
H(50B)	4597	2446	978	41

Table S12. Torsion angles [º] for **4**.

C(5)-N(1)-C(1)-N(2)	178.03(14)
B(1)-N(1)-C(1)-N(2)	3.1(2)
C(5)-N(1)-C(1)-C(2)	-1.6(2)
B(1)-N(1)-C(1)-C(2)	-176.55(14)
C(5)-N(1)-B(1)-C(11)	7.39(16)
C(1)-N(1)-B(1)-C(11)	-177.27(14)
C(5)-N(1)-B(1)-C(29)	-106.13(15)
C(1)-N(1)-B(1)-C(29)	69.21(18)

C(5)-N(1)-B(1)-C(27)	123.95(15)
C(1)-N(1)-B(1)-C(27)	-60.7(2)
N(2)-Si(1)-Li(1)-O(1)	-143.8(3)
C(12)-Si(1)-Li(1)-O(1)	42.0(2)
C(26)-Si(1)-Li(1)-O(1)	-54.9(3)
C(25)-Si(1)-Li(1)-O(1)	133.3(2)
C(12)-Si(1)-Li(1)-N(2)	-174.15(14)
C(26)-Si(1)-Li(1)-N(2)	88.95(12)
C(25)-Si(1)-Li(1)-N(2)	-82.83(13)
N(2)-Si(1)-Li(1)-C(12)	174.15(14)
C(26)-Si(1)-Li(1)-C(12)	-96.90(11)
C(25)-Si(1)-Li(1)-C(12)	91.32(11)
N(2)-Si(1)-Li(1)-C(13)	144.63(13)
C(12)-Si(1)-Li(1)-C(13)	-29.52(8)
C(26)-Si(1)-Li(1)-C(13)	-126.42(9)
C(25)-Si(1)-Li(1)-C(13)	61.80(12)
N(2)-Si(1)-Li(1)-C(14)	113.95(12)
C(12)-Si(1)-Li(1)-C(14)	-60.20(9)
C(26)-Si(1)-Li(1)-C(14)	-157.11(8)
C(25)-Si(1)-Li(1)-C(14)	31.11(13)
N(1)-C(1)-N(2)-Si(1)	176.21(11)
C(2)-C(1)-N(2)-Si(1)	-4.2(2)
N(1)-C(1)-N(2)-Li(1)	-5.1(3)
C(2)-C(1)-N(2)-Li(1)	174.47(19)
C(12)-Si(1)-N(2)-C(1)	-175.68(14)
C(26)-Si(1)-N(2)-C(1)	63.08(16)
C(25)-Si(1)-N(2)-C(1)	-58.20(15)
Li(1)-Si(1)-N(2)-C(1)	179.11(19)
C(12)-Si(1)-N(2)-Li(1)	5.21(12)
C(26)-Si(1)-N(2)-Li(1)	-116.03(12)
C(25)-Si(1)-N(2)-Li(1)	122.69(12)
O(1)-Li(1)-N(2)-C(1)	-69.3(6)
C(12)-Li(1)-N(2)-C(1)	177.19(19)
C(13)-Li(1)-N(2)-C(1)	148.69(18)
Si(1)-Li(1)-N(2)-C(1)	-178.9(2)
C(14)-Li(1)-N(2)-C(1)	118.1(2)
O(1)-Li(1)-N(2)-Si(1)	109.6(5)
C(12)-Li(1)-N(2)-Si(1)	-3.91(9)
C(13)-Li(1)-N(2)-Si(1)	-32.42(12)

C(14)-Li(1)-N(2)-Si(1)	-63.05(10)
N(2)-C(1)-C(2)-C(3)	-176.83(16)
N(1)-C(1)-C(2)-C(3)	2.8(2)
C(1)-C(2)-C(3)-C(4)	-1.8(3)
C(2)-C(3)-C(4)-C(5)	-0.4(2)
C(1)-N(1)-C(5)-C(4)	-0.5(2)
B(1)-N(1)-C(5)-C(4)	175.12(15)
C(1)-N(1)-C(5)-C(6)	178.83(13)
B(1)-N(1)-C(5)-C(6)	-5.54(17)
C(3)-C(4)-C(5)-N(1)	1.6(2)
C(3)-C(4)-C(5)-C(6)	-177.63(15)
N(1)-C(5)-C(6)-C(7)	-178.41(15)
C(4)-C(5)-C(6)-C(7)	0.9(3)
N(1)-C(5)-C(6)-C(11)	0.63(18)
C(4)-C(5)-C(6)-C(11)	179.94(16)
C(11)-C(6)-C(7)-C(8)	-0.8(3)
C(5)-C(6)-C(7)-C(8)	178.16(16)
C(6)-C(7)-C(8)-C(9)	-0.2(3)
C(7)-C(8)-C(9)-C(10)	0.4(3)
C(8)-C(9)-C(10)-C(11)	0.4(3)
C(7)-C(6)-C(11)-C(10)	1.5(2)
C(5)-C(6)-C(11)-C(10)	-177.59(14)
C(7)-C(6)-C(11)-B(1)	-176.36(15)
C(5)-C(6)-C(11)-B(1)	4.56(18)
C(9)-C(10)-C(11)-C(6)	-1.3(2)
C(9)-C(10)-C(11)-B(1)	176.02(16)
C(29)-B(1)-C(11)-C(6)	104.53(15)
N(1)-B(1)-C(11)-C(6)	-6.89(16)
C(27)-B(1)-C(11)-C(6)	-125.39(14)
C(29)-B(1)-C(11)-C(10)	-72.9(2)
N(1)-B(1)-C(11)-C(10)	175.70(16)
C(27)-B(1)-C(11)-C(10)	57.2(2)
N(2)-Si(1)-C(12)-C(13)	63.77(13)
C(26)-Si(1)-C(12)-C(13)	-174.62(12)
C(25)-Si(1)-C(12)-C(13)	-54.97(14)
Li(1)-Si(1)-C(12)-C(13)	68.09(14)
N(2)-Si(1)-C(12)-C(24)	-127.87(15)
C(26)-Si(1)-C(12)-C(24)	-6.27(18)
C(25)-Si(1)-C(12)-C(24)	113.38(16)

Li(1)-Si(1)-C(12)-C(24)	-123.56(18)
N(2)-Si(1)-C(12)-Li(1)	-4.32(10)
C(26)-Si(1)-C(12)-Li(1)	117.29(10)
C(25)-Si(1)-C(12)-Li(1)	-123.06(10)
O(1)-Li(1)-C(12)-C(13)	78.84(16)
N(2)-Li(1)-C(12)-C(13)	-122.50(14)
Si(1)-Li(1)-C(12)-C(13)	-126.25(12)
C(14)-Li(1)-C(12)-C(13)	-22.25(9)
O(1)-Li(1)-C(12)-C(24)	-21.3(2)
N(2)-Li(1)-C(12)-C(24)	137.37(15)
C(13)-Li(1)-C(12)-C(24)	-100.13(17)
Si(1)-Li(1)-C(12)-C(24)	133.62(17)
C(14)-Li(1)-C(12)-C(24)	-122.38(15)
O(1)-Li(1)-C(12)-Si(1)	-154.91(15)
N(2)-Li(1)-C(12)-Si(1)	3.75(9)
C(13)-Li(1)-C(12)-Si(1)	126.25(12)
C(14)-Li(1)-C(12)-Si(1)	104.00(8)
C(24)-C(12)-C(13)-C(14)	178.54(16)
Si(1)-C(12)-C(13)-C(14)	-10.3(2)
Li(1)-C(12)-C(13)-C(14)	58.55(18)
C(24)-C(12)-C(13)-C(18)	0.54(16)
Si(1)-C(12)-C(13)-C(18)	171.67(11)
Li(1)-C(12)-C(13)-C(18)	-119.45(13)
C(24)-C(12)-C(13)-Li(1)	119.99(13)
Si(1)-C(12)-C(13)-Li(1)	-68.88(12)
O(1)-Li(1)-C(13)-C(14)	111.01(14)
N(2)-Li(1)-C(13)-C(14)	-82.61(14)
C(12)-Li(1)-C(13)-C(14)	-140.00(15)
Si(1)-Li(1)-C(13)-C(14)	-104.38(10)
O(1)-Li(1)-C(13)-C(12)	-108.99(15)
N(2)-Li(1)-C(13)-C(12)	57.39(14)
Si(1)-Li(1)-C(13)-C(12)	35.61(9)
C(14)-Li(1)-C(13)-C(12)	140.00(15)
O(1)-Li(1)-C(13)-C(18)	-8.2(2)
N(2)-Li(1)-C(13)-C(18)	158.21(16)
C(12)-Li(1)-C(13)-C(18)	100.83(19)
Si(1)-Li(1)-C(13)-C(18)	136.44(16)
C(14)-Li(1)-C(13)-C(18)	-119.18(19)
C(12)-C(13)-C(14)-C(15)	-176.48(16)

C(18)-C(13)-C(14)-C(15)	1.4(2)
Li(1)-C(13)-C(14)-C(15)	-123.51(16)
C(12)-C(13)-C(14)-Li(1)	-52.97(17)
C(18)-C(13)-C(14)-Li(1)	124.91(15)
O(1)-Li(1)-C(14)-C(15)	34.0(2)
N(2)-Li(1)-C(14)-C(15)	-148.92(18)
C(12)-Li(1)-C(14)-C(15)	134.46(19)
C(13)-Li(1)-C(14)-C(15)	110.1(2)
Si(1)-Li(1)-C(14)-C(15)	175.65(18)
O(1)-Li(1)-C(14)-C(13)	-76.08(15)
N(2)-Li(1)-C(14)-C(13)	101.00(14)
C(12)-Li(1)-C(14)-C(13)	24.38(9)
Si(1)-Li(1)-C(14)-C(13)	65.56(10)
C(13)-C(14)-C(15)-C(16)	-0.8(2)
Li(1)-C(14)-C(15)-C(16)	-83.3(2)
C(14)-C(15)-C(16)-C(17)	-0.5(3)
C(15)-C(16)-C(17)-C(18)	1.0(3)
C(16)-C(17)-C(18)-C(19)	177.67(17)
C(16)-C(17)-C(18)-C(13)	-0.4(2)
C(14)-C(13)-C(18)-C(17)	-0.9(2)
C(12)-C(13)-C(18)-C(17)	177.46(14)
Li(1)-C(13)-C(18)-C(17)	100.37(19)
C(14)-C(13)-C(18)-C(19)	-179.34(13)
C(12)-C(13)-C(18)-C(19)	-1.03(17)
Li(1)-C(13)-C(18)-C(19)	-78.11(18)
C(17)-C(18)-C(19)-C(20)	2.9(3)
C(13)-C(18)-C(19)-C(20)	-178.87(16)
C(17)-C(18)-C(19)-C(24)	-177.14(17)
C(13)-C(18)-C(19)-C(24)	1.09(17)
C(18)-C(19)-C(20)-C(21)	179.08(17)
C(24)-C(19)-C(20)-C(21)	-0.9(2)
C(19)-C(20)-C(21)-C(22)	0.7(3)
C(20)-C(21)-C(22)-C(23)	0.2(3)
C(21)-C(22)-C(23)-C(24)	-0.8(3)
C(22)-C(23)-C(24)-C(12)	-178.05(16)
C(22)-C(23)-C(24)-C(19)	0.6(2)
C(13)-C(12)-C(24)-C(23)	178.86(16)
Si(1)-C(12)-C(24)-C(23)	9.1(3)
Li(1)-C(12)-C(24)-C(23)	-96.5(2)

C(13)-C(12)-C(24)-C(19)	0.15(16)
Si(1)-C(12)-C(24)-C(19)	-169.62(12)
Li(1)-C(12)-C(24)-C(19)	84.78(17)
C(20)-C(19)-C(24)-C(23)	0.3(2)
C(18)-C(19)-C(24)-C(23)	-179.72(14)
C(20)-C(19)-C(24)-C(12)	179.18(14)
C(18)-C(19)-C(24)-C(12)	-0.79(17)
C(11)-B(1)-C(27)-C(28)	70.01(17)
C(29)-B(1)-C(27)-C(28)	-163.16(13)
N(1)-B(1)-C(27)-C(28)	-37.70(19)
C(11)-B(1)-C(29)-C(30)	70.31(17)
N(1)-B(1)-C(29)-C(30)	174.45(13)
C(27)-B(1)-C(29)-C(30)	-57.06(19)
N(2)-Li(1)-O(1)-C(31)	-30.0(6)
C(12)-Li(1)-O(1)-C(31)	78.47(19)
C(13)-Li(1)-O(1)-C(31)	112.12(16)
Si(1)-Li(1)-O(1)-C(31)	50.8(3)
C(14)-Li(1)-O(1)-C(31)	142.32(14)
N(2)-Li(1)-O(1)-C(34)	175.7(4)
C(12)-Li(1)-O(1)-C(34)	-75.87(19)
C(13)-Li(1)-O(1)-C(34)	-42.21(19)
Si(1)-Li(1)-O(1)-C(34)	-103.5(3)
C(14)-Li(1)-O(1)-C(34)	-12.0(2)
C(34)-O(1)-C(31)-C(32)	40.53(18)
Li(1)-O(1)-C(31)-C(32)	-117.87(18)
O(1)-C(31)-C(32)-C(33)	-33.11(19)
C(31)-C(32)-C(33)-C(34)	14.00(18)
C(31)-O(1)-C(34)-C(33)	-31.00(17)
Li(1)-O(1)-C(34)-C(33)	127.28(16)
C(32)-C(33)-C(34)-O(1)	9.52(17)
O(5)-Li(2)-O(2)-C(35)	-86.9(2)
O(4)-Li(2)-O(2)-C(35)	154.46(18)
O(3)-Li(2)-O(2)-C(35)	33.7(2)
O(5)-Li(2)-O(2)-C(38)	59.5(2)
O(4)-Li(2)-O(2)-C(38)	-59.1(3)
O(3)-Li(2)-O(2)-C(38)	-179.94(18)
C(38)-O(2)-C(35)-C(36A)	-8.2(4)
Li(2)-O(2)-C(35)-C(36A)	142.2(3)
C(38)-O(2)-C(35)-C(36)	-31.8(3)

Li(2)-O(2)-C(35)-C(36)	118.7(3)
O(2)-C(35)-C(36)-C(37)	49.8(3)
C(36A)-C(35)-C(36)-C(37)	-67.7(11)
O(2)-C(35)-C(36A)-C(37)	12.6(5)
C(36)-C(35)-C(36A)-C(37)	81.4(11)
C(35)-C(36A)-C(37)-C(38)	-11.9(5)
C(35)-C(36A)-C(37)-C(36)	-92.4(11)
C(35)-C(36)-C(37)-C(38)	-48.4(3)
C(35)-C(36)-C(37)-C(36A)	56.5(10)
C(35)-O(2)-C(38)-C(37)	0.2(3)
Li(2)-O(2)-C(38)-C(37)	-149.49(19)
C(36A)-C(37)-C(38)-O(2)	7.1(4)
C(36)-C(37)-C(38)-O(2)	32.9(3)
O(5)-Li(2)-O(3)-C(42)	169.73(17)
O(4)-Li(2)-O(3)-C(42)	-66.4(2)
O(2)-Li(2)-O(3)-C(42)	54.4(2)
O(5)-Li(2)-O(3)-C(39)	-20.8(3)
O(4)-Li(2)-O(3)-C(39)	103.0(2)
O(2)-Li(2)-O(3)-C(39)	-136.17(17)
C(42)-O(3)-C(39)-C(40)	-32.88(19)
Li(2)-O(3)-C(39)-C(40)	156.62(17)
O(3)-C(39)-C(40)-C(41)	16.8(2)
C(39)-C(40)-C(41)-C(42)	4.6(3)
C(39)-O(3)-C(42)-C(41)	35.7(2)
Li(2)-O(3)-C(42)-C(41)	-152.3(2)
C(40)-C(41)-C(42)-O(3)	-24.4(3)
O(5)-Li(2)-O(4)-C(43)	106.06(18)
O(3)-Li(2)-O(4)-C(43)	-20.7(3)
O(2)-Li(2)-O(4)-C(43)	-136.71(16)
O(5)-Li(2)-O(4)-C(46)	-82.1(2)
O(3)-Li(2)-O(4)-C(46)	151.10(16)
O(2)-Li(2)-O(4)-C(46)	35.1(3)
C(46)-O(4)-C(43)-C(44)	19.34(18)
Li(2)-O(4)-C(43)-C(44)	-167.61(17)
O(4)-C(43)-C(44)-C(45)	-34.80(18)
C(43)-C(44)-C(45)-C(46)	36.71(18)
C(43)-O(4)-C(46)-C(45)	4.4(2)
Li(2)-O(4)-C(46)-C(45)	-168.33(17)
C(44)-C(45)-C(46)-O(4)	-26.07(19)

O(4)-Li(2)-O(5)-C(50)	174.97(16)
O(3)-Li(2)-O(5)-C(50)	-59.5(3)
O(2)-Li(2)-O(5)-C(50)	54.3(2)
O(4)-Li(2)-O(5)-C(47A)	-1.9(3)
O(3)-Li(2)-O(5)-C(47A)	123.7(3)
O(2)-Li(2)-O(5)-C(47A)	-122.5(3)
O(4)-Li(2)-O(5)-C(47)	26.7(3)
O(3)-Li(2)-O(5)-C(47)	152.2(3)
O(2)-Li(2)-O(5)-C(47)	-94.0(3)
C(50)-O(5)-C(47)-C(48)	5.8(5)
C(47A)-O(5)-C(47)-C(48)	-66.4(6)
Li(2)-O(5)-C(47)-C(48)	159.0(3)
C(50)-O(5)-C(47A)-C(48)	-44.2(3)
C(47)-O(5)-C(47A)-C(48)	71.8(6)
Li(2)-O(5)-C(47A)-C(48)	133.2(3)
O(5)-C(47A)-C(48)-C(47)	-72.4(6)
O(5)-C(47A)-C(48)-C(49)	30.9(4)
O(5)-C(47)-C(48)-C(47A)	66.3(5)
O(5)-C(47)-C(48)-C(49)	-19.1(5)
C(47A)-C(48)-C(49)-C(50)	-6.3(3)
C(47)-C(48)-C(49)-C(50)	25.0(4)
C(47A)-O(5)-C(50)-C(49)	38.5(3)
C(47)-O(5)-C(50)-C(49)	9.7(3)
Li(2)-O(5)-C(50)-C(49)	-139.11(18)
C(48)-C(49)-C(50)-O(5)	-20.7(2)

Table S13. Crystal data and structure refinement for **Zr-1**.

Empirical formula	C34H39BCl2N2OSiZr
Formula weight	692.69
Temperature	110(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 8.8424(6) Å α = 105.517(4) º.
	b = 12.4631(9) Å β = 91.645(3) º.
	c = 16.1075(12) Å γ = 106.554(3)º.
Volume	1628.9(2) Å ^{3}
Z, Calculated density	2, 1.412 mg/m^3

Absorption coefficient	0.568 mm^{-1}
F(000)	716
Crystal size	0.40 × 0.38 × 0.23 mm
Theta range for data collection	1.78 to 30.66 º.
Limiting indices	-12<=h<=12, -17<=k<=17, -23<=l<=23
Reflections collected / unique	35338 / 9935 [R(int) = 0.0250]
Completeness to theta = 30.66	98.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7461 and 0.7030
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9935 / 12 / 402
Goodness-of-fit on F^2	1.038
Final R indices [I>2σ(I)]	R1 = 0.0259, wR2 = 0.0629
R indices (all data)	R1 = 0.0341, wR2 = 0.0659
Extinction coefficient	0.0064(4)
Largest diff. peak and hole	0.573 and -0.349 $e.A^{-3}$

Table S14. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($A^2 \times 10^3$) for **Zr-1**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)	
Zr(1)	1904(1)	6604(1)	2217(1)	13(1)	
Cl(1)	1619(1)	5181(1)	855(1)	22(1)	
Cl(2)	-128(1)	7059(1)	3092(1)	20(1)	
Si(1)	4910(1)	6518(1)	2933(1)	14(1)	
N(1)	1567(1)	4392(1)	3653(1)	13(1)	
O(1)	1299(1)	7749(1)	1475(1)	17(1)	
B(1)	615(2)	3428(1)	2738(1)	14(1)	
N(2)	2889(1)	5961(1)	3093(1)	13(1)	
C(1)	2449(1)	5523(1)	3792(1)	14(1)	
C(2)	2918(2)	6242(1)	4648(1)	18(1)	
C(3)	2561(2)	5795(1)	5340(1)	19(1)	
C(4)	1738(2)	4623(1)	5191(1)	18(1)	
C(5)	1241(1)	3942(1)	4340(1)	15(1)	
C(6)	314(2)	2710(1)	4039(1)	16(1)	
C(7)	-116(1)	2364(1)	3139(1)	15(1)	
C(8)	-987(2)	1197(1)	2754(1)	19(1)	

C(9)	-1382(2)	413(1)	3243(1)	21(1)
C(10)	-925(2)	782(1)	4136(1)	22(1)
C(11)	-84(2)	1940(1)	4544(1)	20(1)
C(12)	-721(2)	3954(1)	2422(1)	17(1)
C(13)	-1984(2)	3084(1)	1708(1)	26(1)
C(14)	1821(2)	3122(1)	2040(1)	16(1)
C(15)	3106(2)	2690(1)	2373(1)	22(1)
C(16)	4816(2)	9499(1)	2397(1)	17(1)
C(17)	4747(2)	10625(1)	2756(1)	22(1)
C(18)	4161(2)	10899(1)	3551(1)	24(1)
C(19)	3652(2)	10061(1)	3987(1)	22(1)
C(20)	3744(2)	8932(1)	3650(1)	17(1)
C(21)	4344(1)	8641(1)	2849(1)	15(1)
C(22)	4549(1)	7527(1)	2333(1)	15(1)
C(23)	5201(1)	7786(1)	1551(1)	17(1)
C(24)	5346(2)	8960(1)	1589(1)	18(1)
C(25)	5877(2)	9401(1)	901(1)	25(1)
C(26)	6265(2)	8674(2)	185(1)	30(1)
C(27)	6141(2)	7517(1)	147(1)	29(1)
C(28)	5605(2)	7065(1)	821(1)	23(1)
C(29)	5714(2)	5387(1)	2271(1)	22(1)
C(30)	6245(2)	7323(1)	3961(1)	22(1)
C(31)	748(2)	8770(1)	1856(1)	23(1)
C(32)	1180(3)	9515(2)	1235(1)	23(1)
C(33)	790(3)	8571(2)	355(1)	23(1)
C(32A)	534(15)	9250(12)	1136(9)	31(3)
C(33A)	1460(20)	8834(14)	527(10)	45(3)
C(34)	1431(2)	7638(1)	544(1)	20(1)

Table S15. Bond lengths [Å] and angles [°] for **Zr-1**.

Zr(1)-N(2)	2.0795(10)
Zr(1)-O(1)	2.2502(9)
Zr(1)-C(22)	2.2704(12)
Zr(1)-Cl(1)	2.3779(4)
Zr(1)-Cl(2)	2.4151(3)
Zr(1)-C(21)	2.7393(13)
Zr(1)-Si(1)	2.9084(4)

Si(1)-N(2)	1.7779(11)
Si(1)-C(29)	1.8540(14)
Si(1)-C(30)	1.8624(14)
Si(1)-C(22)	1.8645(13)
N(1)-C(1)	1.3565(16)
N(1)-C(5)	1.3721(15)
N(1)-B(1)	1.6520(17)
O(1)-C(31)	1.4778(16)
O(1)-C(34)	1.4798(15)
B(1)-C(7)	1.6085(19)
B(1)-C(14)	1.6181(19)
B(1)-C(12)	1.6333(19)
N(2)-C(1)	1.3953(15)
C(1)-C(2)	1.4039(17)
C(2)-C(3)	1.3803(18)
C(2)-H(2)	0.9500
C(3)-C(4)	1.3840(19)
C(3)-H(3)	0.9500
C(4)-C(5)	1.3865(18)
C(4)-H(4)	0.9500
C(5)-C(6)	1.4585(18)
C(6)-C(11)	1.3958(18)
C(6)-C(7)	1.4039(17)
C(7)-C(8)	1.3951(18)
C(8)-C(9)	1.3896(19)
C(8)-H(8)	0.9500
C(9)-C(10)	1.396(2)
C(9)-H(9)	0.9500
C(10)-C(11)	1.386(2)
C(10)-H(10)	0.9500
C(11)-H(11)	0.9500
C(12)-C(13)	1.5209(19)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-C(15)	1.5284(18)
C(14)-H(14A)	0.9900

C(14)-H(14B)	0.9900
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-C(17)	1.3873(19)
C(16)-C(21)	1.4242(18)
C(16)-C(24)	1.4529(18)
C(17)-C(18)	1.388(2)
C(17)-H(17)	0.9500
C(18)-C(19)	1.390(2)
C(18)-H(18)	0.9500
C(19)-C(20)	1.3924(19)
C(19)-H(19)	0.9500
C(20)-C(21)	1.4047(17)
C(20)-H(20)	0.9500
C(21)-C(22)	1.4789(17)
C(22)-C(23)	1.4749(17)
C(23)-C(28)	1.4008(18)
C(23)-C(24)	1.4167(19)
C(24)-C(25)	1.3992(19)
C(25)-C(26)	1.382(2)
C(25)-H(25)	0.9500
C(26)-C(27)	1.398(2)
C(26)-H(26)	0.9500
C(27)-C(28)	1.387(2)
C(27)-H(27)	0.9500
C(28)-H(28)	0.9500
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-C(32A)	1.469(13)
C(31)-C(32)	1.524(3)
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(32)-C(33)	1.537(3)
C(32)-H(32A)	0.9900

C(32)-H(32B)	0.9900
C(33)-C(34)	1.524(2)
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(32A)-C(33A)	1.38(2)
C(32A)-H(32C)	0.9900
C(32A)-H(32D)	0.9900
C(33A)-C(34)	1.492(15)
C(33A)-H(33C)	0.9900
C(33A)-H(33D)	0.9900
C(34)-H(34A)	0.9900
C(34)-H(34B)	0.9900

N(2)-Zr(1)-O(1)	164.84(4)
N(2)-Zr(1)-C(22)	76.12(4)
O(1)-Zr(1)-C(22)	92.57(4)
N(2)-Zr(1)-Cl(1)	104.63(3)
O(1)-Zr(1)-Cl(1)	86.91(3)
C(22)-Zr(1)-Cl(1)	99.18(3)
N(2)-Zr(1)-Cl(2)	95.21(3)
O(1)-Zr(1)-Cl(2)	84.64(3)
C(22)-Zr(1)-Cl(2)	131.36(3)
Cl(1)-Zr(1)-Cl(2)	128.976(13)
N(2)-Zr(1)-C(21)	87.09(4)
O(1)-Zr(1)-C(21)	78.06(4)
C(22)-Zr(1)-C(21)	32.66(4)
Cl(1)-Zr(1)-C(21)	126.67(3)
Cl(2)-Zr(1)-C(21)	100.43(3)
N(2)-Zr(1)-Si(1)	37.30(3)
O(1)-Zr(1)-Si(1)	132.43(3)
C(22)-Zr(1)-Si(1)	39.86(3)
Cl(1)-Zr(1)-Si(1)	98.439(12)
Cl(2)-Zr(1)-Si(1)	123.534(12)
C(21)-Zr(1)-Si(1)	60.89(3)
N(2)-Si(1)-C(29)	113.30(6)
N(2)-Si(1)-C(30)	113.48(6)
C(29)-Si(1)-C(30)	109.57(6)
N(2)-Si(1)-C(22)	94.99(5)
C(29)-Si(1)-C(22)	112.98(6)

C(30)-Si(1)-C(22)	111.96(6)
N(2)-Si(1)-Zr(1)	45.14(3)
C(29)-Si(1)-Zr(1)	115.99(5)
C(30)-Si(1)-Zr(1)	134.38(4)
C(22)-Si(1)-Zr(1)	51.30(4)
C(1)-N(1)-C(5)	120.13(11)
C(1)-N(1)-B(1)	128.95(10)
C(5)-N(1)-B(1)	110.65(10)
C(31)-O(1)-C(34)	108.78(9)
C(31)-O(1)-Zr(1)	124.89(8)
C(34)-O(1)-Zr(1)	126.30(7)
C(7)-B(1)-C(14)	111.42(10)
C(7)-B(1)-C(12)	113.36(10)
C(14)-B(1)-C(12)	115.60(10)
C(7)-B(1)-N(1)	96.88(9)
C(14)-B(1)-N(1)	111.91(10)
C(12)-B(1)-N(1)	105.97(10)
C(1)-N(2)-Si(1)	122.07(8)
C(1)-N(2)-Zr(1)	138.35(8)
Si(1)-N(2)-Zr(1)	97.57(5)
N(1)-C(1)-N(2)	120.37(11)
N(1)-C(1)-C(2)	118.97(11)
N(2)-C(1)-C(2)	120.65(11)
C(3)-C(2)-C(1)	120.72(12)
C(3)-C(2)-H(2)	119.6
C(1)-C(2)-H(2)	119.6
C(2)-C(3)-C(4)	119.86(12)
C(2)-C(3)-H(3)	120.1
C(4)-C(3)-H(3)	120.1
C(3)-C(4)-C(5)	118.22(12)
C(3)-C(4)-H(4)	120.9
C(5)-C(4)-H(4)	120.9
N(1)-C(5)-C(4)	121.91(12)
N(1)-C(5)-C(6)	110.69(11)
C(4)-C(5)-C(6)	127.39(12)
C(11)-C(6)-C(7)	122.87(12)
C(11)-C(6)-C(5)	126.55(12)
C(7)-C(6)-C(5)	110.56(11)
C(8)-C(7)-C(6)	117.05(12)

C(8)-C(7)-B(1) 132.03(11)
C(6)-C(7)-B(1) 110.82(11)
C(9)-C(8)-C(7) 121.05(12)
C(9)-C(8)-H(8) 119.5
C(7)-C(8)-H(8) 119.5
C(8)-C(9)-C(10) 120.45(13)
C(8)-C(9)-H(9) 119.8
C(10)-C(9)-H(9) 119.8
C(11)-C(10)-C(9) 120.20(13)
C(11)-C(10)-H(10) 119.9
C(9)-C(10)-H(10) 119.9
C(10)-C(11)-C(6) 118.36(12)
C(10)-C(11)-H(11) 120.8
C(6)-C(11)-H(11) 120.8
C(13)-C(12)-B(1) 114.63(11)
C(13)-C(12)-H(12A) 108.6
B(1)-C(12)-H(12A) 108.6
C(13)-C(12)-H(12B) 108.6
B(1)-C(12)-H(12B) 108.6
H(12A)-C(12)-H(12B) 107.6
C(12)-C(13)-H(13A) 109.5
C(12)-C(13)-H(13B) 109.5
H(13A)-C(13)-H(13B) 109.5
C(12)-C(13)-H(13C) 109.5
H(13A)-C(13)-H(13C) 109.5
H(13B)-C(13)-H(13C) 109.5
C(15)-C(14)-B(1) 114.22(11)
C(15)-C(14)-H(14A) 108.7
B(1)-C(14)-H(14A) 108.7
C(15)-C(14)-H(14B) 108.7
B(1)-C(14)-H(14B) 108.7
H(14A)-C(14)-H(14B) 107.6
C(14)-C(15)-H(15A) 109.5
C(14)-C(15)-H(15B) 109.5
H(15A)-C(15)-H(15B) 109.5
C(14)-C(15)-H(15C) 109.5
H(15A)-C(15)-H(15C) 109.5
H(15B)-C(15)-H(15C) 109.5
C(17)-C(16)-C(21) 120.56(12)

C(17)-C(16)-C(24)	131.67(12)
C(21)-C(16)-C(24)	107.76(11)
C(16)-C(17)-C(18)	119.31(13)
C(16)-C(17)-H(17)	120.3
C(18)-C(17)-H(17)	120.3
C(17)-C(18)-C(19)	120.69(13)
C(17)-C(18)-H(18)	119.7
C(19)-C(18)-H(18)	119.7
C(18)-C(19)-C(20)	121.09(13)
C(18)-C(19)-H(19)	119.5
C(20)-C(19)-H(19)	119.5
C(19)-C(20)-C(21)	119.00(12)
C(19)-C(20)-H(20)	120.5
C(21)-C(20)-H(20)	120.5
C(20)-C(21)-C(16)	119.29(12)
C(20)-C(21)-C(22)	130.93(12)
C(16)-C(21)-C(22)	109.75(11)
C(20)-C(21)-Zr(1)	93.17(8)
C(16)-C(21)-Zr(1)	123.46(8)
C(22)-C(21)-Zr(1)	55.95(6)
C(23)-C(22)-C(21)	104.30(11)
C(23)-C(22)-Si(1)	130.13(9)
C(21)-C(22)-Si(1)	117.50(9)
C(23)-C(22)-Zr(1)	117.27(8)
C(21)-C(22)-Zr(1)	91.38(7)
Si(1)-C(22)-Zr(1)	88.84(5)
C(28)-C(23)-C(24)	119.53(12)
C(28)-C(23)-C(22)	130.55(12)
C(24)-C(23)-C(22)	109.88(11)
C(25)-C(24)-C(23)	120.61(13)
C(25)-C(24)-C(16)	131.05(13)
C(23)-C(24)-C(16)	108.30(11)
C(26)-C(25)-C(24)	118.94(14)
C(26)-C(25)-H(25)	120.5
C(24)-C(25)-H(25)	120.5
C(25)-C(26)-C(27)	120.78(14)
C(25)-C(26)-H(26)	119.6
C(27)-C(26)-H(26)	119.6
C(28)-C(27)-C(26)	120.99(14)

C(28)-C(27)-H(27)	119.5
C(26)-C(27)-H(27)	119.5
C(27)-C(28)-C(23)	119.14(14)
C(27)-C(28)-H(28)	120.4
C(23)-C(28)-H(28)	120.4
Si(1)-C(29)-H(29A)	109.5
Si(1)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
Si(1)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
Si(1)-C(30)-H(30A)	109.5
Si(1)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
Si(1)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(32A)-C(31)-O(1)	105.5(5)
C(32A)-C(31)-C(32)	21.7(5)
O(1)-C(31)-C(32)	103.90(13)
C(32A)-C(31)-H(31A)	127.6
O(1)-C(31)-H(31A)	111.0
C(32)-C(31)-H(31A)	111.0
C(32A)-C(31)-H(31B)	90.8
O(1)-C(31)-H(31B)	111.0
C(32)-C(31)-H(31B)	111.0
H(31A)-C(31)-H(31B)	109.0
C(31)-C(32)-C(33)	101.22(17)
C(31)-C(32)-H(32A)	111.5
C(33)-C(32)-H(32A)	111.5
C(31)-C(32)-H(32B)	111.5
C(33)-C(32)-H(32B)	111.5
H(32A)-C(32)-H(32B)	109.3
C(34)-C(33)-C(32)	102.25(15)
C(34)-C(33)-H(33A)	111.3
C(32)-C(33)-H(33A)	111.3
C(34)-C(33)-H(33B)	111.3
C(32)-C(33)-H(33B)	111.3
H(33A)-C(33)-H(33B)	109.2

C(33A)-C(32A)-C(31)	104.9(10)
C(33A)-C(32A)-H(32C)	110.8
C(31)-C(32A)-H(32C)	110.8
C(33A)-C(32A)-H(32D)	110.8
C(31)-C(32A)-H(32D)	110.8
H(32C)-C(32A)-H(32D)	108.8
C(32A)-C(33A)-C(34)	109.3(11)
C(32A)-C(33A)-H(33C)	109.8
C(34)-C(33A)-H(33C)	109.8
C(32A)-C(33A)-H(33D)	109.8
C(34)-C(33A)-H(33D)	109.8
H(33C)-C(33A)-H(33D)	108.3
O(1)-C(34)-C(33A)	100.1(6)
O(1)-C(34)-C(33)	105.45(12)
C(33A)-C(34)-C(33)	23.0(6)
O(1)-C(34)-H(34A)	110.7
C(33A)-C(34)-H(34A)	132.1
C(33)-C(34)-H(34A)	110.7
O(1)-C(34)-H(34B)	110.7
C(33A)-C(34)-H(34B)	92.6
C(33)-C(34)-H(34B)	110.7
H(34A)-C(34)-H(34B)	108.8

Table S16. Anisotropic displacement parameters ($A^2 \times 10^3$) for **Zr-1**. The anisotropic displacement factor exponent takes the form: $-2\ pi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
Zr(1)	12(1)	16(1)	14(1)	5(1)	2(1)	4(1)
Cl(1)	30(1)	17(1)	17(1)	3(1)	-2(1)	6(1)
Cl(2)	16(1)	24(1)	21(1)	6(1)	7(1)	6(1)
Si(1)	11(1)	13(1)	16(1)	2(1)	1(1)	4(1)
N(1)	13(1)	14(1)	13(1)	5(1)	2(1)	5(1)
O(1)	20(1)	19(1)	15(1)	6(1)	3(1)	9(1)
B(1)	16(1)	13(1)	13(1)	3(1)	-1(1)	3(1)
N(2)	13(1)	13(1)	14(1)	4(1)	1(1)	4(1)
C(1)	13(1)	15(1)	14(1)	4(1)	1(1)	5(1)
C(2)	20(1)	15(1)	16(1)	2(1)	0(1)	4(1)

C(3)	23(1)	19(1)	14(1)	2(1)	0(1)	6(1)
C(4)	22(1)	20(1)	14(1)	6(1)	2(1)	8(1)
C(5)	15(1)	17(1)	14(1)	6(1)	2(1)	6(1)
C(6)	17(1)	16(1)	16(1)	5(1)	3(1)	6(1)
C(7)	14(1)	16(1)	16(1)	5(1)	2(1)	5(1)
C(8)	19(1)	19(1)	18(1)	4(1)	2(1)	4(1)
C(9)	19(1)	16(1)	26(1)	6(1)	3(1)	2(1)
C(10)	24(1)	20(1)	25(1)	13(1)	5(1)	6(1)
C(11)	23(1)	22(1)	17(1)	9(1)	3(1)	6(1)
C(12)	17(1)	17(1)	16(1)	4(1)	1(1)	6(1)
C(13)	26(1)	24(1)	25(1)	2(1)	-7(1)	9(1)
C(14)	18(1)	15(1)	15(1)	4(1)	3(1)	6(1)
C(15)	23(1)	22(1)	26(1)	9(1)	6(1)	12(1)
C(16)	14(1)	16(1)	19(1)	6(1)	1(1)	2(1)
C(17)	24(1)	16(1)	26(1)	9(1)	2(1)	5(1)
C(18)	31(1)	16(1)	26(1)	3(1)	2(1)	10(1)
C(19)	26(1)	20(1)	20(1)	3(1)	4(1)	10(1)
C(20)	18(1)	17(1)	18(1)	5(1)	3(1)	6(1)
C(21)	13(1)	14(1)	17(1)	4(1)	1(1)	3(1)
C(22)	14(1)	14(1)	16(1)	3(1)	3(1)	3(1)
C(23)	13(1)	17(1)	17(1)	4(1)	2(1)	1(1)
C(24)	15(1)	19(1)	18(1)	6(1)	2(1)	0(1)
C(25)	27(1)	21(1)	23(1)	9(1)	4(1)	-1(1)
C(26)	32(1)	32(1)	20(1)	10(1)	9(1)	-2(1)
C(27)	29(1)	30(1)	19(1)	2(1)	10(1)	2(1)
C(28)	21(1)	21(1)	21(1)	2(1)	6(1)	2(1)
C(29)	17(1)	19(1)	27(1)	2(1)	4(1)	8(1)
C(30)	15(1)	24(1)	22(1)	1(1)	-2(1)	7(1)
C(31)	31(1)	23(1)	22(1)	7(1)	6(1)	17(1)
C(32)	33(1)	20(1)	20(1)	7(1)	2(1)	12(1)
C(33)	31(1)	22(1)	17(1)	7(1)	-3(1)	12(1)
C(32A)	36(5)	23(5)	36(5)	13(4)	-6(5)	11(4)
C(33A)	63(7)	43(6)	39(6)	24(5)	7(5)	21(5)
C(34)	26(1)	19(1)	13(1)	5(1)	2(1)	7(1)

Table S17. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($A^2 \times 10^3$) for **Zr-1**.

	x	y	z	U(eq)

H(2)	3487	7046	4752	21
H(3)	2879	6289	5917	23
H(4)	1519	4295	5659	22
H(8)	-1316	934	2148	23
H(9)	-1967	-381	2968	25
H(10)	-1192	239	4464	27
H(11)	214	2203	5153	24
H(12A)	-1251	4248	2929	20
H(12B)	-177	4629	2214	20
H(13A)	-1473	2771	1207	39
H(13B)	-2700	3478	1535	39
H(13C)	-2591	2443	1923	39
H(14A)	1199	2515	1517	19
H(14B)	2341	3830	1864	19
H(15A)	3725	3282	2894	33
H(15B)	3810	2551	1924	33
H(15C)	2607	1961	2513	33
H(17)	5098	11202	2462	26
H(18)	4108	11668	3798	29
H(19)	3235	10261	4524	26
H(20)	3407	8368	3956	21
H(25)	5968	10187	925	30
H(26)	6621	8963	-287	36
H(27)	6428	7034	-347	34
H(28)	5513	6275	787	27
H(29A)	5873	4880	2616	32
H(29B)	6731	5765	2093	32
H(29C)	4962	4917	1756	32
H(30A)	5878	7970	4284	32
H(30B)	7330	7633	3828	32
H(30C)	6231	6790	4313	32
H(31A)	1296	9202	2446	28
H(31B)	-413	8526	1885	28
H(32A)	2318	9976	1343	28
H(32B)	525	10049	1278	28
H(33A)	-368	8265	174	27
H(33B)	1333	8876	-101	27
H(32C)	-596	8979	893	37

H(32D)	895	10115	1334	37
H(33C)	2561	9363	657	54
H(33D)	1036	8806	-58	54
H(34A)	795	6850	183	23
H(34B)	2551	7771	425	23

Table S18. Torsion angles [º] for **Zr-1**.

O(1)-Zr(1)-Si(1)-N(2)	163.35(6)
C(22)-Zr(1)-Si(1)-N(2)	162.66(7)
Cl(1)-Zr(1)-Si(1)-N(2)	-103.11(5)
Cl(2)-Zr(1)-Si(1)-N(2)	46.34(5)
C(21)-Zr(1)-Si(1)-N(2)	129.42(6)
N(2)-Zr(1)-Si(1)-C(29)	97.80(7)
O(1)-Zr(1)-Si(1)-C(29)	-98.86(6)
C(22)-Zr(1)-Si(1)-C(29)	-99.55(7)
Cl(1)-Zr(1)-Si(1)-C(29)	-5.31(5)
Cl(2)-Zr(1)-Si(1)-C(29)	144.14(5)
C(21)-Zr(1)-Si(1)-C(29)	-132.78(6)
N(2)-Zr(1)-Si(1)-C(30)	-79.18(8)
O(1)-Zr(1)-Si(1)-C(30)	84.16(8)
C(22)-Zr(1)-Si(1)-C(30)	83.47(9)
Cl(1)-Zr(1)-Si(1)-C(30)	177.71(7)
Cl(2)-Zr(1)-Si(1)-C(30)	-32.84(7)
C(21)-Zr(1)-Si(1)-C(30)	50.24(8)
N(2)-Zr(1)-Si(1)-C(22)	-162.66(7)
O(1)-Zr(1)-Si(1)-C(22)	0.69(6)
Cl(1)-Zr(1)-Si(1)-C(22)	94.24(5)
Cl(2)-Zr(1)-Si(1)-C(22)	-116.31(5)
C(21)-Zr(1)-Si(1)-C(22)	-33.23(6)
N(2)-Zr(1)-O(1)-C(31)	-58.36(18)
C(22)-Zr(1)-O(1)-C(31)	-99.54(10)
Cl(1)-Zr(1)-O(1)-C(31)	161.40(10)
Cl(2)-Zr(1)-O(1)-C(31)	31.78(10)
C(21)-Zr(1)-O(1)-C(31)	-70.09(10)
Si(1)-Zr(1)-O(1)-C(31)	-99.98(10)
N(2)-Zr(1)-O(1)-C(34)	119.55(15)
C(22)-Zr(1)-O(1)-C(34)	78.37(10)

Cl(1)-Zr(1)-O(1)-C(34)	-20.69(9)
Cl(2)-Zr(1)-O(1)-C(34)	-150.31(10)
C(21)-Zr(1)-O(1)-C(34)	107.82(10)
Si(1)-Zr(1)-O(1)-C(34)	77.93(10)
C(1)-N(1)-B(1)-C(7)	-178.98(11)
C(5)-N(1)-B(1)-C(7)	-5.01(12)
C(1)-N(1)-B(1)-C(14)	64.59(15)
C(5)-N(1)-B(1)-C(14)	-121.43(11)
C(1)-N(1)-B(1)-C(12)	-62.24(15)
C(5)-N(1)-B(1)-C(12)	111.73(11)
C(29)-Si(1)-N(2)-C(1)	89.25(11)
C(30)-Si(1)-N(2)-C(1)	-36.53(12)
C(22)-Si(1)-N(2)-C(1)	-153.09(10)
Zr(1)-Si(1)-N(2)-C(1)	-166.60(12)
C(29)-Si(1)-N(2)-Zr(1)	-104.16(6)
C(30)-Si(1)-N(2)-Zr(1)	130.06(6)
C(22)-Si(1)-N(2)-Zr(1)	13.51(5)
O(1)-Zr(1)-N(2)-C(1)	108.82(16)
C(22)-Zr(1)-N(2)-C(1)	151.46(13)
Cl(1)-Zr(1)-N(2)-C(1)	-112.50(12)
Cl(2)-Zr(1)-N(2)-C(1)	20.08(13)
C(21)-Zr(1)-N(2)-C(1)	120.30(13)
Si(1)-Zr(1)-N(2)-C(1)	162.81(15)
O(1)-Zr(1)-N(2)-Si(1)	-53.99(16)
C(22)-Zr(1)-N(2)-Si(1)	-11.35(5)
Cl(1)-Zr(1)-N(2)-Si(1)	84.69(4)
Cl(2)-Zr(1)-N(2)-Si(1)	-142.73(4)
C(21)-Zr(1)-N(2)-Si(1)	-42.51(5)
C(5)-N(1)-C(1)-N(2)	174.96(10)
B(1)-N(1)-C(1)-N(2)	-11.56(18)
C(5)-N(1)-C(1)-C(2)	-4.74(17)
B(1)-N(1)-C(1)-C(2)	168.74(11)
Si(1)-N(2)-C(1)-N(1)	-118.69(11)
Zr(1)-N(2)-C(1)-N(1)	81.54(16)
Si(1)-N(2)-C(1)-C(2)	61.00(14)
Zr(1)-N(2)-C(1)-C(2)	-98.77(14)
N(1)-C(1)-C(2)-C(3)	3.37(19)
N(2)-C(1)-C(2)-C(3)	-176.33(11)
C(1)-C(2)-C(3)-C(4)	0.3(2)

C(2)-C(3)-C(4)-C(5)	-2.5(2)
C(1)-N(1)-C(5)-C(4)	2.58(18)
B(1)-N(1)-C(5)-C(4)	-172.00(11)
C(1)-N(1)-C(5)-C(6)	-178.60(10)
B(1)-N(1)-C(5)-C(6)	6.82(13)
C(3)-C(4)-C(5)-N(1)	1.09(19)
C(3)-C(4)-C(5)-C(6)	-177.51(12)
N(1)-C(5)-C(6)-C(11)	172.58(12)
C(4)-C(5)-C(6)-C(11)	-8.7(2)
N(1)-C(5)-C(6)-C(7)	-5.81(14)
C(4)-C(5)-C(6)-C(7)	172.92(12)
C(11)-C(6)-C(7)-C(8)	0.43(19)
C(5)-C(6)-C(7)-C(8)	178.90(11)
C(11)-C(6)-C(7)-B(1)	-176.27(12)
C(5)-C(6)-C(7)-B(1)	2.19(14)
C(14)-B(1)-C(7)-C(8)	-57.73(17)
C(12)-B(1)-C(7)-C(8)	74.73(17)
N(1)-B(1)-C(7)-C(8)	-174.54(13)
C(14)-B(1)-C(7)-C(6)	118.32(12)
C(12)-B(1)-C(7)-C(6)	-109.22(12)
N(1)-B(1)-C(7)-C(6)	1.51(12)
C(6)-C(7)-C(8)-C(9)	-1.10(19)
B(1)-C(7)-C(8)-C(9)	174.75(13)
C(7)-C(8)-C(9)-C(10)	0.6(2)
C(8)-C(9)-C(10)-C(11)	0.6(2)
C(9)-C(10)-C(11)-C(6)	-1.2(2)
C(7)-C(6)-C(11)-C(10)	0.7(2)
C(5)-C(6)-C(11)-C(10)	-177.48(13)
C(7)-B(1)-C(12)-C(13)	-61.37(15)
C(14)-B(1)-C(12)-C(13)	69.03(15)
N(1)-B(1)-C(12)-C(13)	-166.39(11)
C(7)-B(1)-C(14)-C(15)	-51.58(14)
C(12)-B(1)-C(14)-C(15)	177.10(11)
N(1)-B(1)-C(14)-C(15)	55.67(14)
C(21)-C(16)-C(17)-C(18)	-2.16(19)
C(24)-C(16)-C(17)-C(18)	179.38(13)
C(16)-C(17)-C(18)-C(19)	0.3(2)
C(17)-C(18)-C(19)-C(20)	1.3(2)
C(18)-C(19)-C(20)-C(21)	-0.9(2)

C(19)-C(20)-C(21)-C(16)	-1.03(18)
C(19)-C(20)-C(21)-C(22)	-178.69(13)
C(19)-C(20)-C(21)-Zr(1)	-132.65(11)
C(17)-C(16)-C(21)-C(20)	2.56(18)
C(24)-C(16)-C(21)-C(20)	-178.65(11)
C(17)-C(16)-C(21)-C(22)	-179.31(12)
C(24)-C(16)-C(21)-C(22)	-0.52(14)
C(17)-C(16)-C(21)-Zr(1)	119.09(12)
C(24)-C(16)-C(21)-Zr(1)	-62.11(12)
N(2)-Zr(1)-C(21)-C(20)	-70.42(8)
O(1)-Zr(1)-C(21)-C(20)	106.53(8)
C(22)-Zr(1)-C(21)-C(20)	-138.97(12)
Cl(1)-Zr(1)-C(21)-C(20)	-176.53(6)
Cl(2)-Zr(1)-C(21)-C(20)	24.34(8)
Si(1)-Zr(1)-C(21)-C(20)	-98.37(8)
N(2)-Zr(1)-C(21)-C(16)	160.97(10)
O(1)-Zr(1)-C(21)-C(16)	-22.08(10)
C(22)-Zr(1)-C(21)-C(16)	92.42(12)
Cl(1)-Zr(1)-C(21)-C(16)	54.86(11)
Cl(2)-Zr(1)-C(21)-C(16)	-104.26(10)
Si(1)-Zr(1)-C(21)-C(16)	133.02(11)
N(2)-Zr(1)-C(21)-C(22)	68.55(8)
O(1)-Zr(1)-C(21)-C(22)	-114.50(8)
Cl(1)-Zr(1)-C(21)-C(22)	-37.56(8)
Cl(2)-Zr(1)-C(21)-C(22)	163.31(7)
Si(1)-Zr(1)-C(21)-C(22)	40.60(7)
C(20)-C(21)-C(22)-C(23)	178.79(13)
C(16)-C(21)-C(22)-C(23)	0.96(13)
Zr(1)-C(21)-C(22)-C(23)	118.63(9)
C(20)-C(21)-C(22)-Si(1)	-29.24(17)
C(16)-C(21)-C(22)-Si(1)	152.92(9)
Zr(1)-C(21)-C(22)-Si(1)	-89.41(8)
C(20)-C(21)-C(22)-Zr(1)	60.16(14)
C(16)-C(21)-C(22)-Zr(1)	-117.67(9)
N(2)-Si(1)-C(22)-C(23)	-137.86(12)
C(29)-Si(1)-C(22)-C(23)	-19.93(14)
C(30)-Si(1)-C(22)-C(23)	104.35(12)
Zr(1)-Si(1)-C(22)-C(23)	-125.61(13)
N(2)-Si(1)-C(22)-C(21)	78.71(10)

C(29)-Si(1)-C(22)-C(21)	-163.37(9)
C(30)-Si(1)-C(22)-C(21)	-39.09(11)
Zr(1)-Si(1)-C(22)-C(21)	90.95(9)
N(2)-Si(1)-C(22)-Zr(1)	-12.25(5)
C(29)-Si(1)-C(22)-Zr(1)	105.68(6)
C(30)-Si(1)-C(22)-Zr(1)	-130.04(5)
N(2)-Zr(1)-C(22)-C(23)	146.36(10)
O(1)-Zr(1)-C(22)-C(23)	-43.86(10)
Cl(1)-Zr(1)-C(22)-C(23)	43.43(10)
Cl(2)-Zr(1)-C(22)-C(23)	-128.98(8)
C(21)-Zr(1)-C(22)-C(23)	-106.88(12)
Si(1)-Zr(1)-C(22)-C(23)	135.63(12)
N(2)-Zr(1)-C(22)-C(21)	-106.76(8)
O(1)-Zr(1)-C(22)-C(21)	63.02(7)
Cl(1)-Zr(1)-C(22)-C(21)	150.31(7)
Cl(2)-Zr(1)-C(22)-C(21)	-22.10(9)
Si(1)-Zr(1)-C(22)-C(21)	-117.49(9)
N(2)-Zr(1)-C(22)-Si(1)	10.72(4)
O(1)-Zr(1)-C(22)-Si(1)	-179.49(4)
Cl(1)-Zr(1)-C(22)-Si(1)	-92.20(4)
Cl(2)-Zr(1)-C(22)-Si(1)	95.39(5)
C(21)-Zr(1)-C(22)-Si(1)	117.49(9)
C(21)-C(22)-C(23)-C(28)	-178.47(13)
Si(1)-C(22)-C(23)-C(28)	34.6(2)
Zr(1)-C(22)-C(23)-C(28)	-79.30(16)
C(21)-C(22)-C(23)-C(24)	-1.05(13)
Si(1)-C(22)-C(23)-C(24)	-148.01(11)
Zr(1)-C(22)-C(23)-C(24)	98.12(11)
C(28)-C(23)-C(24)-C(25)	0.50(19)
C(22)-C(23)-C(24)-C(25)	-177.25(12)
C(28)-C(23)-C(24)-C(16)	178.52(11)
C(22)-C(23)-C(24)-C(16)	0.77(14)
C(17)-C(16)-C(24)-C(25)	-3.8(2)
C(21)-C(16)-C(24)-C(25)	177.59(14)
C(17)-C(16)-C(24)-C(23)	178.45(14)
C(21)-C(16)-C(24)-C(23)	-0.15(14)
C(23)-C(24)-C(25)-C(26)	-0.3(2)
C(16)-C(24)-C(25)-C(26)	-177.85(14)
C(24)-C(25)-C(26)-C(27)	-0.3(2)

C(25)-C(26)-C(27)-C(28)	0.9(2)
C(26)-C(27)-C(28)-C(23)	-0.7(2)
C(24)-C(23)-C(28)-C(27)	0.0(2)
C(22)-C(23)-C(28)-C(27)	177.24(13)
C(34)-O(1)-C(31)-C(32A)	0.8(5)
Zr(1)-O(1)-C(31)-C(32A)	179.0(5)
C(34)-O(1)-C(31)-C(32)	-21.59(16)
Zr(1)-O(1)-C(31)-C(32)	156.63(11)
C(32A)-C(31)-C(32)-C(33)	-57.9(16)
O(1)-C(31)-C(32)-C(33)	39.01(18)
C(31)-C(32)-C(33)-C(34)	-41.70(19)
O(1)-C(31)-C(32A)-C(33A)	-21.1(11)
C(32)-C(31)-C(32A)-C(33A)	67.7(16)
C(31)-C(32A)-C(33A)-C(34)	34.4(14)
C(31)-O(1)-C(34)-C(33A)	17.9(7)
Zr(1)-O(1)-C(34)-C(33A)	-160.2(7)
C(31)-O(1)-C(34)-C(33)	-5.00(16)
Zr(1)-O(1)-C(34)-C(33)	176.81(11)
C(32A)-C(33A)-C(34)-O(1)	-32.6(12)
C(32A)-C(33A)-C(34)-C(33)	73.2(17)
C(32)-C(33)-C(34)-O(1)	29.21(19)
C(32)-C(33)-C(34)-C(33A)	-50.1(15)

Table S19. Crystal data and structure refinement for **Hf-1**.

Empirical formula	C34H39BCl2HfN2OSi
Formula weight	779.96
Temperature	110(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 8.8119(5) Å α = 105.491(3) º.
	b = 12.4637(7) Å β= 91.532(3) º.
	c = 16.1223(9) Å γ= 106.268(2) º.
Volume	1628.15(16) Å ^{3}
Z, Calculated density	2, 1.591 mg/m^3
Absorption coefficient	3.435 mm^{-1}
F(000)	780
Crystal size	0.41 × 0.33 ×0.25 mm

Theta range for data collection	1.78 to 28.39 º.
Limiting indices	-11<=h<=11, -16<=k<=16, -21<=l<=20
Reflections collected / unique	27305 / 8030 [R(int) = 0.0216]
Completeness to theta = 28.39	98.2 %
Absorption correction	Numerical
Max. and min. transmission	0.5836 and 0.2816
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8030 / 12 / 401
Goodness-of-fit on F^2	1.041
Final R indices [I>2σ(I)]	R1 = 0.0242, wR2 = 0.0521
R indices (all data)	R1 = 0.0314, wR2 = 0.0542
Largest diff. peak and hole	2.331 and -1.091 e.A^{-3}

Table S20. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($A^2 \times 10^3$) for **Hf-1**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Hf(1)	1907(1)	6599(1)	2210(1)	16(1)
Cl(1)	-106(1)	7066(1)	3081(1)	24(1)
Cl(2)	1543(1)	5171(1)	876(1)	27(1)
Si(1)	4910(1)	6517(1)	2923(1)	16(1)
C(1)	2447(3)	5520(2)	3780(2)	16(1)
N(1)	2889(2)	5955(2)	3081(1)	15(1)
B(1)	628(3)	3420(2)	2742(2)	17(1)
N(2)	1572(2)	4387(2)	3647(1)	15(1)
C(2)	2912(3)	6236(2)	4631(2)	20(1)
C(3)	2557(3)	5795(2)	5324(2)	22(1)
C(4)	1747(3)	4631(2)	5181(2)	20(1)
C(5)	1252(3)	3948(2)	4338(2)	17(1)
C(6)	332(3)	2715(2)	4043(2)	18(1)
C(7)	-83(3)	2362(2)	3149(2)	18(1)
C(8)	-945(3)	1195(2)	2772(2)	22(1)
C(9)	-1344(3)	421(2)	3268(2)	26(1)
C(10)	-909(3)	795(3)	4152(2)	26(1)
C(11)	-76(3)	1955(2)	4554(2)	23(1)
C(12)	4521(3)	7524(2)	2327(2)	16(1)
C(13)	4355(3)	8653(2)	2855(2)	16(1)
C(14)	3771(3)	8955(2)	3656(2)	19(1)

C(15)	3718(3)	10090(2)	3998(2)	23(1)
C(16)	4231(4)	10915(3)	3564(2)	25(1)
C(17)	4805(3)	10644(2)	2771(2)	24(1)
C(18)	4851(3)	9511(2)	2402(2)	19(1)
C(19)	5194(3)	7788(2)	1550(2)	19(1)
C(20)	5586(3)	7066(2)	816(2)	25(1)
C(21)	6134(4)	7517(3)	145(2)	32(1)
C(22)	6283(4)	8674(3)	191(2)	32(1)
C(23)	5907(4)	9401(3)	905(2)	27(1)
C(24)	5369(3)	8963(2)	1591(2)	20(1)
C(25)	5731(3)	5399(2)	2257(2)	25(1)
C(26)	6246(3)	7310(2)	3947(2)	24(1)
C(27)	1841(3)	3122(2)	2045(2)	19(1)
C(28)	3142(3)	2705(3)	2373(2)	25(1)
C(29)	-741(3)	3928(2)	2432(2)	20(1)
C(30)	-1938(4)	3076(3)	1688(2)	30(1)
O(1)	1327(2)	7751(2)	1490(1)	20(1)
C(31)	1455(3)	7635(2)	557(2)	23(1)
C(32)	819(6)	8573(5)	366(3)	26(1)
C(33)	1234(6)	9527(4)	1248(3)	24(1)
C(32A)	1390(30)	8790(20)	515(17)	37(6)
C(33A)	590(30)	9240(20)	1146(17)	38(6)
C(34)	791(4)	8786(3)	1870(2)	27(1)

Table S21. Bond lengths [Å] and angles [º] for **Hf-1**.

Hf(1)-N(1)	2.071(2)
Hf(1)-O(1)	2.2229(18)
Hf(1)-C(12)	2.246(2)
Hf(1)-Cl(2)	2.3441(7)
Hf(1)-Cl(1)	2.3939(7)
Hf(1)-C(13)	2.767(2)
Hf(1)-Si(1)	2.8954(7)
Si(1)-N(1)	1.774(2)
Si(1)-C(25)	1.850(3)
Si(1)-C(26)	1.861(3)
Si(1)-C(12)	1.865(3)

C(1)-N(2)	1.362(3)
C(1)-N(1)	1.396(3)
C(1)-C(2)	1.399(4)
B(1)-C(7)	1.607(4)
B(1)-C(27)	1.615(4)
B(1)-C(29)	1.634(4)
B(1)-N(2)	1.646(3)
N(2)-C(5)	1.369(3)
C(2)-C(3)	1.378(4)
C(2)-H(2)	0.9500
C(3)-C(4)	1.378(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.379(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.462(4)
C(6)-C(7)	1.395(4)
C(6)-C(11)	1.396(4)
C(7)-C(8)	1.395(4)
C(8)-C(9)	1.390(4)
C(8)-H(8)	0.9500
C(9)-C(10)	1.382(4)
C(9)-H(9)	0.9500
C(10)-C(11)	1.388(4)
C(10)-H(10)	0.9500
C(11)-H(11)	0.9500
C(12)-C(19)	1.477(4)
C(12)-C(13)	1.486(3)
C(13)-C(14)	1.399(4)
C(13)-C(18)	1.429(4)
C(14)-C(15)	1.389(4)
C(14)-H(14)	0.9500
C(15)-C(16)	1.375(4)
C(15)-H(15)	0.9500
C(16)-C(17)	1.380(4)
C(16)-H(16)	0.9500
C(17)-C(18)	1.391(4)
C(17)-H(17)	0.9500
C(18)-C(24)	1.453(4)
C(19)-C(20)	1.399(4)

C(19)-C(24)	1.412(4)
C(20)-C(21)	1.385(4)
C(20)-H(20)	0.9500
C(21)-C(22)	1.393(5)
C(21)-H(21)	0.9500
C(22)-C(23)	1.374(4)
C(22)-H(22)	0.9500
C(23)-C(24)	1.397(4)
C(23)-H(23)	0.9500
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-C(28)	1.520(4)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-C(30)	1.517(4)
C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
O(1)-C(31)	1.482(3)
O(1)-C(34)	1.482(3)
C(31)-C(32A)	1.47(3)
C(31)-C(32)	1.525(6)
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(32)-C(33)	1.547(7)
C(32)-H(32A)	0.9900
C(32)-H(32B)	0.9900
C(33)-C(34)	1.525(5)
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900

C(32A)-C(33A)	1.35(4)
C(32A)-H(32C)	0.9900
C(32A)-H(32D)	0.9900
C(33A)-C(34)	1.45(2)
C(33A)-H(33C)	0.9900
C(33A)-H(33D)	0.9900
C(34)-H(34A)	0.9900
C(34)-H(34B)	0.9900

N(1)-Hf(1)-O(1)	164.14(8)
N(1)-Hf(1)-C(12)	76.43(9)
O(1)-Hf(1)-C(12)	91.65(8)
N(1)-Hf(1)-Cl(2)	104.79(6)
O(1)-Hf(1)-Cl(2)	87.66(5)
C(12)-Hf(1)-Cl(2)	101.61(7)
N(1)-Hf(1)-Cl(1)	95.24(6)
O(1)-Hf(1)-Cl(1)	84.49(5)
C(12)-Hf(1)-Cl(1)	130.49(7)
Cl(2)-Hf(1)-Cl(1)	127.39(3)
N(1)-Hf(1)-C(13)	87.04(8)
O(1)-Hf(1)-C(13)	77.41(7)
C(12)-Hf(1)-C(13)	32.42(8)
Cl(2)-Hf(1)-C(13)	129.01(6)
Cl(1)-Hf(1)-C(13)	99.65(6)
N(1)-Hf(1)-Si(1)	37.41(6)
O(1)-Hf(1)-Si(1)	131.74(5)
C(12)-Hf(1)-Si(1)	40.09(7)
Cl(2)-Hf(1)-Si(1)	99.99(2)
Cl(1)-Hf(1)-Si(1)	123.30(2)
C(13)-Hf(1)-Si(1)	60.78(5)
N(1)-Si(1)-C(25)	113.35(12)
N(1)-Si(1)-C(26)	113.79(12)
C(25)-Si(1)-C(26)	109.31(13)
N(1)-Si(1)-C(12)	94.54(11)
C(25)-Si(1)-C(12)	112.92(13)
C(26)-Si(1)-C(12)	112.39(13)
N(1)-Si(1)-Hf(1)	45.16(7)
C(25)-Si(1)-Hf(1)	115.78(10)
C(26)-Si(1)-Hf(1)	134.87(9)

C(12)-Si(1)-Hf(1)	50.85(8)
N(2)-C(1)-N(1)	120.7(2)
N(2)-C(1)-C(2)	118.7(2)
N(1)-C(1)-C(2)	120.6(2)
C(1)-N(1)-Si(1)	122.16(17)
C(1)-N(1)-Hf(1)	138.27(16)
Si(1)-N(1)-Hf(1)	97.42(10)
C(7)-B(1)-C(27)	111.6(2)
C(7)-B(1)-C(29)	112.8(2)
C(27)-B(1)-C(29)	116.0(2)
C(7)-B(1)-N(2)	96.99(19)
C(27)-B(1)-N(2)	111.7(2)
C(29)-B(1)-N(2)	106.0(2)
C(1)-N(2)-C(5)	120.0(2)
C(1)-N(2)-B(1)	129.1(2)
C(5)-N(2)-B(1)	110.7(2)
C(3)-C(2)-C(1)	120.9(2)
C(3)-C(2)-H(2)	119.5
C(1)-C(2)-H(2)	119.5
C(4)-C(3)-C(2)	119.8(3)
C(4)-C(3)-H(3)	120.1
C(2)-C(3)-H(3)	120.1
C(3)-C(4)-C(5)	118.5(2)
C(3)-C(4)-H(4)	120.8
C(5)-C(4)-H(4)	120.8
N(2)-C(5)-C(4)	122.0(2)
N(2)-C(5)-C(6)	110.5(2)
C(4)-C(5)-C(6)	127.5(2)
C(7)-C(6)-C(11)	122.8(3)
C(7)-C(6)-C(5)	110.7(2)
C(11)-C(6)-C(5)	126.6(2)
C(8)-C(7)-C(6)	117.1(2)
C(8)-C(7)-B(1)	132.1(2)
C(6)-C(7)-B(1)	110.8(2)
C(9)-C(8)-C(7)	121.0(3)
C(9)-C(8)-H(8)	119.5
C(7)-C(8)-H(8)	119.5
C(10)-C(9)-C(8)	120.6(3)
C(10)-C(9)-H(9)	119.7

C(8)-C(9)-H(9)	119.7
C(9)-C(10)-C(11)	120.1(3)
C(9)-C(10)-H(10)	119.9
C(11)-C(10)-H(10)	119.9
C(10)-C(11)-C(6)	118.4(3)
C(10)-C(11)-H(11)	120.8
C(6)-C(11)-H(11)	120.8
C(19)-C(12)-C(13)	104.0(2)
C(19)-C(12)-Si(1)	129.28(19)
C(13)-C(12)-Si(1)	117.17(18)
C(19)-C(12)-Hf(1)	117.84(17)
C(13)-C(12)-Hf(1)	93.46(15)
Si(1)-C(12)-Hf(1)	89.06(10)
C(14)-C(13)-C(18)	119.3(2)
C(14)-C(13)-C(12)	131.1(2)
C(18)-C(13)-C(12)	109.6(2)
C(14)-C(13)-Hf(1)	94.29(16)
C(18)-C(13)-Hf(1)	123.70(18)
C(12)-C(13)-Hf(1)	54.12(12)
C(15)-C(14)-C(13)	119.0(2)
C(15)-C(14)-H(14)	120.5
C(13)-C(14)-H(14)	120.5
C(16)-C(15)-C(14)	121.1(3)
C(16)-C(15)-H(15)	119.4
C(14)-C(15)-H(15)	119.4
C(15)-C(16)-C(17)	121.3(3)
C(15)-C(16)-H(16)	119.3
C(17)-C(16)-H(16)	119.3
C(16)-C(17)-C(18)	119.1(3)
C(16)-C(17)-H(17)	120.4
C(18)-C(17)-H(17)	120.4
C(17)-C(18)-C(13)	120.1(2)
C(17)-C(18)-C(24)	132.1(3)
C(13)-C(18)-C(24)	107.8(2)
C(20)-C(19)-C(24)	119.2(2)
C(20)-C(19)-C(12)	130.5(2)
C(24)-C(19)-C(12)	110.3(2)
C(21)-C(20)-C(19)	119.4(3)
C(21)-C(20)-H(20)	120.3

C(19)-C(20)-H(20)	120.3
C(20)-C(21)-C(22)	120.8(3)
C(20)-C(21)-H(21)	119.6
C(22)-C(21)-H(21)	119.6
C(23)-C(22)-C(21)	120.8(3)
C(23)-C(22)-H(22)	119.6
C(21)-C(22)-H(22)	119.6
C(22)-C(23)-C(24)	119.1(3)
C(22)-C(23)-H(23)	120.5
C(24)-C(23)-H(23)	120.5
C(23)-C(24)-C(19)	120.7(3)
C(23)-C(24)-C(18)	130.9(3)
C(19)-C(24)-C(18)	108.4(2)
Si(1)-C(25)-H(25A)	109.5
Si(1)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
Si(1)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
Si(1)-C(26)-H(26A)	109.5
Si(1)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
Si(1)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(28)-C(27)-B(1)	114.4(2)
C(28)-C(27)-H(27A)	108.7
B(1)-C(27)-H(27A)	108.7
C(28)-C(27)-H(27B)	108.7
B(1)-C(27)-H(27B)	108.7
H(27A)-C(27)-H(27B)	107.6
C(27)-C(28)-H(28A)	109.5
C(27)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(27)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(30)-C(29)-B(1)	114.7(2)
C(30)-C(29)-H(29A)	108.6

B(1)-C(29)-H(29A) 108.6
C(30)-C(29)-H(29B) 108.6
B(1)-C(29)-H(29B) 108.6
H(29A)-C(29)-H(29B) 107.6
C(29)-C(30)-H(30A) 109.5
C(29)-C(30)-H(30B) 109.5
H(30A)-C(30)-H(30B) 109.5
C(29)-C(30)-H(30C) 109.5
H(30A)-C(30)-H(30C) 109.5
H(30B)-C(30)-H(30C) 109.5
C(31)-O(1)-C(34) 108.6(2)
C(31)-O(1)-Hf(1) 125.89(15)
C(34)-O(1)-Hf(1) 125.49(16)
C(32A)-C(31)-O(1) 100.9(11)
C(32A)-C(31)-C(32) 19.9(9)
O(1)-C(31)-C(32) 105.6(3)
C(32A)-C(31)-H(31A) 129.2
O(1)-C(31)-H(31A) 110.6
C(32)-C(31)-H(31A) 110.6
C(32A)-C(31)-H(31B) 95.2
O(1)-C(31)-H(31B) 110.6
C(32)-C(31)-H(31B) 110.6
H(31A)-C(31)-H(31B) 108.8
C(31)-C(32)-C(33) 102.0(4)
C(31)-C(32)-H(32A) 111.4
C(33)-C(32)-H(32A) 111.4
C(31)-C(32)-H(32B) 111.4
C(33)-C(32)-H(32B) 111.4
H(32A)-C(32)-H(32B) 109.2
C(34)-C(33)-C(32) 100.9(4)
C(34)-C(33)-H(33A) 111.6
C(32)-C(33)-H(33A) 111.6
C(34)-C(33)-H(33B) 111.6
C(32)-C(33)-H(33B) 111.6
H(33A)-C(33)-H(33B) 109.4
C(33A)-C(32A)-C(31) 110(2)
C(33A)-C(32A)-H(32C) 109.6
C(31)-C(32A)-H(32C) 109.6
C(33A)-C(32A)-H(32D) 109.6

C(31)-C(32A)-H(32D)	109.6
H(32C)-C(32A)-H(32D)	108.1
C(32A)-C(33A)-C(34)	107.8(19)
C(32A)-C(33A)-H(33C)	110.1
C(34)-C(33A)-H(33C)	110.1
C(32A)-C(33A)-H(33D)	110.1
C(34)-C(33A)-H(33D)	110.1
H(33C)-C(33A)-H(33D)	108.5
C(33A)-C(34)-O(1)	104.3(9)
C(33A)-C(34)-C(33)	22.0(8)
O(1)-C(34)-C(33)	104.0(3)
C(33A)-C(34)-H(34A)	128.8
O(1)-C(34)-H(34A)	111.0
C(33)-C(34)-H(34A)	111.0
C(33A)-C(34)-H(34B)	90.9
O(1)-C(34)-H(34B)	111.0
C(33)-C(34)-H(34B)	111.0
H(34A)-C(34)-H(34B)	109.0

Table S22. Anisotropic displacement parameters ($A^2 \times 10^3$) for **Hf-1**. The anisotropic displacement factor exponent takes the form: $-2\,pi^2\,[h^2\,a^{*2}\,U11 + ... + 2\,h\,k\,a^*\,b^*\,U12\,]$

	U11	U22	U33	U23	U13	U12
Hf(1)	13(1)	19(1)	17(1)	7(1)	1(1)	4(1)
Cl(1)	18(1)	30(1)	26(1)	9(1)	8(1)	8(1)
Cl(2)	36(1)	19(1)	21(1)	5(1)	-5(1)	4(1)
Si(1)	13(1)	15(1)	19(1)	2(1)	1(1)	5(1)
C(1)	13(1)	16(1)	19(1)	5(1)	0(1)	6(1)
N(1)	13(1)	17(1)	15(1)	4(1)	0(1)	3(1)
B(1)	19(1)	15(1)	14(1)	2(1)	-2(1)	5(1)
N(2)	14(1)	16(1)	15(1)	4(1)	0(1)	5(1)
C(2)	21(1)	18(1)	19(1)	4(1)	1(1)	5(1)
C(3)	24(1)	25(1)	16(1)	2(1)	1(1)	9(1)
C(4)	24(1)	25(1)	16(1)	9(1)	3(1)	12(1)
C(5)	16(1)	20(1)	17(1)	8(1)	2(1)	9(1)
C(6)	19(1)	19(1)	18(1)	6(1)	2(1)	7(1)

C(7)	18(1)	19(1)	18(1)	7(1)	4(1)	7(1)
C(8)	22(1)	22(1)	19(1)	4(1)	1(1)	5(1)
C(9)	23(1)	20(1)	32(2)	7(1)	2(1)	4(1)
C(10)	27(1)	24(1)	31(2)	17(1)	7(1)	8(1)
C(11)	28(1)	26(1)	19(1)	11(1)	4(1)	10(1)
C(12)	15(1)	16(1)	16(1)	3(1)	3(1)	3(1)
C(13)	14(1)	15(1)	19(1)	3(1)	0(1)	3(1)
C(14)	19(1)	19(1)	19(1)	4(1)	1(1)	5(1)
C(15)	30(2)	24(1)	17(1)	3(1)	6(1)	12(1)
C(16)	32(2)	24(1)	23(2)	2(1)	3(1)	17(1)
C(17)	27(1)	19(1)	27(2)	9(1)	0(1)	7(1)
C(18)	16(1)	18(1)	21(1)	6(1)	2(1)	3(1)
C(19)	14(1)	20(1)	20(1)	5(1)	2(1)	1(1)
C(20)	24(1)	21(1)	24(2)	2(1)	6(1)	3(1)
C(21)	31(2)	33(2)	22(2)	2(1)	11(1)	2(1)
C(22)	36(2)	32(2)	22(2)	10(1)	10(1)	-4(1)
C(23)	28(2)	24(1)	25(2)	8(1)	5(1)	-2(1)
C(24)	16(1)	18(1)	22(1)	4(1)	3(1)	0(1)
C(25)	21(1)	22(1)	32(2)	2(1)	3(1)	10(1)
C(26)	17(1)	26(1)	26(2)	1(1)	-3(1)	9(1)
C(27)	22(1)	17(1)	16(1)	2(1)	5(1)	6(1)
C(28)	28(1)	24(1)	29(2)	8(1)	10(1)	13(1)
C(29)	21(1)	22(1)	16(1)	3(1)	1(1)	8(1)
C(30)	29(2)	29(2)	29(2)	3(1)	-6(1)	9(1)
O(1)	23(1)	22(1)	16(1)	6(1)	3(1)	10(1)
C(31)	30(2)	21(1)	17(1)	6(1)	2(1)	7(1)
C(32)	30(3)	26(2)	26(2)	9(2)	-2(2)	13(2)
C(33)	33(3)	19(2)	21(2)	5(2)	1(2)	10(2)
C(32A)	45(10)	35(9)	34(9)	16(6)	-1(7)	13(7)
C(33A)	41(9)	28(8)	49(9)	11(6)	-2(7)	17(7)
C(34)	35(2)	26(2)	26(2)	7(1)	6(1)	20(1)

Table S23. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($A^2 \times 10^3$) for **Hf-1**.

	x	y	z	U(eq)
H(2)	3481	7037	4732	24

H(3)	2871	6292	5899	26
H(4)	1534	4307	5651	24
H(8)	-1265	925	2166	26
H(9)	-1920	-373	2997	31
H(10)	-1179	258	4485	31
H(11)	209	2225	5163	28
H(14)	3415	8392	3961	23
H(15)	3322	10300	4541	28
H(16)	4188	11686	3815	30
H(17)	5165	11225	2481	29
H(20)	5478	6274	778	29
H(21)	6410	7031	-352	38
H(22)	6651	8965	-279	39
H(23)	6012	10189	932	33
H(25A)	5896	4889	2597	38
H(25B)	6748	5782	2080	38
H(25C)	4983	4934	1742	38
H(26A)	5876	7957	4272	36
H(26B)	7332	7618	3812	36
H(26C)	6233	6774	4296	36
H(27A)	1225	2512	1525	22
H(27B)	2346	3829	1866	22
H(28A)	3766	3304	2887	38
H(28B)	3839	2559	1920	38
H(28C)	2658	1983	2525	38
H(29A)	-1320	4168	2932	24
H(29B)	-214	4634	2256	24
H(30A)	-1377	2812	1194	45
H(30B)	-2673	3463	1520	45
H(30C)	-2536	2403	1871	45
H(31A)	815	6851	199	27
H(31B)	2576	7760	434	27
H(32A)	-344	8278	195	31
H(32B)	1356	8867	-95	31
H(33A)	2378	9971	1349	29
H(33B)	592	10073	1294	29
H(32C)	2489	9317	580	44
H(32D)	867	8710	-56	44
H(33C)	-553	9011	934	46

H(33D)	1006	10100	1328	46
H(34A)	1344	9214	2458	32
H(34B)	-371	8556	1904	32

Table **S24**. Torsion angles [º] for **Hf-1**.

O(1)-Hf(1)-Si(1)-N(1)	162.84(11)
C(12)-Hf(1)-Si(1)-N(1)	162.46(14)
Cl(2)-Hf(1)-Si(1)-N(1)	-101.34(10)
Cl(1)-Hf(1)-Si(1)-N(1)	47.25(10)
C(13)-Hf(1)-Si(1)-N(1)	129.33(12)
N(1)-Hf(1)-Si(1)-C(25)	98.07(15)
O(1)-Hf(1)-Si(1)-C(25)	-99.09(13)
C(12)-Hf(1)-Si(1)-C(25)	-99.47(15)
Cl(2)-Hf(1)-Si(1)-C(25)	-3.26(11)
Cl(1)-Hf(1)-Si(1)-C(25)	145.32(11)
C(13)-Hf(1)-Si(1)-C(25)	-132.60(13)
N(1)-Hf(1)-Si(1)-C(26)	-79.21(17)
O(1)-Hf(1)-Si(1)-C(26)	83.63(16)
C(12)-Hf(1)-Si(1)-C(26)	83.25(17)
Cl(2)-Hf(1)-Si(1)-C(26)	179.46(14)
Cl(1)-Hf(1)-Si(1)-C(26)	-31.96(15)
C(13)-Hf(1)-Si(1)-C(26)	50.12(15)
N(1)-Hf(1)-Si(1)-C(12)	-162.46(14)
O(1)-Hf(1)-Si(1)-C(12)	0.38(12)
Cl(2)-Hf(1)-Si(1)-C(12)	96.20(10)
Cl(1)-Hf(1)-Si(1)-C(12)	-115.21(10)
C(13)-Hf(1)-Si(1)-C(12)	-33.13(12)
N(2)-C(1)-N(1)-Si(1)	-118.8(2)
C(2)-C(1)-N(1)-Si(1)	60.4(3)
N(2)-C(1)-N(1)-Hf(1)	82.1(3)
C(2)-C(1)-N(1)-Hf(1)	-98.7(3)
C(25)-Si(1)-N(1)-C(1)	90.0(2)
C(26)-Si(1)-N(1)-C(1)	-35.7(2)
C(12)-Si(1)-N(1)-C(1)	-152.6(2)
Hf(1)-Si(1)-N(1)-C(1)	-166.1(2)
C(25)-Si(1)-N(1)-Hf(1)	-103.81(13)

C(26)-Si(1)-N(1)-Hf(1)	130.47(12)
C(12)-Si(1)-N(1)-Hf(1)	13.56(11)
O(1)-Hf(1)-N(1)-C(1)	108.6(3)
C(12)-Hf(1)-N(1)-C(1)	150.7(3)
Cl(2)-Hf(1)-N(1)-C(1)	-110.6(2)
Cl(1)-Hf(1)-N(1)-C(1)	20.3(3)
C(13)-Hf(1)-N(1)-C(1)	119.7(3)
Si(1)-Hf(1)-N(1)-C(1)	162.3(3)
O(1)-Hf(1)-N(1)-Si(1)	-53.7(3)
C(12)-Hf(1)-N(1)-Si(1)	-11.52(9)
Cl(2)-Hf(1)-N(1)-Si(1)	87.13(8)
Cl(1)-Hf(1)-N(1)-Si(1)	-141.96(8)
C(13)-Hf(1)-N(1)-Si(1)	-42.53(9)
N(1)-C(1)-N(2)-C(5)	175.0(2)
C(2)-C(1)-N(2)-C(5)	-4.2(3)
N(1)-C(1)-N(2)-B(1)	-11.9(4)
C(2)-C(1)-N(2)-B(1)	169.0(2)
C(7)-B(1)-N(2)-C(1)	-179.2(2)
C(27)-B(1)-N(2)-C(1)	64.2(3)
C(29)-B(1)-N(2)-C(1)	-63.0(3)
C(7)-B(1)-N(2)-C(5)	-5.5(2)
C(27)-B(1)-N(2)-C(5)	-122.1(2)
C(29)-B(1)-N(2)-C(5)	110.7(2)
N(2)-C(1)-C(2)-C(3)	2.9(4)
N(1)-C(1)-C(2)-C(3)	-176.3(2)
C(1)-C(2)-C(3)-C(4)	0.6(4)
C(2)-C(3)-C(4)-C(5)	-2.8(4)
C(1)-N(2)-C(5)-C(4)	2.1(4)
B(1)-N(2)-C(5)-C(4)	-172.2(2)
C(1)-N(2)-C(5)-C(6)	-178.8(2)
B(1)-N(2)-C(5)-C(6)	6.9(3)
C(3)-C(4)-C(5)-N(2)	1.4(4)
C(3)-C(4)-C(5)-C(6)	-177.6(2)
N(2)-C(5)-C(6)-C(7)	-5.4(3)
C(4)-C(5)-C(6)-C(7)	173.7(3)
N(2)-C(5)-C(6)-C(11)	173.3(3)
C(4)-C(5)-C(6)-C(11)	-7.6(4)
C(11)-C(6)-C(7)-C(8)	0.2(4)
C(5)-C(6)-C(7)-C(8)	179.0(2)

C(11)-C(6)-C(7)-B(1)	-177.3(2)
C(5)-C(6)-C(7)-B(1)	1.4(3)
C(27)-B(1)-C(7)-C(8)	-58.1(4)
C(29)-B(1)-C(7)-C(8)	74.6(4)
N(2)-B(1)-C(7)-C(8)	-174.8(3)
C(27)-B(1)-C(7)-C(6)	118.9(2)
C(29)-B(1)-C(7)-C(6)	-108.4(3)
N(2)-B(1)-C(7)-C(6)	2.2(3)
C(6)-C(7)-C(8)-C(9)	-1.1(4)
B(1)-C(7)-C(8)-C(9)	175.8(3)
C(7)-C(8)-C(9)-C(10)	0.8(4)
C(8)-C(9)-C(10)-C(11)	0.5(4)
C(9)-C(10)-C(11)-C(6)	-1.4(4)
C(7)-C(6)-C(11)-C(10)	1.0(4)
C(5)-C(6)-C(11)-C(10)	-177.6(3)
N(1)-Si(1)-C(12)-C(19)	-138.5(2)
C(25)-Si(1)-C(12)-C(19)	-20.8(3)
C(26)-Si(1)-C(12)-C(19)	103.4(2)
Hf(1)-Si(1)-C(12)-C(19)	-126.2(3)
N(1)-Si(1)-C(12)-C(13)	81.03(19)
C(25)-Si(1)-C(12)-C(13)	-161.25(18)
C(26)-Si(1)-C(12)-C(13)	-37.0(2)
Hf(1)-Si(1)-C(12)-C(13)	93.41(19)
N(1)-Si(1)-C(12)-Hf(1)	-12.38(10)
C(25)-Si(1)-C(12)-Hf(1)	105.34(12)
C(26)-Si(1)-C(12)-Hf(1)	-130.43(11)
N(1)-Hf(1)-C(12)-C(19)	145.9(2)
O(1)-Hf(1)-C(12)-C(19)	-44.70(19)
Cl(2)-Hf(1)-C(12)-C(19)	43.25(19)
Cl(1)-Hf(1)-C(12)-C(19)	-128.85(17)
C(13)-Hf(1)-C(12)-C(19)	-107.8(3)
Si(1)-Hf(1)-C(12)-C(19)	135.0(2)
N(1)-Hf(1)-C(12)-C(13)	-106.31(16)
O(1)-Hf(1)-C(12)-C(13)	63.12(15)
Cl(2)-Hf(1)-C(12)-C(13)	151.07(14)
Cl(1)-Hf(1)-C(12)-C(13)	-21.03(19)
Si(1)-Hf(1)-C(12)-C(13)	-117.16(18)
N(1)-Hf(1)-C(12)-Si(1)	10.86(9)
O(1)-Hf(1)-C(12)-Si(1)	-179.72(9)

Cl(2)-Hf(1)-C(12)-Si(1)	-91.77(8)
Cl(1)-Hf(1)-C(12)-Si(1)	96.13(9)
C(13)-Hf(1)-C(12)-Si(1)	117.16(18)
C(19)-C(12)-C(13)-C(14)	179.2(3)
Si(1)-C(12)-C(13)-C(14)	-31.3(4)
Hf(1)-C(12)-C(13)-C(14)	59.4(3)
C(19)-C(12)-C(13)-C(18)	1.8(3)
Si(1)-C(12)-C(13)-C(18)	151.26(19)
Hf(1)-C(12)-C(13)-C(18)	-118.02(19)
C(19)-C(12)-C(13)-Hf(1)	119.8(2)
Si(1)-C(12)-C(13)-Hf(1)	-90.72(16)
N(1)-Hf(1)-C(13)-C(14)	-70.34(16)
O(1)-Hf(1)-C(13)-C(14)	106.56(16)
C(12)-Hf(1)-C(13)-C(14)	-139.4(2)
Cl(2)-Hf(1)-C(13)-C(14)	-177.02(13)
Cl(1)-Hf(1)-C(13)-C(14)	24.48(16)
Si(1)-Hf(1)-C(13)-C(14)	-98.41(16)
N(1)-Hf(1)-C(13)-C(18)	159.9(2)
O(1)-Hf(1)-C(13)-C(18)	-23.2(2)
C(12)-Hf(1)-C(13)-C(18)	90.8(3)
Cl(2)-Hf(1)-C(13)-C(18)	53.2(2)
Cl(1)-Hf(1)-C(13)-C(18)	-105.3(2)
Si(1)-Hf(1)-C(13)-C(18)	131.8(2)
N(1)-Hf(1)-C(13)-C(12)	69.11(16)
O(1)-Hf(1)-C(13)-C(12)	-114.00(16)
Cl(2)-Hf(1)-C(13)-C(12)	-37.58(17)
Cl(1)-Hf(1)-C(13)-C(12)	163.93(15)
Si(1)-Hf(1)-C(13)-C(12)	41.04(14)
C(18)-C(13)-C(14)-C(15)	-1.3(4)
C(12)-C(13)-C(14)-C(15)	-178.5(3)
Hf(1)-C(13)-C(14)-C(15)	-134.1(2)
C(13)-C(14)-C(15)-C(16)	-0.1(4)
C(14)-C(15)-C(16)-C(17)	0.4(5)
C(15)-C(16)-C(17)-C(18)	0.6(4)
C(16)-C(17)-C(18)-C(13)	-2.0(4)
C(16)-C(17)-C(18)-C(24)	179.6(3)
C(14)-C(13)-C(18)-C(17)	2.4(4)
C(12)-C(13)-C(18)-C(17)	-179.9(2)
Hf(1)-C(13)-C(18)-C(17)	120.9(2)

C(14)-C(13)-C(18)-C(24)	-178.9(2)
C(12)-C(13)-C(18)-C(24)	-1.1(3)
Hf(1)-C(13)-C(18)-C(24)	-60.4(3)
C(13)-C(12)-C(19)-C(20)	-178.9(3)
Si(1)-C(12)-C(19)-C(20)	36.9(4)
Hf(1)-C(12)-C(19)-C(20)	-77.2(3)
C(13)-C(12)-C(19)-C(24)	-1.9(3)
Si(1)-C(12)-C(19)-C(24)	-146.1(2)
Hf(1)-C(12)-C(19)-C(24)	99.8(2)
C(24)-C(19)-C(20)-C(21)	-0.1(4)
C(12)-C(19)-C(20)-C(21)	176.7(3)
C(19)-C(20)-C(21)-C(22)	-0.6(5)
C(20)-C(21)-C(22)-C(23)	0.6(5)
C(21)-C(22)-C(23)-C(24)	0.0(5)
C(22)-C(23)-C(24)-C(19)	-0.7(4)
C(22)-C(23)-C(24)-C(18)	-178.0(3)
C(20)-C(19)-C(24)-C(23)	0.8(4)
C(12)-C(19)-C(24)-C(23)	-176.6(3)
C(20)-C(19)-C(24)-C(18)	178.6(2)
C(12)-C(19)-C(24)-C(18)	1.3(3)
C(17)-C(18)-C(24)-C(23)	-3.9(5)
C(13)-C(18)-C(24)-C(23)	177.5(3)
C(17)-C(18)-C(24)-C(19)	178.5(3)
C(13)-C(18)-C(24)-C(19)	-0.1(3)
C(7)-B(1)-C(27)-C(28)	-51.6(3)
C(29)-B(1)-C(27)-C(28)	177.3(2)
N(2)-B(1)-C(27)-C(28)	55.8(3)
C(7)-B(1)-C(29)-C(30)	-65.2(3)
C(27)-B(1)-C(29)-C(30)	65.3(3)
N(2)-B(1)-C(29)-C(30)	-170.1(2)
N(1)-Hf(1)-O(1)-C(31)	120.4(3)
C(12)-Hf(1)-O(1)-C(31)	79.6(2)
Cl(2)-Hf(1)-O(1)-C(31)	-21.91(18)
Cl(1)-Hf(1)-O(1)-C(31)	-149.82(19)
C(13)-Hf(1)-O(1)-C(31)	108.99(19)
Si(1)-Hf(1)-O(1)-C(31)	79.4(2)
N(1)-Hf(1)-O(1)-C(34)	-57.7(4)
C(12)-Hf(1)-O(1)-C(34)	-98.5(2)
Cl(2)-Hf(1)-O(1)-C(34)	160.0(2)

Cl(1)-Hf(1)-O(1)-C(34)	32.1(2)
C(13)-Hf(1)-O(1)-C(34)	-69.1(2)
Si(1)-Hf(1)-O(1)-C(34)	-98.7(2)
C(34)-O(1)-C(31)-C(32A)	14.4(10)
Hf(1)-O(1)-C(31)-C(32A)	-163.9(10)
C(34)-O(1)-C(31)-C(32)	-5.4(3)
Hf(1)-O(1)-C(31)-C(32)	176.2(2)
C(32A)-C(31)-C(32)-C(33)	-49(3)
O(1)-C(31)-C(32)-C(33)	29.7(4)
C(31)-C(32)-C(33)-C(34)	-42.2(4)
O(1)-C(31)-C(32A)-C(33A)	-27(2)
C(32)-C(31)-C(32A)-C(33A)	79(4)
C(31)-C(32A)-C(33A)-C(34)	29(2)
C(32A)-C(33A)-C(34)-O(1)	-18(2)
C(32A)-C(33A)-C(34)-C(33)	74(3)
C(31)-O(1)-C(34)-C(33A)	1.1(10)
Hf(1)-O(1)-C(34)-C(33A)	179.5(10)
C(31)-O(1)-C(34)-C(33)	-21.7(3)
Hf(1)-O(1)-C(34)-C(33)	156.7(2)
C(32)-C(33)-C(34)-C(33A)	-54(3)
C(32)-C(33)-C(34)-O(1)	39.3(4)

Table S25. Crystal data and structure refinement for **Zr-2**.

Empirical formula	C40H47BCl2N2SiZr
Formula weight	756.82
Temperature	110(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 9.9361(7) Å α = 84.293(3)º.
	b = 12.4723(8) Å β = 73.108(3) º.
	c = 15.9000(11) Å γ= 83.935(3) º.
Volume	1870.0(2) Å^3
Z, Calculated density	2, 1.344 Mg/m^3
Absorption coefficient	0.500 mm^{-1}
F(000)	788
Crystal size	0.45 x 0.36 x 0.32 mm
Theta range for data collection	2.05 to 30.66 º.

Limiting indices	-14<=h<=14, -17<=k<=17, -22<=l<=22
Reflections collected / unique	79591 / 11477 [R(int) = 0.0198]
Completeness to theta = 30.66	99.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7461 and 0.7149
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11477 / 0 / 436
Goodness-of-fit on F^2	1.052
Final R indices [I>2σ(I)]	R1 = 0.0253, wR2 = 0.0659
R indices (all data)	R1 = 0.0304, wR2 = 0.0685
Largest diff. peak and hole	0.484 and -0.309 e.A^{-3}

Table S26. Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (A^2 × 10^3) for **Zr-2**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Zr(1)	4418(1)	7901(1)	3455(1)	15(1)
Si(1)	2633(1)	6075(1)	3239(1)	17(1)
Cl(1)	4098(1)	9596(1)	4106(1)	29(1)
Cl(2)	6793(1)	7662(1)	2484(1)	24(1)
C(1)	3124(1)	8081(1)	2111(1)	16(1)
B(1)	2412(1)	12091(1)	1526(1)	15(1)
N(1)	3016(1)	7373(1)	2840(1)	19(1)
N(2)	3810(1)	8943(1)	2173(1)	15(1)
C(2)	2646(1)	7960(1)	1384(1)	19(1)
C(3)	2878(1)	8766(1)	708(1)	19(1)
C(4)	3517(1)	9680(1)	787(1)	17(1)
C(5)	3957(1)	9756(1)	1533(1)	14(1)
C(6)	4629(1)	10732(1)	1626(1)	14(1)
C(7)	4022(1)	11789(1)	1469(1)	15(1)
C(8)	4810(1)	12656(1)	1486(1)	17(1)
C(9)	6071(1)	12506(1)	1710(1)	19(1)
C(10)	6605(1)	11467(1)	1905(1)	20(1)
C(11)	5902(1)	10586(1)	1842(1)	18(1)
C(12)	3501(1)	6169(1)	4128(1)	16(1)
C(13)	2954(1)	6958(1)	4778(1)	18(1)

C(14)	4074(2)	7232(1)	5079(1)	22(1)
C(15)	5325(1)	6654(1)	4608(1)	22(1)
C(16)	4980(1)	5987(1)	4040(1)	19(1)
C(17)	1444(2)	7412(1)	5095(1)	28(1)
C(18)	3950(2)	7926(1)	5821(1)	34(1)
C(19)	6754(2)	6649(1)	4751(1)	34(1)
C(20)	6015(1)	5178(1)	3501(1)	28(1)
C(21)	3493(2)	5061(1)	2432(1)	30(1)
C(22)	722(2)	5849(1)	3631(1)	33(1)
C(23)	1351(1)	11299(1)	2145(1)	15(1)
C(24)	463(1)	10742(1)	1826(1)	17(1)
C(25)	-388(1)	9990(1)	2385(1)	19(1)
C(26)	-421(1)	9801(1)	3269(1)	20(1)
C(27)	431(1)	10376(1)	3585(1)	19(1)
C(28)	1315(1)	11117(1)	3042(1)	16(1)
C(29)	394(1)	10946(1)	885(1)	22(1)
C(30)	-1374(2)	9006(1)	3864(1)	29(1)
C(31)	2159(1)	11755(1)	3440(1)	20(1)
C(32)	1913(1)	13215(1)	1120(1)	16(1)
C(33)	720(1)	13857(1)	1607(1)	18(1)
C(34)	427(1)	14918(1)	1294(1)	20(1)
C(35)	1227(1)	15373(1)	499(1)	21(1)
C(36)	2334(1)	14731(1)	-3(1)	23(1)
C(37)	2687(1)	13673(1)	289(1)	20(1)
C(38)	-293(1)	13463(1)	2462(1)	26(1)
C(39)	849(2)	16508(1)	177(1)	27(1)
C(40)	3870(2)	13044(1)	-342(1)	30(1)

Table S27. Bond lengths [Å] and angles [°] for **Zr-2**.

Zr(1)-N(1)	2.1085(10)
Zr(1)-Cl(1)	2.3960(3)
Zr(1)-Cl(2)	2.4219(4)
Zr(1)-C(13)	2.4526(11)
Zr(1)-C(12)	2.4560(11)
Zr(1)-N(2)	2.4961(9)
Zr(1)-C(16)	2.5407(11)

Zr(1)-C(14)	2.5692(12)
Zr(1)-C(15)	2.5866(12)
Zr(1)-C(1)	2.7765(11)
Zr(1)-Si(1)	3.1332(4)
Si(1)-N(1)	1.7187(10)
Si(1)-C(21)	1.8529(14)
Si(1)-C(22)	1.8618(15)
Si(1)-C(12)	1.8757(12)
C(1)-N(2)	1.3583(14)
C(1)-N(1)	1.3703(14)
C(1)-C(2)	1.3974(16)
B(1)-C(23)	1.5747(17)
B(1)-C(32)	1.5769(16)
B(1)-C(7)	1.5822(16)
N(2)-C(5)	1.3509(13)
C(2)-C(3)	1.3815(16)
C(2)-H(2)	0.9500
C(3)-C(4)	1.3941(16)
C(3)-H(3)	0.9500
C(4)-C(5)	1.3917(15)
C(4)-H(4)	0.9500
C(5)-C(6)	1.4886(15)
C(6)-C(11)	1.3935(15)
C(6)-C(7)	1.4212(14)
C(7)-C(8)	1.4072(15)
C(8)-C(9)	1.3880(16)
C(8)-H(8)	0.9500
C(9)-C(10)	1.3879(16)
C(9)-H(9)	0.9500
C(10)-C(11)	1.3904(16)
C(10)-H(10)	0.9500
C(11)-H(11)	0.9500
C(12)-C(16)	1.4306(16)
C(12)-C(13)	1.4464(16)
C(13)-C(14)	1.4166(17)
C(13)-C(17)	1.5048(18)
C(14)-C(15)	1.4153(19)
C(14)-C(18)	1.5009(18)
C(15)-C(16)	1.4204(18)

C(15)-C(19)	1.5004(18)
C(16)-C(20)	1.5006(17)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-C(24)	1.4064(16)
C(23)-C(28)	1.4122(15)
C(24)-C(25)	1.3956(16)
C(24)-C(29)	1.5124(16)
C(25)-C(26)	1.3930(17)
C(25)-H(25)	0.9500
C(26)-C(27)	1.3886(17)
C(26)-C(30)	1.5060(17)
C(27)-C(28)	1.3938(16)
C(27)-H(27)	0.9500
C(28)-C(31)	1.5126(16)
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800

C(31)-H(31C)	0.9800
C(32)-C(37)	1.4197(16)
C(32)-C(33)	1.4264(16)
C(33)-C(34)	1.3986(15)
C(33)-C(38)	1.5098(17)
C(34)-C(35)	1.3869(18)
C(34)-H(34)	0.9500
C(35)-C(36)	1.3857(18)
C(35)-C(39)	1.5033(16)
C(36)-C(37)	1.3981(16)
C(36)-H(36)	0.9500
C(37)-C(40)	1.5093(18)
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800

N(1)-Zr(1)-Cl(1)	124.37(3)
N(1)-Zr(1)-Cl(2)	108.44(3)
Cl(1)-Zr(1)-Cl(2)	109.597(13)
N(1)-Zr(1)-C(13)	83.79(4)
Cl(1)-Zr(1)-C(13)	94.35(3)
Cl(2)-Zr(1)-C(13)	137.27(3)
N(1)-Zr(1)-C(12)	67.35(4)
Cl(1)-Zr(1)-C(12)	128.59(3)
Cl(2)-Zr(1)-C(12)	111.96(3)
C(13)-Zr(1)-C(12)	34.28(4)
N(1)-Zr(1)-N(2)	57.42(3)
Cl(1)-Zr(1)-N(2)	86.51(2)
Cl(2)-Zr(1)-N(2)	86.10(2)
C(13)-Zr(1)-N(2)	131.51(4)
C(12)-Zr(1)-N(2)	124.76(3)
N(1)-Zr(1)-C(16)	91.75(4)
Cl(1)-Zr(1)-C(16)	131.41(3)

Cl(2)-Zr(1)-C(16)	83.40(3)
C(13)-Zr(1)-C(16)	54.82(4)
C(12)-Zr(1)-C(16)	33.22(4)
N(2)-Zr(1)-C(16)	141.96(4)
N(1)-Zr(1)-C(14)	116.14(4)
Cl(1)-Zr(1)-C(14)	79.89(3)
Cl(2)-Zr(1)-C(14)	116.41(3)
C(13)-Zr(1)-C(14)	32.67(4)
C(12)-Zr(1)-C(14)	55.16(4)
N(2)-Zr(1)-C(14)	156.54(4)
C(16)-Zr(1)-C(14)	53.56(4)
N(1)-Zr(1)-C(15)	121.19(4)
Cl(1)-Zr(1)-C(15)	100.21(3)
Cl(2)-Zr(1)-C(15)	86.52(3)
C(13)-Zr(1)-C(15)	53.91(4)
C(12)-Zr(1)-C(15)	54.60(4)
N(2)-Zr(1)-C(15)	171.36(4)
C(16)-Zr(1)-C(15)	32.15(4)
C(14)-Zr(1)-C(15)	31.86(4)
N(1)-Zr(1)-C(1)	28.63(3)
Cl(1)-Zr(1)-C(1)	109.65(2)
Cl(2)-Zr(1)-C(1)	94.81(3)
C(13)-Zr(1)-C(1)	110.14(4)
C(12)-Zr(1)-C(1)	95.70(4)
N(2)-Zr(1)-C(1)	29.24(3)
C(16)-Zr(1)-C(1)	115.77(4)
C(14)-Zr(1)-C(1)	142.71(4)
C(15)-Zr(1)-C(1)	147.62(4)
N(1)-Zr(1)-Si(1)	31.14(3)
Cl(1)-Zr(1)-Si(1)	139.795(13)
Cl(2)-Zr(1)-Si(1)	109.756(11)
C(13)-Zr(1)-Si(1)	60.92(3)
C(12)-Zr(1)-Si(1)	36.76(3)
N(2)-Zr(1)-Si(1)	88.22(2)
C(16)-Zr(1)-Si(1)	61.66(3)
C(14)-Zr(1)-Si(1)	89.94(3)
C(15)-Zr(1)-Si(1)	90.05(3)
C(1)-Zr(1)-Si(1)	59.02(2)
N(1)-Si(1)-C(21)	112.90(6)

N(1)-Si(1)-C(22)	115.42(6)
C(21)-Si(1)-C(22)	107.16(7)
N(1)-Si(1)-C(12)	90.15(5)
C(21)-Si(1)-C(12)	115.48(6)
C(22)-Si(1)-C(12)	115.33(6)
N(1)-Si(1)-Zr(1)	39.38(3)
C(21)-Si(1)-Zr(1)	118.26(5)
C(22)-Si(1)-Zr(1)	133.87(5)
C(12)-Si(1)-Zr(1)	51.59(3)
N(2)-C(1)-N(1)	110.20(10)
N(2)-C(1)-C(2)	122.89(10)
N(1)-C(1)-C(2)	126.90(10)
N(2)-C(1)-Zr(1)	63.86(6)
N(1)-C(1)-Zr(1)	47.50(5)
C(2)-C(1)-Zr(1)	167.55(8)
C(23)-B(1)-C(32)	122.79(10)
C(23)-B(1)-C(7)	115.49(9)
C(32)-B(1)-C(7)	120.88(10)
C(1)-N(1)-Si(1)	142.52(9)
C(1)-N(1)-Zr(1)	103.87(7)
Si(1)-N(1)-Zr(1)	109.48(5)
C(5)-N(2)-C(1)	118.75(10)
C(5)-N(2)-Zr(1)	153.37(8)
C(1)-N(2)-Zr(1)	86.90(6)
C(3)-C(2)-C(1)	117.76(11)
C(3)-C(2)-H(2)	121.1
C(1)-C(2)-H(2)	121.1
C(2)-C(3)-C(4)	119.64(11)
C(2)-C(3)-H(3)	120.2
C(4)-C(3)-H(3)	120.2
C(5)-C(4)-C(3)	119.75(10)
C(5)-C(4)-H(4)	120.1
C(3)-C(4)-H(4)	120.1
N(2)-C(5)-C(4)	120.99(10)
N(2)-C(5)-C(6)	118.88(10)
C(4)-C(5)-C(6)	120.12(10)
C(11)-C(6)-C(7)	120.44(10)
C(11)-C(6)-C(5)	118.29(9)
C(7)-C(6)-C(5)	121.23(10)

C(8)-C(7)-C(6)	116.81(10)
C(8)-C(7)-B(1)	116.01(9)
C(6)-C(7)-B(1)	125.12(10)
C(9)-C(8)-C(7)	122.33(10)
C(9)-C(8)-H(8)	118.8
C(7)-C(8)-H(8)	118.8
C(10)-C(9)-C(8)	119.64(11)
C(10)-C(9)-H(9)	120.2
C(8)-C(9)-H(9)	120.2
C(9)-C(10)-C(11)	119.70(11)
C(9)-C(10)-H(10)	120.1
C(11)-C(10)-H(10)	120.1
C(10)-C(11)-C(6)	120.88(10)
C(10)-C(11)-H(11)	119.6
C(6)-C(11)-H(11)	119.6
C(16)-C(12)-C(13)	106.15(10)
C(16)-C(12)-Si(1)	125.92(9)
C(13)-C(12)-Si(1)	120.47(8)
C(16)-C(12)-Zr(1)	76.65(6)
C(13)-C(12)-Zr(1)	72.73(6)
Si(1)-C(12)-Zr(1)	91.66(4)
C(14)-C(13)-C(12)	108.86(11)
C(14)-C(13)-C(17)	125.00(11)
C(12)-C(13)-C(17)	126.14(11)
C(14)-C(13)-Zr(1)	78.20(7)
C(12)-C(13)-Zr(1)	72.99(6)
C(17)-C(13)-Zr(1)	115.79(8)
C(15)-C(14)-C(13)	107.73(11)
C(15)-C(14)-C(18)	125.47(13)
C(13)-C(14)-C(18)	126.58(13)
C(15)-C(14)-Zr(1)	74.74(7)
C(13)-C(14)-Zr(1)	69.14(6)
C(18)-C(14)-Zr(1)	125.84(8)
C(14)-C(15)-C(16)	108.57(11)
C(14)-C(15)-C(19)	126.01(13)
C(16)-C(15)-C(19)	125.10(13)
C(14)-C(15)-Zr(1)	73.39(7)
C(16)-C(15)-Zr(1)	72.15(6)
C(19)-C(15)-Zr(1)	125.48(8)

C(15)-C(16)-C(12)	108.64(11)
C(15)-C(16)-C(20)	123.77(11)
C(12)-C(16)-C(20)	127.45(11)
C(15)-C(16)-Zr(1)	75.70(6)
C(12)-C(16)-Zr(1)	70.14(6)
C(20)-C(16)-Zr(1)	123.73(8)
C(13)-C(17)-H(17A)	109.5
C(13)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(13)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(14)-C(18)-H(18A)	109.5
C(14)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(14)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(15)-C(19)-H(19A)	109.5
C(15)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(15)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(16)-C(20)-H(20A)	109.5
C(16)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(16)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
Si(1)-C(21)-H(21A)	109.5
Si(1)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
Si(1)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
Si(1)-C(22)-H(22A)	109.5
Si(1)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5

Si(1)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(24)-C(23)-C(28)	118.77(10)
C(24)-C(23)-B(1)	121.99(10)
C(28)-C(23)-B(1)	119.21(10)
C(25)-C(24)-C(23)	119.91(10)
C(25)-C(24)-C(29)	118.74(11)
C(23)-C(24)-C(29)	121.35(10)
C(26)-C(25)-C(24)	121.53(11)
C(26)-C(25)-H(25)	119.2
C(24)-C(25)-H(25)	119.2
C(27)-C(26)-C(25)	118.22(11)
C(27)-C(26)-C(30)	121.26(11)
C(25)-C(26)-C(30)	120.51(12)
C(26)-C(27)-C(28)	121.83(11)
C(26)-C(27)-H(27)	119.1
C(28)-C(27)-H(27)	119.1
C(27)-C(28)-C(23)	119.69(11)
C(27)-C(28)-C(31)	118.97(10)
C(23)-C(28)-C(31)	121.25(10)
C(24)-C(29)-H(29A)	109.5
C(24)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(24)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(26)-C(30)-H(30A)	109.5
C(26)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(26)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(28)-C(31)-H(31A)	109.5
C(28)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(28)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5

C(37)-C(32)-C(33)	116.94(10)
C(37)-C(32)-B(1)	121.86(10)
C(33)-C(32)-B(1)	121.02(10)
C(34)-C(33)-C(32)	119.99(11)
C(34)-C(33)-C(38)	115.98(11)
C(32)-C(33)-C(38)	124.03(10)
C(35)-C(34)-C(33)	122.46(11)
C(35)-C(34)-H(34)	118.8
C(33)-C(34)-H(34)	118.8
C(36)-C(35)-C(34)	117.73(11)
C(36)-C(35)-C(39)	121.56(12)
C(34)-C(35)-C(39)	120.63(12)
C(35)-C(36)-C(37)	121.94(11)
C(35)-C(36)-H(36)	119.0
C(37)-C(36)-H(36)	119.0
C(36)-C(37)-C(32)	120.74(11)
C(36)-C(37)-C(40)	116.47(11)
C(32)-C(37)-C(40)	122.72(10)
C(33)-C(38)-H(38A)	109.5
C(33)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(33)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(35)-C(39)-H(39A)	109.5
C(35)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(35)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(37)-C(40)-H(40A)	109.5
C(37)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(37)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5

Table S28. Anisotropic displacement parameters ($A^2 \times 10^3$) for **Zr-2**. The anisotropic displacement factor exponent takes the form: $-2\,pi^2\,[\,h^2\,a^{*2}\,U11 + ... + 2\,h\,k\,a^*\,b^*\,U12\,]$

	U11	U22	U33	U23	U13	U12
Zr(1)	19(1)	11(1)	16(1)	1(1)	-7(1)	-3(1)
Si(1)	21(1)	13(1)	20(1)	-1(1)	-6(1)	-5(1)
Cl(1)	54(1)	13(1)	25(1)	-2(1)	-18(1)	-3(1)
Cl(2)	21(1)	23(1)	25(1)	4(1)	-4(1)	-1(1)
C(1)	17(1)	13(1)	18(1)	-2(1)	-7(1)	-1(1)
B(1)	17(1)	14(1)	14(1)	-1(1)	-6(1)	1(1)
N(1)	27(1)	14(1)	21(1)	2(1)	-12(1)	-6(1)
N(2)	18(1)	13(1)	17(1)	0(1)	-7(1)	-1(1)
C(2)	23(1)	17(1)	20(1)	-3(1)	-9(1)	-3(1)
C(3)	23(1)	20(1)	17(1)	-4(1)	-9(1)	-1(1)
C(4)	19(1)	17(1)	15(1)	-1(1)	-5(1)	0(1)
C(5)	14(1)	13(1)	16(1)	-1(1)	-4(1)	1(1)
C(6)	15(1)	13(1)	14(1)	1(1)	-3(1)	-1(1)
C(7)	15(1)	14(1)	14(1)	0(1)	-4(1)	-1(1)
C(8)	19(1)	14(1)	18(1)	0(1)	-4(1)	-1(1)
C(9)	19(1)	17(1)	22(1)	-1(1)	-5(1)	-5(1)
C(10)	16(1)	21(1)	22(1)	0(1)	-7(1)	-2(1)
C(11)	16(1)	16(1)	20(1)	1(1)	-6(1)	0(1)
C(12)	20(1)	11(1)	17(1)	1(1)	-4(1)	-3(1)
C(13)	24(1)	14(1)	16(1)	1(1)	-4(1)	-2(1)
C(14)	35(1)	15(1)	18(1)	4(1)	-11(1)	-7(1)
C(15)	26(1)	19(1)	25(1)	8(1)	-13(1)	-7(1)
C(16)	20(1)	13(1)	22(1)	4(1)	-6(1)	-1(1)
C(17)	27(1)	27(1)	24(1)	-5(1)	0(1)	3(1)
C(18)	61(1)	23(1)	22(1)	-1(1)	-19(1)	-10(1)
C(19)	33(1)	33(1)	44(1)	17(1)	-25(1)	-13(1)
C(20)	24(1)	19(1)	33(1)	3(1)	-3(1)	4(1)
C(21)	42(1)	22(1)	29(1)	-10(1)	-12(1)	-1(1)
C(22)	26(1)	39(1)	37(1)	-1(1)	-10(1)	-13(1)
C(23)	14(1)	15(1)	16(1)	0(1)	-4(1)	1(1)
C(24)	15(1)	18(1)	18(1)	-1(1)	-6(1)	1(1)
C(25)	17(1)	19(1)	23(1)	-1(1)	-7(1)	-2(1)

C(26)	17(1)	18(1)	22(1)	2(1)	-3(1)	-2(1)
C(27)	20(1)	19(1)	16(1)	0(1)	-4(1)	0(1)
C(28)	16(1)	15(1)	16(1)	-2(1)	-5(1)	1(1)
C(29)	23(1)	25(1)	21(1)	1(1)	-11(1)	-2(1)
C(30)	28(1)	29(1)	29(1)	7(1)	-6(1)	-12(1)
C(31)	23(1)	22(1)	17(1)	-2(1)	-7(1)	-3(1)
C(32)	17(1)	15(1)	17(1)	0(1)	-7(1)	0(1)
C(33)	18(1)	17(1)	19(1)	0(1)	-7(1)	1(1)
C(34)	21(1)	17(1)	25(1)	-2(1)	-11(1)	2(1)
C(35)	25(1)	17(1)	26(1)	2(1)	-16(1)	-2(1)
C(36)	26(1)	21(1)	22(1)	6(1)	-9(1)	-3(1)
C(37)	21(1)	20(1)	18(1)	2(1)	-6(1)	0(1)
C(38)	23(1)	23(1)	26(1)	2(1)	1(1)	7(1)
C(39)	36(1)	17(1)	33(1)	4(1)	-20(1)	-2(1)
C(40)	33(1)	32(1)	18(1)	3(1)	0(1)	7(1)

Table S29. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($A^2 \times 10^3$) for **Zr-2**.

	x	y	z	U(eq)
H(2)	2177	7345	1356	23
H(3)	2604	8698	192	23
H(4)	3651	10248	334	21
H(8)	4468	13369	1340	21
H(9)	6565	13110	1730	23
H(10)	7448	11359	2081	24
H(11)	6294	9874	1947	21
H(17A)	1362	7938	5530	42
H(17B)	842	6825	5367	42
H(17C)	1143	7771	4595	42
H(18A)	3086	8412	5907	50
H(18B)	4769	8355	5677	50
H(18C)	3913	7466	6362	50
H(19A)	6904	6019	5144	52
H(19B)	6808	7311	5020	52
H(19C)	7482	6613	4184	52

H(20A)	6648	5555	2993	41
H(20B)	5504	4678	3293	41
H(20C)	6569	4771	3864	41
H(21A)	2976	5080	1990	45
H(21B)	3488	4339	2738	45
H(21C)	4469	5227	2140	45
H(22A)	217	6411	4022	50
H(22B)	599	5138	3954	50
H(22C)	342	5878	3125	50
H(25)	-957	9599	2158	23
H(27)	411	10260	4188	23
H(29A)	228	10273	675	33
H(29B)	1288	11203	512	33
H(29C)	-379	11494	860	33
H(30A)	-1145	8880	4427	44
H(30B)	-1237	8321	3584	44
H(30C)	-2359	9297	3968	44
H(31A)	1764	11714	4082	30
H(31B)	2116	12511	3208	30
H(31C)	3143	11452	3288	30
H(34)	-349	15342	1640	24
H(36)	2868	15017	-562	28
H(38A)	-1020	14044	2678	40
H(38B)	223	13247	2900	40
H(38C)	-739	12841	2363	40
H(39A)	338	16487	-263	40
H(39B)	1712	16876	-91	40
H(39C)	250	16900	674	40
H(40A)	3737	13143	-932	45
H(40B)	3868	12275	-143	45
H(40C)	4774	13306	-359	45

Table S30. Torsion angles [°] for **Zr-2**.

Cl(1)-Zr(1)-Si(1)-N(1)	74.50(6)
Cl(2)-Zr(1)-Si(1)-N(1)	-93.18(6)
C(13)-Zr(1)-Si(1)-N(1)	132.92(7)

C(12)-Zr(1)-Si(1)-N(1)	166.26(8)
N(2)-Zr(1)-Si(1)-N(1)	-7.97(6)
C(16)-Zr(1)-Si(1)-N(1)	-163.76(7)
C(14)-Zr(1)-Si(1)-N(1)	148.64(7)
C(15)-Zr(1)-Si(1)-N(1)	-179.50(7)
C(1)-Zr(1)-Si(1)-N(1)	-9.60(6)
N(1)-Zr(1)-Si(1)-C(21)	92.37(8)
Cl(1)-Zr(1)-Si(1)-C(21)	166.87(5)
Cl(2)-Zr(1)-Si(1)-C(21)	-0.81(6)
C(13)-Zr(1)-Si(1)-C(21)	-134.71(6)
C(12)-Zr(1)-Si(1)-C(21)	-101.37(7)
N(2)-Zr(1)-Si(1)-C(21)	84.40(6)
C(16)-Zr(1)-Si(1)-C(21)	-71.39(6)
C(14)-Zr(1)-Si(1)-C(21)	-118.99(6)
C(15)-Zr(1)-Si(1)-C(21)	-87.13(6)
C(1)-Zr(1)-Si(1)-C(21)	82.78(6)
N(1)-Zr(1)-Si(1)-C(22)	-76.54(9)
Cl(1)-Zr(1)-Si(1)-C(22)	-2.03(8)
Cl(2)-Zr(1)-Si(1)-C(22)	-169.72(7)
C(13)-Zr(1)-Si(1)-C(22)	56.39(8)
C(12)-Zr(1)-Si(1)-C(22)	89.72(8)
N(2)-Zr(1)-Si(1)-C(22)	-84.51(8)
C(16)-Zr(1)-Si(1)-C(22)	119.70(8)
C(14)-Zr(1)-Si(1)-C(22)	72.10(8)
C(15)-Zr(1)-Si(1)-C(22)	103.96(8)
C(1)-Zr(1)-Si(1)-C(22)	-86.13(8)
N(1)-Zr(1)-Si(1)-C(12)	-166.26(8)
Cl(1)-Zr(1)-Si(1)-C(12)	-91.76(5)
Cl(2)-Zr(1)-Si(1)-C(12)	100.56(5)
C(13)-Zr(1)-Si(1)-C(12)	-33.34(5)
N(2)-Zr(1)-Si(1)-C(12)	-174.23(5)
C(16)-Zr(1)-Si(1)-C(12)	29.98(5)
C(14)-Zr(1)-Si(1)-C(12)	-17.62(5)
C(15)-Zr(1)-Si(1)-C(12)	14.24(5)
C(1)-Zr(1)-Si(1)-C(12)	-175.85(5)
N(1)-Zr(1)-C(1)-N(2)	166.31(11)
Cl(1)-Zr(1)-C(1)-N(2)	39.66(7)
Cl(2)-Zr(1)-C(1)-N(2)	-73.14(6)
C(13)-Zr(1)-C(1)-N(2)	142.17(6)

C(12)-Zr(1)-C(1)-N(2)	174.18(7)
C(16)-Zr(1)-C(1)-N(2)	-158.12(6)
C(14)-Zr(1)-C(1)-N(2)	138.93(7)
C(15)-Zr(1)-C(1)-N(2)	-164.22(7)
Si(1)-Zr(1)-C(1)-N(2)	176.67(7)
Cl(1)-Zr(1)-C(1)-N(1)	-126.65(7)
Cl(2)-Zr(1)-C(1)-N(1)	120.55(8)
C(13)-Zr(1)-C(1)-N(1)	-24.14(8)
C(12)-Zr(1)-C(1)-N(1)	7.87(8)
N(2)-Zr(1)-C(1)-N(1)	-166.31(11)
C(16)-Zr(1)-C(1)-N(1)	35.57(9)
C(14)-Zr(1)-C(1)-N(1)	-27.38(10)
C(15)-Zr(1)-C(1)-N(1)	29.47(11)
Si(1)-Zr(1)-C(1)-N(1)	10.36(7)
N(1)-Zr(1)-C(1)-C(2)	-68.1(4)
Cl(1)-Zr(1)-C(1)-C(2)	165.3(4)
Cl(2)-Zr(1)-C(1)-C(2)	52.5(4)
C(13)-Zr(1)-C(1)-C(2)	-92.2(4)
C(12)-Zr(1)-C(1)-C(2)	-60.2(4)
N(2)-Zr(1)-C(1)-C(2)	125.6(4)
C(16)-Zr(1)-C(1)-C(2)	-32.5(4)
C(14)-Zr(1)-C(1)-C(2)	-95.4(4)
C(15)-Zr(1)-C(1)-C(2)	-38.6(4)
Si(1)-Zr(1)-C(1)-C(2)	-57.7(4)
N(2)-C(1)-N(1)-Si(1)	-165.56(11)
C(2)-C(1)-N(1)-Si(1)	13.1(2)
Zr(1)-C(1)-N(1)-Si(1)	-152.47(17)
N(2)-C(1)-N(1)-Zr(1)	-13.09(11)
C(2)-C(1)-N(1)-Zr(1)	165.52(10)
C(21)-Si(1)-N(1)-C(1)	44.40(17)
C(22)-Si(1)-N(1)-C(1)	-79.34(16)
C(12)-Si(1)-N(1)-C(1)	162.31(15)
Zr(1)-Si(1)-N(1)-C(1)	151.58(18)
C(21)-Si(1)-N(1)-Zr(1)	-107.18(7)
C(22)-Si(1)-N(1)-Zr(1)	129.08(7)
C(12)-Si(1)-N(1)-Zr(1)	10.73(6)
Cl(1)-Zr(1)-N(1)-C(1)	66.26(8)
Cl(2)-Zr(1)-N(1)-C(1)	-64.76(8)
C(13)-Zr(1)-N(1)-C(1)	157.28(8)

C(12)-Zr(1)-N(1)-C(1)	-171.51(9)
N(2)-Zr(1)-N(1)-C(1)	7.89(7)
C(16)-Zr(1)-N(1)-C(1)	-148.39(8)
C(14)-Zr(1)-N(1)-C(1)	161.92(7)
C(15)-Zr(1)-N(1)-C(1)	-162.06(7)
Si(1)-Zr(1)-N(1)-C(1)	-162.65(11)
Cl(1)-Zr(1)-N(1)-Si(1)	-131.10(4)
Cl(2)-Zr(1)-N(1)-Si(1)	97.88(5)
C(13)-Zr(1)-N(1)-Si(1)	-40.07(6)
C(12)-Zr(1)-N(1)-Si(1)	-8.86(5)
N(2)-Zr(1)-N(1)-Si(1)	170.53(7)
C(16)-Zr(1)-N(1)-Si(1)	14.25(6)
C(14)-Zr(1)-N(1)-Si(1)	-35.43(7)
C(15)-Zr(1)-N(1)-Si(1)	0.58(8)
C(1)-Zr(1)-N(1)-Si(1)	162.65(11)
N(1)-C(1)-N(2)-C(5)	-176.81(10)
C(2)-C(1)-N(2)-C(5)	4.51(17)
Zr(1)-C(1)-N(2)-C(5)	172.47(11)
N(1)-C(1)-N(2)-Zr(1)	10.72(9)
C(2)-C(1)-N(2)-Zr(1)	-167.96(11)
N(1)-Zr(1)-N(2)-C(5)	-172.89(18)
Cl(1)-Zr(1)-N(2)-C(5)	51.87(17)
Cl(2)-Zr(1)-N(2)-C(5)	-58.07(17)
C(13)-Zr(1)-N(2)-C(5)	144.59(16)
C(12)-Zr(1)-N(2)-C(5)	-172.21(16)
C(16)-Zr(1)-N(2)-C(5)	-132.16(16)
C(14)-Zr(1)-N(2)-C(5)	106.26(18)
C(15)-Zr(1)-N(2)-C(5)	-89.4(3)
C(1)-Zr(1)-N(2)-C(5)	-165.2(2)
Si(1)-Zr(1)-N(2)-C(5)	-168.01(17)
N(1)-Zr(1)-N(2)-C(1)	-7.73(6)
Cl(1)-Zr(1)-N(2)-C(1)	-142.98(6)
Cl(2)-Zr(1)-N(2)-C(1)	107.09(6)
C(13)-Zr(1)-N(2)-C(1)	-50.25(8)
C(12)-Zr(1)-N(2)-C(1)	-7.05(8)
C(16)-Zr(1)-N(2)-C(1)	32.99(9)
C(14)-Zr(1)-N(2)-C(1)	-88.58(10)
C(15)-Zr(1)-N(2)-C(1)	75.7(2)
Si(1)-Zr(1)-N(2)-C(1)	-2.85(6)

N(2)-C(1)-C(2)-C(3)	-0.64(18)
N(1)-C(1)-C(2)-C(3)	-179.08(12)
Zr(1)-C(1)-C(2)-C(3)	-120.3(4)
C(1)-C(2)-C(3)-C(4)	-2.67(18)
C(2)-C(3)-C(4)-C(5)	2.12(17)
C(1)-N(2)-C(5)-C(4)	-5.05(16)
Zr(1)-N(2)-C(5)-C(4)	157.99(13)
C(1)-N(2)-C(5)-C(6)	176.26(10)
Zr(1)-N(2)-C(5)-C(6)	-20.7(2)
C(3)-C(4)-C(5)-N(2)	1.82(17)
C(3)-C(4)-C(5)-C(6)	-179.50(10)
N(2)-C(5)-C(6)-C(11)	48.87(15)
C(4)-C(5)-C(6)-C(11)	-129.83(11)
N(2)-C(5)-C(6)-C(7)	-133.41(11)
C(4)-C(5)-C(6)-C(7)	47.88(15)
C(11)-C(6)-C(7)-C(8)	3.97(16)
C(5)-C(6)-C(7)-C(8)	-173.69(10)
C(11)-C(6)-C(7)-B(1)	-159.01(11)
C(5)-C(6)-C(7)-B(1)	23.32(16)
C(23)-B(1)-C(7)-C(8)	-137.81(10)
C(32)-B(1)-C(7)-C(8)	32.01(15)
C(23)-B(1)-C(7)-C(6)	25.29(16)
C(32)-B(1)-C(7)-C(6)	-164.89(10)
C(6)-C(7)-C(8)-C(9)	-4.71(17)
B(1)-C(7)-C(8)-C(9)	159.84(11)
C(7)-C(8)-C(9)-C(10)	1.60(18)
C(8)-C(9)-C(10)-C(11)	2.40(18)
C(9)-C(10)-C(11)-C(6)	-3.08(18)
C(7)-C(6)-C(11)-C(10)	-0.20(17)
C(5)-C(6)-C(11)-C(10)	177.53(10)
N(1)-Si(1)-C(12)-C(16)	-83.34(10)
C(21)-Si(1)-C(12)-C(16)	32.27(12)
C(22)-Si(1)-C(12)-C(16)	158.23(10)
Zr(1)-Si(1)-C(12)-C(16)	-74.67(9)
N(1)-Si(1)-C(12)-C(13)	62.21(9)
C(21)-Si(1)-C(12)-C(13)	177.82(9)
C(22)-Si(1)-C(12)-C(13)	-56.21(11)
Zr(1)-Si(1)-C(12)-C(13)	70.88(8)
N(1)-Si(1)-C(12)-Zr(1)	-8.67(5)

C(21)-Si(1)-C(12)-Zr(1)	106.94(6)
C(22)-Si(1)-C(12)-Zr(1)	-127.10(6)
N(1)-Zr(1)-C(12)-C(16)	134.26(8)
Cl(1)-Zr(1)-C(12)-C(16)	-109.03(7)
Cl(2)-Zr(1)-C(12)-C(16)	32.65(7)
C(13)-Zr(1)-C(12)-C(16)	-111.91(10)
N(2)-Zr(1)-C(12)-C(16)	133.64(7)
C(14)-Zr(1)-C(12)-C(16)	-75.04(8)
C(15)-Zr(1)-C(12)-C(16)	-35.83(7)
C(1)-Zr(1)-C(12)-C(16)	130.18(7)
Si(1)-Zr(1)-C(12)-C(16)	126.61(9)
N(1)-Zr(1)-C(12)-C(13)	-113.84(8)
Cl(1)-Zr(1)-C(12)-C(13)	2.88(8)
Cl(2)-Zr(1)-C(12)-C(13)	144.55(6)
N(2)-Zr(1)-C(12)-C(13)	-114.46(7)
C(16)-Zr(1)-C(12)-C(13)	111.91(10)
C(14)-Zr(1)-C(12)-C(13)	36.87(7)
C(15)-Zr(1)-C(12)-C(13)	76.08(7)
C(1)-Zr(1)-C(12)-C(13)	-117.91(7)
Si(1)-Zr(1)-C(12)-C(13)	-121.49(8)
N(1)-Zr(1)-C(12)-Si(1)	7.65(4)
Cl(1)-Zr(1)-C(12)-Si(1)	124.36(3)
Cl(2)-Zr(1)-C(12)-Si(1)	-93.96(4)
C(13)-Zr(1)-C(12)-Si(1)	121.49(8)
N(2)-Zr(1)-C(12)-Si(1)	7.03(6)
C(16)-Zr(1)-C(12)-Si(1)	-126.61(9)
C(14)-Zr(1)-C(12)-Si(1)	158.36(7)
C(15)-Zr(1)-C(12)-Si(1)	-162.43(7)
C(1)-Zr(1)-C(12)-Si(1)	3.57(5)
C(16)-C(12)-C(13)-C(14)	-0.69(12)
Si(1)-C(12)-C(13)-C(14)	-152.20(8)
Zr(1)-C(12)-C(13)-C(14)	-70.70(8)
C(16)-C(12)-C(13)-C(17)	179.89(11)
Si(1)-C(12)-C(13)-C(17)	28.37(15)
Zr(1)-C(12)-C(13)-C(17)	109.88(11)
C(16)-C(12)-C(13)-Zr(1)	70.01(7)
Si(1)-C(12)-C(13)-Zr(1)	-81.50(7)
N(1)-Zr(1)-C(13)-C(14)	172.27(7)
Cl(1)-Zr(1)-C(13)-C(14)	-63.59(7)

Cl(2)-Zr(1)-C(13)-C(14)	61.72(8)
C(12)-Zr(1)-C(13)-C(14)	114.16(10)
N(2)-Zr(1)-C(13)-C(14)	-152.78(7)
C(16)-Zr(1)-C(13)-C(14)	75.70(8)
C(15)-Zr(1)-C(13)-C(14)	35.88(7)
C(1)-Zr(1)-C(13)-C(14)	-176.36(7)
Si(1)-Zr(1)-C(13)-C(14)	149.88(8)
N(1)-Zr(1)-C(13)-C(12)	58.12(7)
Cl(1)-Zr(1)-C(13)-C(12)	-177.74(6)
Cl(2)-Zr(1)-C(13)-C(12)	-52.44(8)
N(2)-Zr(1)-C(13)-C(12)	93.07(7)
C(16)-Zr(1)-C(13)-C(12)	-38.45(6)
C(14)-Zr(1)-C(13)-C(12)	-114.16(10)
C(15)-Zr(1)-C(13)-C(12)	-78.28(7)
C(1)-Zr(1)-C(13)-C(12)	69.48(7)
Si(1)-Zr(1)-C(13)-C(12)	35.73(6)
N(1)-Zr(1)-C(13)-C(17)	-64.37(9)
Cl(1)-Zr(1)-C(13)-C(17)	59.77(9)
Cl(2)-Zr(1)-C(13)-C(17)	-174.92(7)
C(12)-Zr(1)-C(13)-C(17)	-122.48(12)
N(2)-Zr(1)-C(13)-C(17)	-29.42(11)
C(16)-Zr(1)-C(13)-C(17)	-160.94(11)
C(14)-Zr(1)-C(13)-C(17)	123.36(12)
C(15)-Zr(1)-C(13)-C(17)	159.24(11)
C(1)-Zr(1)-C(13)-C(17)	-53.00(10)
Si(1)-Zr(1)-C(13)-C(17)	-86.76(9)
C(12)-C(13)-C(14)-C(15)	1.90(13)
C(17)-C(13)-C(14)-C(15)	-178.67(11)
Zr(1)-C(13)-C(14)-C(15)	-65.32(8)
C(12)-C(13)-C(14)-C(18)	-172.95(11)
C(17)-C(13)-C(14)-C(18)	6.48(19)
Zr(1)-C(13)-C(14)-C(18)	119.83(12)
C(12)-C(13)-C(14)-Zr(1)	67.22(8)
C(17)-C(13)-C(14)-Zr(1)	-113.35(12)
N(1)-Zr(1)-C(14)-C(15)	107.66(7)
Cl(1)-Zr(1)-C(14)-C(15)	-128.90(7)
Cl(2)-Zr(1)-C(14)-C(15)	-21.93(8)
C(13)-Zr(1)-C(14)-C(15)	116.22(10)
C(12)-Zr(1)-C(14)-C(15)	77.46(7)

N(2)-Zr(1)-C(14)-C(15)	175.58(8)
C(16)-Zr(1)-C(14)-C(15)	36.32(7)
C(1)-Zr(1)-C(14)-C(15)	121.86(8)
Si(1)-Zr(1)-C(14)-C(15)	90.21(7)
N(1)-Zr(1)-C(14)-C(13)	-8.56(8)
Cl(1)-Zr(1)-C(14)-C(13)	114.89(7)
Cl(2)-Zr(1)-C(14)-C(13)	-138.15(6)
C(12)-Zr(1)-C(14)-C(13)	-38.76(7)
N(2)-Zr(1)-C(14)-C(13)	59.37(12)
C(16)-Zr(1)-C(14)-C(13)	-79.90(7)
C(15)-Zr(1)-C(14)-C(13)	-116.22(10)
C(1)-Zr(1)-C(14)-C(13)	5.65(10)
Si(1)-Zr(1)-C(14)-C(13)	-26.01(7)
N(1)-Zr(1)-C(14)-C(18)	-129.32(12)
Cl(1)-Zr(1)-C(14)-C(18)	-5.87(12)
Cl(2)-Zr(1)-C(14)-C(18)	101.10(12)
C(13)-Zr(1)-C(14)-C(18)	-120.76(16)
C(12)-Zr(1)-C(14)-C(18)	-159.52(14)
N(2)-Zr(1)-C(14)-C(18)	-61.39(17)
C(16)-Zr(1)-C(14)-C(18)	159.34(14)
C(15)-Zr(1)-C(14)-C(18)	123.03(16)
C(1)-Zr(1)-C(14)-C(18)	-115.11(12)
Si(1)-Zr(1)-C(14)-C(18)	-146.77(12)
C(13)-C(14)-C(15)-C(16)	-2.39(13)
C(18)-C(14)-C(15)-C(16)	172.53(11)
Zr(1)-C(14)-C(15)-C(16)	-64.04(8)
C(13)-C(14)-C(15)-C(19)	-176.20(11)
C(18)-C(14)-C(15)-C(19)	-1.28(19)
Zr(1)-C(14)-C(15)-C(19)	122.14(12)
C(13)-C(14)-C(15)-Zr(1)	61.66(8)
C(18)-C(14)-C(15)-Zr(1)	-123.42(12)
N(1)-Zr(1)-C(15)-C(14)	-90.09(8)
Cl(1)-Zr(1)-C(15)-C(14)	51.12(7)
Cl(2)-Zr(1)-C(15)-C(14)	160.42(7)
C(13)-Zr(1)-C(15)-C(14)	-36.81(7)
C(12)-Zr(1)-C(15)-C(14)	-79.38(8)
N(2)-Zr(1)-C(15)-C(14)	-168.2(2)
C(16)-Zr(1)-C(15)-C(14)	-116.44(10)
C(1)-Zr(1)-C(15)-C(14)	-106.09(9)

Si(1)-Zr(1)-C(15)-C(14)	-89.79(7)
N(1)-Zr(1)-C(15)-C(16)	26.35(9)
Cl(1)-Zr(1)-C(15)-C(16)	167.56(7)
Cl(2)-Zr(1)-C(15)-C(16)	-83.14(7)
C(13)-Zr(1)-C(15)-C(16)	79.63(8)
C(12)-Zr(1)-C(15)-C(16)	37.06(7)
N(2)-Zr(1)-C(15)-C(16)	-51.8(3)
C(14)-Zr(1)-C(15)-C(16)	116.44(10)
C(1)-Zr(1)-C(15)-C(16)	10.35(12)
Si(1)-Zr(1)-C(15)-C(16)	26.65(7)
N(1)-Zr(1)-C(15)-C(19)	147.17(12)
Cl(1)-Zr(1)-C(15)-C(19)	-71.61(13)
Cl(2)-Zr(1)-C(15)-C(19)	37.68(12)
C(13)-Zr(1)-C(15)-C(19)	-159.55(14)
C(12)-Zr(1)-C(15)-C(19)	157.88(14)
N(2)-Zr(1)-C(15)-C(19)	69.0(3)
C(16)-Zr(1)-C(15)-C(19)	120.82(16)
C(14)-Zr(1)-C(15)-C(19)	-122.74(16)
C(1)-Zr(1)-C(15)-C(19)	131.18(12)
Si(1)-Zr(1)-C(15)-C(19)	147.47(12)
C(14)-C(15)-C(16)-C(12)	1.98(13)
C(19)-C(15)-C(16)-C(12)	175.86(11)
Zr(1)-C(15)-C(16)-C(12)	-62.87(8)
C(14)-C(15)-C(16)-C(20)	-173.89(11)
C(19)-C(15)-C(16)-C(20)	-0.01(18)
Zr(1)-C(15)-C(16)-C(20)	121.26(11)
C(14)-C(15)-C(16)-Zr(1)	64.85(8)
C(19)-C(15)-C(16)-Zr(1)	-121.27(12)
C(13)-C(12)-C(16)-C(15)	-0.79(12)
Si(1)-C(12)-C(16)-C(15)	148.71(9)
Zr(1)-C(12)-C(16)-C(15)	66.49(8)
C(13)-C(12)-C(16)-C(20)	174.89(11)
Si(1)-C(12)-C(16)-C(20)	-35.61(16)
Zr(1)-C(12)-C(16)-C(20)	-117.84(12)
C(13)-C(12)-C(16)-Zr(1)	-67.27(7)
Si(1)-C(12)-C(16)-Zr(1)	82.23(8)
N(1)-Zr(1)-C(16)-C(15)	-157.68(8)
Cl(1)-Zr(1)-C(16)-C(15)	-16.41(9)
Cl(2)-Zr(1)-C(16)-C(15)	93.96(7)

C(13)-Zr(1)-C(16)-C(15)	-76.54(8)
C(12)-Zr(1)-C(16)-C(15)	-116.28(10)
N(2)-Zr(1)-C(16)-C(15)	168.95(7)
C(14)-Zr(1)-C(16)-C(15)	-35.98(7)
C(1)-Zr(1)-C(16)-C(15)	-173.87(7)
Si(1)-Zr(1)-C(16)-C(15)	-149.36(8)
N(1)-Zr(1)-C(16)-C(12)	-41.40(7)
Cl(1)-Zr(1)-C(16)-C(12)	99.87(7)
Cl(2)-Zr(1)-C(16)-C(12)	-149.76(7)
C(13)-Zr(1)-C(16)-C(12)	39.74(7)
N(2)-Zr(1)-C(16)-C(12)	-74.77(9)
C(14)-Zr(1)-C(16)-C(12)	80.29(8)
C(15)-Zr(1)-C(16)-C(12)	116.28(10)
C(1)-Zr(1)-C(16)-C(12)	-57.59(8)
Si(1)-Zr(1)-C(16)-C(12)	-33.08(6)
N(1)-Zr(1)-C(16)-C(20)	81.02(11)
Cl(1)-Zr(1)-C(16)-C(20)	-137.72(9)
Cl(2)-Zr(1)-C(16)-C(20)	-27.34(10)
C(13)-Zr(1)-C(16)-C(20)	162.16(12)
C(12)-Zr(1)-C(16)-C(20)	122.42(14)
N(2)-Zr(1)-C(16)-C(20)	47.65(13)
C(14)-Zr(1)-C(16)-C(20)	-157.29(12)
C(15)-Zr(1)-C(16)-C(20)	-121.30(14)
C(1)-Zr(1)-C(16)-C(20)	64.83(11)
Si(1)-Zr(1)-C(16)-C(20)	89.34(10)
C(32)-B(1)-C(23)-C(24)	69.87(15)
C(7)-B(1)-C(23)-C(24)	-120.53(11)
C(32)-B(1)-C(23)-C(28)	-112.00(12)
C(7)-B(1)-C(23)-C(28)	57.60(14)
C(28)-C(23)-C(24)-C(25)	-2.68(16)
B(1)-C(23)-C(24)-C(25)	175.46(10)
C(28)-C(23)-C(24)-C(29)	176.65(10)
B(1)-C(23)-C(24)-C(29)	-5.21(16)
C(23)-C(24)-C(25)-C(26)	2.31(17)
C(29)-C(24)-C(25)-C(26)	-177.04(11)
C(24)-C(25)-C(26)-C(27)	-0.61(17)
C(24)-C(25)-C(26)-C(30)	178.54(12)
C(25)-C(26)-C(27)-C(28)	-0.68(17)
C(30)-C(26)-C(27)-C(28)	-179.82(11)

C(26)-C(27)-C(28)-C(23)	0.26(17)
C(26)-C(27)-C(28)-C(31)	176.97(11)
C(24)-C(23)-C(28)-C(27)	1.43(16)
B(1)-C(23)-C(28)-C(27)	-176.76(10)
C(24)-C(23)-C(28)-C(31)	-175.20(10)
B(1)-C(23)-C(28)-C(31)	6.61(15)
C(23)-B(1)-C(32)-C(37)	-149.03(11)
C(7)-B(1)-C(32)-C(37)	41.91(16)
C(23)-B(1)-C(32)-C(33)	36.01(16)
C(7)-B(1)-C(32)-C(33)	-133.05(12)
C(37)-C(32)-C(33)-C(34)	-5.15(17)
B(1)-C(32)-C(33)-C(34)	170.05(11)
C(37)-C(32)-C(33)-C(38)	174.42(12)
B(1)-C(32)-C(33)-C(38)	-10.38(18)
C(32)-C(33)-C(34)-C(35)	2.57(18)
C(38)-C(33)-C(34)-C(35)	-177.03(12)
C(33)-C(34)-C(35)-C(36)	1.45(18)
C(33)-C(34)-C(35)-C(39)	178.34(11)
C(34)-C(35)-C(36)-C(37)	-2.73(19)
C(39)-C(35)-C(36)-C(37)	-179.59(12)
C(35)-C(36)-C(37)-C(32)	-0.02(19)
C(35)-C(36)-C(37)-C(40)	177.17(13)
C(33)-C(32)-C(37)-C(36)	3.94(17)
B(1)-C(32)-C(37)-C(36)	-171.22(11)
C(33)-C(32)-C(37)-C(40)	-173.07(12)
B(1)-C(32)-C(37)-C(40)	11.77(18)