Electronic Supplementary Material (ESI) for Polymer Chemistry.


# Supporting Information

to

# Tandem Vinyl Insertion-/Ring-Opening Metathesis Copolymerization with *ansa*-6-[2-(Dimesitylboryl)-phenyl]pyrid-2-ylamido Zirconium Complexes: Role of Trialkylaluminum and MAO

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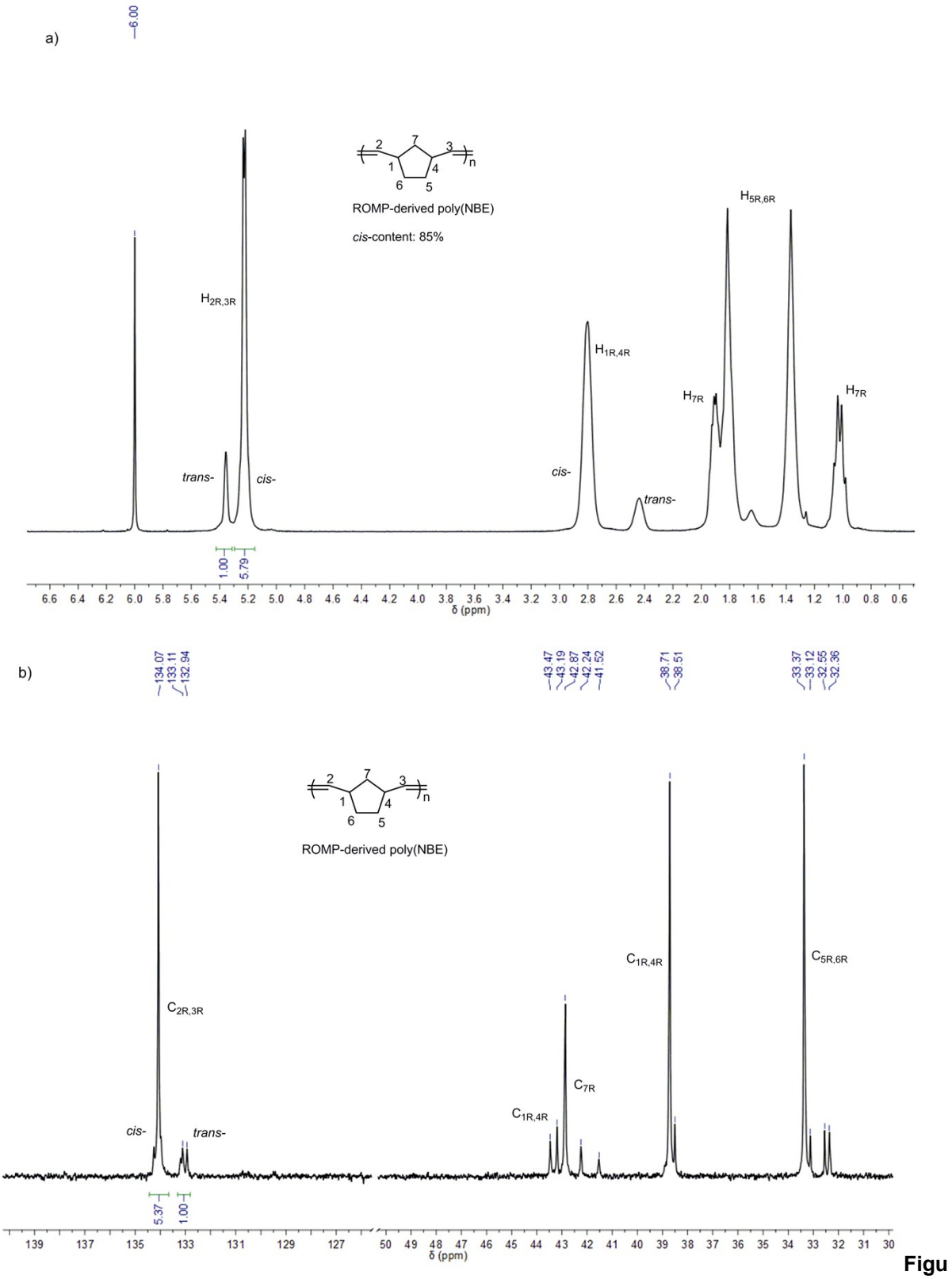



**Figure S1.** a) $^{1}H$ NMR and b) $^{13}C$ NMR spectra of poly(NBE)$_{ROMP}$ produced by **L´Zr(CH$_3$)$_2$**/[Ph$_3$C]$^+$[B(C$_6$F$_5$)$_4$]$^-$ at 50 ºC (1,1,2,2-tetrachloroethane-d$_2$) (Table 2, entry 1).

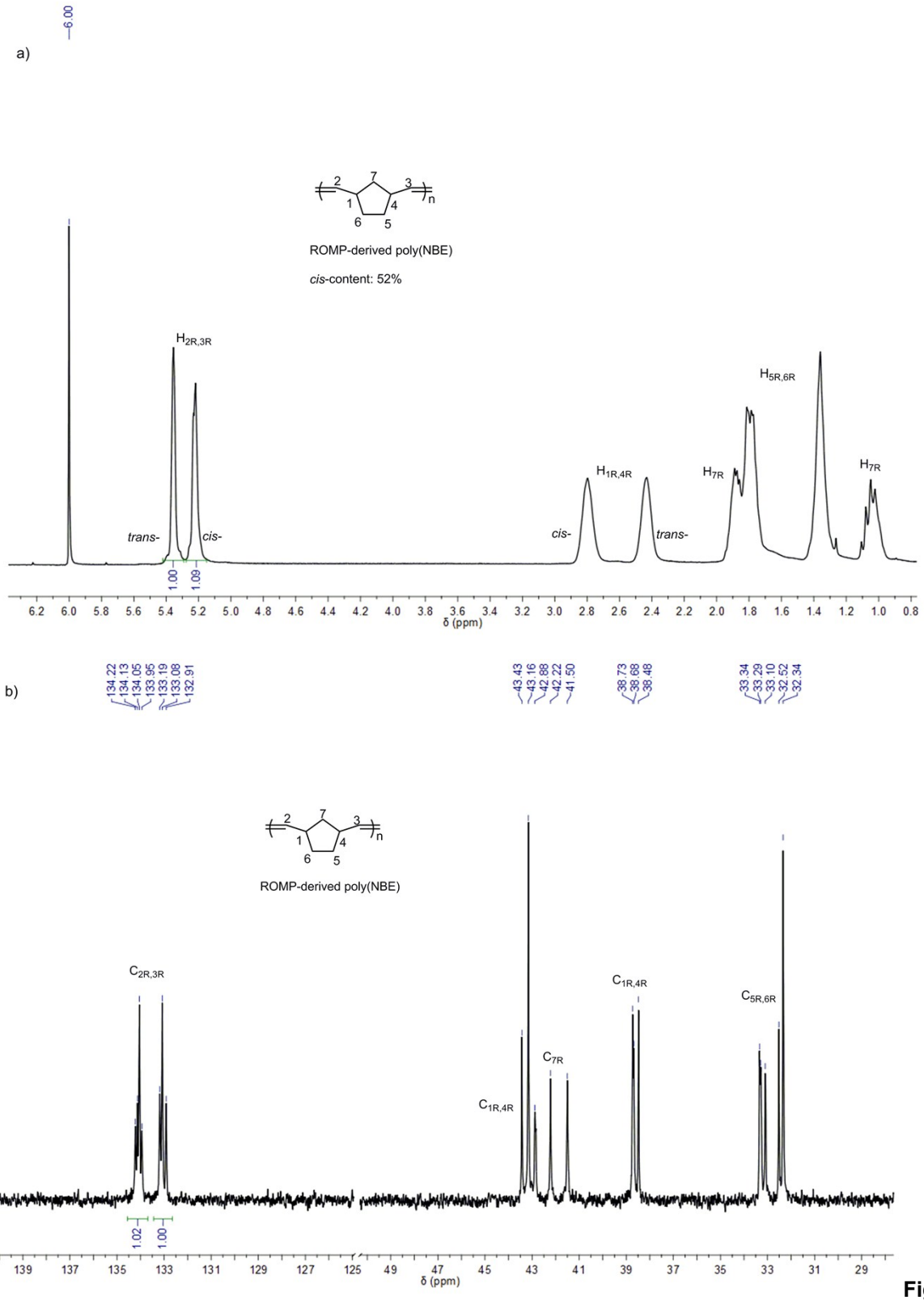



**Figure S2.** a) $^{1}H$ NMR and b) $^{13}C$ NMR spectra of poly(NBE)$_{ROMP}$ produced by **L´Zr(CH$_3$)$_2$**/[Ph$_3$C]$^+$[B(C$_6$F$_5$)$_4$]$^-$ at 80 ºC (1,1,2,2-tetrachloroethane-d$_2$) (Table 2, entry 3).

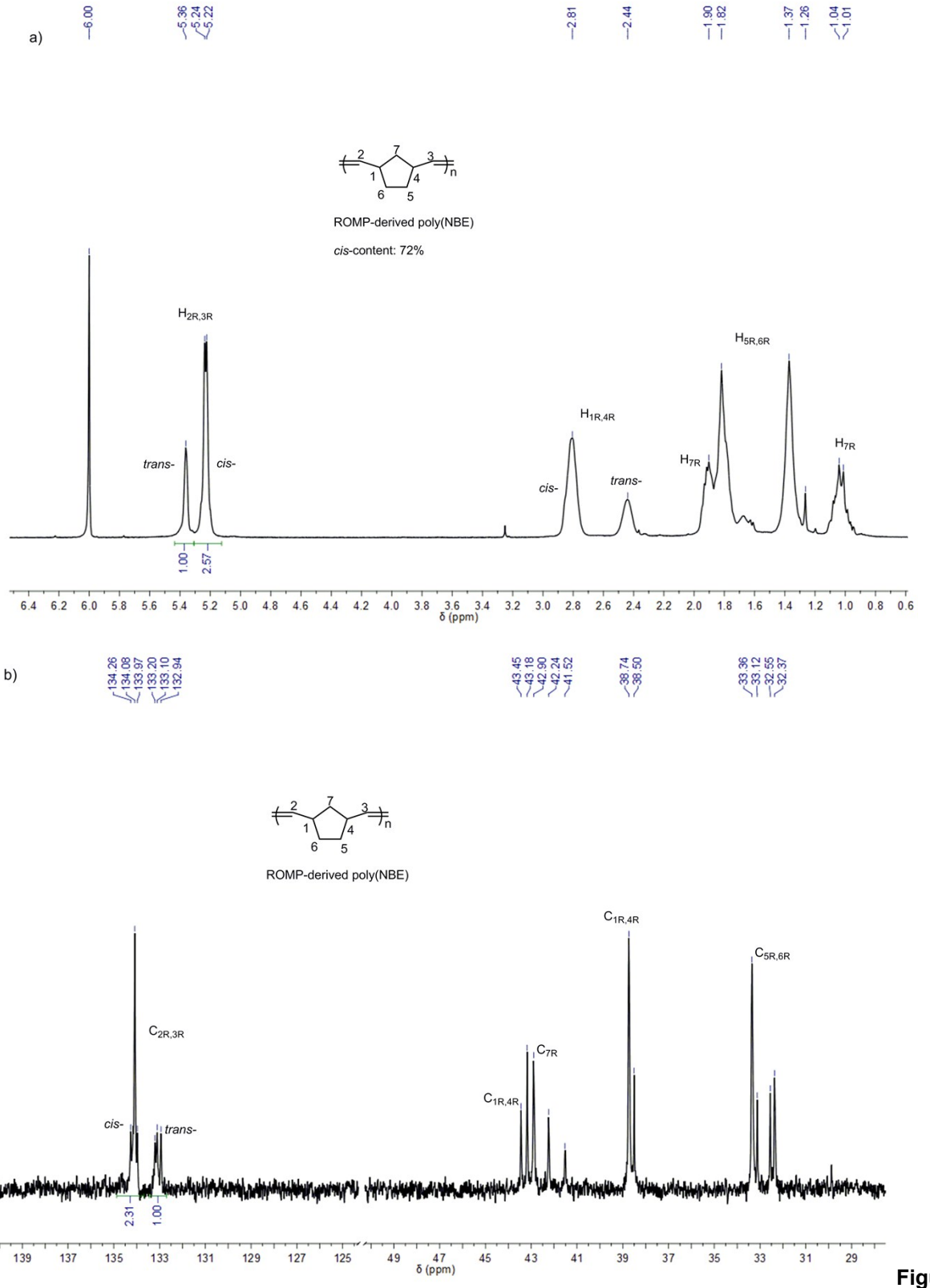



**Figure S3.** a) $^{1}H$ NMR and b) $^{13}C$ NMR spectra of poly(NBE)$_{ROMP}$ produced by **L´Zr(Bn)$_2$**/[$Ph_3C$]$^+$[$B(C_6F_5)_4$]$^-$ at 80 ºC (1,1,2,2-tetrachloroethane-$d_2$) (Table 2, entry 6).

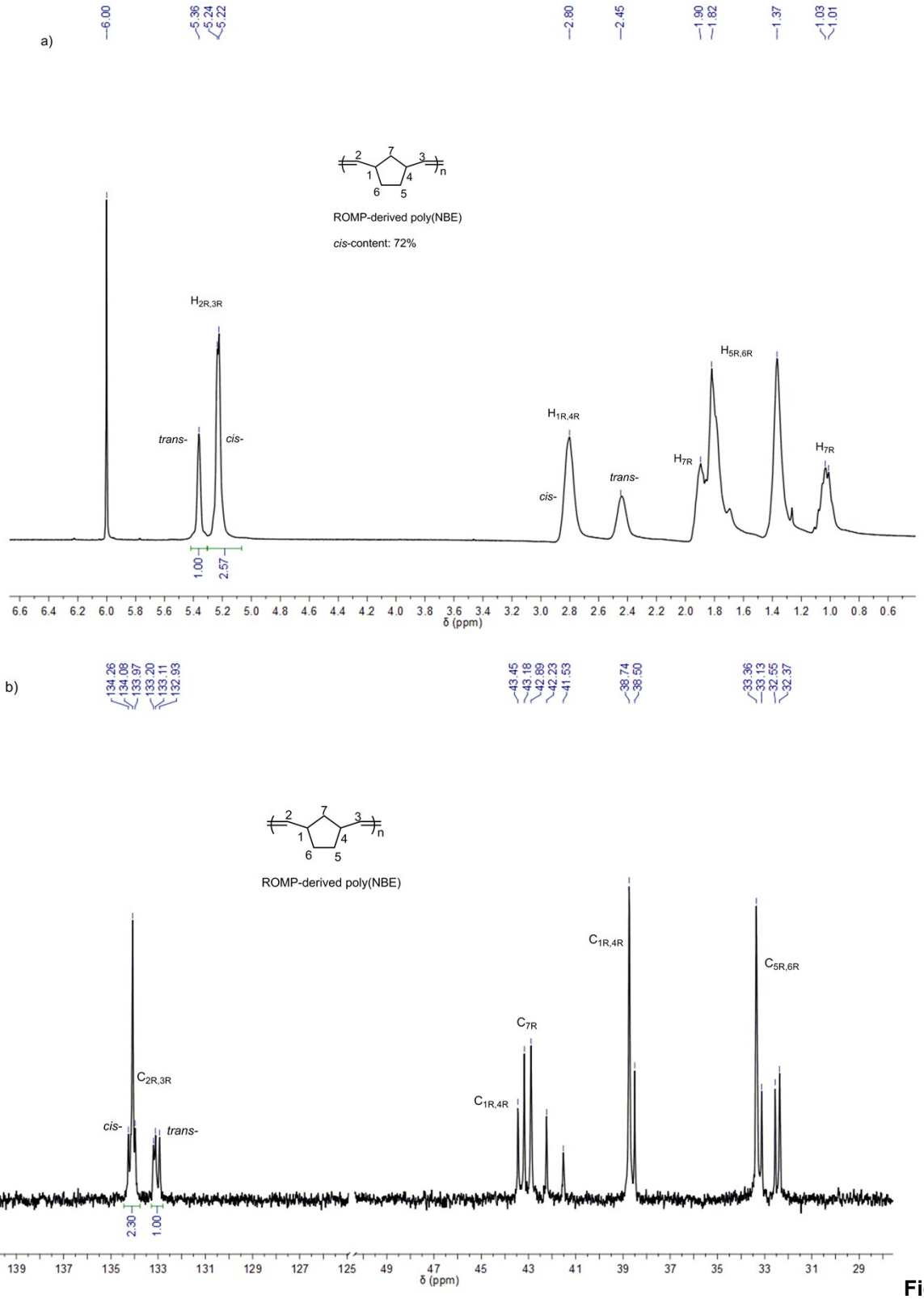



**Figure S4.** a) $^{1}H$ NMR and b) $^{13}C$ NMR spectra of poly(NBE)$_{ROMP}$ produced by **L´Zr(CH$_2$SiMe$_3$)$_2$**/$[Ph_3C]^+[B(C_6F_5)_4]^-$ at 50 ºC (1,1,2,2-tetrachloroethane-$d_2$) (Table 2, entry 7).

$$C_{NBE}\,(\%) = \frac{1/3(I_{2,3} + I_{1,4} + 2I_7)}{I_{CH_2}} * 100$$

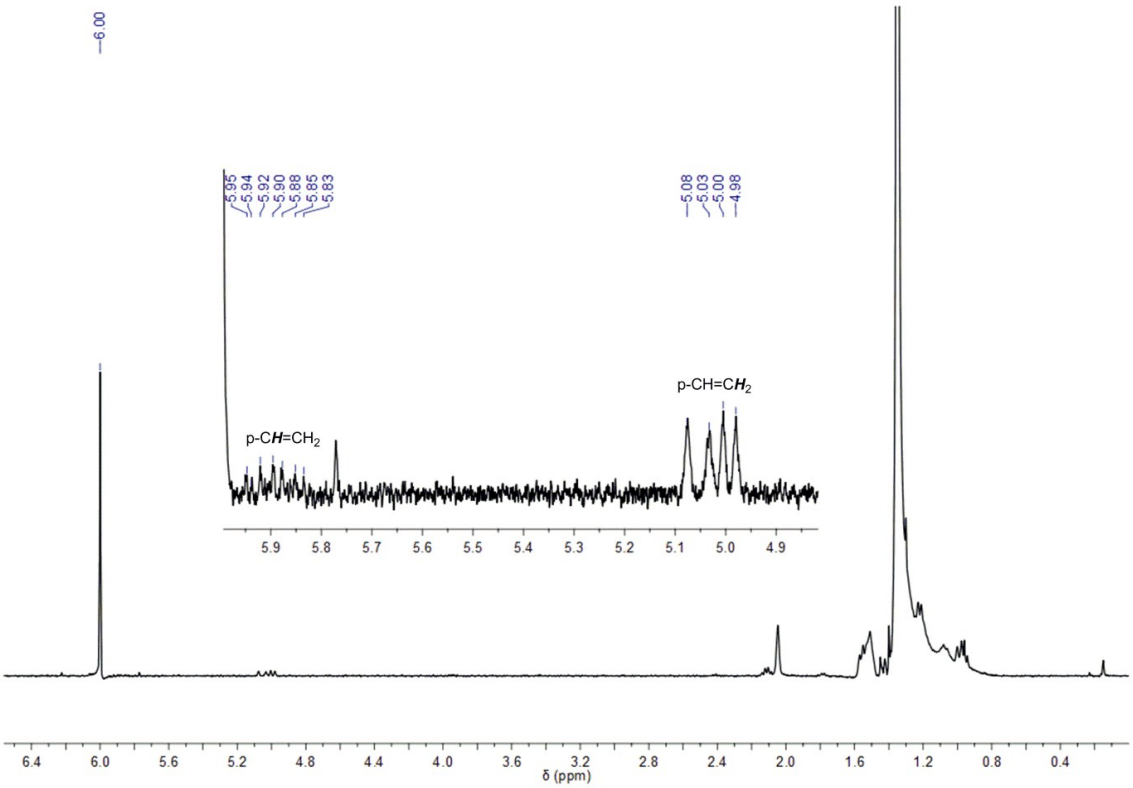



**Figure S5.** $^1$H NMR spectrum of poly(E)-*co*-poly(NBE)$_{VIP}$ produced by **L´Zr(CH$_3$)$_2$**/[Ph$_3$C]$^+$[B(C$_6$F$_5$)$_4$]$^-$ /Al$^i$Bu$_3$ at 80 ºC (1,1,2,2-tetrachloroethane-d$_2$) (Table 3, entry 4).

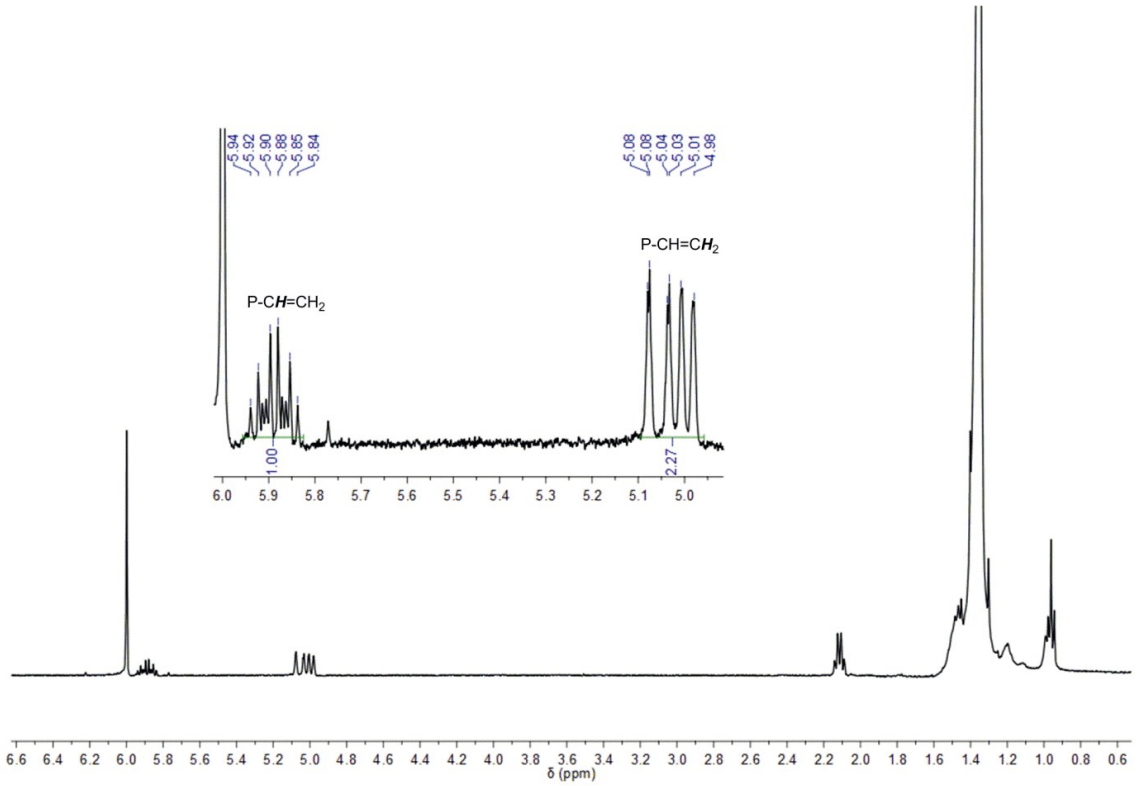



**Figure S6.** $^{1}$H NMR spectrum of PE produced by **L´Zr(CH$_3$)$_2$**/[Ph$_3$C]$^+$[B(C$_6$F$_5$)$_4$]$^-$/Al$^i$Bu$_3$ at 50 ºC (1,1,2,2-tetrachloroethane-d$_2$) (Table 3, entry 1).

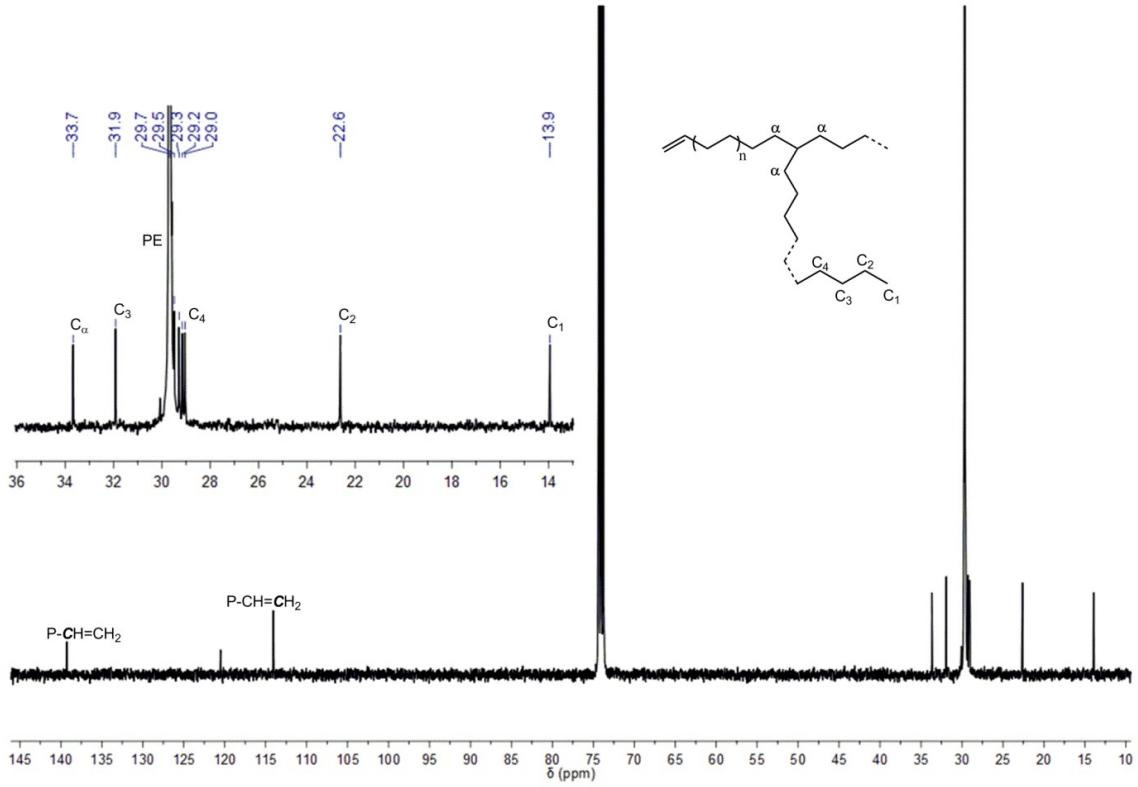



**Figure S7.** $^{13}$C NMR spectrum of PE produced by **L´Zr(CH$_3$)$_2$**/[Ph$_3$C]$^+$[B(C$_6$F$_5$)$_4$]$^-$/Al$^i$Bu$_3$ at 50 ºC (1,1,2,2-tetrachloroethane-d$_2$) (Table 3, entry 1).

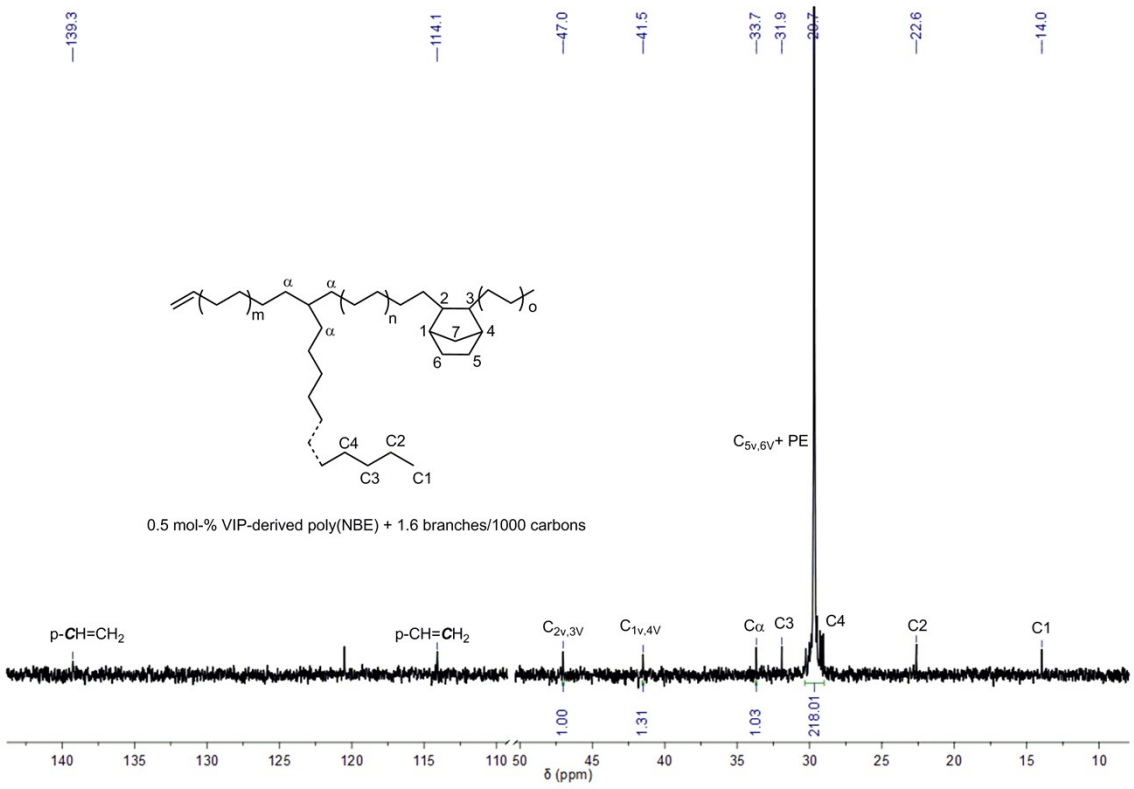



**Figure S8.** $^{13}$C NMR spectrum of poly(E)-*co*-poly(NBE)$_{VIP}$ produced by **L´Zr(Bn)$_2$**/[Ph$_3$C]$^+$[B(C$_6$F$_5$)$_4$]$^-$ /Al$^i$Bu$_3$ at 50 ºC (1,1,2,2-tetrachloroethane-d$_2$) (Table 3, entry 5).

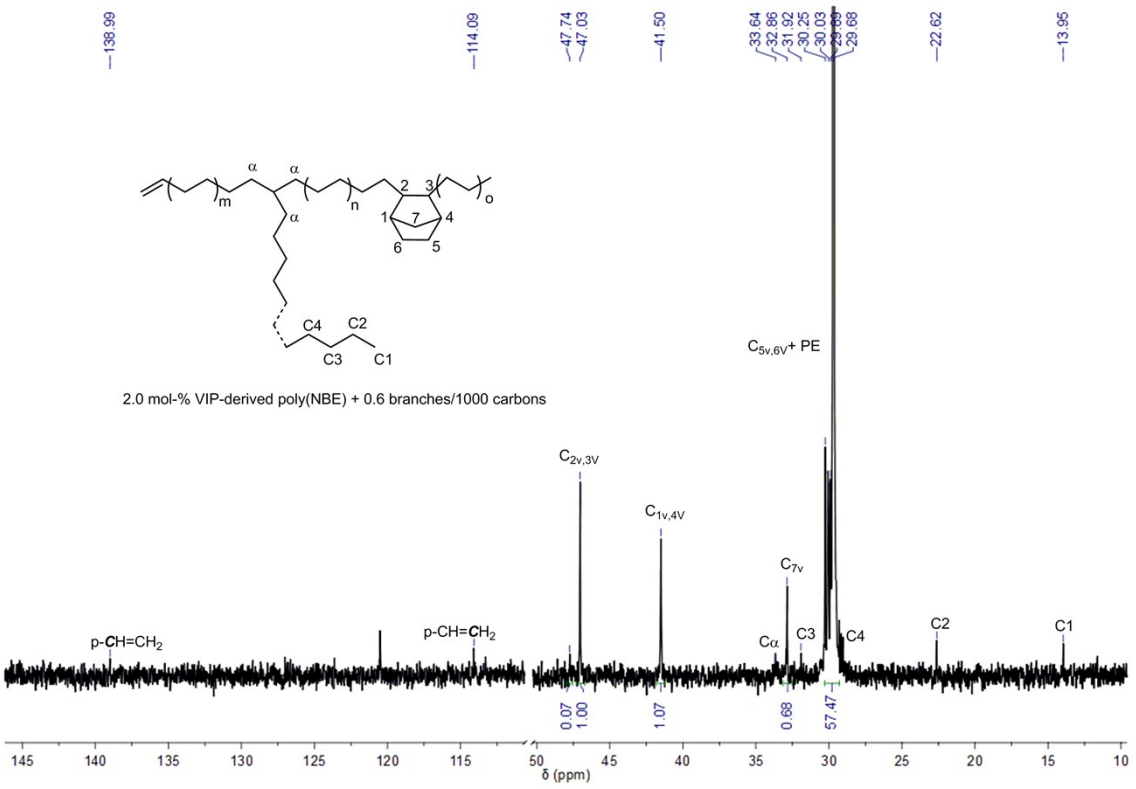



**Figure S9.** $^{13}$C NMR spectrum of poly(E)-*co*-poly(NBE)$_{VIP}$ produced by **L´Zr(CH$_2$SiMe$_3$)$_2$**/[Ph$_3$C]$^+$[B(C$_6$F$_5$)$_4$]$^-$ /Al$^i$Bu$_3$ at 50 ºC (1,1,2,2-tetrachloroethane-d$_2$) (Table 3, entry 6).

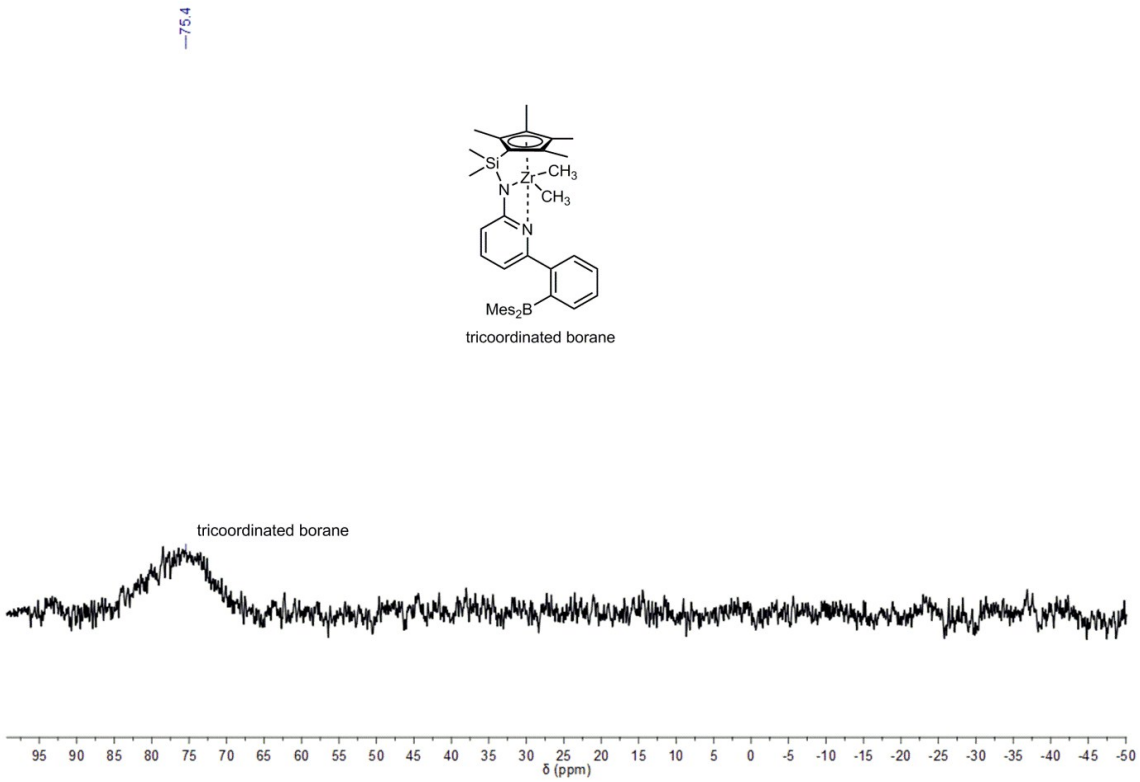



**Figure S10.** $^{11}B$ NMR spectrum of **L´Zr(CH$_3$)$_2$** in toluene-d$_8$ at 298.3 K.

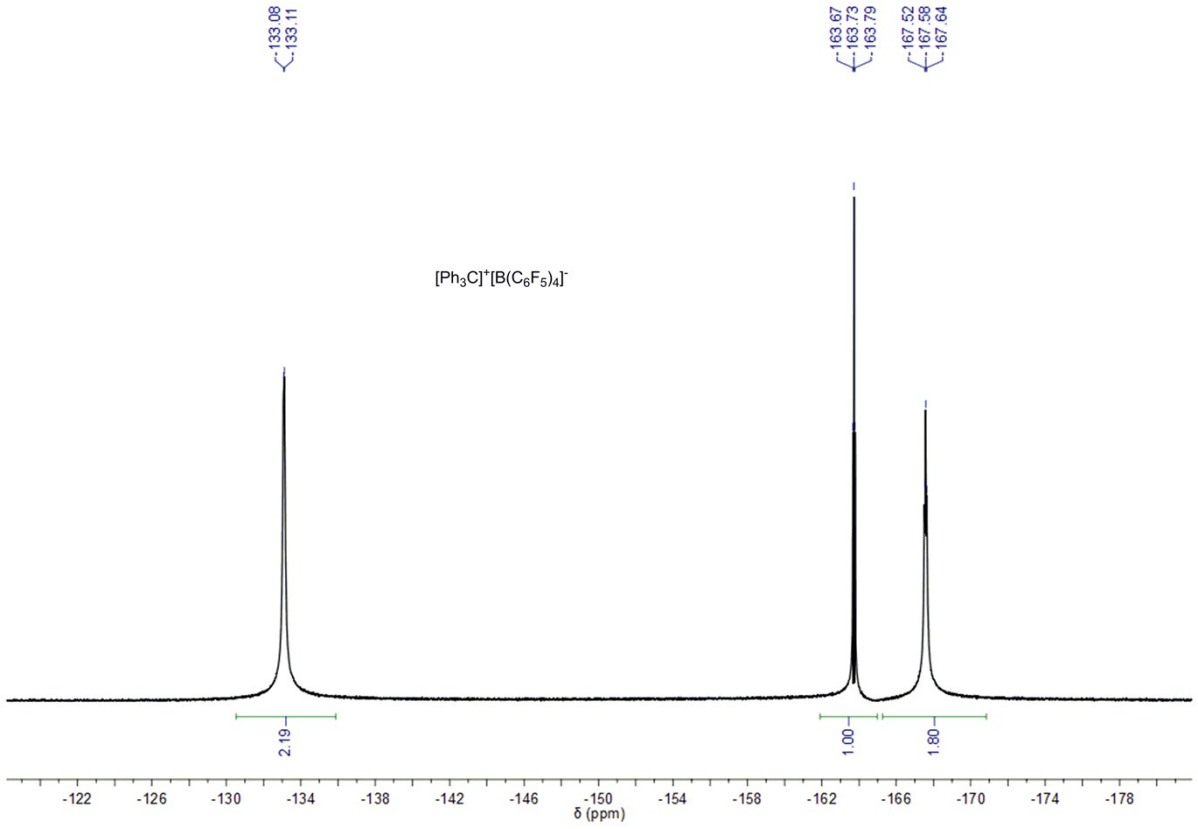



**Figure S11.** $^{19}F$ NMR spectrum of **[Ph$_3$C]$^+$[B(C$_6$F$_5$)$_4$]$^-$** in $CD_2Cl_2$.

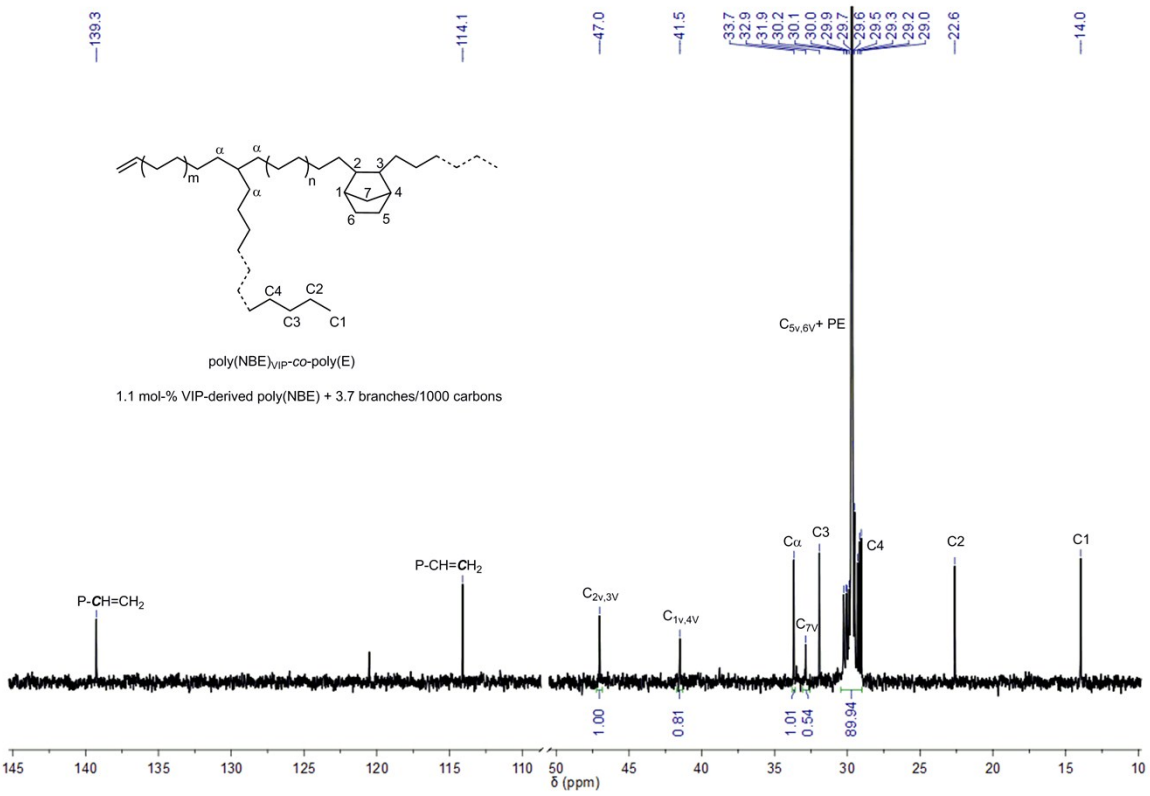



**Figure S12.** $^{13}$C NMR spectrum of poly(E)-*co*-poly(NBE)$_{VIP}$ produced by **L´Zr(CH$_3$)$_2$**/MAO at 50 ºC (1,1,2,2-tetrachloroethane-d$_2$) (Table 3, entry 7).

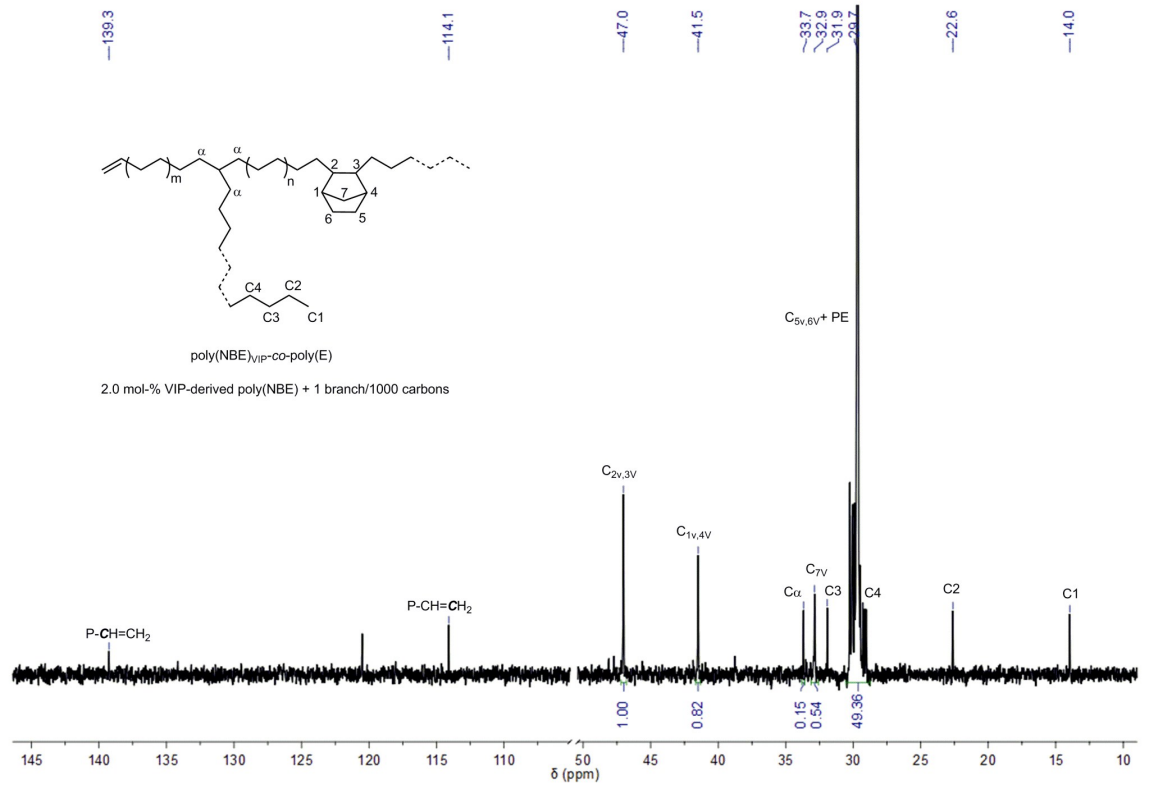



**Figure S13.** $^{13}$C NMR spectrum of poly(E)-*co*-poly(NBE)$_{VIP}$ produced by **L´Zr(Bn)$_2$**/MAO at 50 ºC (1,1,2,2-tetrachloroethane-d$_2$) (Table 3, entry 8).

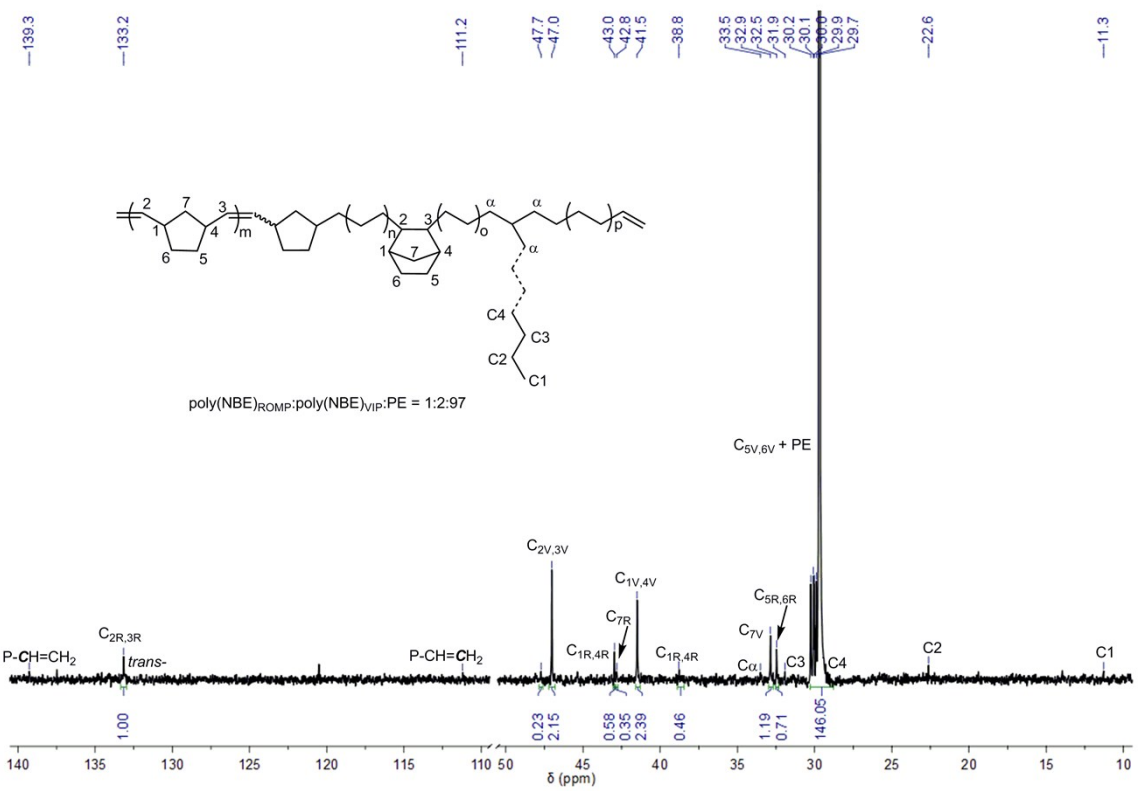



**Figure S14.** $^{13}$C NMR spectrum of poly(NBE)$_{ROMP}$-*co*-poly(NBE)$_{VIP}$-*co*-PE produced by **L´Zr(CH$_2$SiMe$_3$)$_2$**/MAO at 30 ºC (1,1,2,2-tetrachloroethane-d$_2$) (Table 3, entry 9).

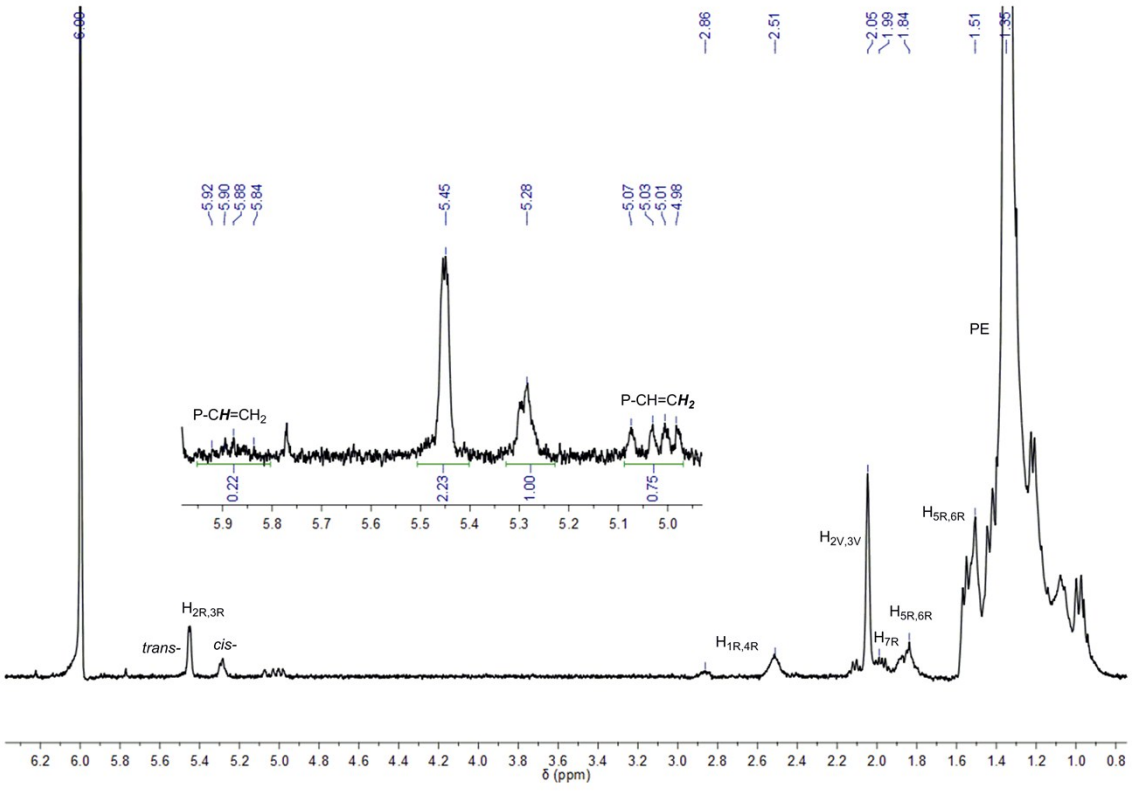



**Figure S15.** $^{1}$H NMR spectrum of poly(NBE)$_{ROMP}$-*co*-poly(NBE)$_{VIP}$-*co*-PE produced by produced by **L´Zr(CH$_2$SiMe$_3$)$_2$**/MAO at 30 ºC (1,1,2,2-tetrachloroethane-d$_2$) (Table 3, entry 9).

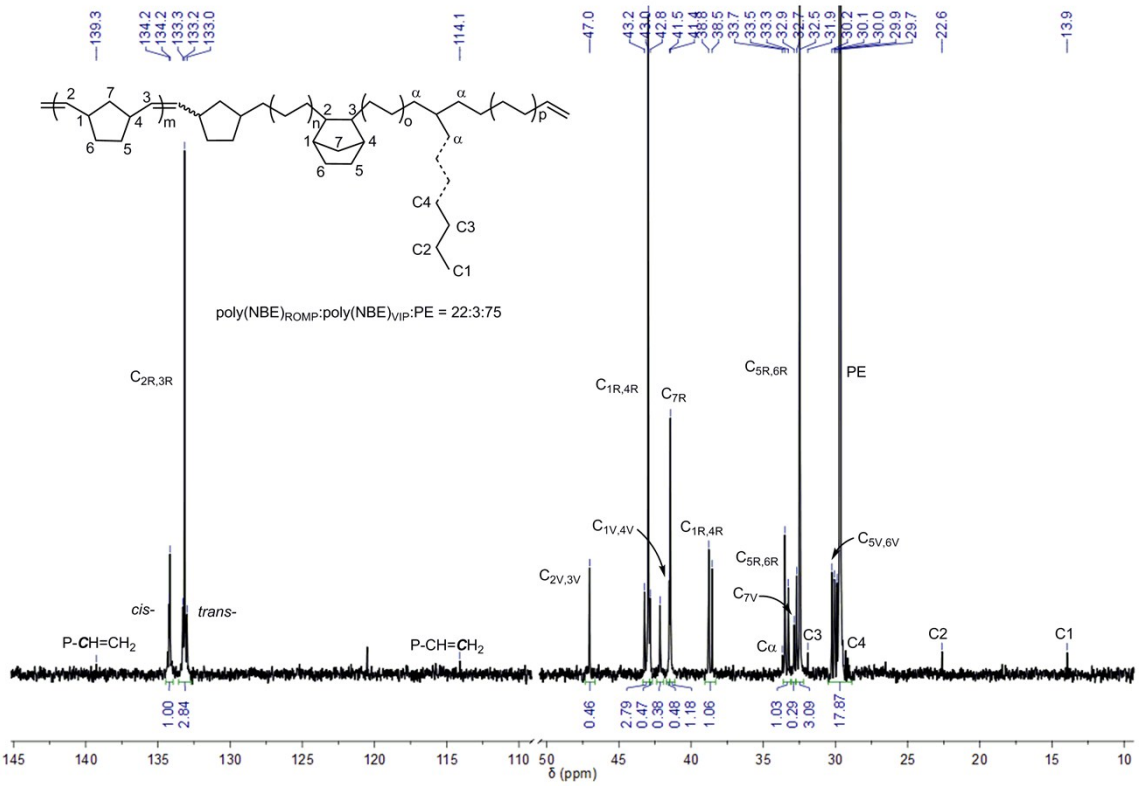



**Figure S16.** $^{13}$C NMR spectrum of poly(NBE)$_{ROMP}$-*co*-poly(NBE)$_{VIP}$-*co*-PE produced by **L´Zr(CH$_2$SiMe$_3$)$_2$**/MAO at 50 ºC (1,1,2,2-tetrachloroethane-d$_2$) (Table 3, entry 10).

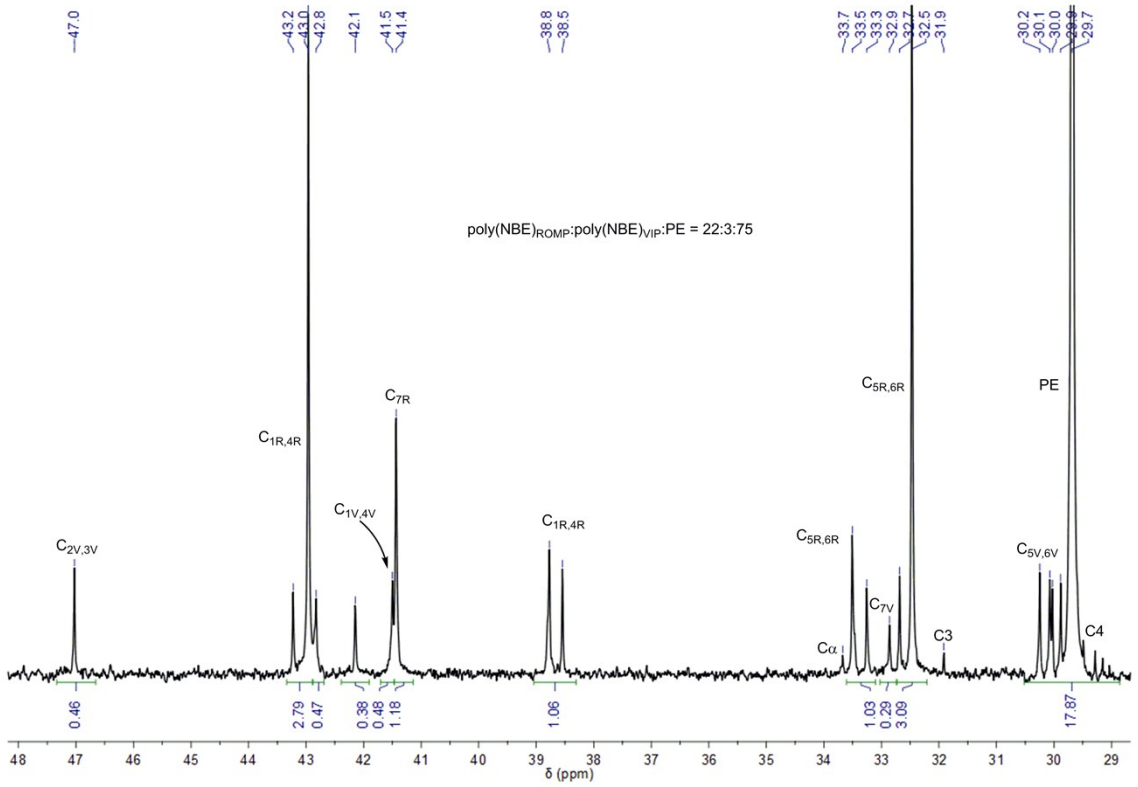



**Figure S17.** $^{13}$C NMR spectrum of poly(NBE)$_{ROMP}$-*co*-poly(NBE)$_{VIP}$-*co*-PE produced by **L´Zr(CH$_2$SiMe$_3$)$_2$**/MAO at 50 ºC (1,1,2,2-tetrachloroethane-d$_2$) (29-48 ppm, Table 3, entry 10).

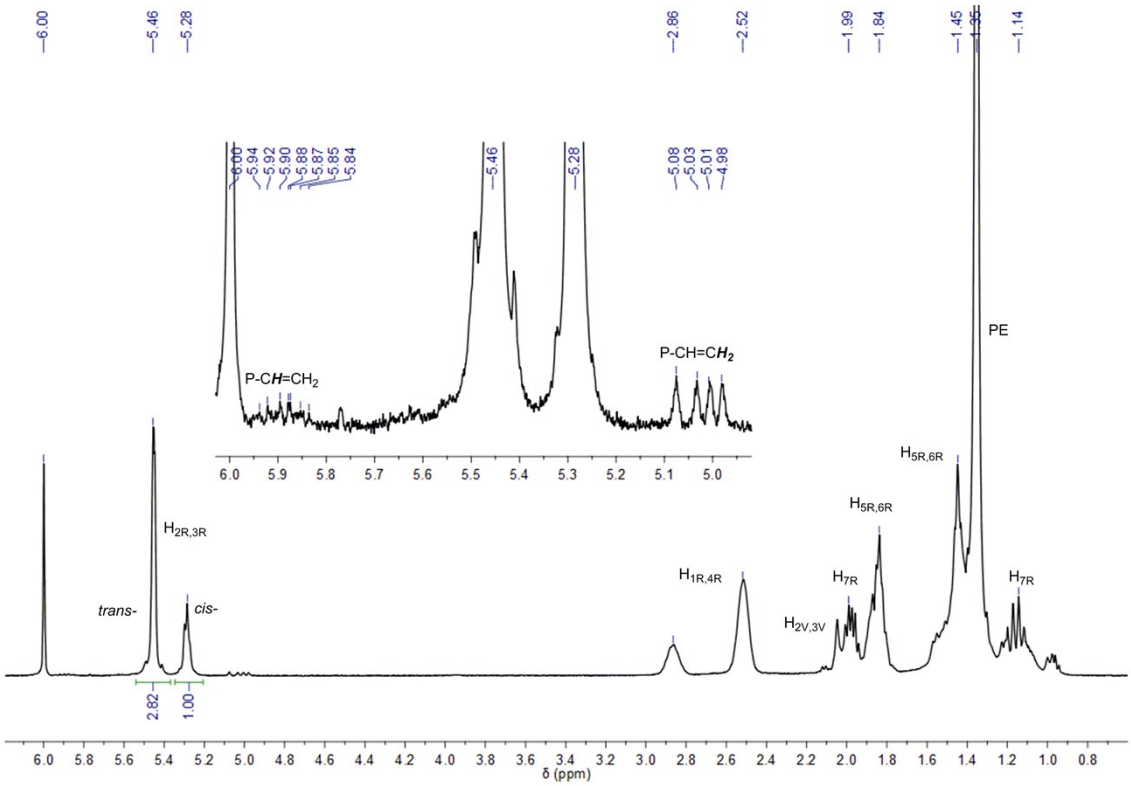



**Figure S18.** $^{1}$H NMR spectrum of poly(NBE)$_{ROMP}$-*co*-poly(NBE)$_{VIP}$-*co*-PE produced by produced by **L´Zr(CH$_2$SiMe$_3$)$_2$**/MAO at 50 ºC (1,1,2,2-tetrachloroethane-d$_2$) (Table 3, entry 10).

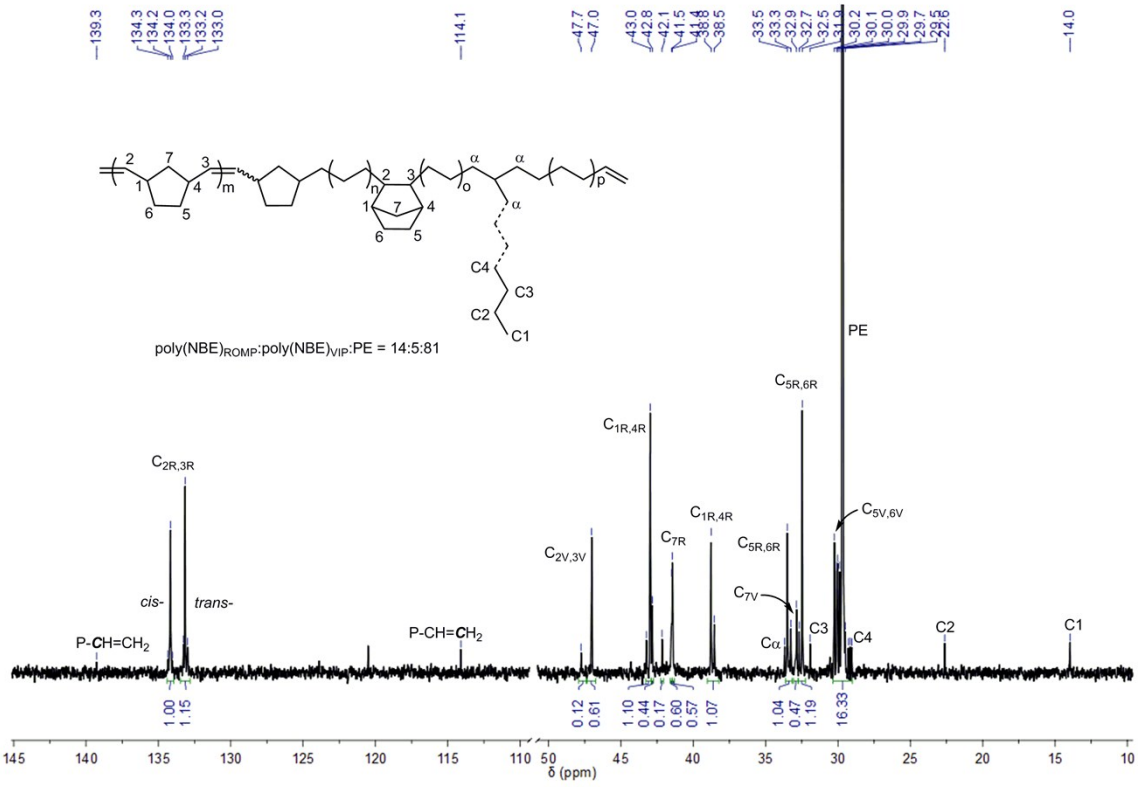



**Figure S19.** $^{13}$C NMR spectrum of poly(NBE)$_{ROMP}$-*co*-poly(NBE)$_{VIP}$-*co*-PE produced by **L´Zr(CH$_2$SiMe$_3$)$_2$**/MAO at 80 ºC (1,1,2,2-tetrachloroethane-d$_2$) (Table 3, entry 11).

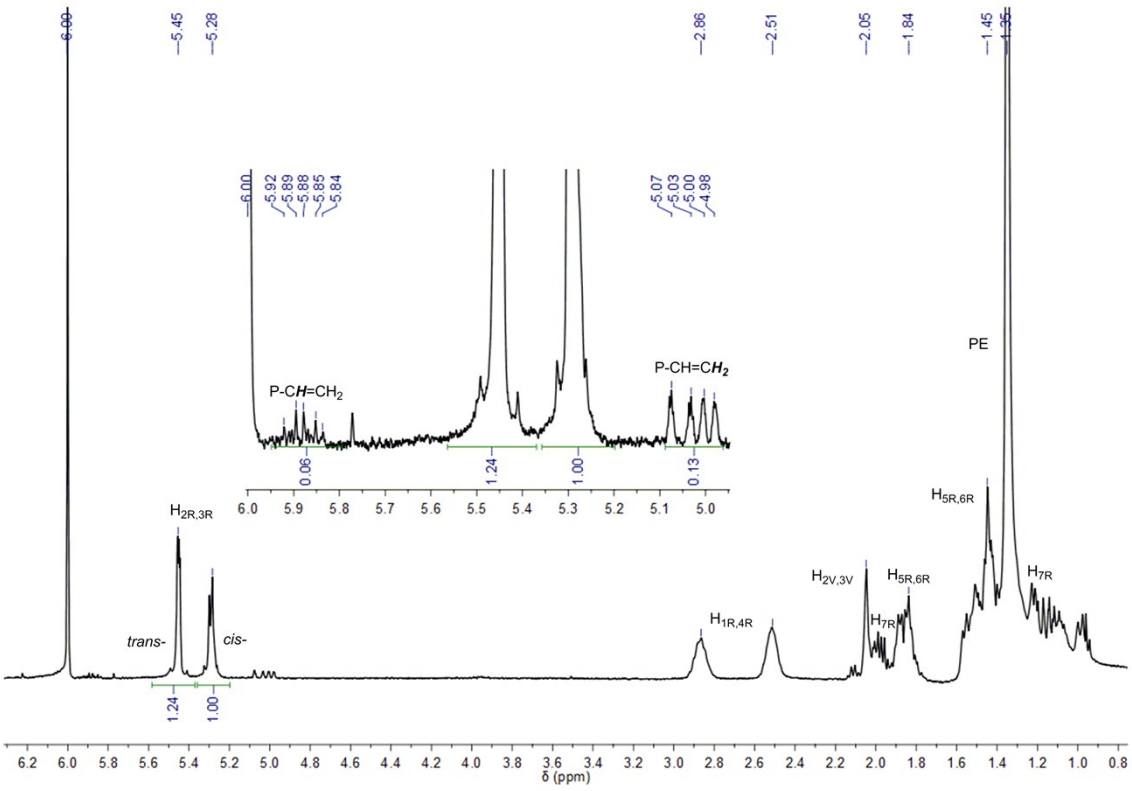



**Figure S20.** $^1$H NMR spectrum of poly(NBE)$_{ROMP}$-*co*-poly(NBE)$_{VIP}$-*co*-PE produced by produced by **L´Zr(CH$_2$SiMe$_3$)$_2$**/MAO at 80 ºC (1,1,2,2-tetrachloroethane-d$_2$) (Table 3, entry 11).

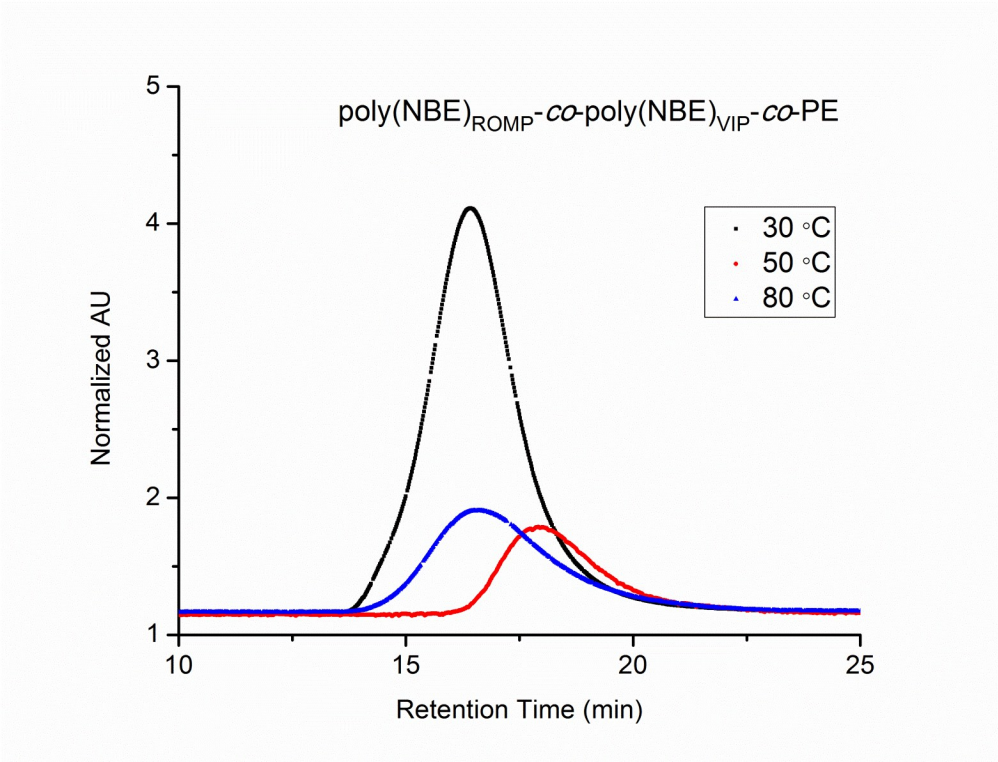
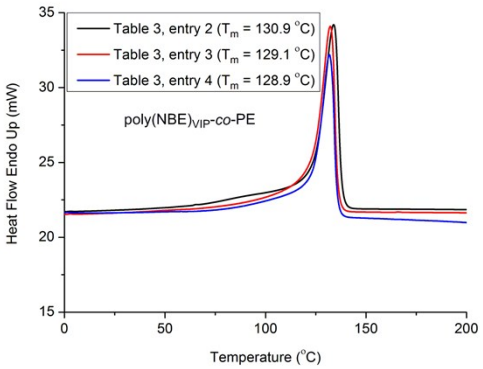
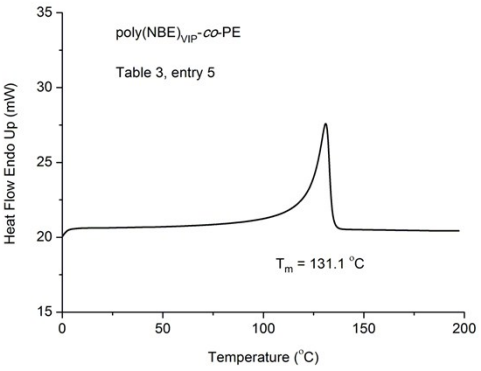
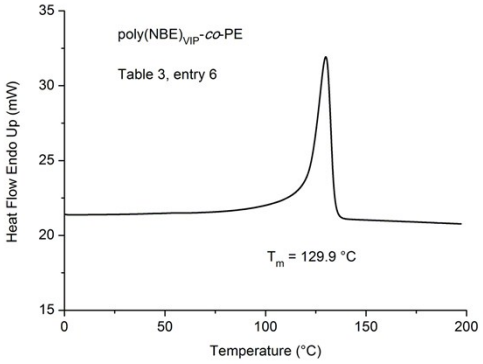
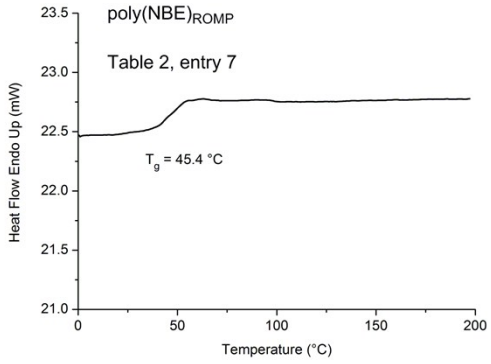


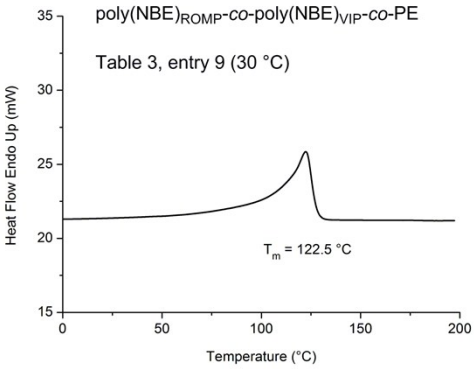

**Figure S21.** HT-GPC traces of poly(NBE)$_{ROMP}$-*co*-poly(NBE)$_{VIP}$-*co*-PE produced by **L´Zr(CH$_2$SiMe$_3$)$_2$**/MAO at 30, 50 and 80 ºC (Table 3, entries 9-11).

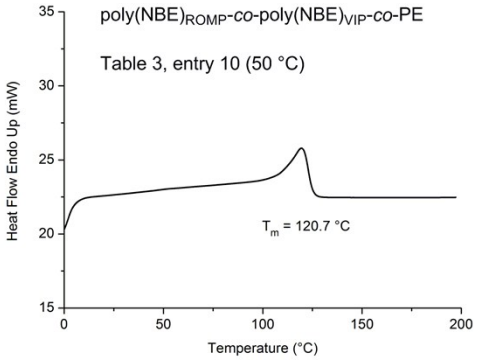


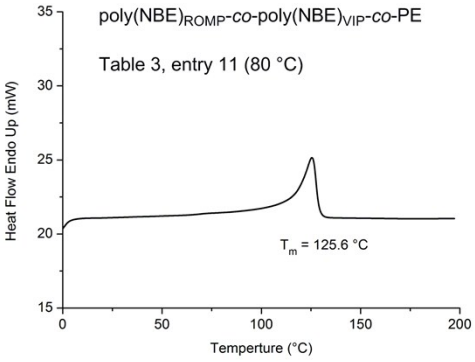




**Figure S22.** DSC curves for poly(NBE)$_{ROMP}$, poly(NBE)$_{VIP}$-*co*-PE and poly(NBE)$_{ROMP}$-*co*-poly(NBE)$_{VIP}$-*co*-PE.

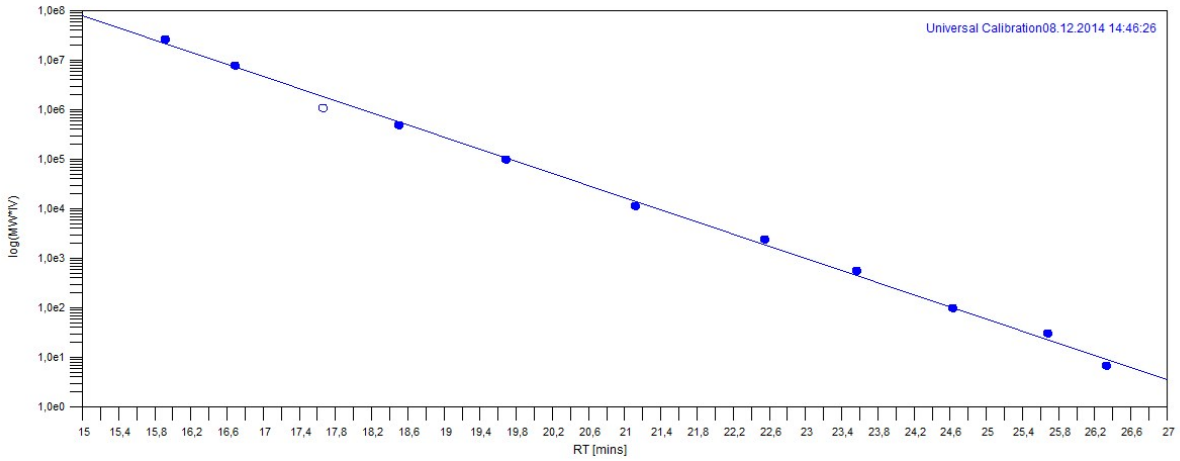



**Figure S23.** HT-GPC calibration curve with poly(stryrene) standards (162-6,035,000 g mol$^{-1}$).

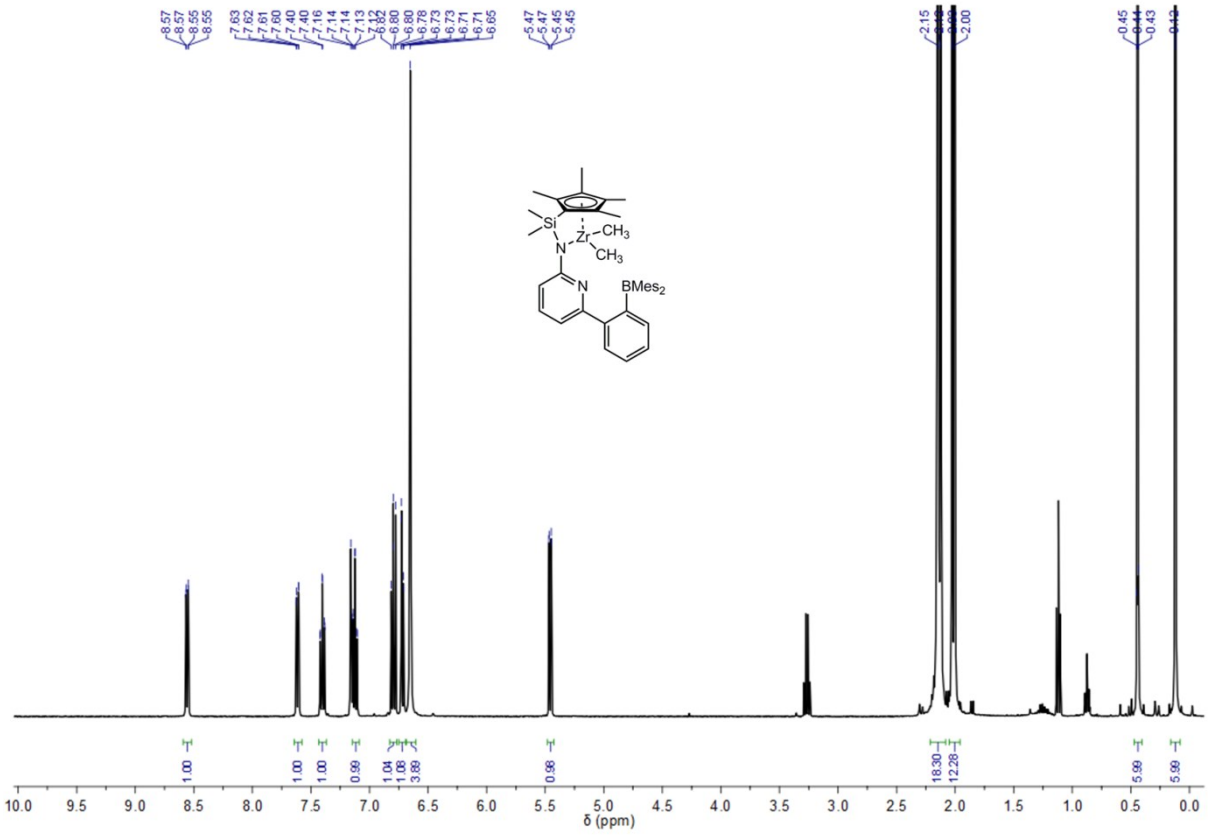



**Figure S24.** $^{1}$H NMR spectrum of **L´Zr(CH$_3$)$_2$** in $C_6D_6$.

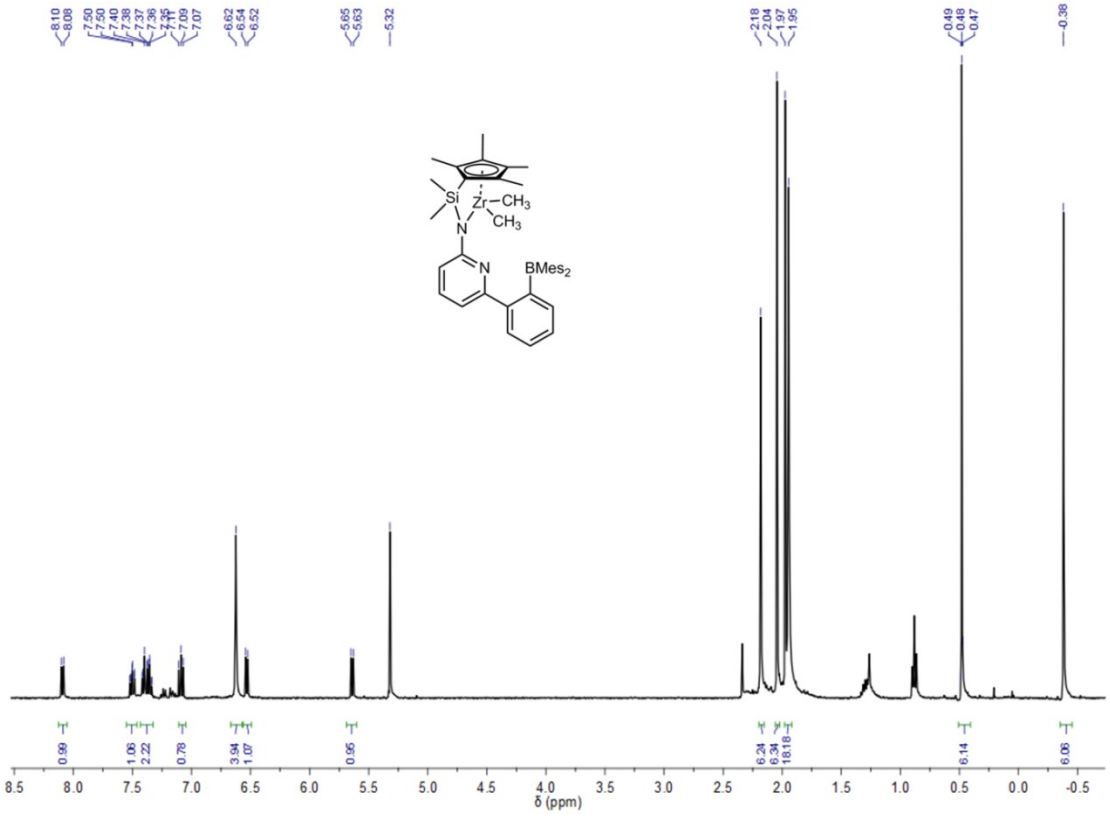



**Figure S25.** $^{1}$H NMR spectrum of **L´Zr(CH$_3$)$_2$** in $CD_2Cl_2$.

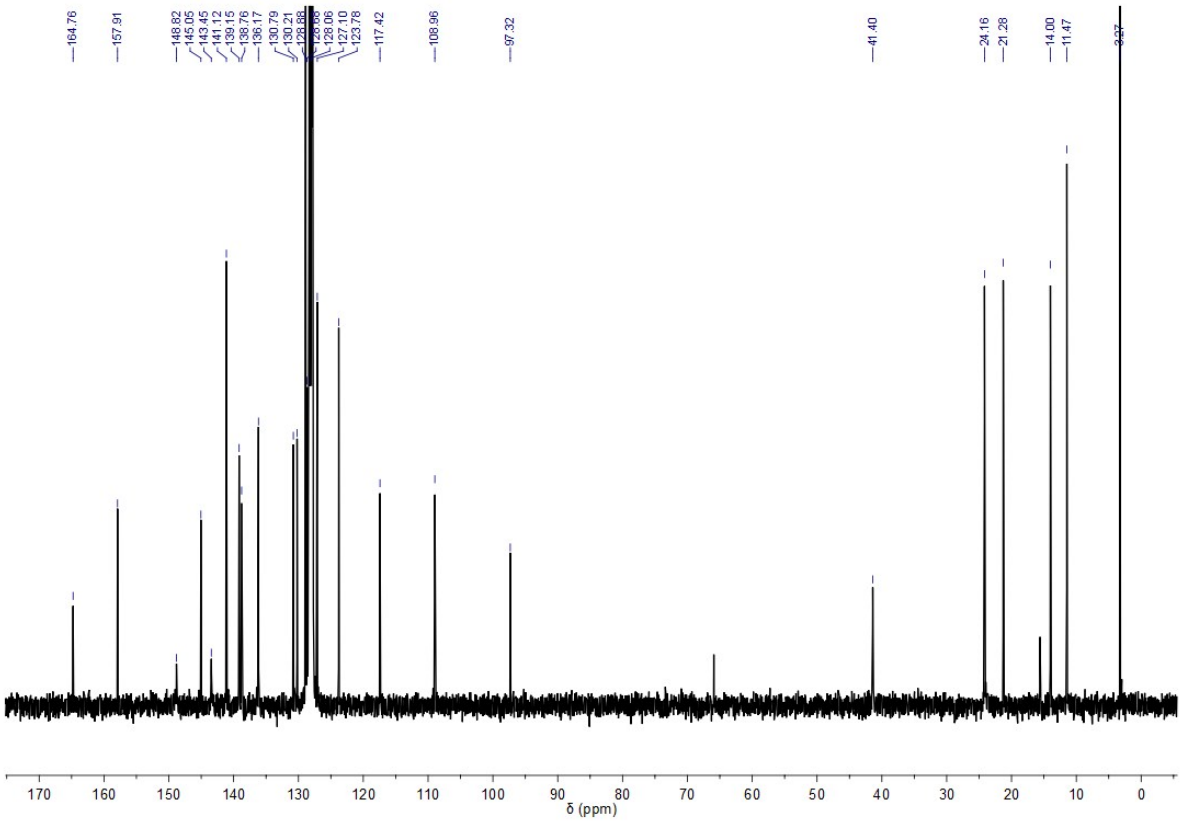



**Figure S26.** $^{13}$C NMR spectrum of **L´Zr(CH$_3$)$_2$** in $C_6D_6$.

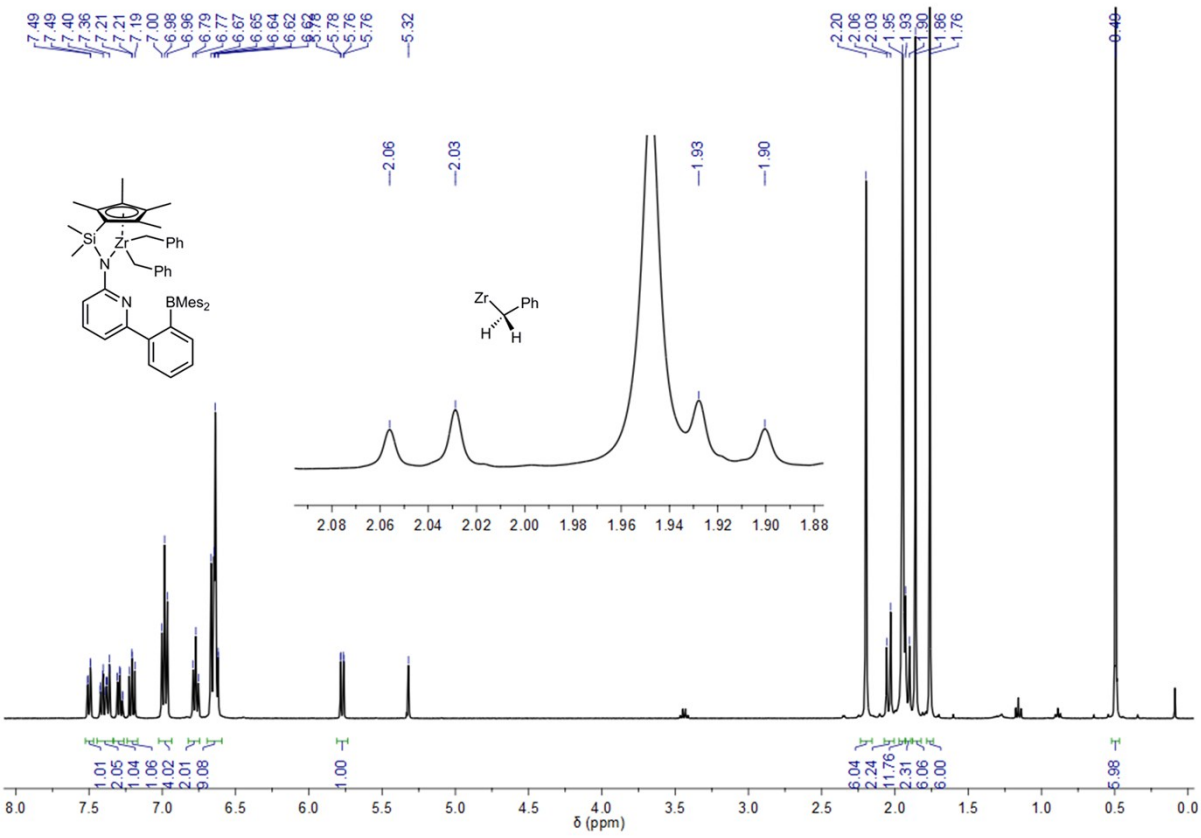



**Figure S27.** $^{1}$H NMR spectrum of **L´Zr(Bn)$_2$** in $CD_2Cl_2$.

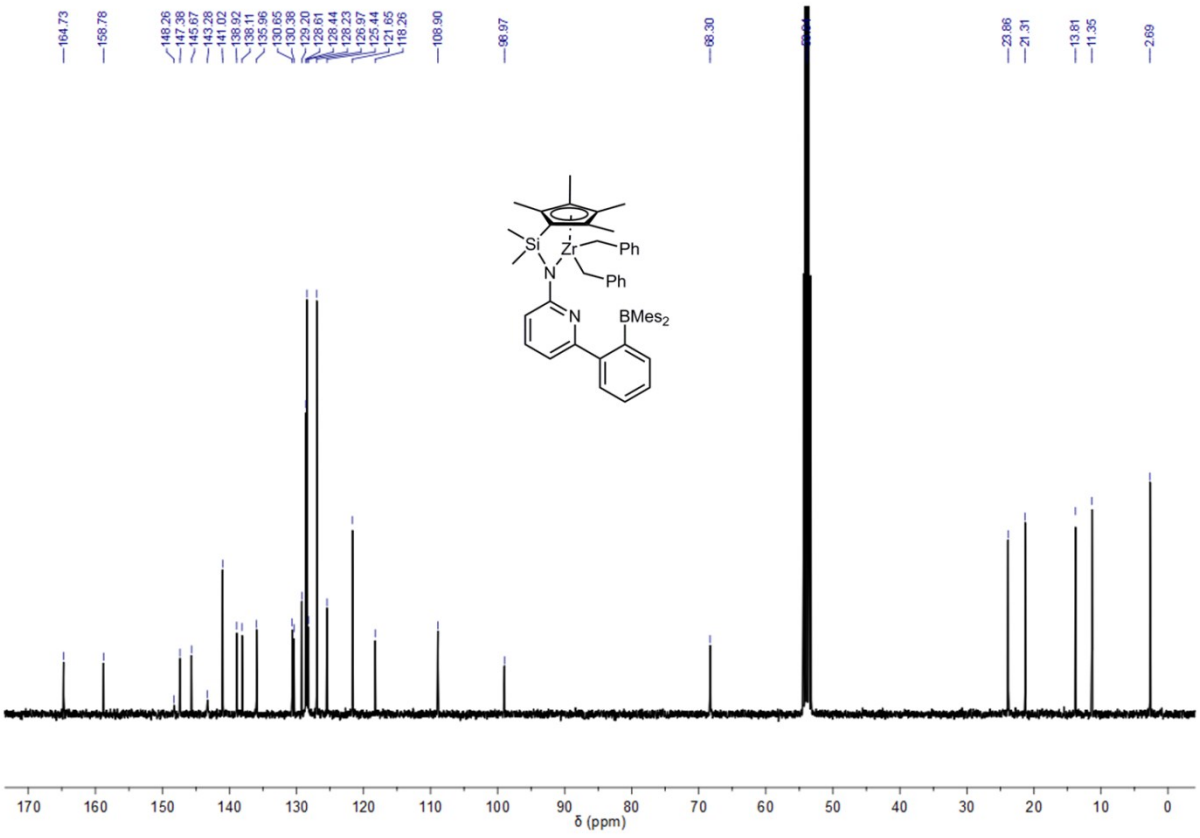



**Figure S28.** $^{13}$C NMR spectrum of **L´Zr(Bn)$_2$** in $CD_2Cl_2$.

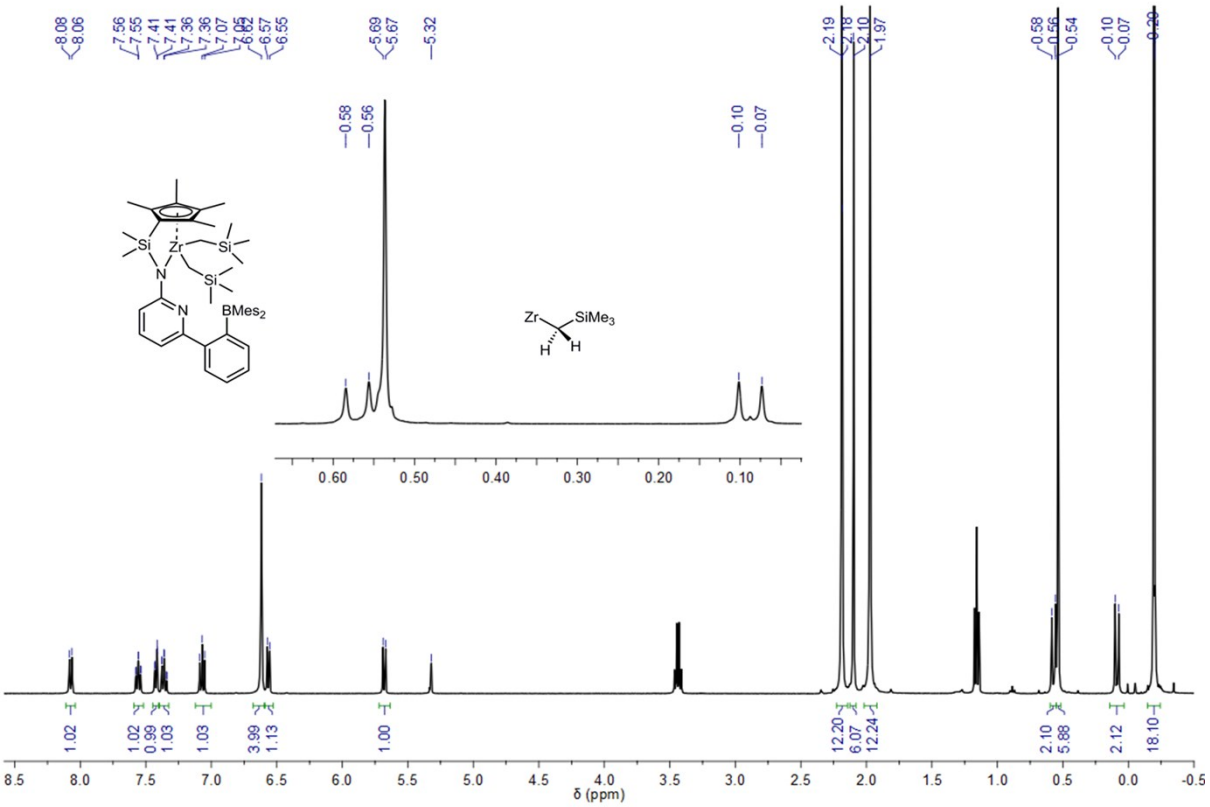



**Figure S29.** $^{1}$H NMR spectrum of **L´Zr(CH$_2$SiMe$_3$)$_2$** in $CD_2Cl_2$.

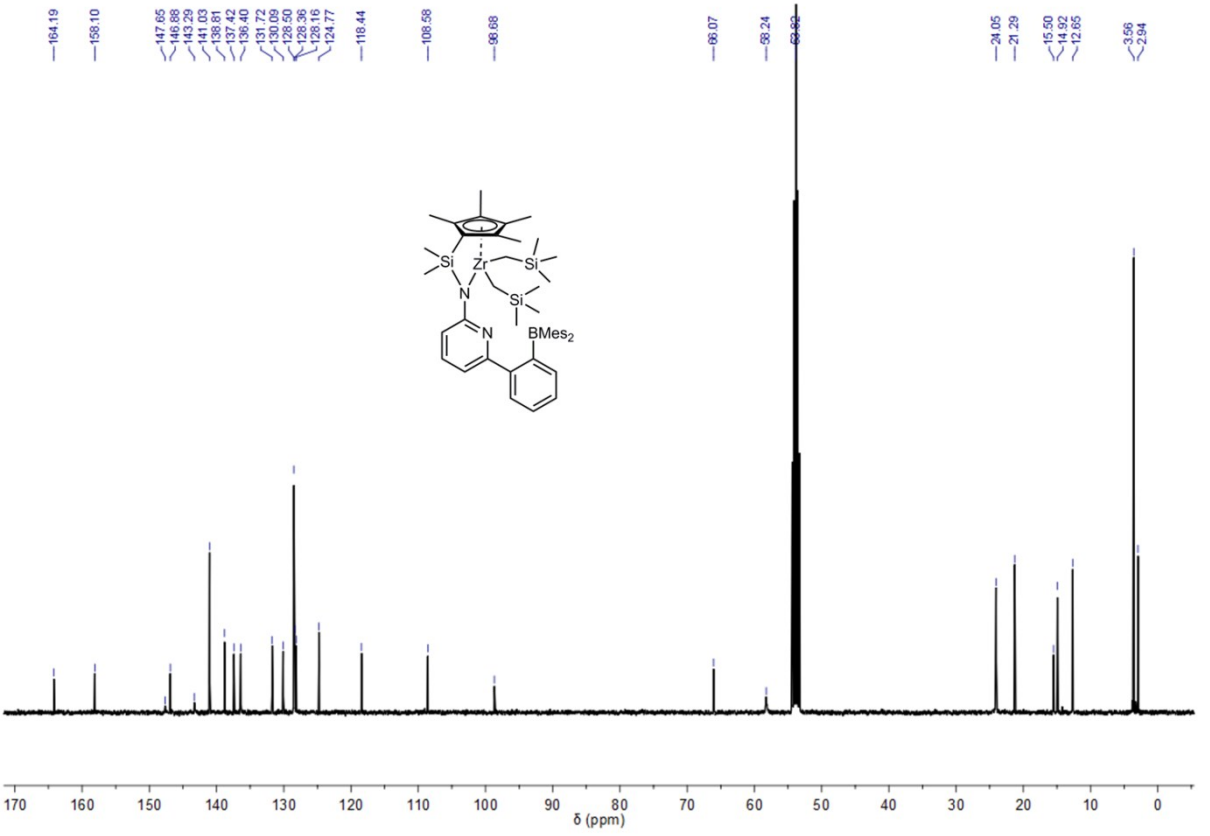



**Figure S30.** $^{13}$C NMR spectrum of **L´Zr(CH$_2$SiMe$_3$)$_2$** in $CD_2Cl_2$.

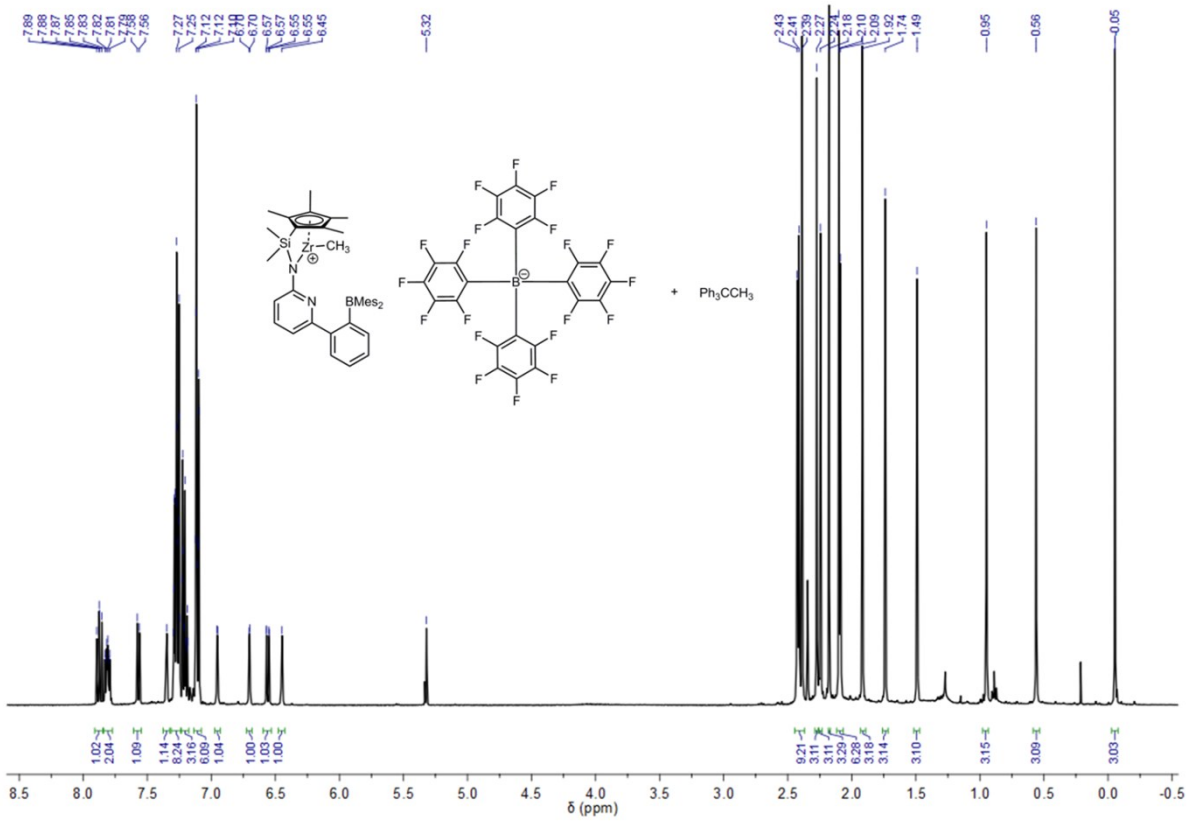



**Figure S31.** $^{1}$H NMR spectrum of the formation of **[L´Zr(CH$_3$)]$^+$[B(C$_6$F$_5$)$_4$]$^-$** *in situ* in $CD_2Cl_2$.

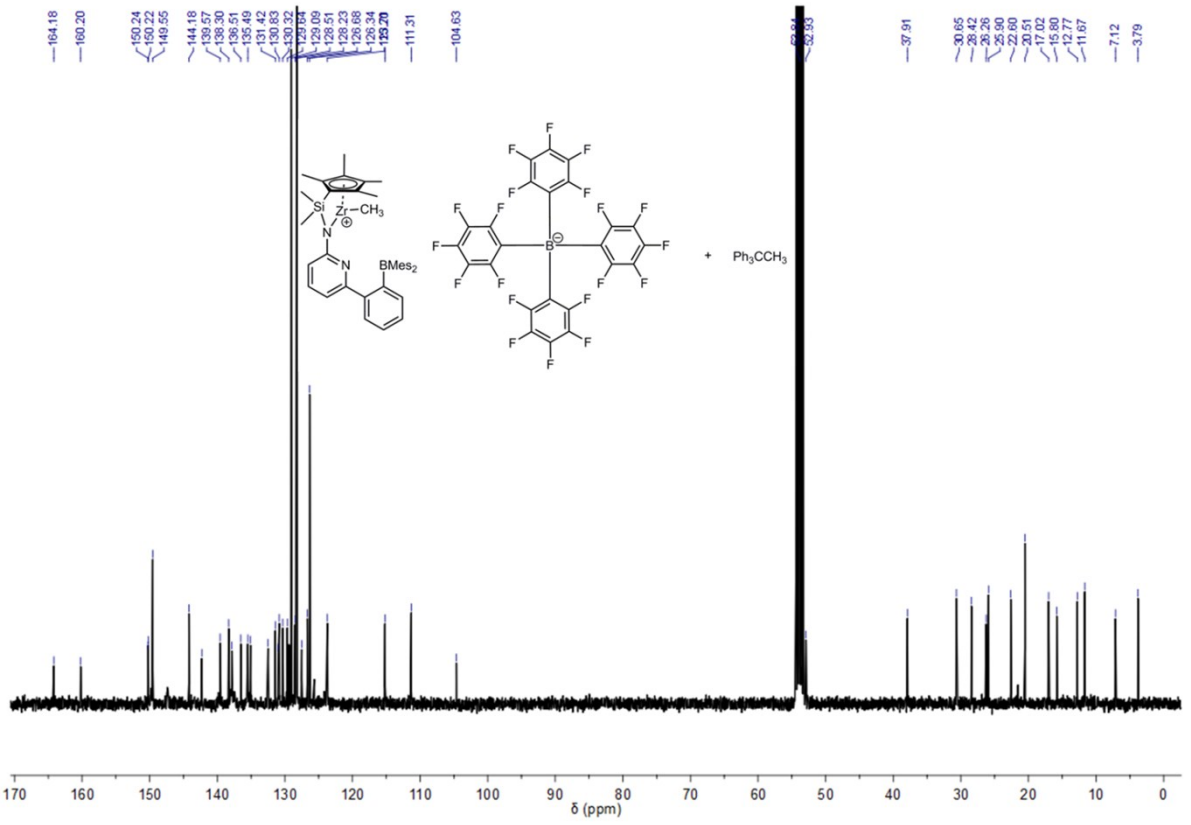



**Figure S32.** $^{13}$C NMR spectrum of the formation of **[L´Zr(CH$_3$)]$^+$[B(C$_6$F$_5$)$_4$]$^-$** *in situ* in $CD_2Cl_2$.

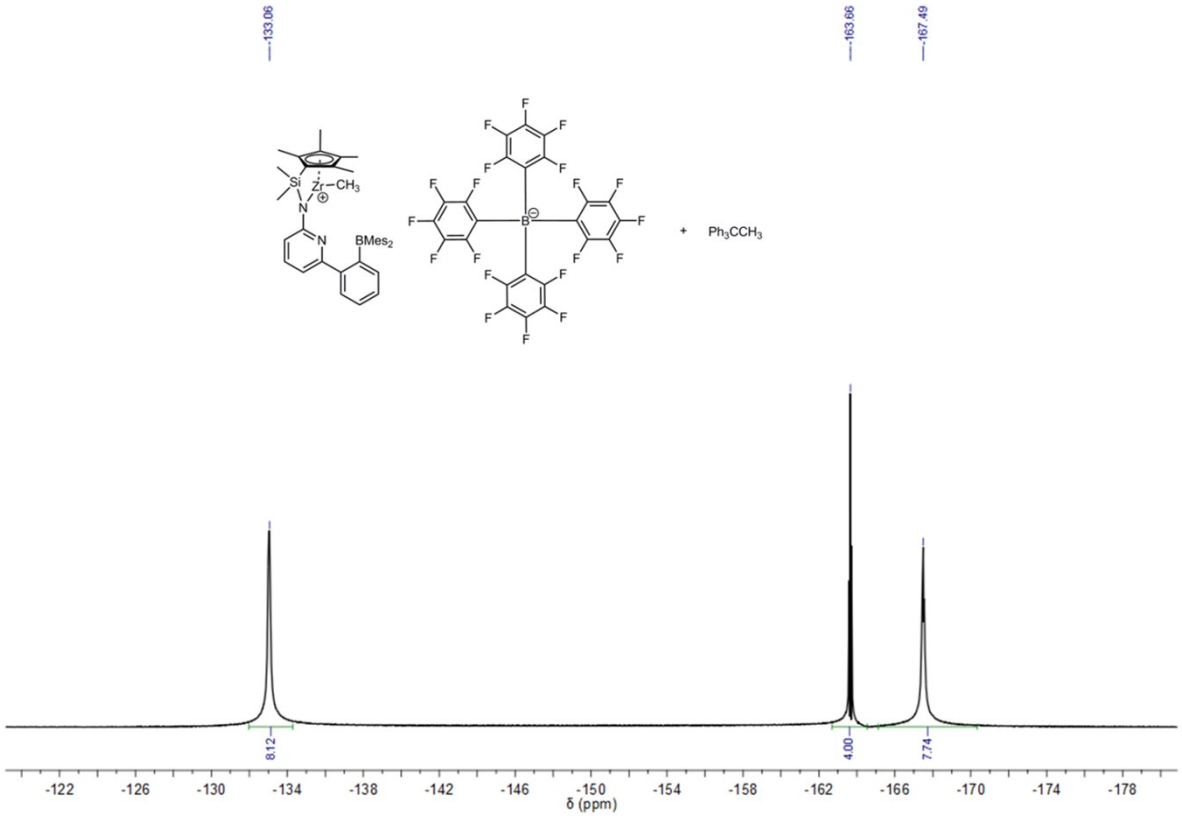



**Figure S33.** $^{19}F$ NMR spectrum of the formation of **[L´Zr(CH$_3$)]$^+$[B(C$_6$F$_5$)$_4$]$^-$** *in situ* in $CD_2Cl_2$.

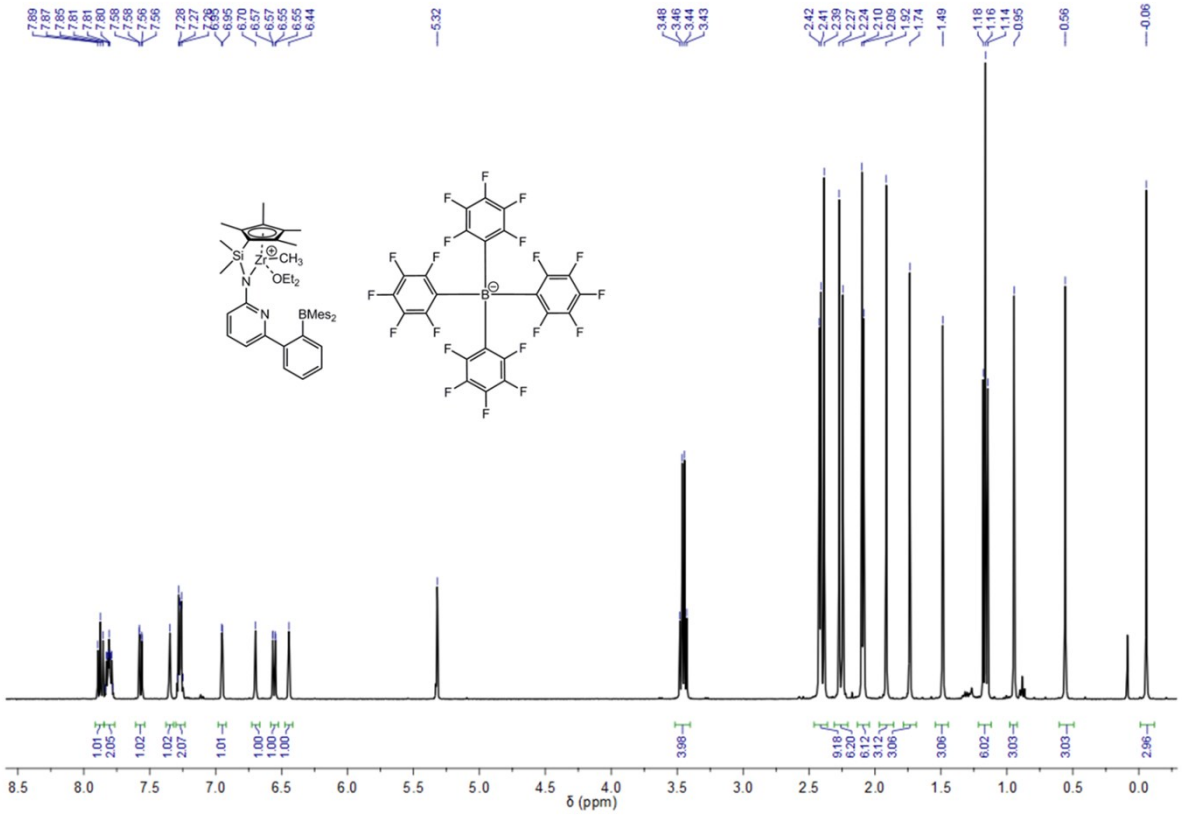



**Figure S34.** $^1H$ NMR spectrum of **[L´Zr(CH$_3$)Et$_2$O]$^+$[B(C$_6$F$_5$)$_4$]$^-$** in $CD_2Cl_2$.

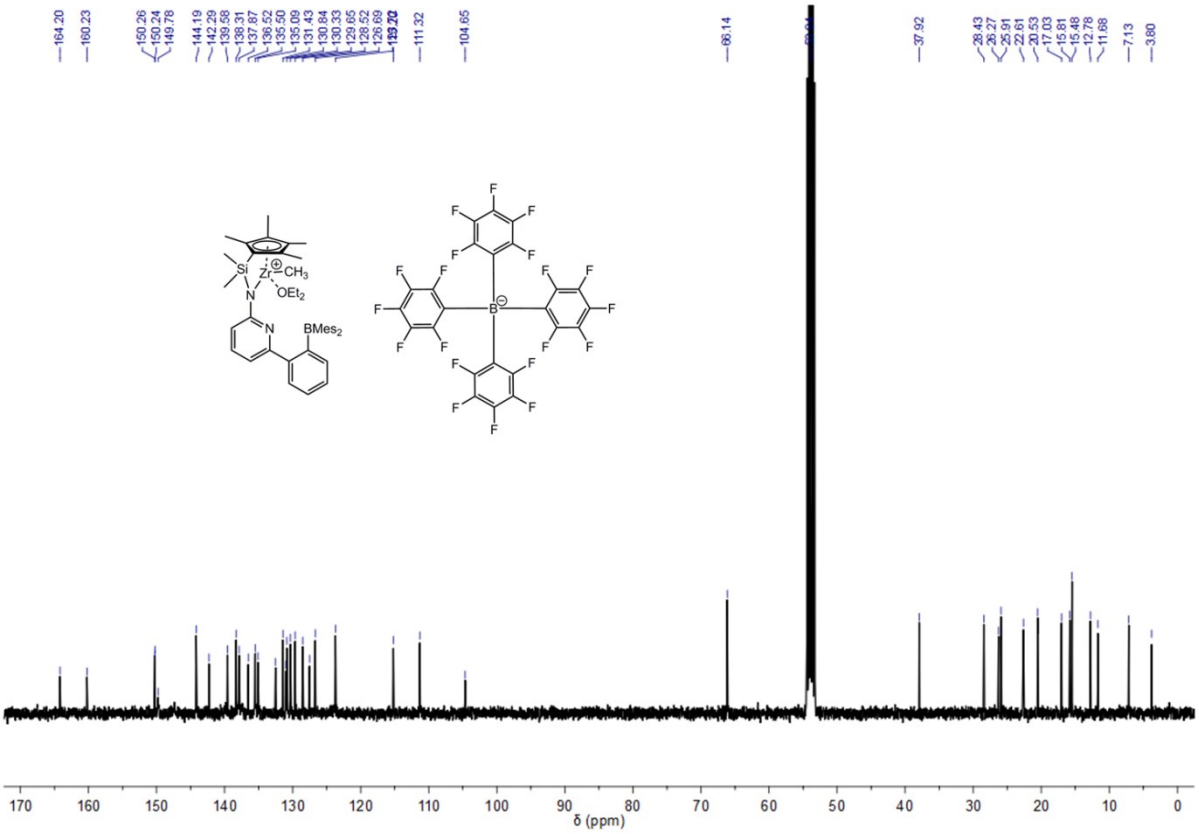



**Figure S35.** $^{13}C$ NMR spectrum of **[L´Zr(CH$_3$)Et$_2$O]$^+$[B(C$_6$F$_5$)$_4$]$^-$** in $CD_2Cl_2$.

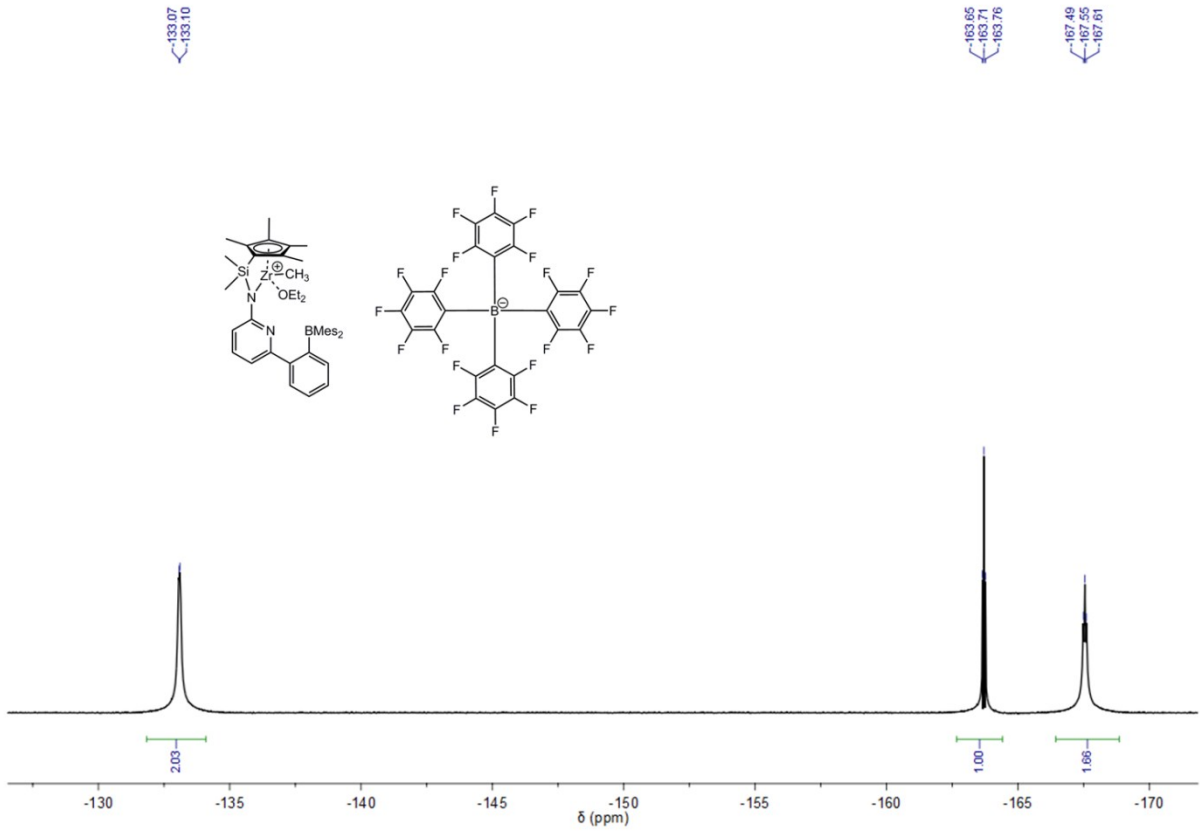



**Figure S36.** $^{19}F$ NMR spectrum of **[L´Zr(CH$_3$)Et$_2$O]$^+$[B(C$_6$F$_5$)$_4$]$^-$** in $CD_2Cl_2$.

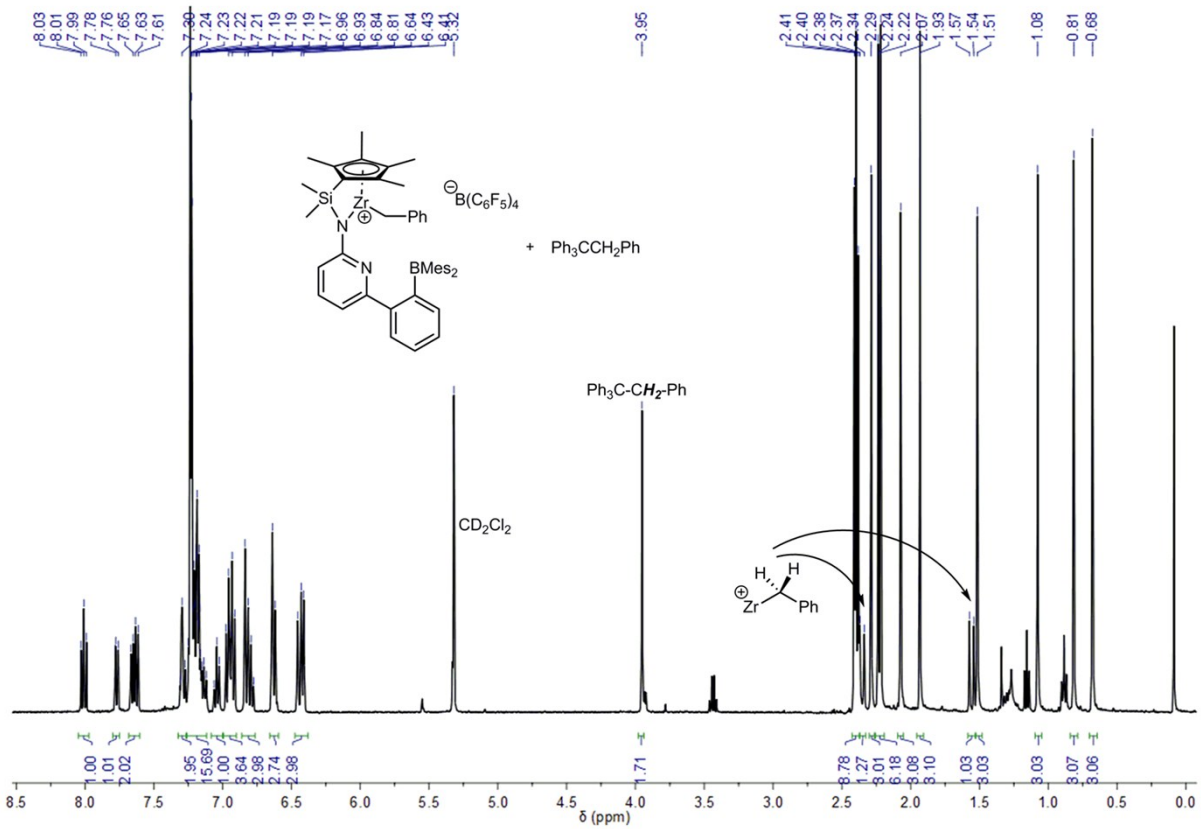



**Figure S37.** $^{1}$H NMR spectrum of the *in situ* formation of **[L´Zr(Bn)]$^{+}$[B(C$_6$F$_5$)$_4$]$^{-}$** in $CD_2Cl_2$.

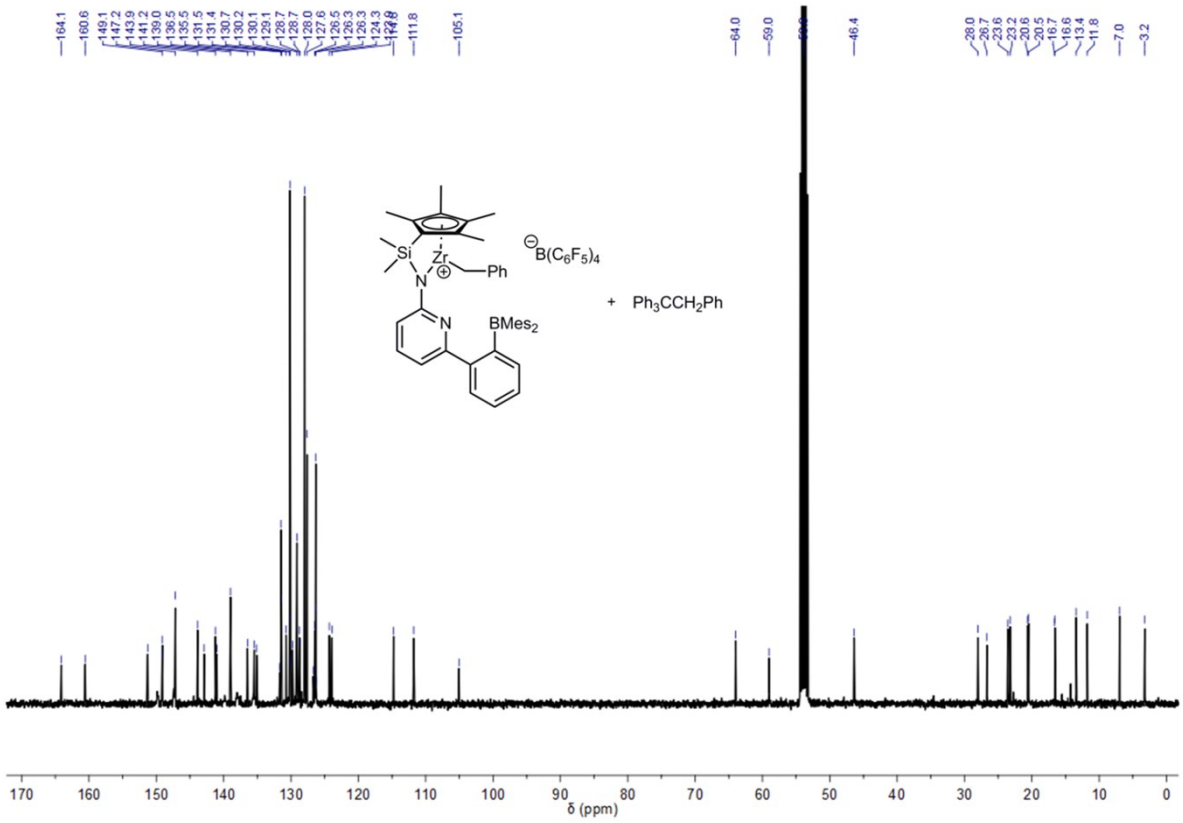



**Figure S38.** $^{13}$C NMR spectrum of the *in situ* formation of **[L´Zr(Bn)]$^{+}$[B(C$_6$F$_5$)$_4$]$^{-}$** in $CD_2Cl_2$.

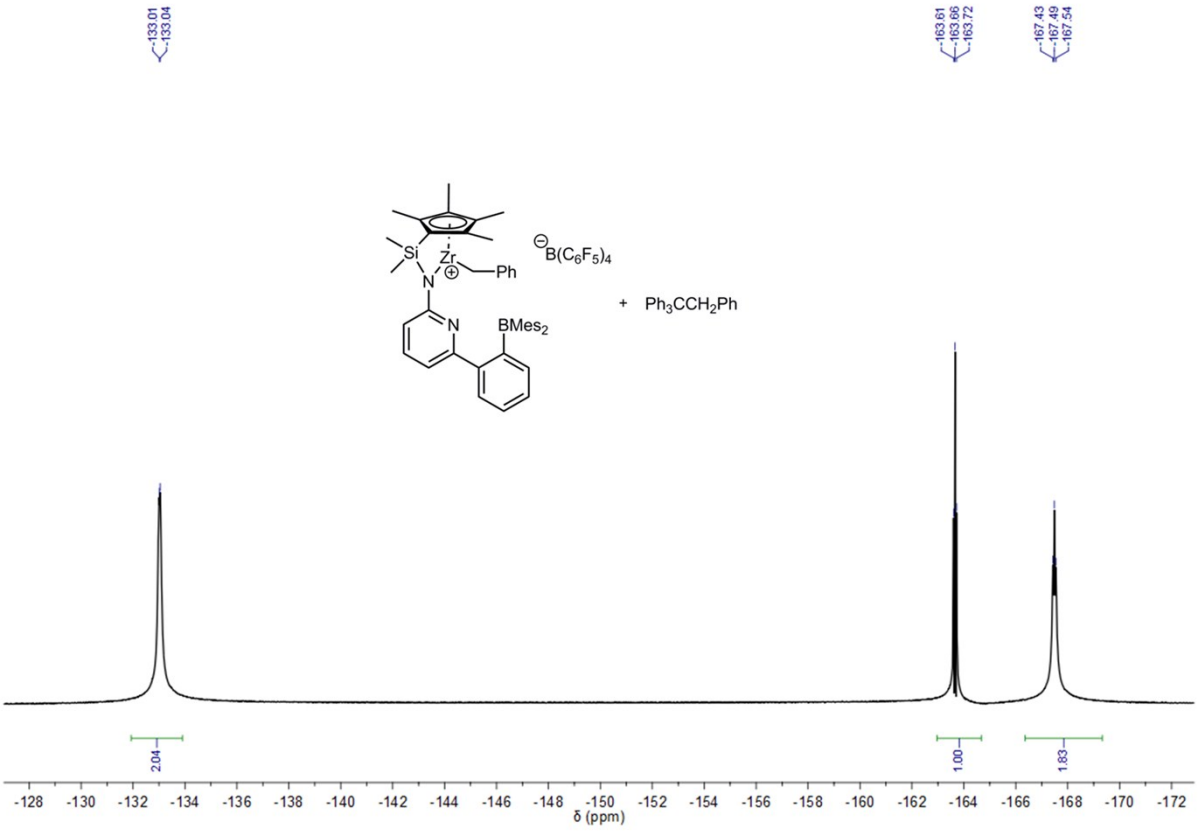
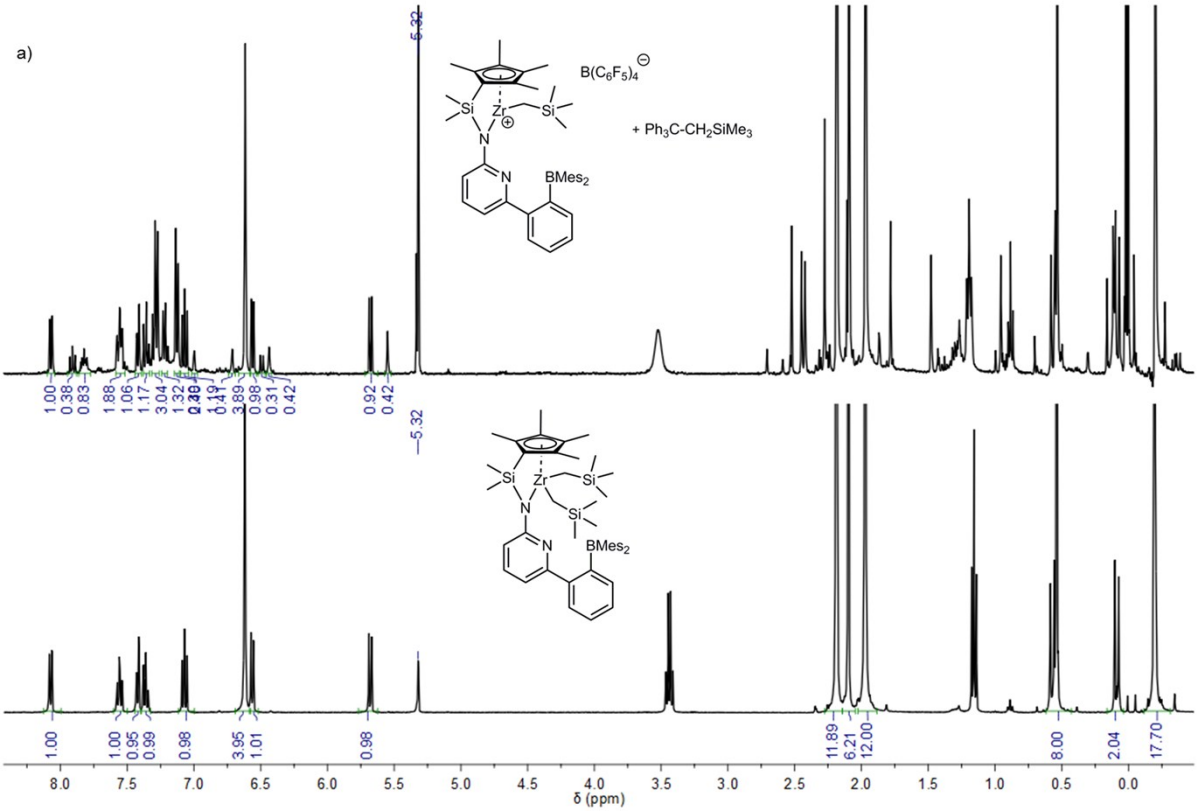



**Figure S39.** $^{19}F$ NMR spectrum of the *in situ* formation of **[L´Zr(Bn)]$^+$[B(C$_6$F$_5$)$_4$]$^-$** in $CD_2Cl_2$.



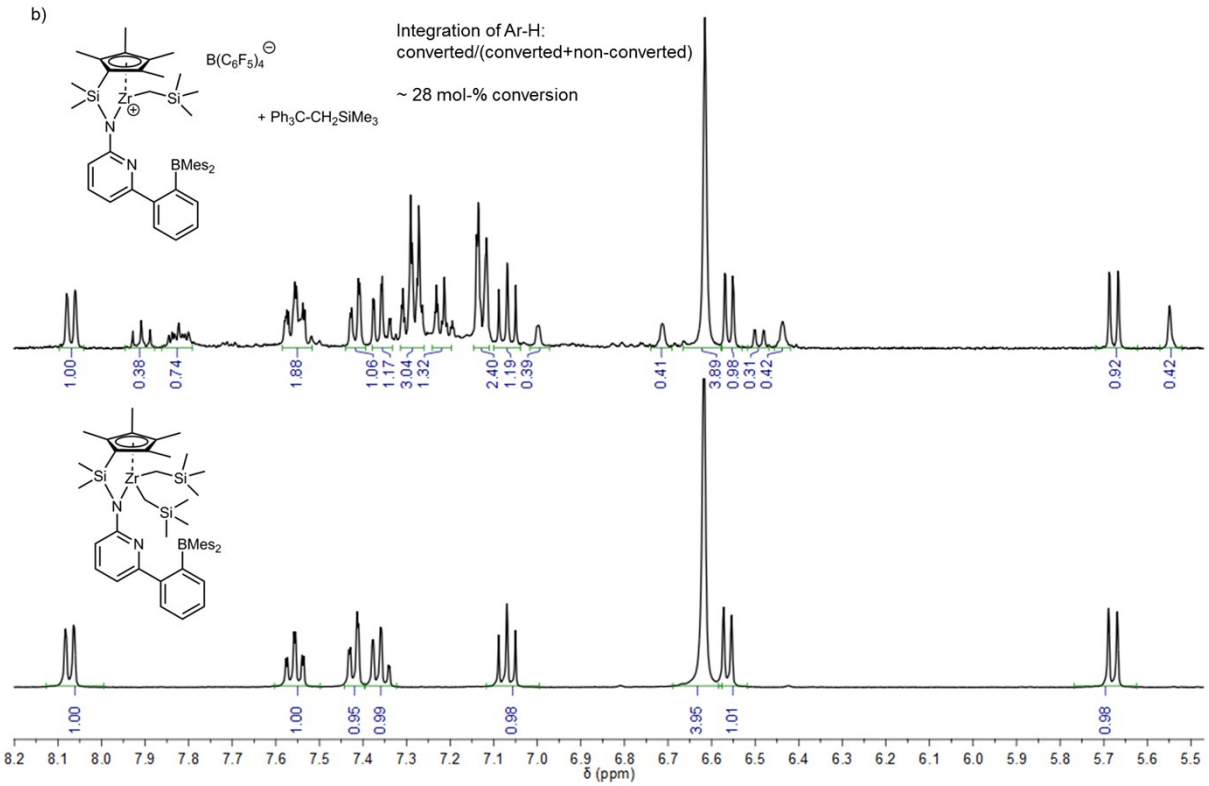



**Figure S40.** $^{1}$H NMR spectra of the *in situ* formation of **[L´Zr($CH_2SiMe_3$)]$^+$[$B(C_6F_5)_4$]$^-$** in $CD_2Cl_2$ a) -0.5-8.5 ppm and b) 5.5-8.2 ppm.

**Table S1.** Crystal data and structure refinement for **L´Zr(CH$_3$)$_2$**.

| | |
|---|---|
| Empirical formula | C42H53BN2SiZr |
| Formula weight | 715.98 |
| Temperature | 110(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, space group | Triclinic, P-1 |
| Unit cell dimensions | a = 8.6885(10) Å α = 79.834(5)°. |
| | b = 12.1849(12) Å β = 85.356(6)°. |
| | c = 18.105(2) Å γ= 81.823(5)°. |
| Volume | 1864.4(4) Å$^3$ |
| Z, Calculated density | 2, 1.275 mg/m$^3$ |
| Absorption coefficient | 0.358 mm$^{-1}$ |
| F(000) | 756 |
| Crystal size | 0.21 x 0.16 x 0.09 mm |
| Theta range for data collection | 1.71 to 26.45°. |
| Limiting indices | -10<=h<=10, -15<=k<=10, -22<=l<=22 |
| Reflections collected / unique | 27284 / 7603 [R(int) = 0.0573] |
| Completeness to theta = 26.45 | 98.9 % |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.7454 and 0.7066 |
| Refinement method | Full-matrix least-squares on F$^2$ |
| Data / restraints / parameters | 7603 / 0 / 438 |
| Goodness-of-fit on F$^2$ | 1.041 |
| Final R indices [I>2σ(I)] | R1 = 0.0423, wR2 = 0.0769 |
| R indices (all data) | R1 = 0.0738, wR2 = 0.0833 |
| Largest diff. peak and hole | 0.431 and -0.419 e.A$^{-3}$ |

**Table S2.** Atomic coordinates (×10$^4$) and equivalent isotropic displacement parameters (A$^2$ × 10$^3$) for **L´Zr(CH$_3$)$_2$**. U(eq) is defined as one third of the trace of the orthogonalized U$_{ij}$ tensor.

| x | y | z | U(eq) |
|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| Zr(1) | 1992(1) | 139(1) | 2071(1) | 15(1) |
| Si(1) | 2650(1) | 1251(1) | 374(1) | 18(1) |
| B(1) | -1114(3) | 4323(2) | 3361(2) | 13(1) |
| N(1) | 1272(3) | 1356(2) | 1102(1) | 26(1) |
| C(1) | 21(3) | 2021(2) | 1360(2) | 18(1) |
| N(2) | -170(2) | 1766(2) | 2125(1) | 16(1) |
| C(2) | -1321(3) | 2377(2) | 2485(1) | 14(1) |
| C(3) | -2359(3) | 3199(2) | 2092(2) | 17(1) |
| C(4) | -2179(3) | 3432(2) | 1311(2) | 19(1) |
| C(5) | -975(3) | 2847(2) | 942(2) | 19(1) |
| C(6) | -1404(3) | 2173(2) | 3318(2) | 14(1) |
| C(7) | -1416(3) | 3080(2) | 3715(1) | 13(1) |
| C(8) | -1533(3) | 2824(2) | 4503(1) | 17(1) |
| C(9) | -1595(3) | 1737(2) | 4887(2) | 20(1) |
| C(10) | -1604(3) | 867(2) | 4487(2) | 20(1) |
| C(11) | -1513(3) | 1087(2) | 3708(2) | 17(1) |
| C(12) | 80(3) | 4560(2) | 2661(1) | 13(1) |
| C(13) | 1633(3) | 4005(2) | 2667(2) | 15(1) |
| C(14) | 2679(3) | 4254(2) | 2054(2) | 17(1) |
| C(15) | 2261(3) | 5020(2) | 1422(2) | 20(1) |
| C(16) | 734(3) | 5565(2) | 1414(2) | 18(1) |
| C(17) | -341(3) | 5367(2) | 2023(1) | 15(1) |
| C(18) | 2217(3) | 3199(2) | 3343(2) | 22(1) |
| C(19) | 3430(3) | 5277(2) | 769(2) | 31(1) |
| C(20) | -1941(3) | 6029(2) | 1974(2) | 21(1) |
| C(21) | -1931(3) | 5317(2) | 3771(1) | 14(1) |
| C(22) | -3564(3) | 5462(2) | 3957(1) | 14(1) |
| C(23) | -4235(3) | 6338(2) | 4329(1) | 16(1) |
| C(24) | -3363(3) | 7091(2) | 4538(1) | 16(1) |
| C(25) | -1779(3) | 6948(2) | 4358(1) | 18(1) |
| C(26) | -1049(3) | 6096(2) | 3978(1) | 15(1) |
| C(27) | -4649(3) | 4742(2) | 3715(2) | 17(1) |

| | | | | |
|---|---|---|---|---|
| C(28) | -4122(3) | 8047(2) | 4928(2) | 22(1) |
| C(29) | 702(3) | 6024(2) | 3825(2) | 24(1) |
| C(30) | 240(3) | -1084(2) | 2318(2) | 24(1) |
| C(31) | 2616(3) | 304(2) | 3236(2) | 22(1) |
| C(32) | 3573(4) | 2562(2) | 84(2) | 34(1) |
| C(33) | 1962(3) | 955(2) | -502(2) | 26(1) |
| C(34) | 3833(3) | 41(2) | 962(1) | 15(1) |
| C(35) | 4734(3) | 156(2) | 1565(2) | 18(1) |
| C(36) | 4822(3) | -851(2) | 2103(2) | 16(1) |
| C(37) | 3940(3) | -1594(2) | 1847(2) | 17(1) |
| C(38) | 3343(3) | -1056(2) | 1152(2) | 16(1) |
| C(39) | 5505(3) | 1160(2) | 1641(2) | 23(1) |
| C(40) | 5798(3) | -1152(2) | 2770(2) | 23(1) |
| C(41) | 3774(3) | -2774(2) | 2236(2) | 23(1) |
| C(42) | 2358(3) | -1566(2) | 687(2) | 24(1) |

**Table S3.** Bond lengths [Å] and angles [º] for **L´Zr($CH_3$)$_2$**.

| | |
|---|---|
| Zr(1)-N(1) | 2.160(2) |
| Zr(1)-C(30) | 2.244(2) |
| Zr(1)-C(31) | 2.269(3) |
| Zr(1)-C(34) | 2.473(2) |
| Zr(1)-C(35) | 2.484(3) |
| Zr(1)-C(38) | 2.514(2) |
| Zr(1)-N(2) | 2.539(2) |
| Zr(1)-C(36) | 2.581(3) |
| Zr(1)-C(37) | 2.581(2) |
| Zr(1)-C(1) | 2.837(3) |
| Zr(1)-Si(1) | 3.1731(8) |
| Si(1)-N(1) | 1.716(2) |
| Si(1)-C(33) | 1.849(3) |
| Si(1)-C(32) | 1.864(3) |
| Si(1)-C(34) | 1.885(3) |

| | |
|---|---|
| B(1)-C(12) | 1.584(4) |
| B(1)-C(21) | 1.584(4) |
| B(1)-C(7) | 1.586(4) |
| N(1)-C(1) | 1.363(3) |
| C(1)-N(2) | 1.367(3) |
| C(1)-C(5) | 1.386(4) |
| N(2)-C(2) | 1.354(3) |
| C(2)-C(3) | 1.384(4) |
| C(2)-C(6) | 1.483(4) |
| C(3)-C(4) | 1.392(4) |
| C(3)-H(3) | 0.9500 |
| C(4)-C(5) | 1.375(4) |
| C(4)-H(4) | 0.9500 |
| C(5)-H(5) | 0.9500 |
| C(6)-C(11) | 1.398(3) |
| C(6)-C(7) | 1.417(3) |
| C(7)-C(8) | 1.404(3) |
| C(8)-C(9) | 1.389(3) |
| C(8)-H(8) | 0.9500 |
| C(9)-C(10) | 1.387(4) |
| C(9)-H(9) | 0.9500 |
| C(10)-C(11) | 1.385(4) |
| C(10)-H(10) | 0.9500 |
| C(11)-H(11) | 0.9500 |
| C(12)-C(17) | 1.415(4) |
| C(12)-C(13) | 1.420(4) |
| C(13)-C(14) | 1.396(3) |
| C(13)-C(18) | 1.501(4) |
| C(14)-C(15) | 1.381(4) |
| C(14)-H(14) | 0.9500 |
| C(15)-C(16) | 1.396(4) |
| C(15)-C(19) | 1.514(4) |
| C(16)-C(17) | 1.397(3) |

| | |
|---|---|
| C(16)-H(16) | 0.9500 |
| C(17)-C(20) | 1.506(4) |
| 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)-C(26) | 1.417(3) |
| C(21)-C(22) | 1.425(3) |
| C(22)-C(23) | 1.396(3) |
| C(22)-C(27) | 1.512(3) |
| C(23)-C(24) | 1.388(3) |
| C(23)-H(23) | 0.9500 |
| C(24)-C(25) | 1.382(4) |
| C(24)-C(28) | 1.512(3) |
| C(25)-C(26) | 1.396(3) |
| C(25)-H(25) | 0.9500 |
| C(26)-C(29) | 1.517(4) |
| C(27)-H(27A) | 0.9800 |
| C(27)-H(27B) | 0.9800 |
| C(27)-H(27C) | 0.9800 |
| C(28)-H(28A) | 0.9800 |
| C(28)-H(28B) | 0.9800 |
| C(28)-H(28C) | 0.9800 |
| 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)-H(32A) | 0.9800 |
| C(32)-H(32B) | 0.9800 |
| C(32)-H(32C) | 0.9800 |
| C(33)-H(33A) | 0.9800 |
| C(33)-H(33B) | 0.9800 |
| C(33)-H(33C) | 0.9800 |
| C(34)-C(35) | 1.431(4) |
| C(34)-C(38) | 1.436(3) |
| C(35)-C(36) | 1.423(4) |
| C(35)-C(39) | 1.507(3) |
| C(36)-C(37) | 1.422(3) |
| C(36)-C(40) | 1.494(4) |
| C(37)-C(38) | 1.413(4) |
| C(37)-C(41) | 1.507(3) |
| C(38)-C(42) | 1.510(4) |
| 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 |
| C(41)-H(41A) | 0.9800 |
| C(41)-H(41B) | 0.9800 |
| C(41)-H(41C) | 0.9800 |
| C(42)-H(42A) | 0.9800 |
| C(42)-H(42B) | 0.9800 |
| C(42)-H(42C) | 0.9800 |

| | |
|---|---|
| N(1)-Zr(1)-C(30) | 107.52(10) |

| | |
|---|---|
| N(1)-Zr(1)-C(31) | 132.95(9) |
| C(30)-Zr(1)-C(31) | 102.70(10) |
| N(1)-Zr(1)-C(34) | 67.08(9) |
| C(30)-Zr(1)-C(34) | 118.48(9) |
| C(31)-Zr(1)-C(34) | 125.83(9) |
| N(1)-Zr(1)-C(35) | 88.81(9) |
| C(30)-Zr(1)-C(35) | 137.90(9) |
| C(31)-Zr(1)-C(35) | 92.27(9) |
| C(34)-Zr(1)-C(35) | 33.56(8) |
| N(1)-Zr(1)-C(38) | 86.45(9) |
| C(30)-Zr(1)-C(38) | 87.24(9) |
| C(31)-Zr(1)-C(38) | 130.67(9) |
| C(34)-Zr(1)-C(38) | 33.46(8) |
| C(35)-Zr(1)-C(38) | 54.53(8) |
| N(1)-Zr(1)-N(2) | 56.29(7) |
| C(30)-Zr(1)-N(2) | 90.31(8) |
| C(31)-Zr(1)-N(2) | 88.90(8) |
| C(34)-Zr(1)-N(2) | 122.15(8) |
| C(35)-Zr(1)-N(2) | 129.58(7) |
| C(38)-Zr(1)-N(2) | 139.86(8) |
| N(1)-Zr(1)-C(36) | 119.75(8) |
| C(30)-Zr(1)-C(36) | 112.42(9) |
| C(31)-Zr(1)-C(36) | 78.52(9) |
| C(34)-Zr(1)-C(36) | 54.79(9) |
| C(35)-Zr(1)-C(36) | 32.56(8) |
| C(38)-Zr(1)-C(36) | 53.58(8) |
| N(2)-Zr(1)-C(36) | 155.85(7) |
| N(1)-Zr(1)-C(37) | 117.85(8) |
| C(30)-Zr(1)-C(37) | 84.69(9) |
| C(31)-Zr(1)-C(37) | 99.90(9) |
| C(34)-Zr(1)-C(37) | 54.63(8) |
| C(35)-Zr(1)-C(37) | 53.81(8) |
| C(38)-Zr(1)-C(37) | 32.18(8) |

| | |
|---|---|
| N(2)-Zr(1)-C(37) | 170.64(8) |
| C(36)-Zr(1)-C(37) | 32.00(8) |
| N(1)-Zr(1)-C(1) | 27.64(8) |
| C(30)-Zr(1)-C(1) | 98.17(9) |
| C(31)-Zr(1)-C(1) | 113.78(9) |
| C(34)-Zr(1)-C(1) | 94.49(8) |
| C(35)-Zr(1)-C(1) | 111.44(8) |
| C(38)-Zr(1)-C(1) | 112.28(8) |
| N(2)-Zr(1)-C(1) | 28.79(7) |
| C(36)-Zr(1)-C(1) | 143.99(8) |
| C(37)-Zr(1)-C(1) | 144.43(8) |
| N(1)-Zr(1)-Si(1) | 30.69(6) |
| C(30)-Zr(1)-Si(1) | 118.20(8) |
| C(31)-Zr(1)-Si(1) | 138.79(7) |
| C(34)-Zr(1)-Si(1) | 36.41(6) |
| C(35)-Zr(1)-Si(1) | 61.16(7) |
| C(38)-Zr(1)-Si(1) | 60.39(6) |
| N(2)-Zr(1)-Si(1) | 86.22(5) |
| C(36)-Zr(1)-Si(1) | 89.79(6) |
| C(37)-Zr(1)-Si(1) | 89.18(6) |
| C(1)-Zr(1)-Si(1) | 58.10(5) |
| N(1)-Si(1)-C(33) | 116.14(13) |
| N(1)-Si(1)-C(32) | 112.21(13) |
| C(33)-Si(1)-C(32) | 104.97(14) |
| N(1)-Si(1)-C(34) | 91.07(11) |
| C(33)-Si(1)-C(34) | 116.16(12) |
| C(32)-Si(1)-C(34) | 116.41(13) |
| N(1)-Si(1)-Zr(1) | 39.96(8) |
| C(33)-Si(1)-Zr(1) | 130.23(9) |
| C(32)-Si(1)-Zr(1) | 124.00(10) |
| C(34)-Si(1)-Zr(1) | 51.15(8) |
| C(12)-B(1)-C(21) | 120.5(2) |
| C(12)-B(1)-C(7) | 121.3(2) |

| | |
|---|---|
| C(21)-B(1)-C(7) | 118.0(2) |
| C(1)-N(1)-Si(1) | 144.3(2) |
| C(1)-N(1)-Zr(1) | 105.03(17) |
| Si(1)-N(1)-Zr(1) | 109.35(11) |
| N(1)-C(1)-N(2) | 110.4(2) |
| N(1)-C(1)-C(5) | 127.7(2) |
| N(2)-C(1)-C(5) | 121.9(2) |
| N(1)-C(1)-Zr(1) | 47.33(13) |
| N(2)-C(1)-Zr(1) | 63.41(14) |
| C(5)-C(1)-Zr(1) | 172.07(19) |
| C(2)-N(2)-C(1) | 118.7(2) |
| C(2)-N(2)-Zr(1) | 153.31(18) |
| C(1)-N(2)-Zr(1) | 87.80(15) |
| N(2)-C(2)-C(3) | 121.4(2) |
| N(2)-C(2)-C(6) | 118.0(2) |
| C(3)-C(2)-C(6) | 120.6(2) |
| C(2)-C(3)-C(4) | 119.3(2) |
| C(2)-C(3)-H(3) | 120.3 |
| C(4)-C(3)-H(3) | 120.3 |
| C(5)-C(4)-C(3) | 119.7(3) |
| C(5)-C(4)-H(4) | 120.2 |
| C(3)-C(4)-H(4) | 120.2 |
| C(4)-C(5)-C(1) | 118.9(3) |
| C(4)-C(5)-H(5) | 120.6 |
| C(1)-C(5)-H(5) | 120.6 |
| C(11)-C(6)-C(7) | 120.4(2) |
| C(11)-C(6)-C(2) | 119.4(2) |
| C(7)-C(6)-C(2) | 120.1(2) |
| C(8)-C(7)-C(6) | 116.8(2) |
| C(8)-C(7)-B(1) | 116.5(2) |
| C(6)-C(7)-B(1) | 126.3(2) |
| C(9)-C(8)-C(7) | 122.5(2) |
| C(9)-C(8)-H(8) | 118.8 |

| | |
|---|---|
| C(7)-C(8)-H(8) | 118.8 |
| C(10)-C(9)-C(8) | 119.7(2) |
| C(10)-C(9)-H(9) | 120.2 |
| C(8)-C(9)-H(9) | 120.2 |
| C(11)-C(10)-C(9) | 119.6(2) |
| C(11)-C(10)-H(10) | 120.2 |
| C(9)-C(10)-H(10) | 120.2 |
| C(10)-C(11)-C(6) | 121.0(2) |
| C(10)-C(11)-H(11) | 119.5 |
| C(6)-C(11)-H(11) | 119.5 |
| C(17)-C(12)-C(13) | 117.7(2) |
| C(17)-C(12)-B(1) | 121.2(2) |
| C(13)-C(12)-B(1) | 121.1(2) |
| C(14)-C(13)-C(12) | 120.1(2) |
| C(14)-C(13)-C(18) | 118.4(2) |
| C(12)-C(13)-C(18) | 121.4(2) |
| C(15)-C(14)-C(13) | 122.4(3) |
| C(15)-C(14)-H(14) | 118.8 |
| C(13)-C(14)-H(14) | 118.8 |
| C(14)-C(15)-C(16) | 117.6(2) |
| C(14)-C(15)-C(19) | 121.0(3) |
| C(16)-C(15)-C(19) | 121.3(3) |
| C(15)-C(16)-C(17) | 122.0(3) |
| C(15)-C(16)-H(16) | 119.0 |
| C(17)-C(16)-H(16) | 119.0 |
| C(16)-C(17)-C(12) | 120.1(2) |
| C(16)-C(17)-C(20) | 118.1(2) |
| C(12)-C(17)-C(20) | 121.7(2) |
| C(13)-C(18)-H(18A) | 109.5 |
| C(13)-C(18)-H(18B) | 109.5 |
| H(18A)-C(18)-H(18B) | 109.5 |
| C(13)-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(17)-C(20)-H(20A) | 109.5 |
| C(17)-C(20)-H(20B) | 109.5 |
| H(20A)-C(20)-H(20B) | 109.5 |
| C(17)-C(20)-H(20C) | 109.5 |
| H(20A)-C(20)-H(20C) | 109.5 |
| H(20B)-C(20)-H(20C) | 109.5 |
| C(26)-C(21)-C(22) | 117.1(2) |
| C(26)-C(21)-B(1) | 120.8(2) |
| C(22)-C(21)-B(1) | 122.1(2) |
| C(23)-C(22)-C(21) | 120.3(2) |
| C(23)-C(22)-C(27) | 117.4(2) |
| C(21)-C(22)-C(27) | 122.2(2) |
| C(24)-C(23)-C(22) | 122.3(2) |
| C(24)-C(23)-H(23) | 118.8 |
| C(22)-C(23)-H(23) | 118.8 |
| C(25)-C(24)-C(23) | 117.2(2) |
| C(25)-C(24)-C(28) | 121.4(2) |
| C(23)-C(24)-C(28) | 121.3(2) |
| C(24)-C(25)-C(26) | 122.9(2) |
| C(24)-C(25)-H(25) | 118.6 |
| C(26)-C(25)-H(25) | 118.6 |
| C(25)-C(26)-C(21) | 120.2(2) |
| C(25)-C(26)-C(29) | 117.5(2) |
| C(21)-C(26)-C(29) | 122.3(2) |
| C(22)-C(27)-H(27A) | 109.5 |
| C(22)-C(27)-H(27B) | 109.5 |

| | |
|---|---|
| H(27A)-C(27)-H(27B) | 109.5 |
| C(22)-C(27)-H(27C) | 109.5 |
| H(27A)-C(27)-H(27C) | 109.5 |
| H(27B)-C(27)-H(27C) | 109.5 |
| C(24)-C(28)-H(28A) | 109.5 |
| C(24)-C(28)-H(28B) | 109.5 |
| H(28A)-C(28)-H(28B) | 109.5 |
| C(24)-C(28)-H(28C) | 109.5 |
| H(28A)-C(28)-H(28C) | 109.5 |
| H(28B)-C(28)-H(28C) | 109.5 |
| C(26)-C(29)-H(29A) | 109.5 |
| C(26)-C(29)-H(29B) | 109.5 |
| H(29A)-C(29)-H(29B) | 109.5 |
| C(26)-C(29)-H(29C) | 109.5 |
| H(29A)-C(29)-H(29C) | 109.5 |
| H(29B)-C(29)-H(29C) | 109.5 |
| Zr(1)-C(30)-H(30A) | 109.5 |
| Zr(1)-C(30)-H(30B) | 109.5 |
| H(30A)-C(30)-H(30B) | 109.5 |
| Zr(1)-C(30)-H(30C) | 109.5 |
| H(30A)-C(30)-H(30C) | 109.5 |
| H(30B)-C(30)-H(30C) | 109.5 |
| Zr(1)-C(31)-H(31A) | 109.5 |
| Zr(1)-C(31)-H(31B) | 109.5 |
| H(31A)-C(31)-H(31B) | 109.5 |
| Zr(1)-C(31)-H(31C) | 109.5 |
| H(31A)-C(31)-H(31C) | 109.5 |
| H(31B)-C(31)-H(31C) | 109.5 |
| Si(1)-C(32)-H(32A) | 109.5 |
| Si(1)-C(32)-H(32B) | 109.5 |
| H(32A)-C(32)-H(32B) | 109.5 |
| Si(1)-C(32)-H(32C) | 109.5 |
| H(32A)-C(32)-H(32C) | 109.5 |

| | |
|---|---|
| H(32B)-C(32)-H(32C) | 109.5 |
| Si(1)-C(33)-H(33A) | 109.5 |
| Si(1)-C(33)-H(33B) | 109.5 |
| H(33A)-C(33)-H(33B) | 109.5 |
| Si(1)-C(33)-H(33C) | 109.5 |
| H(33A)-C(33)-H(33C) | 109.5 |
| H(33B)-C(33)-H(33C) | 109.5 |
| C(35)-C(34)-C(38) | 106.0(2) |
| C(35)-C(34)-Si(1) | 124.19(18) |
| C(38)-C(34)-Si(1) | 122.25(19) |
| C(35)-C(34)-Zr(1) | 73.61(14) |
| C(38)-C(34)-Zr(1) | 74.80(14) |
| Si(1)-C(34)-Zr(1) | 92.44(10) |
| C(36)-C(35)-C(34) | 109.3(2) |
| C(36)-C(35)-C(39) | 123.6(2) |
| C(34)-C(35)-C(39) | 127.2(2) |
| C(36)-C(35)-Zr(1) | 77.47(14) |
| C(34)-C(35)-Zr(1) | 72.83(14) |
| C(39)-C(35)-Zr(1) | 116.87(17) |
| C(37)-C(36)-C(35) | 107.4(2) |
| C(37)-C(36)-C(40) | 124.9(2) |
| C(35)-C(36)-C(40) | 127.3(2) |
| C(37)-C(36)-Zr(1) | 74.01(15) |
| C(35)-C(36)-Zr(1) | 69.97(14) |
| C(40)-C(36)-Zr(1) | 126.75(17) |
| C(38)-C(37)-C(36) | 108.2(2) |
| C(38)-C(37)-C(41) | 126.8(2) |
| C(36)-C(37)-C(41) | 124.9(3) |
| C(38)-C(37)-Zr(1) | 71.29(14) |
| C(36)-C(37)-Zr(1) | 74.00(14) |
| C(41)-C(37)-Zr(1) | 123.48(17) |
| C(37)-C(38)-C(34) | 109.1(2) |
| C(37)-C(38)-C(42) | 125.0(2) |

| | |
|---|---|
| C(34)-C(38)-C(42) | 125.9(2) |
| C(37)-C(38)-Zr(1) | 76.53(15) |
| C(34)-C(38)-Zr(1) | 71.74(14) |
| C(42)-C(38)-Zr(1) | 118.44(17) |
| 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(36)-C(40)-H(40A) | 109.5 |
| C(36)-C(40)-H(40B) | 109.5 |
| H(40A)-C(40)-H(40B) | 109.5 |
| C(36)-C(40)-H(40C) | 109.5 |
| H(40A)-C(40)-H(40C) | 109.5 |
| H(40B)-C(40)-H(40C) | 109.5 |
| C(37)-C(41)-H(41A) | 109.5 |
| C(37)-C(41)-H(41B) | 109.5 |
| H(41A)-C(41)-H(41B) | 109.5 |
| C(37)-C(41)-H(41C) | 109.5 |
| H(41A)-C(41)-H(41C) | 109.5 |
| H(41B)-C(41)-H(41C) | 109.5 |
| C(38)-C(42)-H(42A) | 109.5 |
| C(38)-C(42)-H(42B) | 109.5 |
| H(42A)-C(42)-H(42B) | 109.5 |
| C(38)-C(42)-H(42C) | 109.5 |
| H(42A)-C(42)-H(42C) | 109.5 |
| H(42B)-C(42)-H(42C) | 109.5 |

**Table S4.** Anisotropic displacement parameters ($A^2 \times 10^3$) for **L´Zr(CH$_3$)$_2$**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [ h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$.

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

| | | | | | | |
|---|---|---|---|---|---|---|
| C(26) | 15(2) | 17(1) | 11(1) | 1(1) | -1(1) | -1(1) |
| C(27) | 13(2) | 19(1) | 19(2) | -1(1) | 1(1) | -2(1) |
| C(28) | 22(2) | 21(1) | 23(2) | -5(1) | -1(1) | 2(1) |
| C(29) | 19(2) | 30(2) | 29(2) | -15(1) | 3(1) | -9(1) |
| C(30) | 15(2) | 28(2) | 30(2) | -7(1) | 1(1) | -1(1) |
| C(31) | 23(2) | 22(1) | 20(2) | -3(1) | 1(1) | 3(1) |
| C(32) | 44(2) | 23(2) | 33(2) | 4(1) | -10(2) | -7(2) |
| C(33) | 21(2) | 30(2) | 24(2) | -2(1) | -1(1) | 6(1) |
| C(34) | 12(1) | 19(1) | 14(2) | -5(1) | 3(1) | -1(1) |
| C(35) | 14(2) | 19(1) | 20(2) | -7(1) | 5(1) | 0(1) |
| C(36) | 11(1) | 20(1) | 17(2) | -4(1) | 1(1) | 1(1) |
| C(37) | 11(2) | 16(1) | 22(2) | -5(1) | 4(1) | 2(1) |
| C(38) | 13(1) | 17(1) | 18(2) | -6(1) | 2(1) | 0(1) |
| C(39) | 22(2) | 26(2) | 22(2) | -4(1) | -2(1) | -7(1) |
| C(40) | 14(2) | 27(2) | 28(2) | -3(1) | -1(1) | -3(1) |
| C(41) | 18(2) | 19(1) | 30(2) | -1(1) | 0(1) | 1(1) |
| C(42) | 23(2) | 21(1) | 28(2) | -8(1) | 2(1) | -3(1) |

**Table S5.** Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($A^2 \times 10^3$) for **L´Zr($CH_3$)$_2$**.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(3) | -3185 | 3599 | 2352 | 20 |
| H(4) | -2885 | 3992 | 1035 | 23 |
| H(5) | -829 | 3005 | 410 | 23 |
| H(8) | -1570 | 3417 | 4784 | 20 |
| H(9) | -1632 | 1591 | 5420 | 24 |
| H(10) | -1671 | 124 | 4745 | 24 |
| H(11) | -1525 | 490 | 3435 | 21 |
| H(14) | 3717 | 3883 | 2072 | 21 |

| | | | | |
|---|---|---|---|---|
| H(16) | 418 | 6086 | 981 | 22 |
| H(18A) | 3340 | 2980 | 3267 | 33 |
| H(18B) | 1682 | 2529 | 3414 | 33 |
| H(18C) | 2009 | 3562 | 3789 | 33 |
| H(19A) | 4039 | 5848 | 870 | 47 |
| H(19B) | 2879 | 5561 | 309 | 47 |
| H(19C) | 4129 | 4590 | 707 | 47 |
| H(20A) | -2025 | 6624 | 2280 | 32 |
| H(20B) | -2725 | 5527 | 2161 | 32 |
| H(20C) | -2114 | 6365 | 1450 | 32 |
| H(23) | -5328 | 6422 | 4444 | 19 |
| H(25) | -1160 | 7452 | 4499 | 21 |
| H(27A) | -5669 | 4863 | 3982 | 26 |
| H(27B) | -4216 | 3948 | 3833 | 26 |
| H(27C) | -4765 | 4950 | 3172 | 26 |
| H(28A) | -3342 | 8301 | 5198 | 33 |
| H(28B) | -4956 | 7788 | 5285 | 33 |
| H(28C) | -4559 | 8672 | 4554 | 33 |
| H(29A) | 1061 | 6701 | 3935 | 37 |
| H(29B) | 964 | 5963 | 3296 | 37 |
| H(29C) | 1211 | 5360 | 4145 | 37 |
| H(30A) | -767 | -715 | 2134 | 36 |
| H(30B) | 127 | -1339 | 2862 | 36 |
| H(30C) | 594 | -1731 | 2066 | 36 |
| H(31A) | 3465 | 766 | 3192 | 33 |
| H(31B) | 2949 | -444 | 3518 | 33 |
| H(31C) | 1704 | 662 | 3500 | 33 |
| H(32A) | 2777 | 3188 | -91 | 51 |
| H(32B) | 4366 | 2460 | -324 | 51 |
| H(32C) | 4062 | 2729 | 514 | 51 |
| H(33A) | 1356 | 321 | -383 | 39 |
| H(33B) | 2860 | 768 | -842 | 39 |
| H(33C) | 1306 | 1621 | -745 | 39 |

| | | | | |
|---|---|---|---|---|
| H(39A) | 4707 | 1803 | 1686 | 34 |
| H(39B) | 6200 | 1346 | 1196 | 34 |
| H(39C) | 6110 | 983 | 2091 | 34 |
| H(40A) | 5314 | -1689 | 3154 | 34 |
| H(40B) | 5881 | -472 | 2975 | 34 |
| H(40C) | 6840 | -1492 | 2617 | 34 |
| H(41A) | 2789 | -2984 | 2112 | 35 |
| H(41B) | 3781 | -2812 | 2780 | 35 |
| H(41C) | 4643 | -3295 | 2067 | 35 |
| H(42A) | 2139 | -2303 | 958 | 35 |
| H(42B) | 2921 | -1656 | 205 | 35 |
| H(42C) | 1377 | -1071 | 596 | 35 |

**Table S6.** Torsion angles [°] for **L´Zr($CH_3$)$_2$**.

| | |
|---|---|
| C(30)-Zr(1)-Si(1)-N(1) | 76.44(15) |
| C(31)-Zr(1)-Si(1)-N(1) | -95.87(17) |
| C(34)-Zr(1)-Si(1)-N(1) | 177.07(16) |
| C(35)-Zr(1)-Si(1)-N(1) | -151.81(14) |
| C(38)-Zr(1)-Si(1)-N(1) | 144.87(14) |
| N(2)-Zr(1)-Si(1)-N(1) | -11.88(13) |
| C(36)-Zr(1)-Si(1)-N(1) | -168.04(14) |
| C(37)-Zr(1)-Si(1)-N(1) | 159.97(14) |
| C(1)-Zr(1)-Si(1)-N(1) | -5.28(14) |
| N(1)-Zr(1)-Si(1)-C(33) | -83.62(18) |
| C(30)-Zr(1)-Si(1)-C(33) | -7.18(15) |
| C(31)-Zr(1)-Si(1)-C(33) | -179.49(16) |
| C(34)-Zr(1)-Si(1)-C(33) | 93.45(15) |
| C(35)-Zr(1)-Si(1)-C(33) | 124.57(14) |
| C(38)-Zr(1)-Si(1)-C(33) | 61.25(14) |
| N(2)-Zr(1)-Si(1)-C(33) | -95.50(13) |
| C(36)-Zr(1)-Si(1)-C(33) | 108.34(13) |
| C(37)-Zr(1)-Si(1)-C(33) | 76.35(14) |

| | |
|---|---|
| C(1)-Zr(1)-Si(1)-C(33) | -88.91(14) |
| N(1)-Zr(1)-Si(1)-C(32) | 84.55(18) |
| C(30)-Zr(1)-Si(1)-C(32) | 160.99(15) |
| C(31)-Zr(1)-Si(1)-C(32) | -11.32(17) |
| C(34)-Zr(1)-Si(1)-C(32) | -98.38(16) |
| C(35)-Zr(1)-Si(1)-C(32) | -67.26(14) |
| C(38)-Zr(1)-Si(1)-C(32) | -130.58(14) |
| N(2)-Zr(1)-Si(1)-C(32) | 72.67(13) |
| C(36)-Zr(1)-Si(1)-C(32) | -83.49(14) |
| C(37)-Zr(1)-Si(1)-C(32) | -115.48(14) |
| C(1)-Zr(1)-Si(1)-C(32) | 79.27(14) |
| N(1)-Zr(1)-Si(1)-C(34) | -177.07(16) |
| C(30)-Zr(1)-Si(1)-C(34) | -100.63(13) |
| C(31)-Zr(1)-Si(1)-C(34) | 87.06(14) |
| C(35)-Zr(1)-Si(1)-C(34) | 31.12(11) |
| C(38)-Zr(1)-Si(1)-C(34) | -32.20(11) |
| N(2)-Zr(1)-Si(1)-C(34) | 171.05(11) |
| C(36)-Zr(1)-Si(1)-C(34) | 14.89(11) |
| C(37)-Zr(1)-Si(1)-C(34) | -17.10(11) |
| C(1)-Zr(1)-Si(1)-C(34) | 177.64(11) |
| C(33)-Si(1)-N(1)-C(1) | -73.9(4) |
| C(32)-Si(1)-N(1)-C(1) | 46.9(4) |
| C(34)-Si(1)-N(1)-C(1) | 166.1(4) |
| Zr(1)-Si(1)-N(1)-C(1) | 163.8(4) |
| C(33)-Si(1)-N(1)-Zr(1) | 122.31(13) |
| C(32)-Si(1)-N(1)-Zr(1) | -116.95(14) |
| C(34)-Si(1)-N(1)-Zr(1) | 2.28(12) |
| C(30)-Zr(1)-N(1)-C(1) | 73.64(18) |
| C(31)-Zr(1)-N(1)-C(1) | -53.9(2) |
| C(34)-Zr(1)-N(1)-C(1) | -172.19(19) |
| C(35)-Zr(1)-N(1)-C(1) | -145.85(17) |
| C(38)-Zr(1)-N(1)-C(1) | 159.62(18) |
| N(2)-Zr(1)-N(1)-C(1) | -4.59(15) |

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| C(36)-Zr(1)-N(1)-C(1) | -156.49(16) |
| C(37)-Zr(1)-N(1)-C(1) | 166.91(15) |
| Si(1)-Zr(1)-N(1)-C(1) | -170.3(3) |
| C(30)-Zr(1)-N(1)-Si(1) | -116.05(13) |
| C(31)-Zr(1)-N(1)-Si(1) | 116.45(13) |
| C(34)-Zr(1)-N(1)-Si(1) | -1.89(10) |
| C(35)-Zr(1)-N(1)-Si(1) | 24.45(12) |
| C(38)-Zr(1)-N(1)-Si(1) | -30.08(12) |
| N(2)-Zr(1)-N(1)-Si(1) | 165.71(16) |
| C(36)-Zr(1)-N(1)-Si(1) | 13.81(16) |
| C(37)-Zr(1)-N(1)-Si(1) | -22.79(15) |
| C(1)-Zr(1)-N(1)-Si(1) | 170.3(3) |
| Si(1)-N(1)-C(1)-N(2) | -156.6(3) |
| Zr(1)-N(1)-C(1)-N(2) | 7.6(2) |
| Si(1)-N(1)-C(1)-C(5) | 24.0(5) |
| Zr(1)-N(1)-C(1)-C(5) | -171.9(2) |
| Si(1)-N(1)-C(1)-Zr(1) | -164.2(4) |
| C(30)-Zr(1)-C(1)-N(1) | -112.42(18) |
| C(31)-Zr(1)-C(1)-N(1) | 139.77(18) |
| C(34)-Zr(1)-C(1)-N(1) | 7.21(18) |
| C(35)-Zr(1)-C(1)-N(1) | 37.08(19) |
| C(38)-Zr(1)-C(1)-N(1) | -22.07(19) |
| N(2)-Zr(1)-C(1)-N(1) | 172.0(3) |
| C(36)-Zr(1)-C(1)-N(1) | 36.1(2) |
| C(37)-Zr(1)-C(1)-N(1) | -20.1(2) |
| Si(1)-Zr(1)-C(1)-N(1) | 5.81(15) |
| N(1)-Zr(1)-C(1)-N(2) | -172.0(3) |
| C(30)-Zr(1)-C(1)-N(2) | 75.53(15) |
| C(31)-Zr(1)-C(1)-N(2) | -32.28(16) |
| C(34)-Zr(1)-C(1)-N(2) | -164.84(14) |
| C(35)-Zr(1)-C(1)-N(2) | -134.96(14) |
| C(38)-Zr(1)-C(1)-N(2) | 165.88(13) |
| C(36)-Zr(1)-C(1)-N(2) | -135.96(15) |

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| C(37)-Zr(1)-C(1)-N(2) | 167.82(14) |
| Si(1)-Zr(1)-C(1)-N(2) | -166.24(16) |
| N(1)-Zr(1)-C(1)-C(5) | 54.3(13) |
| C(30)-Zr(1)-C(1)-C(5) | -58.1(14) |
| C(31)-Zr(1)-C(1)-C(5) | -166.0(14) |
| C(34)-Zr(1)-C(1)-C(5) | 61.5(14) |
| C(35)-Zr(1)-C(1)-C(5) | 91.4(14) |
| C(38)-Zr(1)-C(1)-C(5) | 32.2(14) |
| N(2)-Zr(1)-C(1)-C(5) | -133.7(14) |
| C(36)-Zr(1)-C(1)-C(5) | 90.4(14) |
| C(37)-Zr(1)-C(1)-C(5) | 34.1(14) |
| Si(1)-Zr(1)-C(1)-C(5) | 60.1(14) |
| N(1)-C(1)-N(2)-C(2) | 177.2(2) |
| C(5)-C(1)-N(2)-C(2) | -3.3(4) |
| Zr(1)-C(1)-N(2)-C(2) | -176.6(2) |
| N(1)-C(1)-N(2)-Zr(1) | -6.2(2) |
| C(5)-C(1)-N(2)-Zr(1) | 173.2(2) |
| N(1)-Zr(1)-N(2)-C(2) | 177.7(4) |
| C(30)-Zr(1)-N(2)-C(2) | 66.7(4) |
| C(31)-Zr(1)-N(2)-C(2) | -36.0(4) |
| C(34)-Zr(1)-N(2)-C(2) | -168.8(3) |
| C(35)-Zr(1)-N(2)-C(2) | -128.0(3) |
| C(38)-Zr(1)-N(2)-C(2) | 152.8(3) |
| C(36)-Zr(1)-N(2)-C(2) | -94.0(4) |
| C(37)-Zr(1)-N(2)-C(2) | 124.3(5) |
| C(1)-Zr(1)-N(2)-C(2) | 173.3(4) |
| Si(1)-Zr(1)-N(2)-C(2) | -175.0(4) |
| N(1)-Zr(1)-N(2)-C(1) | 4.42(14) |
| C(30)-Zr(1)-N(2)-C(1) | -106.57(15) |
| C(31)-Zr(1)-N(2)-C(1) | 150.74(15) |
| C(34)-Zr(1)-N(2)-C(1) | 17.94(17) |
| C(35)-Zr(1)-N(2)-C(1) | 58.70(17) |
| C(38)-Zr(1)-N(2)-C(1) | -20.49(19) |

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| C(36)-Zr(1)-N(2)-C(1) | 92.7(2) |
| C(37)-Zr(1)-N(2)-C(1) | -49.0(5) |
| Si(1)-Zr(1)-N(2)-C(1) | 11.68(13) |
| C(1)-N(2)-C(2)-C(3) | 4.2(3) |
| Zr(1)-N(2)-C(2)-C(3) | -168.1(3) |
| C(1)-N(2)-C(2)-C(6) | -173.4(2) |
| Zr(1)-N(2)-C(2)-C(6) | 14.2(5) |
| N(2)-C(2)-C(3)-C(4) | -2.5(4) |
| C(6)-C(2)-C(3)-C(4) | 175.1(2) |
| C(2)-C(3)-C(4)-C(5) | -0.2(4) |
| C(3)-C(4)-C(5)-C(1) | 1.0(4) |
| N(1)-C(1)-C(5)-C(4) | -179.9(2) |
| N(2)-C(1)-C(5)-C(4) | 0.7(4) |
| Zr(1)-C(1)-C(5)-C(4) | 131.1(13) |
| N(2)-C(2)-C(6)-C(11) | -56.1(3) |
| C(3)-C(2)-C(6)-C(11) | 126.2(3) |
| N(2)-C(2)-C(6)-C(7) | 125.6(2) |
| C(3)-C(2)-C(6)-C(7) | -52.1(3) |
| C(11)-C(6)-C(7)-C(8) | 0.3(4) |
| C(2)-C(6)-C(7)-C(8) | 178.6(2) |
| C(11)-C(6)-C(7)-B(1) | 172.7(2) |
| C(2)-C(6)-C(7)-B(1) | -9.1(4) |
| C(12)-B(1)-C(7)-C(8) | 138.0(3) |
| C(21)-B(1)-C(7)-C(8) | -36.7(3) |
| C(12)-B(1)-C(7)-C(6) | -34.3(4) |
| C(21)-B(1)-C(7)-C(6) | 151.0(2) |
| C(6)-C(7)-C(8)-C(9) | 1.5(4) |
| B(1)-C(7)-C(8)-C(9) | -171.6(2) |
| C(7)-C(8)-C(9)-C(10) | -2.5(4) |
| C(8)-C(9)-C(10)-C(11) | 1.5(4) |
| C(9)-C(10)-C(11)-C(6) | 0.3(4) |
| C(7)-C(6)-C(11)-C(10) | -1.3(4) |
| C(2)-C(6)-C(11)-C(10) | -179.6(2) |

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| C(21)-B(1)-C(12)-C(17) | -55.1(3) |
| C(7)-B(1)-C(12)-C(17) | 130.4(3) |
| C(21)-B(1)-C(12)-C(13) | 122.1(3) |
| C(7)-B(1)-C(12)-C(13) | -52.5(3) |
| C(17)-C(12)-C(13)-C(14) | -0.7(3) |
| B(1)-C(12)-C(13)-C(14) | -178.0(2) |
| C(17)-C(12)-C(13)-C(18) | 175.5(2) |
| B(1)-C(12)-C(13)-C(18) | -1.7(3) |
| C(12)-C(13)-C(14)-C(15) | -1.0(4) |
| C(18)-C(13)-C(14)-C(15) | -177.3(2) |
| C(13)-C(14)-C(15)-C(16) | 0.9(4) |
| C(13)-C(14)-C(15)-C(19) | 179.4(2) |
| C(14)-C(15)-C(16)-C(17) | 1.0(4) |
| C(19)-C(15)-C(16)-C(17) | -177.6(2) |
| C(15)-C(16)-C(17)-C(12) | -2.7(4) |
| C(15)-C(16)-C(17)-C(20) | 177.6(2) |
| C(13)-C(12)-C(17)-C(16) | 2.5(3) |
| B(1)-C(12)-C(17)-C(16) | 179.7(2) |
| C(13)-C(12)-C(17)-C(20) | -177.8(2) |
| B(1)-C(12)-C(17)-C(20) | -0.6(4) |
| C(12)-B(1)-C(21)-C(26) | -48.0(4) |
| C(7)-B(1)-C(21)-C(26) | 126.7(3) |
| C(12)-B(1)-C(21)-C(22) | 132.9(3) |
| C(7)-B(1)-C(21)-C(22) | -52.4(3) |
| C(26)-C(21)-C(22)-C(23) | -0.2(4) |
| B(1)-C(21)-C(22)-C(23) | 179.0(2) |
| C(26)-C(21)-C(22)-C(27) | 175.2(2) |
| B(1)-C(21)-C(22)-C(27) | -5.6(4) |
| C(21)-C(22)-C(23)-C(24) | -0.5(4) |
| C(27)-C(22)-C(23)-C(24) | -176.2(2) |
| C(22)-C(23)-C(24)-C(25) | 0.4(4) |
| C(22)-C(23)-C(24)-C(28) | 178.8(2) |
| C(23)-C(24)-C(25)-C(26) | 0.4(4) |

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| C(28)-C(24)-C(25)-C(26) | -178.0(2) |
| C(24)-C(25)-C(26)-C(21) | -1.1(4) |
| C(24)-C(25)-C(26)-C(29) | -179.2(3) |
| C(22)-C(21)-C(26)-C(25) | 1.0(4) |
| B(1)-C(21)-C(26)-C(25) | -178.2(2) |
| C(22)-C(21)-C(26)-C(29) | 178.9(2) |
| B(1)-C(21)-C(26)-C(29) | -0.2(4) |
| N(1)-Si(1)-C(34)-C(35) | -73.7(2) |
| C(33)-Si(1)-C(34)-C(35) | 166.3(2) |
| C(32)-Si(1)-C(34)-C(35) | 41.9(3) |
| Zr(1)-Si(1)-C(34)-C(35) | -71.8(2) |
| N(1)-Si(1)-C(34)-C(38) | 71.7(2) |
| C(33)-Si(1)-C(34)-C(38) | -48.3(2) |
| C(32)-Si(1)-C(34)-C(38) | -172.8(2) |
| Zr(1)-Si(1)-C(34)-C(38) | 73.54(19) |
| N(1)-Si(1)-C(34)-Zr(1) | -1.88(10) |
| C(33)-Si(1)-C(34)-Zr(1) | -121.89(12) |
| C(32)-Si(1)-C(34)-Zr(1) | 113.68(13) |
| N(1)-Zr(1)-C(34)-C(35) | 126.63(16) |
| C(30)-Zr(1)-C(34)-C(35) | -135.18(15) |
| C(31)-Zr(1)-C(34)-C(35) | -0.75(19) |
| C(38)-Zr(1)-C(34)-C(35) | -112.2(2) |
| N(2)-Zr(1)-C(34)-C(35) | 114.45(15) |
| C(36)-Zr(1)-C(34)-C(35) | -36.66(14) |
| C(37)-Zr(1)-C(34)-C(35) | -76.12(16) |
| C(1)-Zr(1)-C(34)-C(35) | 123.01(15) |
| Si(1)-Zr(1)-C(34)-C(35) | 125.01(18) |
| N(1)-Zr(1)-C(34)-C(38) | -121.19(17) |
| C(30)-Zr(1)-C(34)-C(38) | -23.01(19) |
| C(31)-Zr(1)-C(34)-C(38) | 111.43(16) |
| C(35)-Zr(1)-C(34)-C(38) | 112.2(2) |
| N(2)-Zr(1)-C(34)-C(38) | -133.38(15) |
| C(36)-Zr(1)-C(34)-C(38) | 75.52(16) |

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| C(37)-Zr(1)-C(34)-C(38) | 36.05(14) |
| C(1)-Zr(1)-C(34)-C(38) | -124.82(15) |
| Si(1)-Zr(1)-C(34)-C(38) | -122.81(19) |
| N(1)-Zr(1)-C(34)-Si(1) | 1.62(9) |
| C(30)-Zr(1)-C(34)-Si(1) | 99.81(12) |
| C(31)-Zr(1)-C(34)-Si(1) | -125.76(11) |
| C(35)-Zr(1)-C(34)-Si(1) | -125.01(18) |
| C(38)-Zr(1)-C(34)-Si(1) | 122.81(19) |
| N(2)-Zr(1)-C(34)-Si(1) | -10.56(13) |
| C(36)-Zr(1)-C(34)-Si(1) | -161.67(13) |
| C(37)-Zr(1)-C(34)-Si(1) | 158.86(13) |
| C(1)-Zr(1)-C(34)-Si(1) | -2.01(10) |
| C(38)-C(34)-C(35)-C(36) | 1.2(3) |
| Si(1)-C(34)-C(35)-C(36) | 151.19(19) |
| Zr(1)-C(34)-C(35)-C(36) | 69.60(18) |
| C(38)-C(34)-C(35)-C(39) | -179.4(2) |
| Si(1)-C(34)-C(35)-C(39) | -29.5(4) |
| Zr(1)-C(34)-C(35)-C(39) | -111.1(3) |
| C(38)-C(34)-C(35)-Zr(1) | -68.38(17) |
| Si(1)-C(34)-C(35)-Zr(1) | 81.59(18) |
| N(1)-Zr(1)-C(35)-C(36) | -162.67(15) |
| C(30)-Zr(1)-C(35)-C(36) | -47.4(2) |
| C(31)-Zr(1)-C(35)-C(36) | 64.40(15) |
| C(34)-Zr(1)-C(35)-C(36) | -115.0(2) |
| C(38)-Zr(1)-C(35)-C(36) | -76.18(15) |
| N(2)-Zr(1)-C(35)-C(36) | 154.84(13) |
| C(37)-Zr(1)-C(35)-C(36) | -36.22(14) |
| C(1)-Zr(1)-C(35)-C(36) | -178.92(14) |
| Si(1)-Zr(1)-C(35)-C(36) | -148.71(16) |
| N(1)-Zr(1)-C(35)-C(34) | -47.67(15) |
| C(30)-Zr(1)-C(35)-C(34) | 67.6(2) |
| C(31)-Zr(1)-C(35)-C(34) | 179.39(15) |
| C(38)-Zr(1)-C(35)-C(34) | 38.82(14) |

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| N(2)-Zr(1)-C(35)-C(34) | -90.16(16) |
| C(36)-Zr(1)-C(35)-C(34) | 115.0(2) |
| C(37)-Zr(1)-C(35)-C(34) | 78.78(16) |
| C(1)-Zr(1)-C(35)-C(34) | -63.92(16) |
| Si(1)-Zr(1)-C(35)-C(34) | -33.71(13) |
| N(1)-Zr(1)-C(35)-C(39) | 75.9(2) |
| C(30)-Zr(1)-C(35)-C(39) | -168.93(19) |
| C(31)-Zr(1)-C(35)-C(39) | -57.1(2) |
| C(34)-Zr(1)-C(35)-C(39) | 123.5(3) |
| C(38)-Zr(1)-C(35)-C(39) | 162.3(2) |
| N(2)-Zr(1)-C(35)-C(39) | 33.4(2) |
| C(36)-Zr(1)-C(35)-C(39) | -121.5(3) |
| C(37)-Zr(1)-C(35)-C(39) | -157.7(2) |
| C(1)-Zr(1)-C(35)-C(39) | 59.6(2) |
| Si(1)-Zr(1)-C(35)-C(39) | 89.8(2) |
| C(34)-C(35)-C(36)-C(37) | -1.5(3) |
| C(39)-C(35)-C(36)-C(37) | 179.2(2) |
| Zr(1)-C(35)-C(36)-C(37) | 65.06(18) |
| C(34)-C(35)-C(36)-C(40) | 171.9(2) |
| C(39)-C(35)-C(36)-C(40) | -7.4(4) |
| Zr(1)-C(35)-C(36)-C(40) | -121.5(3) |
| C(34)-C(35)-C(36)-Zr(1) | -66.54(18) |
| C(39)-C(35)-C(36)-Zr(1) | 114.1(2) |
| N(1)-Zr(1)-C(36)-C(37) | -95.78(16) |
| C(30)-Zr(1)-C(36)-C(37) | 31.87(18) |
| C(31)-Zr(1)-C(36)-C(37) | 131.01(16) |
| C(34)-Zr(1)-C(36)-C(37) | -78.02(16) |
| C(35)-Zr(1)-C(36)-C(37) | -115.8(2) |
| C(38)-Zr(1)-C(36)-C(37) | -36.47(14) |
| N(2)-Zr(1)-C(36)-C(37) | -169.04(17) |
| C(1)-Zr(1)-C(36)-C(37) | -114.13(17) |
| Si(1)-Zr(1)-C(36)-C(37) | -88.78(15) |
| N(1)-Zr(1)-C(36)-C(35) | 20.07(17) |

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| C(30)-Zr(1)-C(36)-C(35) | 147.71(15) |
| C(31)-Zr(1)-C(36)-C(35) | -113.15(16) |
| C(34)-Zr(1)-C(36)-C(35) | 37.82(14) |
| C(38)-Zr(1)-C(36)-C(35) | 79.38(16) |
| N(2)-Zr(1)-C(36)-C(35) | -53.2(3) |
| C(37)-Zr(1)-C(36)-C(35) | 115.8(2) |
| C(1)-Zr(1)-C(36)-C(35) | 1.7(2) |
| Si(1)-Zr(1)-C(36)-C(35) | 27.06(14) |
| N(1)-Zr(1)-C(36)-C(40) | 142.25(19) |
| C(30)-Zr(1)-C(36)-C(40) | -90.1(2) |
| C(31)-Zr(1)-C(36)-C(40) | 9.0(2) |
| C(34)-Zr(1)-C(36)-C(40) | 160.0(2) |
| C(35)-Zr(1)-C(36)-C(40) | 122.2(3) |
| C(38)-Zr(1)-C(36)-C(40) | -158.4(2) |
| N(2)-Zr(1)-C(36)-C(40) | 69.0(3) |
| C(37)-Zr(1)-C(36)-C(40) | -122.0(3) |
| C(1)-Zr(1)-C(36)-C(40) | 123.9(2) |
| Si(1)-Zr(1)-C(36)-C(40) | 149.2(2) |
| C(35)-C(36)-C(37)-C(38) | 1.2(3) |
| C(40)-C(36)-C(37)-C(38) | -172.5(2) |
| Zr(1)-C(36)-C(37)-C(38) | 63.55(18) |
| C(35)-C(36)-C(37)-C(41) | 177.6(2) |
| C(40)-C(36)-C(37)-C(41) | 4.0(4) |
| Zr(1)-C(36)-C(37)-C(41) | -120.0(2) |
| C(35)-C(36)-C(37)-Zr(1) | -62.39(17) |
| C(40)-C(36)-C(37)-Zr(1) | 124.0(3) |
| N(1)-Zr(1)-C(37)-C(38) | -13.77(17) |
| C(30)-Zr(1)-C(37)-C(38) | 93.26(16) |
| C(31)-Zr(1)-C(37)-C(38) | -164.75(15) |
| C(34)-Zr(1)-C(37)-C(38) | -37.53(14) |
| C(35)-Zr(1)-C(37)-C(38) | -79.21(16) |
| N(2)-Zr(1)-C(37)-C(38) | 35.3(5) |
| C(36)-Zr(1)-C(37)-C(38) | -116.1(2) |

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| C(1)-Zr(1)-C(37)-C(38) | -3.4(2) |
| Si(1)-Zr(1)-C(37)-C(38) | -25.17(14) |
| N(1)-Zr(1)-C(37)-C(36) | 102.33(16) |
| C(30)-Zr(1)-C(37)-C(36) | -150.65(17) |
| C(31)-Zr(1)-C(37)-C(36) | -48.65(16) |
| C(34)-Zr(1)-C(37)-C(36) | 78.57(16) |
| C(35)-Zr(1)-C(37)-C(36) | 36.89(15) |
| C(38)-Zr(1)-C(37)-C(36) | 116.1(2) |
| N(2)-Zr(1)-C(37)-C(36) | 151.4(4) |
| C(1)-Zr(1)-C(37)-C(36) | 112.73(17) |
| Si(1)-Zr(1)-C(37)-C(36) | 90.93(15) |
| N(1)-Zr(1)-C(37)-C(41) | -136.0(2) |
| C(30)-Zr(1)-C(37)-C(41) | -29.0(2) |
| C(31)-Zr(1)-C(37)-C(41) | 73.0(2) |
| C(34)-Zr(1)-C(37)-C(41) | -159.8(3) |
| C(35)-Zr(1)-C(37)-C(41) | 158.5(3) |
| C(38)-Zr(1)-C(37)-C(41) | -122.3(3) |
| N(2)-Zr(1)-C(37)-C(41) | -86.9(5) |
| C(36)-Zr(1)-C(37)-C(41) | 121.6(3) |
| C(1)-Zr(1)-C(37)-C(41) | -125.6(2) |
| Si(1)-Zr(1)-C(37)-C(41) | -147.4(2) |
| C(36)-C(37)-C(38)-C(34) | -0.4(3) |
| C(41)-C(37)-C(38)-C(34) | -176.8(2) |
| Zr(1)-C(37)-C(38)-C(34) | 64.91(17) |
| C(36)-C(37)-C(38)-C(42) | 179.2(2) |
| C(41)-C(37)-C(38)-C(42) | 2.8(4) |
| Zr(1)-C(37)-C(38)-C(42) | -115.5(3) |
| C(36)-C(37)-C(38)-Zr(1) | -65.32(18) |
| C(41)-C(37)-C(38)-Zr(1) | 118.3(3) |
| C(35)-C(34)-C(38)-C(37) | -0.5(3) |
| Si(1)-C(34)-C(38)-C(37) | -151.19(19) |
| Zr(1)-C(34)-C(38)-C(37) | -68.04(18) |
| C(35)-C(34)-C(38)-C(42) | 179.9(2) |

| | |
|---|---|
| Si(1)-C(34)-C(38)-C(42) | 29.2(4) |
| Zr(1)-C(34)-C(38)-C(42) | 112.4(2) |
| C(35)-C(34)-C(38)-Zr(1) | 67.54(17) |
| Si(1)-C(34)-C(38)-Zr(1) | -83.15(17) |
| N(1)-Zr(1)-C(38)-C(37) | 167.83(15) |
| C(30)-Zr(1)-C(38)-C(37) | -84.42(15) |
| C(31)-Zr(1)-C(38)-C(37) | 19.98(19) |
| C(34)-Zr(1)-C(38)-C(37) | 115.7(2) |
| C(35)-Zr(1)-C(38)-C(37) | 76.76(16) |
| N(2)-Zr(1)-C(38)-C(37) | -171.61(13) |
| C(36)-Zr(1)-C(38)-C(37) | 36.25(14) |
| C(1)-Zr(1)-C(38)-C(37) | 177.89(13) |
| Si(1)-Zr(1)-C(38)-C(37) | 150.72(16) |
| N(1)-Zr(1)-C(38)-C(34) | 52.13(16) |
| C(30)-Zr(1)-C(38)-C(34) | 159.88(17) |
| C(31)-Zr(1)-C(38)-C(34) | -95.72(18) |
| C(35)-Zr(1)-C(38)-C(34) | -38.94(15) |
| N(2)-Zr(1)-C(38)-C(34) | 72.69(18) |
| C(36)-Zr(1)-C(38)-C(34) | -79.45(16) |
| C(37)-Zr(1)-C(38)-C(34) | -115.7(2) |
| C(1)-Zr(1)-C(38)-C(34) | 62.19(16) |
| Si(1)-Zr(1)-C(38)-C(34) | 35.02(13) |
| N(1)-Zr(1)-C(38)-C(42) | -69.4(2) |
| C(30)-Zr(1)-C(38)-C(42) | 38.3(2) |
| C(31)-Zr(1)-C(38)-C(42) | 142.73(19) |
| C(34)-Zr(1)-C(38)-C(42) | -121.5(3) |
| C(35)-Zr(1)-C(38)-C(42) | -160.5(2) |
| N(2)-Zr(1)-C(38)-C(42) | -48.9(2) |
| C(36)-Zr(1)-C(38)-C(42) | 159.0(2) |
| C(37)-Zr(1)-C(38)-C(42) | 122.8(3) |
| C(1)-Zr(1)-C(38)-C(42) | -59.4(2) |
| Si(1)-Zr(1)-C(38)-C(42) | -86.53(19) |

**Table S7.** Crystal data and structure refinement for **L´Zr(Bn)$_2$**.

| | |
|---|---|
| Empirical formula | C54H61BN2SiZr |
| Formula weight | 868.17 |
| Temperature | 110(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, space group | Monoclinic, P 21/c |
| Unit cell dimensions | a = 27.914(2) Å α = 90º. |
| | b = 16.0147(9) Å β= 95.322(4)º. |
| | c = 10.2151(7) Å γ= 90º. |
| Volume | 4546.8(5) Å$^3$ |
| Z, Calculated density | 4, 1.268 mg/m$^3$ |
| Absorption coefficient | 0.307 mm$^{-1}$ |
| F(000) | 1832 |
| Crystal size | 0.15 x 0.15 x 0.08 mm |
| Theta range for data collection | 1.47 to 25.06º. |
| Limiting indices | -31<=h<=33, -17<=k<=19, -12<=l<=11 |
| Reflections collected / unique | 29530 / 8047 [R(int) = 0.1167] |
| Completeness to theta = 25.06 | 99.7 % |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.7452 and 0.6702 |
| Refinement method | Full-matrix least-squares on F$^2$ |
| Data / restraints / parameters | 8047 / 36 / 544 |
| Goodness-of-fit on F$^2$ | 1.061 |
| Final R indices [I>2σ (I)] | R1 = 0.0651, wR2 = 0.1143 |
| R indices (all data) | R1 = 0.2007, wR2 = 0.1337 |
| Largest diff. peak and hole | 0.901 and -0.892 e.A$^{-3}$ |

**Table S8.** Atomic coordinates (×$10^4$) and equivalent isotropic displacement parameters ($A^2$ × $10^3$) for **L´Zr(Bn)$_2$**. U(eq) is defined as one third of the trace of the orthogonalized $U_{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Zr(1) | 1541(1) | 4517(1) | 760(1) | 36(1) |
| Si(1) | 2139(1) | 4165(1) | 3380(2) | 65(1) |
| B(1) | 3730(3) | 5749(4) | -1719(7) | 41(2) |
| N(1) | 2169(2) | 4766(3) | 1973(4) | 45(2) |
| N(2) | 2514(2) | 5560(3) | 397(4) | 28(1) |
| C(1) | 2540(3) | 5278(3) | 1654(5) | 36(2) |
| C(2) | 2880(2) | 6031(3) | 19(5) | 28(2) |
| C(3) | 3266(3) | 6253(3) | 869(6) | 47(2) |
| C(4) | 3300(3) | 5968(4) | 2164(7) | 65(2) |
| C(5) | 2932(3) | 5485(5) | 2551(6) | 65(2) |
| C(6) | 2851(2) | 6307(3) | -1373(5) | 28(2) |
| C(7) | 3240(2) | 6224(3) | -2144(5) | 34(2) |
| C(8) | 3171(2) | 6509(3) | -3440(6) | 44(2) |
| C(9) | 2748(2) | 6865(3) | -3976(6) | 42(2) |
| C(10) | 2375(2) | 6958(3) | -3193(6) | 36(2) |
| C(11) | 2429(2) | 6690(3) | -1900(5) | 30(2) |
| C(12) | 4186(3) | 6095(4) | -2321(7) | 56(2) |
| C(13) | 4441(3) | 5636(6) | -3141(9) | 91(3) |
| C(14) | 4818(3) | 6000(8) | -3777(9) | 123(4) |
| C(15) | 4950(4) | 6786(7) | -3581(10) | 109(4) |
| C(16) | 4733(3) | 7272(5) | -2724(8) | 81(3) |
| C(17) | 4340(3) | 6933(5) | -2100(8) | 70(2) |
| C(18) | 4313(4) | 4725(6) | -3397(10) | 149(5) |
| C(19) | 5348(4) | 7225(6) | -4313(9) | 138(4) |
| C(20) | 4109(3) | 7489(4) | -1146(9) | 90(3) |
| C(21) | 3738(2) | 4923(3) | -904(6) | 40(2) |
| C(22) | 4084(2) | 4782(3) | 186(6) | 42(2) |
| C(23) | 4080(2) | 4055(4) | 925(6) | 40(2) |

| | | | | |
|---|---|---|---|---|
| C(24) | 3745(3) | 3442(3) | 629(6) | 40(2) |
| C(25) | 3410(2) | 3549(3) | -456(6) | 38(2) |
| C(26) | 3399(2) | 4276(3) | -1215(5) | 33(2) |
| C(27) | 4452(2) | 5445(4) | 646(7) | 64(2) |
| C(28) | 3728(3) | 2650(3) | 1441(6) | 55(2) |
| C(29) | 3024(2) | 4330(3) | -2378(5) | 37(2) |
| C(30) | 2656(3) | 3430(5) | 3694(7) | 100(3) |
| C(31) | 2110(3) | 4800(4) | 4906(5) | 66(2) |
| C(32) | 1564(3) | 3660(4) | 2732(5) | 45(2) |
| C(33) | 1518(3) | 3081(3) | 1648(6) | 50(2) |
| C(34) | 1068(3) | 3136(3) | 1009(6) | 53(2) |
| C(35) | 814(3) | 3777(3) | 1626(6) | 51(2) |
| C(36) | 1112(3) | 4075(3) | 2704(6) | 42(2) |
| C(37) | 1920(3) | 2492(4) | 1296(7) | 106(4) |
| C(38) | 842(3) | 2545(3) | -34(6) | 98(4) |
| C(39) | 311(3) | 4020(4) | 1252(6) | 67(3) |
| C(40) | 952(2) | 4670(3) | 3743(5) | 36(2) |
| C(41) | 1177(2) | 5791(3) | 592(5) | 29(2) |
| C(42) | 1045(2) | 6282(3) | 1745(5) | 25(2) |
| C(43) | 1396(2) | 6598(3) | 2673(5) | 26(2) |
| C(44) | 1275(2) | 7036(3) | 3770(5) | 34(2) |
| C(45) | 799(3) | 7179(3) | 3965(5) | 35(2) |
| C(46) | 447(2) | 6880(3) | 3062(5) | 33(2) |
| C(47) | 565(2) | 6443(3) | 1965(5) | 29(2) |
| C(48) | 1729(3) | 3907(3) | -1123(5) | 51(2) |
| C(49) | 1385(2) | 4444(3) | -1907(5) | 33(2) |
| C(50) | 1519(3) | 5261(3) | -2241(5) | 38(2) |
| C(51) | 1196(3) | 5799(4) | -2877(5) | 39(2) |
| C(52) | 723(3) | 5561(4) | -3191(5) | 47(2) |
| C(53) | 577(3) | 4768(4) | -2873(6) | 57(2) |
| C(54) | 898(3) | 4239(4) | -2226(6) | 46(2) |

**Table S9.** Bond lengths [Å] and angles [º] for **L´Zr(Bn)$_2$**.

| | |
|---|---|
| Zr(1)-N(1) | 2.089(6) |
| Zr(1)-C(48) | 2.262(5) |
| Zr(1)-C(41) | 2.279(5) |
| Zr(1)-C(32) | 2.433(5) |
| Zr(1)-C(33) | 2.474(5) |
| Zr(1)-C(36) | 2.514(5) |
| Zr(1)-C(35) | 2.577(7) |
| Zr(1)-C(34) | 2.600(6) |
| Zr(1)-C(49) | 2.722(5) |
| Zr(1)-Si(1) | 3.071(2) |
| Si(1)-N(1) | 1.738(4) |
| Si(1)-C(32) | 1.862(7) |
| Si(1)-C(30) | 1.867(7) |
| Si(1)-C(31) | 1.869(6) |
| B(1)-C(21) | 1.562(8) |
| B(1)-C(12) | 1.565(9) |
| B(1)-C(7) | 1.588(9) |
| N(1)-C(1) | 1.384(7) |
| N(2)-C(2) | 1.355(7) |
| N(2)-C(1) | 1.357(6) |
| C(1)-C(5) | 1.401(9) |
| C(2)-C(3) | 1.367(8) |
| C(2)-C(6) | 1.484(7) |
| C(3)-C(4) | 1.395(8) |
| C(3)-H(3) | 0.9500 |
| C(4)-C(5) | 1.370(9) |
| C(4)-H(4) | 0.9500 |
| C(5)-H(5) | 0.9500 |
| C(6)-C(11) | 1.392(8) |
| C(6)-C(7) | 1.407(7) |
| C(7)-C(8) | 1.397(7) |
| C(8)-C(9) | 1.379(8) |

| | |
|---|---|
| C(8)-H(8) | 0.9500 |
| C(9)-C(10) | 1.378(7) |
| C(9)-H(9) | 0.9500 |
| C(10)-C(11) | 1.384(7) |
| C(10)-H(10) | 0.9500 |
| C(11)-H(11) | 0.9500 |
| C(12)-C(13) | 1.365(10) |
| C(12)-C(17) | 1.421(10) |
| C(13)-C(14) | 1.411(10) |
| C(13)-C(18) | 1.518(11) |
| C(14)-C(15) | 1.321(12) |
| C(14)-H(14) | 0.9500 |
| C(15)-C(16) | 1.356(12) |
| C(15)-C(19) | 1.563(11) |
| C(16)-C(17) | 1.426(9) |
| C(16)-H(16) | 0.9500 |
| C(17)-C(20) | 1.508(10) |
| 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)-C(26) | 1.419(8) |
| C(21)-C(22) | 1.423(8) |
| C(22)-C(23) | 1.389(7) |
| C(22)-C(27) | 1.520(8) |
| C(23)-C(24) | 1.370(8) |
| C(23)-H(23) | 0.9500 |
| C(24)-C(25) | 1.392(8) |

| | |
|---|---|
| C(24)-C(28) | 1.519(7) |
| C(25)-C(26) | 1.397(7) |
| C(25)-H(25) | 0.9500 |
| C(26)-C(29) | 1.512(8) |
| C(27)-H(27A) | 0.9800 |
| C(27)-H(27B) | 0.9800 |
| C(27)-H(27C) | 0.9800 |
| C(28)-H(28A) | 0.9800 |
| C(28)-H(28B) | 0.9800 |
| C(28)-H(28C) | 0.9800 |
| 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(36) | 1.425(8) |
| C(32)-C(33) | 1.441(8) |
| C(33)-C(34) | 1.365(9) |
| C(33)-C(37) | 1.533(9) |
| C(34)-C(35) | 1.426(8) |
| C(34)-C(38) | 1.519(9) |
| C(35)-C(36) | 1.401(9) |
| C(35)-C(39) | 1.472(9) |
| C(36)-C(40) | 1.524(7) |
| C(37)-H(37A) | 0.9800 |
| C(37)-H(37B) | 0.9800 |
| C(37)-H(37C) | 0.9800 |
| 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 |
| C(41)-C(42) | 1.490(6) |
| C(41)-H(41A) | 0.9900 |
| C(41)-H(41B) | 0.9900 |
| C(42)-C(43) | 1.394(7) |
| C(42)-C(47) | 1.403(7) |
| C(43)-C(44) | 1.391(6) |
| C(43)-H(43) | 0.9500 |
| C(44)-C(45) | 1.380(8) |
| C(44)-H(44) | 0.9500 |
| C(45)-C(46) | 1.370(8) |
| C(45)-H(45) | 0.9500 |
| C(46)-C(47) | 1.387(6) |
| C(46)-H(46) | 0.9500 |
| C(47)-H(47) | 0.9500 |
| C(48)-C(49) | 1.471(8) |
| C(48)-H(48A) | 0.9900 |
| C(48)-H(48B) | 0.9900 |
| C(49)-C(54) | 1.406(8) |
| C(49)-C(50) | 1.413(7) |
| C(50)-C(51) | 1.367(8) |
| C(50)-H(50) | 0.9500 |
| C(51)-C(52) | 1.384(8) |
| C(51)-H(51) | 0.9500 |
| C(52)-C(53) | 1.382(8) |
| C(52)-H(52) | 0.9500 |
| C(53)-C(54) | 1.360(9) |

| | |
|---|---|
| C(53)-H(53) | 0.9500 |
| C(54)-H(54) | 0.9500 |

| | |
|---|---|
| N(1)-Zr(1)-C(48) | 109.8(2) |
| N(1)-Zr(1)-C(41) | 102.59(19) |
| C(48)-Zr(1)-C(41) | 117.38(19) |
| N(1)-Zr(1)-C(32) | 70.1(2) |
| C(48)-Zr(1)-C(32) | 118.0(2) |
| C(41)-Zr(1)-C(32) | 123.00(18) |
| N(1)-Zr(1)-C(33) | 90.5(2) |
| C(48)-Zr(1)-C(33) | 85.78(19) |
| C(41)-Zr(1)-C(33) | 146.40(19) |
| C(32)-Zr(1)-C(33) | 34.13(19) |
| N(1)-Zr(1)-C(36) | 91.2(2) |
| C(48)-Zr(1)-C(36) | 135.66(19) |
| C(41)-Zr(1)-C(36) | 93.99(17) |
| C(32)-Zr(1)-C(36) | 33.43(19) |
| C(33)-Zr(1)-C(36) | 54.45(17) |
| N(1)-Zr(1)-C(35) | 121.9(2) |
| C(48)-Zr(1)-C(35) | 110.2(2) |
| C(41)-Zr(1)-C(35) | 94.4(2) |
| C(32)-Zr(1)-C(35) | 54.4(2) |
| C(33)-Zr(1)-C(35) | 53.1(2) |
| C(36)-Zr(1)-C(35) | 31.9(2) |
| N(1)-Zr(1)-C(34) | 120.7(2) |
| C(48)-Zr(1)-C(34) | 82.90(18) |
| C(41)-Zr(1)-C(34) | 122.8(2) |
| C(32)-Zr(1)-C(34) | 54.1(2) |
| C(33)-Zr(1)-C(34) | 31.1(2) |
| C(36)-Zr(1)-C(34) | 53.10(19) |
| C(35)-Zr(1)-C(34) | 31.98(18) |
| N(1)-Zr(1)-C(49) | 130.51(18) |
| C(48)-Zr(1)-C(49) | 32.71(19) |

| | |
|---|---|
| C(41)-Zr(1)-C(49) | 86.23(17) |
| C(32)-Zr(1)-C(49) | 142.56(19) |
| C(33)-Zr(1)-C(49) | 108.65(19) |
| C(36)-Zr(1)-C(49) | 137.3(2) |
| C(35)-Zr(1)-C(49) | 105.4(2) |
| C(34)-Zr(1)-C(49) | 91.47(19) |
| N(1)-Zr(1)-Si(1) | 32.88(12) |
| C(48)-Zr(1)-Si(1) | 120.76(19) |
| C(41)-Zr(1)-Si(1) | 115.60(14) |
| C(32)-Zr(1)-Si(1) | 37.32(17) |
| C(33)-Zr(1)-Si(1) | 62.7(2) |
| C(36)-Zr(1)-Si(1) | 61.35(19) |
| C(35)-Zr(1)-Si(1) | 89.9(2) |
| C(34)-Zr(1)-Si(1) | 89.93(19) |
| C(49)-Zr(1)-Si(1) | 152.63(14) |
| N(1)-Si(1)-C(32) | 93.0(3) |
| N(1)-Si(1)-C(30) | 113.3(3) |
| C(32)-Si(1)-C(30) | 114.4(4) |
| N(1)-Si(1)-C(31) | 113.5(3) |
| C(32)-Si(1)-C(31) | 115.5(3) |
| C(30)-Si(1)-C(31) | 107.0(3) |
| N(1)-Si(1)-Zr(1) | 40.7(2) |
| C(32)-Si(1)-Zr(1) | 52.40(16) |
| C(30)-Si(1)-Zr(1) | 127.9(2) |
| C(31)-Si(1)-Zr(1) | 124.4(2) |
| C(21)-B(1)-C(12) | 122.5(6) |
| C(21)-B(1)-C(7) | 121.4(5) |
| C(12)-B(1)-C(7) | 115.7(5) |
| C(1)-N(1)-Si(1) | 128.1(5) |
| C(1)-N(1)-Zr(1) | 125.4(4) |
| Si(1)-N(1)-Zr(1) | 106.4(3) |
| C(2)-N(2)-C(1) | 118.6(5) |
| N(2)-C(1)-N(1) | 116.3(6) |

| | |
|---|---|
| N(2)-C(1)-C(5) | 120.7(6) |
| N(1)-C(1)-C(5) | 122.9(6) |
| N(2)-C(2)-C(3) | 122.3(5) |
| N(2)-C(2)-C(6) | 117.6(5) |
| C(3)-C(2)-C(6) | 120.1(6) |
| C(2)-C(3)-C(4) | 119.8(6) |
| C(2)-C(3)-H(3) | 120.1 |
| C(4)-C(3)-H(3) | 120.1 |
| C(5)-C(4)-C(3) | 118.2(7) |
| C(5)-C(4)-H(4) | 120.9 |
| C(3)-C(4)-H(4) | 120.9 |
| C(4)-C(5)-C(1) | 120.3(6) |
| C(4)-C(5)-H(5) | 119.8 |
| C(1)-C(5)-H(5) | 119.8 |
| C(11)-C(6)-C(7) | 119.7(5) |
| C(11)-C(6)-C(2) | 118.1(5) |
| C(7)-C(6)-C(2) | 122.1(6) |
| C(8)-C(7)-C(6) | 116.9(6) |
| C(8)-C(7)-B(1) | 117.1(5) |
| C(6)-C(7)-B(1) | 125.6(5) |
| C(9)-C(8)-C(7) | 123.4(6) |
| C(9)-C(8)-H(8) | 118.3 |
| C(7)-C(8)-H(8) | 118.3 |
| C(10)-C(9)-C(8) | 118.7(5) |
| C(10)-C(9)-H(9) | 120.7 |
| C(8)-C(9)-H(9) | 120.7 |
| C(9)-C(10)-C(11) | 119.9(6) |
| C(9)-C(10)-H(10) | 120.0 |
| C(11)-C(10)-H(10) | 120.0 |
| C(10)-C(11)-C(6) | 121.3(5) |
| C(10)-C(11)-H(11) | 119.4 |
| C(6)-C(11)-H(11) | 119.4 |
| C(13)-C(12)-C(17) | 116.0(7) |

| | |
|---|---|
| C(13)-C(12)-B(1) | 122.8(7) |
| C(17)-C(12)-B(1) | 121.1(7) |
| C(12)-C(13)-C(14) | 120.9(9) |
| C(12)-C(13)-C(18) | 119.6(6) |
| C(14)-C(13)-C(18) | 119.5(9) |
| C(15)-C(14)-C(13) | 122.2(10) |
| C(15)-C(14)-H(14) | 118.9 |
| C(13)-C(14)-H(14) | 118.9 |
| C(14)-C(15)-C(16) | 120.6(9) |
| C(14)-C(15)-C(19) | 123.8(11) |
| C(16)-C(15)-C(19) | 115.5(10) |
| C(15)-C(16)-C(17) | 118.6(9) |
| C(15)-C(16)-H(16) | 120.7 |
| C(17)-C(16)-H(16) | 120.7 |
| C(12)-C(17)-C(16) | 121.5(8) |
| C(12)-C(17)-C(20) | 121.3(6) |
| C(16)-C(17)-C(20) | 117.2(8) |
| C(13)-C(18)-H(18A) | 109.5 |
| C(13)-C(18)-H(18B) | 109.5 |
| H(18A)-C(18)-H(18B) | 109.5 |
| C(13)-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(17)-C(20)-H(20A) | 109.5 |
| C(17)-C(20)-H(20B) | 109.5 |
| H(20A)-C(20)-H(20B) | 109.5 |
| C(17)-C(20)-H(20C) | 109.5 |

| | |
|---|---|
| H(20A)-C(20)-H(20C) | 109.5 |
| H(20B)-C(20)-H(20C) | 109.5 |
| C(26)-C(21)-C(22) | 116.8(5) |
| C(26)-C(21)-B(1) | 121.5(6) |
| C(22)-C(21)-B(1) | 121.7(6) |
| C(23)-C(22)-C(21) | 121.2(6) |
| C(23)-C(22)-C(27) | 117.2(6) |
| C(21)-C(22)-C(27) | 121.5(5) |
| C(24)-C(23)-C(22) | 121.4(6) |
| C(24)-C(23)-H(23) | 119.3 |
| C(22)-C(23)-H(23) | 119.3 |
| C(23)-C(24)-C(25) | 118.8(5) |
| C(23)-C(24)-C(28) | 122.2(7) |
| C(25)-C(24)-C(28) | 119.0(6) |
| C(24)-C(25)-C(26) | 121.5(6) |
| C(24)-C(25)-H(25) | 119.3 |
| C(26)-C(25)-H(25) | 119.3 |
| C(25)-C(26)-C(21) | 120.3(6) |
| C(25)-C(26)-C(29) | 117.5(6) |
| C(21)-C(26)-C(29) | 122.2(5) |
| C(22)-C(27)-H(27A) | 109.5 |
| C(22)-C(27)-H(27B) | 109.5 |
| H(27A)-C(27)-H(27B) | 109.5 |
| C(22)-C(27)-H(27C) | 109.5 |
| H(27A)-C(27)-H(27C) | 109.5 |
| H(27B)-C(27)-H(27C) | 109.5 |
| C(24)-C(28)-H(28A) | 109.5 |
| C(24)-C(28)-H(28B) | 109.5 |
| H(28A)-C(28)-H(28B) | 109.5 |
| C(24)-C(28)-H(28C) | 109.5 |
| H(28A)-C(28)-H(28C) | 109.5 |
| H(28B)-C(28)-H(28C) | 109.5 |
| C(26)-C(29)-H(29A) | 109.5 |

| | |
|---|---|
| C(26)-C(29)-H(29B) | 109.5 |
| H(29A)-C(29)-H(29B) | 109.5 |
| C(26)-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 |
| Si(1)-C(31)-H(31A) | 109.5 |
| Si(1)-C(31)-H(31B) | 109.5 |
| H(31A)-C(31)-H(31B) | 109.5 |
| Si(1)-C(31)-H(31C) | 109.5 |
| H(31A)-C(31)-H(31C) | 109.5 |
| H(31B)-C(31)-H(31C) | 109.5 |
| C(36)-C(32)-C(33) | 105.6(6) |
| C(36)-C(32)-Si(1) | 122.5(5) |
| C(33)-C(32)-Si(1) | 124.4(5) |
| C(36)-C(32)-Zr(1) | 76.4(3) |
| C(33)-C(32)-Zr(1) | 74.5(3) |
| Si(1)-C(32)-Zr(1) | 90.3(2) |
| C(34)-C(33)-C(32) | 109.8(6) |
| C(34)-C(33)-C(37) | 126.1(7) |
| C(32)-C(33)-C(37) | 124.2(8) |
| C(34)-C(33)-Zr(1) | 79.5(4) |
| C(32)-C(33)-Zr(1) | 71.4(3) |
| C(37)-C(33)-Zr(1) | 116.2(4) |
| C(33)-C(34)-C(35) | 108.0(7) |
| C(33)-C(34)-C(38) | 126.9(7) |
| C(35)-C(34)-C(38) | 124.5(8) |
| C(33)-C(34)-Zr(1) | 69.4(4) |

| | |
|---|---|
| C(35)-C(34)-Zr(1) | 73.1(3) |
| C(38)-C(34)-Zr(1) | 130.0(4) |
| C(36)-C(35)-C(34) | 108.0(8) |
| C(36)-C(35)-C(39) | 126.6(5) |
| C(34)-C(35)-C(39) | 125.2(7) |
| C(36)-C(35)-Zr(1) | 71.6(4) |
| C(34)-C(35)-Zr(1) | 74.9(4) |
| C(39)-C(35)-Zr(1) | 123.5(4) |
| C(35)-C(36)-C(32) | 108.5(6) |
| C(35)-C(36)-C(40) | 124.8(6) |
| C(32)-C(36)-C(40) | 126.4(7) |
| C(35)-C(36)-Zr(1) | 76.5(3) |
| C(32)-C(36)-Zr(1) | 70.2(3) |
| C(40)-C(36)-Zr(1) | 124.4(3) |
| C(33)-C(37)-H(37A) | 109.5 |
| C(33)-C(37)-H(37B) | 109.5 |
| H(37A)-C(37)-H(37B) | 109.5 |
| C(33)-C(37)-H(37C) | 109.5 |
| H(37A)-C(37)-H(37C) | 109.5 |
| H(37B)-C(37)-H(37C) | 109.5 |
| C(34)-C(38)-H(38A) | 109.5 |
| C(34)-C(38)-H(38B) | 109.5 |
| H(38A)-C(38)-H(38B) | 109.5 |
| C(34)-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(36)-C(40)-H(40A) | 109.5 |

| | |
|---|---|
| C(36)-C(40)-H(40B) | 109.5 |
| H(40A)-C(40)-H(40B) | 109.5 |
| C(36)-C(40)-H(40C) | 109.5 |
| H(40A)-C(40)-H(40C) | 109.5 |
| H(40B)-C(40)-H(40C) | 109.5 |
| C(42)-C(41)-Zr(1) | 123.6(3) |
| C(42)-C(41)-H(41A) | 106.4 |
| Zr(1)-C(41)-H(41A) | 106.4 |
| C(42)-C(41)-H(41B) | 106.4 |
| Zr(1)-C(41)-H(41B) | 106.4 |
| H(41A)-C(41)-H(41B) | 106.5 |
| C(43)-C(42)-C(47) | 116.5(5) |
| C(43)-C(42)-C(41) | 121.2(5) |
| C(47)-C(42)-C(41) | 122.2(5) |
| C(44)-C(43)-C(42) | 121.5(5) |
| C(44)-C(43)-H(43) | 119.2 |
| C(42)-C(43)-H(43) | 119.2 |
| C(45)-C(44)-C(43) | 120.6(6) |
| C(45)-C(44)-H(44) | 119.7 |
| C(43)-C(44)-H(44) | 119.7 |
| C(46)-C(45)-C(44) | 119.0(5) |
| C(46)-C(45)-H(45) | 120.5 |
| C(44)-C(45)-H(45) | 120.5 |
| C(45)-C(46)-C(47) | 120.8(6) |
| C(45)-C(46)-H(46) | 119.6 |
| C(47)-C(46)-H(46) | 119.6 |
| C(46)-C(47)-C(42) | 121.5(6) |
| C(46)-C(47)-H(47) | 119.2 |
| C(42)-C(47)-H(47) | 119.2 |
| C(49)-C(48)-Zr(1) | 91.1(3) |
| C(49)-C(48)-H(48A) | 113.4 |
| Zr(1)-C(48)-H(48A) | 113.4 |
| C(49)-C(48)-H(48B) | 113.4 |

| | |
|---|---|
| Zr(1)-C(48)-H(48B) | 113.4 |
| H(48A)-C(48)-H(48B) | 110.7 |
| C(54)-C(49)-C(50) | 115.7(6) |
| C(54)-C(49)-C(48) | 124.0(6) |
| C(50)-C(49)-C(48) | 119.8(6) |
| C(54)-C(49)-Zr(1) | 107.7(3) |
| C(50)-C(49)-Zr(1) | 100.4(3) |
| C(48)-C(49)-Zr(1) | 56.2(3) |
| C(51)-C(50)-C(49) | 121.3(6) |
| C(51)-C(50)-H(50) | 119.4 |
| C(49)-C(50)-H(50) | 119.4 |
| C(50)-C(51)-C(52) | 120.7(6) |
| C(50)-C(51)-H(51) | 119.6 |
| C(52)-C(51)-H(51) | 119.6 |
| C(53)-C(52)-C(51) | 119.7(7) |
| C(53)-C(52)-H(52) | 120.2 |
| C(51)-C(52)-H(52) | 120.2 |
| C(54)-C(53)-C(52) | 119.4(7) |
| C(54)-C(53)-H(53) | 120.3 |
| C(52)-C(53)-H(53) | 120.3 |
| C(53)-C(54)-C(49) | 123.1(6) |
| C(53)-C(54)-H(54) | 118.4 |
| C(49)-C(54)-H(54) | 118.4 |

**Table S10.** Anisotropic displacement parameters ($A^2 \times 10^3$) for **L´Zr(Bn)$_2$**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$.

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| Zr(1) | 68(1) | 22(1) | 24(1) | 5(1) | 27(1) | 6(1) |
| Si(1) | 90(2) | 76(1) | 36(1) | 38(1) | 42(1) | 55(1) |
| B(1) | 31(6) | 48(4) | 43(4) | 21(3) | 5(4) | -2(4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N(1) | 59(4) | 47(3) | 31(3) | 15(2) | 24(3) | 15(3) |
| N(2) | 36(3) | 32(2) | 17(2) | 2(2) | 4(2) | 7(3) |
| C(1) | 46(5) | 42(4) | 20(3) | 6(3) | -1(3) | 21(3) |
| C(2) | 29(5) | 25(3) | 30(3) | -2(3) | -4(3) | 8(3) |
| C(3) | 45(6) | 46(4) | 47(4) | -2(3) | -13(4) | 3(4) |
| C(4) | 56(7) | 89(5) | 45(5) | -20(4) | -30(4) | 10(5) |
| C(5) | 53(6) | 116(6) | 24(4) | 6(4) | -7(4) | 18(5) |
| C(6) | 32(5) | 17(3) | 35(3) | 8(2) | 1(3) | -5(3) |
| C(7) | 33(5) | 28(3) | 42(4) | 20(3) | 1(3) | -5(3) |
| C(8) | 32(5) | 45(4) | 56(4) | 32(3) | 13(4) | -2(3) |
| C(9) | 40(5) | 44(4) | 41(4) | 32(3) | 3(4) | -2(4) |
| C(10) | 29(5) | 27(3) | 48(4) | 10(3) | -5(3) | -1(3) |
| C(11) | 41(5) | 11(3) | 37(4) | 2(2) | 5(3) | 2(3) |
| C(12) | 25(5) | 77(5) | 67(5) | 47(4) | 1(4) | -13(4) |
| C(13) | 41(6) | 129(8) | 111(7) | 39(6) | 43(5) | -12(6) |
| C(14) | 73(9) | 200(11) | 104(8) | 23(8) | 47(6) | -22(8) |
| C(15) | 81(6) | 145(6) | 100(6) | 38(5) | 7(5) | -46(5) |
| C(16) | 61(5) | 97(5) | 78(5) | 61(4) | -31(4) | -34(4) |
| C(17) | 33(6) | 92(6) | 83(6) | 63(5) | -13(4) | -23(5) |
| C(18) | 114(10) | 156(10) | 200(11) | -19(8) | 135(9) | -4(8) |
| C(19) | 114(6) | 191(7) | 112(6) | 48(5) | 30(5) | -57(5) |
| C(20) | 62(7) | 60(5) | 144(9) | 39(5) | -16(6) | -41(5) |
| C(21) | 28(5) | 38(4) | 56(4) | 14(3) | 14(4) | 9(3) |
| C(22) | 21(5) | 50(4) | 56(4) | 29(3) | 6(4) | 6(3) |
| C(23) | 27(5) | 45(4) | 50(4) | 23(3) | 6(3) | 16(3) |
| C(24) | 46(5) | 34(3) | 43(4) | 12(3) | 27(4) | 17(4) |
| C(25) | 54(5) | 26(3) | 39(4) | 3(3) | 26(4) | 5(3) |
| C(26) | 30(5) | 30(3) | 42(4) | 11(2) | 24(3) | 13(3) |
| C(27) | 19(5) | 73(5) | 98(6) | 53(4) | -7(4) | 0(4) |
| C(28) | 82(6) | 32(3) | 54(4) | 15(3) | 28(4) | 17(3) |
| C(29) | 35(5) | 37(3) | 41(4) | 9(3) | 15(3) | -1(3) |
| C(30) | 114(8) | 132(7) | 63(5) | 49(5) | 59(5) | 82(6) |
| C(31) | 64(6) | 110(6) | 27(4) | 23(3) | 19(4) | 33(4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(32) | 57(6) | 47(4) | 37(4) | 23(3) | 33(4) | 8(4) |
| C(33) | 85(5) | 31(3) | 40(4) | 12(3) | 46(4) | 11(4) |
| C(34) | 92(5) | 31(3) | 44(4) | 2(3) | 45(4) | -15(4) |
| C(35) | 95(7) | 31(3) | 36(4) | 3(3) | 47(5) | -4(4) |
| C(36) | 73(6) | 31(3) | 28(4) | 12(3) | 32(4) | 5(4) |
| C(37) | 198(10) | 48(4) | 89(6) | 39(4) | 106(7) | 63(5) |
| C(38) | 201(10) | 32(4) | 75(5) | -28(3) | 97(6) | -56(5) |
| C(39) | 106(8) | 59(4) | 42(4) | -24(3) | 46(5) | -41(5) |
| C(40) | 53(5) | 33(3) | 25(3) | 1(2) | 23(3) | 9(3) |
| C(41) | 39(5) | 26(3) | 23(3) | -2(2) | 11(3) | -4(3) |
| C(42) | 39(5) | 22(3) | 14(3) | 3(2) | 5(3) | -2(3) |
| C(43) | 29(4) | 26(3) | 26(3) | 6(2) | 10(3) | 2(3) |
| C(44) | 54(6) | 28(3) | 21(3) | -2(2) | 4(3) | -10(3) |
| C(45) | 58(6) | 24(3) | 26(3) | -7(2) | 16(4) | -5(3) |
| C(46) | 36(5) | 34(3) | 30(3) | -9(3) | 14(3) | -6(3) |
| C(47) | 36(5) | 28(3) | 23(3) | -8(2) | 4(3) | -8(3) |
| C(48) | 91(7) | 30(3) | 38(4) | -4(3) | 45(4) | -8(4) |
| C(49) | 48(4) | 30(3) | 27(3) | -7(3) | 28(3) | -7(3) |
| C(50) | 62(6) | 29(3) | 27(3) | -7(3) | 24(4) | -13(3) |
| C(51) | 56(6) | 40(4) | 24(3) | -5(3) | 21(4) | -15(4) |
| C(52) | 56(6) | 63(4) | 26(3) | -1(3) | 24(3) | -10(4) |
| C(53) | 69(7) | 74(5) | 30(4) | -9(4) | 23(4) | -36(5) |
| C(54) | 71(7) | 43(4) | 30(4) | -21(3) | 30(4) | -31(4) |

**Table S11.** Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($A^2 \times 10^3$) for **L´Zr(Bn)$_2$**.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(3) | 3510 | 6601 | 579 | 56 |
| H(4) | 3569 | 6104 | 2762 | 78 |

| | | | | |
|---|---|---|---|---|
| H(5) | 2944 | 5290 | 3432 | 78 |
| H(8) | 3429 | 6455 | -3979 | 52 |
| H(9) | 2714 | 7042 | -4867 | 50 |
| H(10) | 2081 | 7207 | -3540 | 43 |
| H(11) | 2173 | 6769 | -1361 | 36 |
| H(14) | 4981 | 5670 | -4367 | 148 |
| H(16) | 4840 | 7827 | -2543 | 97 |
| H(18A) | 4253 | 4454 | -2568 | 223 |
| H(18B) | 4579 | 4444 | -3776 | 223 |
| H(18C) | 4023 | 4691 | -4013 | 223 |
| H(19A) | 5623 | 6848 | -4345 | 207 |
| H(19B) | 5452 | 7737 | -3843 | 207 |
| H(19C) | 5218 | 7366 | -5210 | 207 |
| H(20A) | 4166 | 7257 | -257 | 135 |
| H(20B) | 3762 | 7520 | -1397 | 135 |
| H(20C) | 4248 | 8049 | -1165 | 135 |
| H(23) | 4314 | 3981 | 1652 | 48 |
| H(25) | 3183 | 3118 | -685 | 46 |
| H(27A) | 4670 | 5222 | 1369 | 97 |
| H(27B) | 4286 | 5937 | 951 | 97 |
| H(27C) | 4637 | 5603 | -85 | 97 |
| H(28A) | 3610 | 2783 | 2292 | 82 |
| H(28B) | 4051 | 2410 | 1584 | 82 |
| H(28C) | 3511 | 2246 | 973 | 82 |
| H(29A) | 2899 | 3770 | -2599 | 55 |
| H(29B) | 3169 | 4565 | -3133 | 55 |
| H(29C) | 2759 | 4690 | -2155 | 55 |
| H(30A) | 2742 | 3201 | 2857 | 150 |
| H(30B) | 2564 | 2973 | 4259 | 150 |
| H(30C) | 2932 | 3729 | 4131 | 150 |
| H(31A) | 2434 | 4983 | 5230 | 99 |
| H(31B) | 1974 | 4461 | 5580 | 99 |
| H(31C) | 1905 | 5291 | 4708 | 99 |

| | | | | |
|---|---|---|---|---|
| H(37A) | 1957 | 2038 | 1940 | 159 |
| H(37B) | 2222 | 2802 | 1304 | 159 |
| H(37C) | 1836 | 2258 | 417 | 159 |
| H(38A) | 1069 | 2441 | -691 | 146 |
| H(38B) | 548 | 2797 | -462 | 146 |
| H(38C) | 762 | 2017 | 378 | 146 |
| H(39A) | 95 | 3604 | 1583 | 100 |
| H(39B) | 255 | 4052 | 292 | 100 |
| H(39C) | 249 | 4567 | 1633 | 100 |
| H(40A) | 975 | 4388 | 4598 | 53 |
| H(40B) | 619 | 4842 | 3503 | 53 |
| H(40C) | 1161 | 5164 | 3796 | 53 |
| H(41A) | 1388 | 6155 | 113 | 35 |
| H(41B) | 876 | 5715 | 9 | 35 |
| H(43) | 1726 | 6512 | 2552 | 31 |
| H(44) | 1522 | 7239 | 4391 | 41 |
| H(45) | 717 | 7480 | 4714 | 42 |
| H(46) | 119 | 6974 | 3189 | 39 |
| H(47) | 314 | 6247 | 1348 | 35 |
| H(48A) | 2067 | 3998 | -1306 | 61 |
| H(48B) | 1646 | 3306 | -1180 | 61 |
| H(50) | 1841 | 5441 | -2019 | 46 |
| H(51) | 1297 | 6341 | -3107 | 47 |
| H(52) | 499 | 5941 | -3622 | 56 |
| H(53) | 254 | 4594 | -3104 | 68 |
| H(54) | 788 | 3705 | -1978 | 56 |

**Table S12.** Torsion angles [º] for **L´Zr(Bn)$_2$**.

| | |
|---|---|
| C(48)-Zr(1)-Si(1)-N(1) | 78.7(3) |
| C(41)-Zr(1)-Si(1)-N(1) | -72.8(3) |
| C(32)-Zr(1)-Si(1)-N(1) | 175.7(3) |
| C(33)-Zr(1)-Si(1)-N(1) | 144.8(3) |

| | |
|---|---|
| C(36)-Zr(1)-Si(1)-N(1) | -152.8(3) |
| C(35)-Zr(1)-Si(1)-N(1) | -167.7(2) |
| C(34)-Zr(1)-Si(1)-N(1) | 160.4(3) |
| C(49)-Zr(1)-Si(1)-N(1) | 67.3(4) |
| N(1)-Zr(1)-Si(1)-C(32) | -175.7(3) |
| C(48)-Zr(1)-Si(1)-C(32) | -97.0(3) |
| C(41)-Zr(1)-Si(1)-C(32) | 111.6(3) |
| C(33)-Zr(1)-Si(1)-C(32) | -30.8(3) |
| C(36)-Zr(1)-Si(1)-C(32) | 31.6(3) |
| C(35)-Zr(1)-Si(1)-C(32) | 16.7(3) |
| C(34)-Zr(1)-Si(1)-C(32) | -15.3(3) |
| C(49)-Zr(1)-Si(1)-C(32) | -108.4(4) |
| N(1)-Zr(1)-Si(1)-C(30) | -82.1(4) |
| C(48)-Zr(1)-Si(1)-C(30) | -3.5(4) |
| C(41)-Zr(1)-Si(1)-C(30) | -154.9(4) |
| C(32)-Zr(1)-Si(1)-C(30) | 93.5(4) |
| C(33)-Zr(1)-Si(1)-C(30) | 62.7(4) |
| C(36)-Zr(1)-Si(1)-C(30) | 125.1(4) |
| C(35)-Zr(1)-Si(1)-C(30) | 110.2(4) |
| C(34)-Zr(1)-Si(1)-C(30) | 78.2(4) |
| C(49)-Zr(1)-Si(1)-C(30) | -14.8(5) |
| N(1)-Zr(1)-Si(1)-C(31) | 86.8(4) |
| C(48)-Zr(1)-Si(1)-C(31) | 165.5(3) |
| C(41)-Zr(1)-Si(1)-C(31) | 14.0(3) |
| C(32)-Zr(1)-Si(1)-C(31) | -97.5(4) |
| C(33)-Zr(1)-Si(1)-C(31) | -128.3(3) |
| C(36)-Zr(1)-Si(1)-C(31) | -65.9(3) |
| C(35)-Zr(1)-Si(1)-C(31) | -80.8(3) |
| C(34)-Zr(1)-Si(1)-C(31) | -112.8(3) |
| C(49)-Zr(1)-Si(1)-C(31) | 154.1(4) |
| C(32)-Si(1)-N(1)-C(1) | -173.4(5) |
| C(30)-Si(1)-N(1)-C(1) | -55.2(6) |
| C(31)-Si(1)-N(1)-C(1) | 67.1(5) |

| | |
|---|---|
| Zr(1)-Si(1)-N(1)-C(1) | -176.8(6) |
| C(32)-Si(1)-N(1)-Zr(1) | 3.4(3) |
| C(30)-Si(1)-N(1)-Zr(1) | 121.7(4) |
| C(31)-Si(1)-N(1)-Zr(1) | -116.1(3) |
| C(48)-Zr(1)-N(1)-C(1) | 60.5(4) |
| C(41)-Zr(1)-N(1)-C(1) | -65.0(4) |
| C(32)-Zr(1)-N(1)-C(1) | 174.2(5) |
| C(33)-Zr(1)-N(1)-C(1) | 146.2(4) |
| C(36)-Zr(1)-N(1)-C(1) | -159.4(4) |
| C(35)-Zr(1)-N(1)-C(1) | -168.5(4) |
| C(34)-Zr(1)-N(1)-C(1) | 154.0(4) |
| C(49)-Zr(1)-N(1)-C(1) | 30.9(5) |
| Si(1)-Zr(1)-N(1)-C(1) | 177.0(5) |
| C(48)-Zr(1)-N(1)-Si(1) | -116.5(2) |
| C(41)-Zr(1)-N(1)-Si(1) | 118.0(2) |
| C(32)-Zr(1)-N(1)-Si(1) | -2.8(2) |
| C(33)-Zr(1)-N(1)-Si(1) | -30.8(2) |
| C(36)-Zr(1)-N(1)-Si(1) | 23.7(2) |
| C(35)-Zr(1)-N(1)-Si(1) | 14.6(3) |
| C(34)-Zr(1)-N(1)-Si(1) | -23.0(3) |
| C(49)-Zr(1)-N(1)-Si(1) | -146.1(2) |
| C(2)-N(2)-C(1)-N(1) | -176.9(4) |
| C(2)-N(2)-C(1)-C(5) | 1.5(8) |
| Si(1)-N(1)-C(1)-N(2) | 168.4(3) |
| Zr(1)-N(1)-C(1)-N(2) | -7.9(6) |
| Si(1)-N(1)-C(1)-C(5) | -9.9(8) |
| Zr(1)-N(1)-C(1)-C(5) | 173.8(5) |
| C(1)-N(2)-C(2)-C(3) | -2.2(8) |
| C(1)-N(2)-C(2)-C(6) | 177.8(4) |
| N(2)-C(2)-C(3)-C(4) | 2.3(9) |
| C(6)-C(2)-C(3)-C(4) | -177.7(5) |
| C(2)-C(3)-C(4)-C(5) | -1.7(10) |
| C(3)-C(4)-C(5)-C(1) | 1.0(11) |

| | |
|---|---|
| N(2)-C(1)-C(5)-C(4) | -1.0(10) |
| N(1)-C(1)-C(5)-C(4) | 177.3(6) |
| N(2)-C(2)-C(6)-C(11) | 50.6(6) |
| C(3)-C(2)-C(6)-C(11) | -129.3(6) |
| N(2)-C(2)-C(6)-C(7) | -132.1(5) |
| C(3)-C(2)-C(6)-C(7) | 47.9(7) |
| C(11)-C(6)-C(7)-C(8) | -2.5(7) |
| C(2)-C(6)-C(7)-C(8) | -179.7(5) |
| C(11)-C(6)-C(7)-B(1) | -175.6(5) |
| C(2)-C(6)-C(7)-B(1) | 7.2(8) |
| C(21)-B(1)-C(7)-C(8) | -135.2(6) |
| C(12)-B(1)-C(7)-C(8) | 37.2(8) |
| C(21)-B(1)-C(7)-C(6) | 37.9(9) |
| C(12)-B(1)-C(7)-C(6) | -149.8(6) |
| C(6)-C(7)-C(8)-C(9) | 0.4(8) |
| B(1)-C(7)-C(8)-C(9) | 174.1(6) |
| C(7)-C(8)-C(9)-C(10) | 1.1(9) |
| C(8)-C(9)-C(10)-C(11) | -0.6(8) |
| C(9)-C(10)-C(11)-C(6) | -1.5(8) |
| C(7)-C(6)-C(11)-C(10) | 3.0(8) |
| C(2)-C(6)-C(11)-C(10) | -179.6(5) |
| C(21)-B(1)-C(12)-C(13) | 55.5(10) |
| C(7)-B(1)-C(12)-C(13) | -116.8(8) |
| C(21)-B(1)-C(12)-C(17) | -128.4(7) |
| C(7)-B(1)-C(12)-C(17) | 59.4(9) |
| C(17)-C(12)-C(13)-C(14) | -3.4(12) |
| B(1)-C(12)-C(13)-C(14) | 172.9(8) |
| C(17)-C(12)-C(13)-C(18) | 178.0(8) |
| B(1)-C(12)-C(13)-C(18) | -5.7(13) |
| C(12)-C(13)-C(14)-C(15) | 2.2(16) |
| C(18)-C(13)-C(14)-C(15) | -179.1(11) |
| C(13)-C(14)-C(15)-C(16) | 1.5(17) |
| C(13)-C(14)-C(15)-C(19) | -177.1(9) |

| | |
|---|---|
| C(14)-C(15)-C(16)-C(17) | -3.6(15) |
| C(19)-C(15)-C(16)-C(17) | 175.0(7) |
| C(13)-C(12)-C(17)-C(16) | 1.2(11) |
| B(1)-C(12)-C(17)-C(16) | -175.2(7) |
| C(13)-C(12)-C(17)-C(20) | -176.0(8) |
| B(1)-C(12)-C(17)-C(20) | 7.7(11) |
| C(15)-C(16)-C(17)-C(12) | 2.3(12) |
| C(15)-C(16)-C(17)-C(20) | 179.6(8) |
| C(12)-B(1)-C(21)-C(26) | -127.7(7) |
| C(7)-B(1)-C(21)-C(26) | 44.1(8) |
| C(12)-B(1)-C(21)-C(22) | 52.4(9) |
| C(7)-B(1)-C(21)-C(22) | -135.7(6) |
| C(26)-C(21)-C(22)-C(23) | -1.7(8) |
| B(1)-C(21)-C(22)-C(23) | 178.2(5) |
| C(26)-C(21)-C(22)-C(27) | -177.4(5) |
| B(1)-C(21)-C(22)-C(27) | 2.5(9) |
| C(21)-C(22)-C(23)-C(24) | 0.6(8) |
| C(27)-C(22)-C(23)-C(24) | 176.4(5) |
| C(22)-C(23)-C(24)-C(25) | 1.4(8) |
| C(22)-C(23)-C(24)-C(28) | -178.8(5) |
| C(23)-C(24)-C(25)-C(26) | -2.2(8) |
| C(28)-C(24)-C(25)-C(26) | 178.1(4) |
| C(24)-C(25)-C(26)-C(21) | 1.0(7) |
| C(24)-C(25)-C(26)-C(29) | 179.6(5) |
| C(22)-C(21)-C(26)-C(25) | 1.0(7) |
| B(1)-C(21)-C(26)-C(25) | -178.9(5) |
| C(22)-C(21)-C(26)-C(29) | -177.7(5) |
| B(1)-C(21)-C(26)-C(29) | 2.4(8) |
| N(1)-Si(1)-C(32)-C(36) | -76.8(4) |
| C(30)-Si(1)-C(32)-C(36) | 165.9(4) |
| C(31)-Si(1)-C(32)-C(36) | 41.0(5) |
| Zr(1)-Si(1)-C(32)-C(36) | -74.0(4) |
| N(1)-Si(1)-C(32)-C(33) | 68.5(5) |

| | |
|---|---|
| C(30)-Si(1)-C(32)-C(33) | -48.8(5) |
| C(31)-Si(1)-C(32)-C(33) | -173.7(5) |
| Zr(1)-Si(1)-C(32)-C(33) | 71.3(4) |
| N(1)-Si(1)-C(32)-Zr(1) | -2.8(2) |
| C(30)-Si(1)-C(32)-Zr(1) | -120.1(2) |
| C(31)-Si(1)-C(32)-Zr(1) | 115.0(2) |
| N(1)-Zr(1)-C(32)-C(36) | 126.0(4) |
| C(48)-Zr(1)-C(32)-C(36) | -131.6(4) |
| C(41)-Zr(1)-C(32)-C(36) | 33.6(5) |
| C(33)-Zr(1)-C(32)-C(36) | -110.7(6) |
| C(35)-Zr(1)-C(32)-C(36) | -35.9(3) |
| C(34)-Zr(1)-C(32)-C(36) | -75.5(4) |
| C(49)-Zr(1)-C(32)-C(36) | -102.4(5) |
| Si(1)-Zr(1)-C(32)-C(36) | 123.5(5) |
| N(1)-Zr(1)-C(32)-C(33) | -123.3(5) |
| C(48)-Zr(1)-C(32)-C(33) | -20.9(5) |
| C(41)-Zr(1)-C(32)-C(33) | 144.3(4) |
| C(36)-Zr(1)-C(32)-C(33) | 110.7(6) |
| C(35)-Zr(1)-C(32)-C(33) | 74.9(4) |
| C(34)-Zr(1)-C(32)-C(33) | 35.2(4) |
| C(49)-Zr(1)-C(32)-C(33) | 8.3(6) |
| Si(1)-Zr(1)-C(32)-C(33) | -125.8(5) |
| N(1)-Zr(1)-C(32)-Si(1) | 2.50(19) |
| C(48)-Zr(1)-C(32)-Si(1) | 104.9(3) |
| C(41)-Zr(1)-C(32)-Si(1) | -89.9(3) |
| C(33)-Zr(1)-C(32)-Si(1) | 125.8(5) |
| C(36)-Zr(1)-C(32)-Si(1) | -123.5(5) |
| C(35)-Zr(1)-C(32)-Si(1) | -159.3(3) |
| C(34)-Zr(1)-C(32)-Si(1) | 161.0(4) |
| C(49)-Zr(1)-C(32)-Si(1) | 134.1(3) |
| C(36)-C(32)-C(33)-C(34) | -0.4(6) |
| Si(1)-C(32)-C(33)-C(34) | -150.4(5) |
| Zr(1)-C(32)-C(33)-C(34) | -71.0(4) |

| | |
|---|---|
| C(36)-C(32)-C(33)-C(37) | -179.7(5) |
| Si(1)-C(32)-C(33)-C(37) | 30.2(7) |
| Zr(1)-C(32)-C(33)-C(37) | 109.6(5) |
| C(36)-C(32)-C(33)-Zr(1) | 70.7(3) |
| Si(1)-C(32)-C(33)-Zr(1) | -79.4(4) |
| N(1)-Zr(1)-C(33)-C(34) | 167.0(4) |
| C(48)-Zr(1)-C(33)-C(34) | -83.2(4) |
| C(41)-Zr(1)-C(33)-C(34) | 53.0(6) |
| C(32)-Zr(1)-C(33)-C(34) | 115.2(6) |
| C(36)-Zr(1)-C(33)-C(34) | 75.9(4) |
| C(35)-Zr(1)-C(33)-C(34) | 36.1(4) |
| C(49)-Zr(1)-C(33)-C(34) | -59.5(4) |
| Si(1)-Zr(1)-C(33)-C(34) | 148.8(4) |
| N(1)-Zr(1)-C(33)-C(32) | 51.8(4) |
| C(48)-Zr(1)-C(33)-C(32) | 161.6(5) |
| C(41)-Zr(1)-C(33)-C(32) | -62.2(7) |
| C(36)-Zr(1)-C(33)-C(32) | -39.3(4) |
| C(35)-Zr(1)-C(33)-C(32) | -79.1(4) |
| C(34)-Zr(1)-C(33)-C(32) | -115.2(6) |
| C(49)-Zr(1)-C(33)-C(32) | -174.7(4) |
| Si(1)-Zr(1)-C(33)-C(32) | 33.6(4) |
| N(1)-Zr(1)-C(33)-C(37) | -67.8(6) |
| C(48)-Zr(1)-C(33)-C(37) | 41.9(6) |
| C(41)-Zr(1)-C(33)-C(37) | 178.2(5) |
| C(32)-Zr(1)-C(33)-C(37) | -119.7(9) |
| C(36)-Zr(1)-C(33)-C(37) | -158.9(8) |
| C(35)-Zr(1)-C(33)-C(37) | 161.2(7) |
| C(34)-Zr(1)-C(33)-C(37) | 125.2(8) |
| C(49)-Zr(1)-C(33)-C(37) | 65.7(7) |
| Si(1)-Zr(1)-C(33)-C(37) | -86.0(6) |
| C(32)-C(33)-C(34)-C(35) | 2.3(6) |
| C(37)-C(33)-C(34)-C(35) | -178.3(5) |
| Zr(1)-C(33)-C(34)-C(35) | -63.4(4) |

| | |
|---|---|
| C(32)-C(33)-C(34)-C(38) | -169.0(5) |
| C(37)-C(33)-C(34)-C(38) | 10.3(9) |
| Zr(1)-C(33)-C(34)-C(38) | 125.2(5) |
| C(32)-C(33)-C(34)-Zr(1) | 65.7(4) |
| C(37)-C(33)-C(34)-Zr(1) | -114.9(5) |
| N(1)-Zr(1)-C(34)-C(33) | -15.2(4) |
| C(48)-Zr(1)-C(34)-C(33) | 93.6(4) |
| C(41)-Zr(1)-C(34)-C(33) | -148.3(3) |
| C(32)-Zr(1)-C(34)-C(33) | -38.8(3) |
| C(36)-Zr(1)-C(34)-C(33) | -80.6(4) |
| C(35)-Zr(1)-C(34)-C(33) | -117.3(6) |
| C(49)-Zr(1)-C(34)-C(33) | 125.3(4) |
| Si(1)-Zr(1)-C(34)-C(33) | -27.4(3) |
| N(1)-Zr(1)-C(34)-C(35) | 102.2(5) |
| C(48)-Zr(1)-C(34)-C(35) | -149.0(5) |
| C(41)-Zr(1)-C(34)-C(35) | -30.9(6) |
| C(32)-Zr(1)-C(34)-C(35) | 78.6(5) |
| C(33)-Zr(1)-C(34)-C(35) | 117.3(6) |
| C(36)-Zr(1)-C(34)-C(35) | 36.7(4) |
| C(49)-Zr(1)-C(34)-C(35) | -117.4(5) |
| Si(1)-Zr(1)-C(34)-C(35) | 89.9(5) |
| N(1)-Zr(1)-C(34)-C(38) | -136.6(7) |
| C(48)-Zr(1)-C(34)-C(38) | -27.8(7) |
| C(41)-Zr(1)-C(34)-C(38) | 90.3(7) |
| C(32)-Zr(1)-C(34)-C(38) | -160.2(8) |
| C(33)-Zr(1)-C(34)-C(38) | -121.4(9) |
| C(36)-Zr(1)-C(34)-C(38) | 157.9(9) |
| C(35)-Zr(1)-C(34)-C(38) | 121.2(10) |
| C(49)-Zr(1)-C(34)-C(38) | 3.8(7) |
| Si(1)-Zr(1)-C(34)-C(38) | -148.8(7) |
| C(33)-C(34)-C(35)-C(36) | -3.5(6) |
| C(38)-C(34)-C(35)-C(36) | 168.2(5) |
| Zr(1)-C(34)-C(35)-C(36) | -64.4(4) |

| | |
|---|---|
| C(33)-C(34)-C(35)-C(39) | -178.5(5) |
| C(38)-C(34)-C(35)-C(39) | -6.8(9) |
| Zr(1)-C(34)-C(35)-C(39) | 120.6(5) |
| C(33)-C(34)-C(35)-Zr(1) | 61.0(4) |
| C(38)-C(34)-C(35)-Zr(1) | -127.4(5) |
| N(1)-Zr(1)-C(35)-C(36) | 17.4(4) |
| C(48)-Zr(1)-C(35)-C(36) | 148.2(4) |
| C(41)-Zr(1)-C(35)-C(36) | -90.4(4) |
| C(32)-Zr(1)-C(35)-C(36) | 37.6(4) |
| C(33)-Zr(1)-C(35)-C(36) | 80.3(4) |
| C(34)-Zr(1)-C(35)-C(36) | 115.3(7) |
| C(49)-Zr(1)-C(35)-C(36) | -177.7(4) |
| Si(1)-Zr(1)-C(35)-C(36) | 25.3(4) |
| N(1)-Zr(1)-C(35)-C(34) | -97.9(5) |
| C(48)-Zr(1)-C(35)-C(34) | 33.0(5) |
| C(41)-Zr(1)-C(35)-C(34) | 154.3(5) |
| C(32)-Zr(1)-C(35)-C(34) | -77.7(5) |
| C(33)-Zr(1)-C(35)-C(34) | -35.0(4) |
| C(36)-Zr(1)-C(35)-C(34) | -115.3(7) |
| C(49)-Zr(1)-C(35)-C(34) | 67.0(5) |
| Si(1)-Zr(1)-C(35)-C(34) | -90.0(5) |
| N(1)-Zr(1)-C(35)-C(39) | 139.6(5) |
| C(48)-Zr(1)-C(35)-C(39) | -89.6(5) |
| C(41)-Zr(1)-C(35)-C(39) | 31.8(5) |
| C(32)-Zr(1)-C(35)-C(39) | 159.8(6) |
| C(33)-Zr(1)-C(35)-C(39) | -157.5(6) |
| C(36)-Zr(1)-C(35)-C(39) | 122.2(6) |
| C(34)-Zr(1)-C(35)-C(39) | -122.5(8) |
| C(49)-Zr(1)-C(35)-C(39) | -55.5(5) |
| Si(1)-Zr(1)-C(35)-C(39) | 147.4(5) |
| C(34)-C(35)-C(36)-C(32) | 3.2(6) |
| C(39)-C(35)-C(36)-C(32) | 178.2(5) |
| Zr(1)-C(35)-C(36)-C(32) | -63.4(4) |

| | |
|---|---|
| C(34)-C(35)-C(36)-C(40) | -170.7(4) |
| C(39)-C(35)-C(36)-C(40) | 4.3(9) |
| Zr(1)-C(35)-C(36)-C(40) | 122.7(5) |
| C(34)-C(35)-C(36)-Zr(1) | 66.6(4) |
| C(39)-C(35)-C(36)-Zr(1) | -118.5(6) |
| C(33)-C(32)-C(36)-C(35) | -1.8(6) |
| Si(1)-C(32)-C(36)-C(35) | 149.0(4) |
| Zr(1)-C(32)-C(36)-C(35) | 67.5(4) |
| C(33)-C(32)-C(36)-C(40) | 172.0(4) |
| Si(1)-C(32)-C(36)-C(40) | -37.2(7) |
| Zr(1)-C(32)-C(36)-C(40) | -118.7(5) |
| C(33)-C(32)-C(36)-Zr(1) | -69.3(3) |
| Si(1)-C(32)-C(36)-Zr(1) | 81.5(3) |
| N(1)-Zr(1)-C(36)-C(35) | -165.3(4) |
| C(48)-Zr(1)-C(36)-C(35) | -45.0(5) |
| C(41)-Zr(1)-C(36)-C(35) | 92.0(4) |
| C(32)-Zr(1)-C(36)-C(35) | -115.7(6) |
| C(33)-Zr(1)-C(36)-C(35) | -75.6(4) |
| C(34)-Zr(1)-C(36)-C(35) | -36.8(4) |
| C(49)-Zr(1)-C(36)-C(35) | 3.2(5) |
| Si(1)-Zr(1)-C(36)-C(35) | -150.9(4) |
| N(1)-Zr(1)-C(36)-C(32) | -49.6(4) |
| C(48)-Zr(1)-C(36)-C(32) | 70.7(6) |
| C(41)-Zr(1)-C(36)-C(32) | -152.3(4) |
| C(33)-Zr(1)-C(36)-C(32) | 40.2(4) |
| C(35)-Zr(1)-C(36)-C(32) | 115.7(6) |
| C(34)-Zr(1)-C(36)-C(32) | 78.9(4) |
| C(49)-Zr(1)-C(36)-C(32) | 119.0(4) |
| Si(1)-Zr(1)-C(36)-C(32) | -35.2(4) |
| N(1)-Zr(1)-C(36)-C(40) | 71.6(6) |
| C(48)-Zr(1)-C(36)-C(40) | -168.1(5) |
| C(41)-Zr(1)-C(36)-C(40) | -31.2(6) |
| C(32)-Zr(1)-C(36)-C(40) | 121.1(8) |

| | |
|---|---|
| C(33)-Zr(1)-C(36)-C(40) | 161.3(7) |
| C(35)-Zr(1)-C(36)-C(40) | -123.1(8) |
| C(34)-Zr(1)-C(36)-C(40) | -159.9(7) |
| C(49)-Zr(1)-C(36)-C(40) | -119.9(5) |
| Si(1)-Zr(1)-C(36)-C(40) | 85.9(6) |
| N(1)-Zr(1)-C(41)-C(42) | -57.7(5) |
| C(48)-Zr(1)-C(41)-C(42) | -178.0(5) |
| C(32)-Zr(1)-C(41)-C(42) | 16.7(6) |
| C(33)-Zr(1)-C(41)-C(42) | 52.9(7) |
| C(36)-Zr(1)-C(41)-C(42) | 34.4(5) |
| C(35)-Zr(1)-C(41)-C(42) | 66.4(5) |
| C(34)-Zr(1)-C(41)-C(42) | 82.3(5) |
| C(49)-Zr(1)-C(41)-C(42) | 171.6(5) |
| Si(1)-Zr(1)-C(41)-C(42) | -25.6(5) |
| Zr(1)-C(41)-C(42)-C(43) | 65.6(6) |
| Zr(1)-C(41)-C(42)-C(47) | -113.7(5) |
| C(47)-C(42)-C(43)-C(44) | 1.2(7) |
| C(41)-C(42)-C(43)-C(44) | -178.2(4) |
| C(42)-C(43)-C(44)-C(45) | -0.7(7) |
| C(43)-C(44)-C(45)-C(46) | 0.2(7) |
| C(44)-C(45)-C(46)-C(47) | -0.2(8) |
| C(45)-C(46)-C(47)-C(42) | 0.7(8) |
| C(43)-C(42)-C(47)-C(46) | -1.1(7) |
| C(41)-C(42)-C(47)-C(46) | 178.2(4) |
| N(1)-Zr(1)-C(48)-C(49) | -135.9(3) |
| C(41)-Zr(1)-C(48)-C(49) | -19.4(4) |
| C(32)-Zr(1)-C(48)-C(49) | 146.7(4) |
| C(33)-Zr(1)-C(48)-C(49) | 135.1(4) |
| C(36)-Zr(1)-C(48)-C(49) | 110.6(4) |
| C(35)-Zr(1)-C(48)-C(49) | 87.1(4) |
| C(34)-Zr(1)-C(48)-C(49) | 104.0(4) |
| Si(1)-Zr(1)-C(48)-C(49) | -170.3(3) |
| Zr(1)-C(48)-C(49)-C(54) | -89.4(5) |

| | |
|---|---|
| Zr(1)-C(48)-C(49)-C(50) | 82.3(4) |
| N(1)-Zr(1)-C(49)-C(54) | 179.0(4) |
| C(48)-Zr(1)-C(49)-C(54) | 119.5(6) |
| C(41)-Zr(1)-C(49)-C(54) | -77.6(4) |
| C(32)-Zr(1)-C(49)-C(54) | 66.6(6) |
| C(33)-Zr(1)-C(49)-C(54) | 71.5(5) |
| C(36)-Zr(1)-C(49)-C(54) | 14.2(5) |
| C(35)-Zr(1)-C(49)-C(54) | 15.9(5) |
| C(34)-Zr(1)-C(49)-C(54) | 45.1(4) |
| Si(1)-Zr(1)-C(49)-C(54) | 137.8(4) |
| N(1)-Zr(1)-C(49)-C(50) | -59.6(5) |
| C(48)-Zr(1)-C(49)-C(50) | -119.1(6) |
| C(41)-Zr(1)-C(49)-C(50) | 43.7(4) |
| C(32)-Zr(1)-C(49)-C(50) | -172.0(4) |
| C(33)-Zr(1)-C(49)-C(50) | -167.1(4) |
| C(36)-Zr(1)-C(49)-C(50) | 135.5(4) |
| C(35)-Zr(1)-C(49)-C(50) | 137.3(4) |
| C(34)-Zr(1)-C(49)-C(50) | 166.5(4) |
| Si(1)-Zr(1)-C(49)-C(50) | -100.8(4) |
| N(1)-Zr(1)-C(49)-C(48) | 59.5(4) |
| C(41)-Zr(1)-C(49)-C(48) | 162.8(4) |
| C(32)-Zr(1)-C(49)-C(48) | -52.9(5) |
| C(33)-Zr(1)-C(49)-C(48) | -48.0(4) |
| C(36)-Zr(1)-C(49)-C(48) | -105.4(4) |
| C(35)-Zr(1)-C(49)-C(48) | -103.6(4) |
| C(34)-Zr(1)-C(49)-C(48) | -74.4(4) |
| Si(1)-Zr(1)-C(49)-C(48) | 18.3(5) |
| C(54)-C(49)-C(50)-C(51) | -2.3(7) |
| C(48)-C(49)-C(50)-C(51) | -174.7(4) |
| Zr(1)-C(49)-C(50)-C(51) | -117.9(5) |
| C(49)-C(50)-C(51)-C(52) | 1.3(7) |
| C(50)-C(51)-C(52)-C(53) | -0.9(7) |
| C(51)-C(52)-C(53)-C(54) | 1.6(8) |

| | |
|---|---|
| C(52)-C(53)-C(54)-C(49) | -2.9(8) |
| C(50)-C(49)-C(54)-C(53) | 3.2(7) |
| C(48)-C(49)-C(54)-C(53) | 175.2(5) |
| Zr(1)-C(49)-C(54)-C(53) | 114.5(5) |

**Table S13.** Crystal data and structure refinement for **L´Zr($CH_2SiMe_3$)$_2$**.

| | |
|---|---|
| Empirical formula | C50H74BN2O0.50Si3Zr |
| Formula weight | 897.41 |
| Temperature | 110(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, space group | Triclinic, P-1 |
| Unit cell dimensions | a = 11.1492(5) Å α = 89.308(2)º. |
| | b = 11.3188(5) Å β= 82.967(2)º. |
| | c = 20.2772(9) Å γ= 77.549(2)º. |
| Volume | 2479.64(19) $Å^3$ |
| Z, Calculated density | 2, 1.202 $mg/m^3$ |
| Absorption coefficient | 0.329$mm^{-1}$ |
| F(000) | 958 |
| Crystal size | 0.66 x 0.38 x 0.34 mm |
| Theta range for data collection | 1.84 to 30.57º. |
| Limiting indices | -15<=h<=15, -16<=k<=16, -29<=l<=28 |
| Reflections collected / unique | 61402 / 15077 [R(int) = 0.0328] |
| Completeness to theta = 30.57 | 99.2 % |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.7461 and 0.7113 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 15077 / 14 / 558 |
| Goodness-of-fit on $F^2$ | 1.048 |
| Final R indices [I>2σ(I)] | R1 = 0.0309, wR2 = 0.0790 |
| R indices (all data) | R1 = 0.0440, wR2 = 0.0835 |
| Largest diff. peak and hole | 0.452 and -0.507 $e.A^{-3}$ |

**Table S14.** Atomic coordinates (×$10^4$) and equivalent isotropic displacement parameters ($A^2$ × $10^3$) for **L´Zr($CH_2SiMe_3$)$_2$**. U(eq) is defined as one third of the trace of the orthogonalized $U_{ij}$ tensor.

| | x | y | z | |
|---|---|---|---|---|
| Zr(1) | 8178(1) | 3112(1) | 1384(1) | 13(1) |
| Si(1) | 9019(1) | 5463(1) | 1785(1) | 15(1) |
| N(1) | 8365(1) | 4326(1) | 2143(1) | 18(1) |
| C(1) | 7735(1) | 4147(1) | 2742(1) | 15(1) |
| B(1) | 3686(1) | 3164(1) | 3808(1) | 14(1) |
| Si(2) | 10477(1) | 677(1) | 2092(1) | 17(1) |
| N(2) | 7186(1) | 3193(1) | 2737(1) | 14(1) |
| C(2) | 6500(1) | 2951(1) | 3298(1) | 14(1) |
| Si(3) | 6092(1) | 1351(1) | 792(1) | 17(1) |
| C(3) | 6387(1) | 3628(1) | 3880(1) | 19(1) |
| C(4) | 6961(1) | 4599(1) | 3882(1) | 21(1) |
| C(5) | 7637(1) | 4878(1) | 3311(1) | 18(1) |
| C(6) | 5904(1) | 1899(1) | 3293(1) | 16(1) |
| C(7) | 4670(1) | 1966(1) | 3587(1) | 16(1) |
| C(8) | 4225(1) | 894(1) | 3609(1) | 21(1) |
| C(9) | 4945(2) | -190(1) | 3343(1) | 25(1) |
| C(10) | 6147(2) | -238(1) | 3056(1) | 26(1) |
| C(11) | 6623(1) | 800(1) | 3032(1) | 21(1) |
| C(12) | 3655(1) | 4305(1) | 3351(1) | 14(1) |
| C(13) | 3677(1) | 4205(1) | 2654(1) | 15(1) |
| C(14) | 3759(1) | 5199(1) | 2254(1) | 19(1) |
| C(15) | 3807(1) | 6317(1) | 2514(1) | 20(1) |
| C(16) | 3728(1) | 6426(1) | 3201(1) | 20(1) |
| C(17) | 3641(1) | 5458(1) | 3617(1) | 16(1) |
| C(18) | 3508(1) | 3067(1) | 2330(1) | 20(1) |
| C(19) | 3900(2) | 7381(1) | 2071(1) | 30(1) |
| C(20) | 3524(1) | 5674(1) | 4359(1) | 23(1) |

| | | | | |
|---|---|---|---|---|
| C(21) | 2707(1) | 3099(1) | 4433(1) | 15(1) |
| C(22) | 3050(1) | 2541(1) | 5031(1) | 19(1) |
| C(23) | 2147(1) | 2413(1) | 5551(1) | 23(1) |
| C(24) | 896(1) | 2791(1) | 5503(1) | 24(1) |
| C(25) | 552(1) | 3356(1) | 4924(1) | 23(1) |
| C(26) | 1421(1) | 3531(1) | 4397(1) | 18(1) |
| C(27) | 4378(1) | 2090(2) | 5155(1) | 28(1) |
| C(28) | -53(2) | 2545(2) | 6053(1) | 34(1) |
| C(29) | 931(1) | 4151(2) | 3793(1) | 26(1) |
| C(30) | 8029(2) | 7005(1) | 1978(1) | 27(1) |
| C(31) | 10574(1) | 5497(1) | 2020(1) | 26(1) |
| C(32) | 9394(1) | 1275(1) | 1475(1) | 18(1) |
| C(33) | 12121(1) | 624(1) | 1745(1) | 26(1) |
| C(34) | 10354(2) | -912(2) | 2311(1) | 33(1) |
| C(35) | 10159(2) | 1601(2) | 2875(1) | 39(1) |
| C(36) | 6341(1) | 2698(1) | 1233(1) | 19(1) |
| C(37) | 5869(2) | 118(1) | 1386(1) | 31(1) |
| C(38) | 4681(2) | 1770(2) | 352(1) | 31(1) |
| C(39) | 7407(2) | 633(2) | 157(1) | 34(1) |
| C(40) | 9011(1) | 4847(1) | 934(1) | 15(1) |
| C(41) | 9869(1) | 3805(1) | 637(1) | 17(1) |
| C(42) | 9278(1) | 3259(1) | 182(1) | 21(1) |
| C(43) | 8048(1) | 3947(1) | 189(1) | 22(1) |
| C(44) | 7878(1) | 4903(1) | 657(1) | 19(1) |
| C(45) | 11200(1) | 3381(1) | 740(1) | 22(1) |
| C(46) | 9915(2) | 2232(2) | -285(1) | 31(1) |
| C(47) | 7144(2) | 3810(2) | -284(1) | 34(1) |
| C(48) | 6677(1) | 5807(1) | 839(1) | 29(1) |
| O(1X) | 0 | 10000 | 5000 | 35(1) |
| C(1X) | 1224(3) | 9960(3) | 4648(2) | 35(1) |
| C(2X) | 2162(7) | 9257(9) | 5089(4) | 42(2) |
| C(1X1) | 928(3) | 9332(3) | 5351(2) | 40(1) |
| C(2X1) | 2145(7) | 9321(10) | 4895(4) | 51(2) |

**Table S15.** Bond lengths [Å] and angles [º] for **L´Zr($CH_2SiMe_3$)$_2$**.

| | |
|---|---|
| Zr(1)-N(1) | 2.1323(11) |
| Zr(1)-C(32) | 2.2430(13) |
| Zr(1)-C(36) | 2.2550(14) |
| Zr(1)-C(40) | 2.4668(13) |
| Zr(1)-C(44) | 2.4805(13) |
| Zr(1)-C(41) | 2.5247(13) |
| Zr(1)-C(43) | 2.5996(13) |
| Zr(1)-C(42) | 2.6118(13) |
| Zr(1)-Si(1) | 3.1512(4) |
| Si(1)-N(1) | 1.7222(12) |
| Si(1)-C(31) | 1.8619(15) |
| Si(1)-C(30) | 1.8693(14) |
| Si(1)-C(40) | 1.8712(13) |
| N(1)-C(1) | 1.3619(16) |
| C(1)-N(2) | 1.3520(17) |
| C(1)-C(5) | 1.4070(17) |
| B(1)-C(12) | 1.5774(19) |
| B(1)-C(21) | 1.5801(19) |
| B(1)-C(7) | 1.5804(19) |
| Si(2)-C(32) | 1.8652(14) |
| Si(2)-C(35) | 1.8670(16) |
| Si(2)-C(33) | 1.8695(15) |
| Si(2)-C(34) | 1.8768(16) |
| N(2)-C(2) | 1.3498(16) |
| C(2)-C(3) | 1.3920(17) |
| C(2)-C(6) | 1.4843(18) |
| Si(3)-C(36) | 1.8649(14) |
| Si(3)-C(37) | 1.8696(16) |
| Si(3)-C(38) | 1.8723(16) |

| | |
|---|---|
| Si(3)-C(39) | 1.8752(16) |
| C(3)-C(4) | 1.387(2) |
| C(3)-H(3) | 0.9500 |
| C(4)-C(5) | 1.3748(19) |
| C(4)-H(4) | 0.9500 |
| C(5)-H(5) | 0.9500 |
| C(6)-C(11) | 1.3972(18) |
| C(6)-C(7) | 1.4170(18) |
| C(7)-C(8) | 1.4043(19) |
| C(8)-C(9) | 1.388(2) |
| C(8)-H(8) | 0.9500 |
| C(9)-C(10) | 1.384(2) |
| C(9)-H(9) | 0.9500 |
| C(10)-C(11) | 1.388(2) |
| C(10)-H(10) | 0.9500 |
| C(11)-H(11) | 0.9500 |
| C(12)-C(17) | 1.4143(17) |
| C(12)-C(13) | 1.4149(17) |
| C(13)-C(14) | 1.3923(19) |
| C(13)-C(18) | 1.5104(18) |
| C(14)-C(15) | 1.390(2) |
| C(14)-H(14) | 0.9500 |
| C(15)-C(16) | 1.391(2) |
| C(15)-C(19) | 1.508(2) |
| C(16)-C(17) | 1.3879(19) |
| C(16)-H(16) | 0.9500 |
| C(17)-C(20) | 1.5111(18) |
| 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)-C(22) | 1.4172(18) |
| C(21)-C(26) | 1.4211(19) |
| C(22)-C(23) | 1.3946(19) |
| C(22)-C(27) | 1.510(2) |
| C(23)-C(24) | 1.384(2) |
| C(23)-H(23) | 0.9500 |
| C(24)-C(25) | 1.385(2) |
| C(24)-C(28) | 1.507(2) |
| C(25)-C(26) | 1.3948(19) |
| C(25)-H(25) | 0.9500 |
| C(26)-C(29) | 1.507(2) |
| C(27)-H(27A) | 0.9800 |
| C(27)-H(27B) | 0.9800 |
| C(27)-H(27C) | 0.9800 |
| C(28)-H(28A) | 0.9800 |
| C(28)-H(28B) | 0.9800 |
| C(28)-H(28C) | 0.9800 |
| 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)-H(32A) | 0.9900 |
| C(32)-H(32B) | 0.9900 |
| C(33)-H(33A) | 0.9800 |
| C(33)-H(33B) | 0.9800 |

| | |
|---|---|
| C(33)-H(33C) | 0.9800 |
| C(34)-H(34A) | 0.9800 |
| C(34)-H(34B) | 0.9800 |
| C(34)-H(34C) | 0.9800 |
| C(35)-H(35A) | 0.9800 |
| C(35)-H(35B) | 0.9800 |
| C(35)-H(35C) | 0.9800 |
| C(36)-H(36A) | 0.9900 |
| C(36)-H(36B) | 0.9900 |
| C(37)-H(37A) | 0.9800 |
| C(37)-H(37B) | 0.9800 |
| C(37)-H(37C) | 0.9800 |
| 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)-C(44) | 1.4333(19) |
| C(40)-C(41) | 1.4349(17) |
| C(41)-C(42) | 1.4157(19) |
| C(41)-C(45) | 1.4980(19) |
| C(42)-C(43) | 1.422(2) |
| C(42)-C(46) | 1.5023(19) |
| C(43)-C(44) | 1.412(2) |
| C(43)-C(47) | 1.506(2) |
| C(44)-C(48) | 1.508(2) |
| C(45)-H(45A) | 0.9800 |
| C(45)-H(45B) | 0.9800 |
| C(45)-H(45C) | 0.9800 |
| C(46)-H(46A) | 0.9800 |
| C(46)-H(46B) | 0.9800 |
| C(46)-H(46C) | 0.9800 |

| | |
|---|---|
| C(47)-H(47A) | 0.9800 |
| C(47)-H(47B) | 0.9800 |
| C(47)-H(47C) | 0.9800 |
| C(48)-H(48A) | 0.9800 |
| C(48)-H(48B) | 0.9800 |
| C(48)-H(48C) | 0.9800 |
| O(1X)-C(1X1) | 1.407(4) |
| O(1X)-C(1X1)#1 | 1.407(4) |
| O(1X)-C(1X) | 1.452(3) |
| O(1X)-C(1X)#1 | 1.452(3) |
| C(1X)-C(2X) | 1.542(6) |
| C(1X)-H(1X1) | 0.9900 |
| C(1X)-H(1X2) | 0.9900 |
| C(2X)-H(2X1) | 0.9800 |
| C(2X)-H(2X2) | 0.9800 |
| C(2X)-H(2X3) | 0.9800 |
| C(1X1)-C(2X1) | 1.544(7) |
| C(1X1)-H(1X3) | 0.9900 |
| C(1X1)-H(1X4) | 0.9900 |
| C(2X1)-H(2X4) | 0.9800 |
| C(2X1)-H(2X5) | 0.9800 |
| C(2X1)-H(2X6) | 0.9800 |

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|---|---|
| N(1)-Zr(1)-C(32) | 111.58(5) |
| N(1)-Zr(1)-C(36) | 122.44(5) |
| C(32)-Zr(1)-C(36) | 103.35(5) |
| N(1)-Zr(1)-C(40) | 67.41(4) |
| C(32)-Zr(1)-C(40) | 122.06(5) |
| C(36)-Zr(1)-C(40) | 126.52(5) |
| N(1)-Zr(1)-C(44) | 86.24(5) |
| C(32)-Zr(1)-C(44) | 142.36(5) |
| C(36)-Zr(1)-C(44) | 92.95(5) |
| C(40)-Zr(1)-C(44) | 33.68(4) |

| | |
|---|---|
| N(1)-Zr(1)-C(41) | 89.61(4) |
| C(32)-Zr(1)-C(41) | 91.39(5) |
| C(36)-Zr(1)-C(41) | 134.42(5) |
| C(40)-Zr(1)-C(41) | 33.39(4) |
| C(44)-Zr(1)-C(41) | 54.55(4) |
| N(1)-Zr(1)-C(43) | 117.64(5) |
| C(32)-Zr(1)-C(43) | 116.55(5) |
| C(36)-Zr(1)-C(43) | 81.95(5) |
| C(40)-Zr(1)-C(43) | 54.39(4) |
| C(44)-Zr(1)-C(43) | 32.18(5) |
| C(41)-Zr(1)-C(43) | 53.24(5) |
| N(1)-Zr(1)-C(42) | 119.76(4) |
| C(32)-Zr(1)-C(42) | 89.47(5) |
| C(36)-Zr(1)-C(42) | 104.34(5) |
| C(40)-Zr(1)-C(42) | 54.19(4) |
| C(44)-Zr(1)-C(42) | 53.38(5) |
| C(41)-Zr(1)-C(42) | 31.94(4) |
| C(43)-Zr(1)-C(42) | 31.67(5) |
| N(1)-Zr(1)-Si(1) | 31.07(3) |
| C(32)-Zr(1)-Si(1) | 120.76(4) |
| C(36)-Zr(1)-Si(1) | 134.05(4) |
| C(40)-Zr(1)-Si(1) | 36.40(3) |
| C(44)-Zr(1)-Si(1) | 60.37(3) |
| C(41)-Zr(1)-Si(1) | 61.21(3) |
| C(43)-Zr(1)-Si(1) | 88.92(3) |
| C(42)-Zr(1)-Si(1) | 89.23(3) |
| N(1)-Si(1)-C(31) | 114.93(7) |
| N(1)-Si(1)-C(30) | 112.88(6) |
| C(31)-Si(1)-C(30) | 106.51(7) |
| N(1)-Si(1)-C(40) | 91.10(6) |
| C(31)-Si(1)-C(40) | 115.40(6) |
| C(30)-Si(1)-C(40) | 115.83(7) |
| N(1)-Si(1)-Zr(1) | 39.71(4) |

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|---|---|
| C(31)-Si(1)-Zr(1) | 124.93(5) |
| C(30)-Si(1)-Zr(1) | 127.78(5) |
| C(40)-Si(1)-Zr(1) | 51.47(4) |
| C(1)-N(1)-Si(1) | 136.00(9) |
| C(1)-N(1)-Zr(1) | 113.15(9) |
| Si(1)-N(1)-Zr(1) | 109.22(5) |
| N(2)-C(1)-N(1) | 113.08(11) |
| N(2)-C(1)-C(5) | 122.44(12) |
| N(1)-C(1)-C(5) | 124.47(12) |
| C(12)-B(1)-C(21) | 124.08(11) |
| C(12)-B(1)-C(7) | 118.08(11) |
| C(21)-B(1)-C(7) | 117.52(11) |
| C(32)-Si(2)-C(35) | 112.97(7) |
| C(32)-Si(2)-C(33) | 111.35(7) |
| C(35)-Si(2)-C(33) | 107.26(8) |
| C(32)-Si(2)-C(34) | 109.61(7) |
| C(35)-Si(2)-C(34) | 108.22(9) |
| C(33)-Si(2)-C(34) | 107.21(7) |
| C(2)-N(2)-C(1) | 118.46(10) |
| N(2)-C(2)-C(3) | 121.69(12) |
| N(2)-C(2)-C(6) | 118.33(11) |
| C(3)-C(2)-C(6) | 119.93(11) |
| C(36)-Si(3)-C(37) | 111.29(7) |
| C(36)-Si(3)-C(38) | 110.31(7) |
| C(37)-Si(3)-C(38) | 107.98(8) |
| C(36)-Si(3)-C(39) | 114.77(7) |
| C(37)-Si(3)-C(39) | 105.08(8) |
| C(38)-Si(3)-C(39) | 107.05(8) |
| C(4)-C(3)-C(2) | 119.55(12) |
| C(4)-C(3)-H(3) | 120.2 |
| C(2)-C(3)-H(3) | 120.2 |
| C(5)-C(4)-C(3) | 119.49(12) |
| C(5)-C(4)-H(4) | 120.3 |

| | |
|---|---|
| C(3)-C(4)-H(4) | 120.3 |
| C(4)-C(5)-C(1) | 118.34(13) |
| C(4)-C(5)-H(5) | 120.8 |
| C(1)-C(5)-H(5) | 120.8 |
| C(11)-C(6)-C(7) | 120.04(12) |
| C(11)-C(6)-C(2) | 118.08(12) |
| C(7)-C(6)-C(2) | 121.72(11) |
| C(8)-C(7)-C(6) | 117.44(12) |
| C(8)-C(7)-B(1) | 116.14(12) |
| C(6)-C(7)-B(1) | 125.90(12) |
| C(9)-C(8)-C(7) | 121.92(13) |
| C(9)-C(8)-H(8) | 119.0 |
| C(7)-C(8)-H(8) | 119.0 |
| C(10)-C(9)-C(8) | 119.90(14) |
| C(10)-C(9)-H(9) | 120.1 |
| C(8)-C(9)-H(9) | 120.1 |
| C(9)-C(10)-C(11) | 119.75(13) |
| C(9)-C(10)-H(10) | 120.1 |
| C(11)-C(10)-H(10) | 120.1 |
| C(10)-C(11)-C(6) | 120.94(13) |
| C(10)-C(11)-H(11) | 119.5 |
| C(6)-C(11)-H(11) | 119.5 |
| C(17)-C(12)-C(13) | 117.47(12) |
| C(17)-C(12)-B(1) | 121.46(11) |
| C(13)-C(12)-B(1) | 121.04(11) |
| C(14)-C(13)-C(12) | 120.08(12) |
| C(14)-C(13)-C(18) | 118.09(11) |
| C(12)-C(13)-C(18) | 121.64(12) |
| C(15)-C(14)-C(13) | 122.33(12) |
| C(15)-C(14)-H(14) | 118.8 |
| C(13)-C(14)-H(14) | 118.8 |
| C(14)-C(15)-C(16) | 117.37(12) |
| C(14)-C(15)-C(19) | 121.44(13) |

| | |
|---|---|
| C(16)-C(15)-C(19) | 121.16(13) |
| C(17)-C(16)-C(15) | 122.02(12) |
| C(17)-C(16)-H(16) | 119.0 |
| C(15)-C(16)-H(16) | 119.0 |
| C(16)-C(17)-C(12) | 120.57(12) |
| C(16)-C(17)-C(20) | 118.17(12) |
| C(12)-C(17)-C(20) | 121.26(12) |
| C(13)-C(18)-H(18A) | 109.5 |
| C(13)-C(18)-H(18B) | 109.5 |
| H(18A)-C(18)-H(18B) | 109.5 |
| C(13)-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(17)-C(20)-H(20A) | 109.5 |
| C(17)-C(20)-H(20B) | 109.5 |
| H(20A)-C(20)-H(20B) | 109.5 |
| C(17)-C(20)-H(20C) | 109.5 |
| H(20A)-C(20)-H(20C) | 109.5 |
| H(20B)-C(20)-H(20C) | 109.5 |
| C(22)-C(21)-C(26) | 117.13(12) |
| C(22)-C(21)-B(1) | 122.25(12) |
| C(26)-C(21)-B(1) | 120.48(11) |
| C(23)-C(22)-C(21) | 120.41(13) |
| C(23)-C(22)-C(27) | 116.31(12) |
| C(21)-C(22)-C(27) | 123.26(12) |
| C(24)-C(23)-C(22) | 122.16(14) |
| C(24)-C(23)-H(23) | 118.9 |

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|---|---|
| C(22)-C(23)-H(23) | 118.9 |
| C(23)-C(24)-C(25) | 117.77(13) |
| C(23)-C(24)-C(28) | 120.62(15) |
| C(25)-C(24)-C(28) | 121.56(15) |
| C(24)-C(25)-C(26) | 122.13(14) |
| C(24)-C(25)-H(25) | 118.9 |
| C(26)-C(25)-H(25) | 118.9 |
| C(25)-C(26)-C(21) | 120.31(13) |
| C(25)-C(26)-C(29) | 117.08(13) |
| C(21)-C(26)-C(29) | 122.58(12) |
| C(22)-C(27)-H(27A) | 109.5 |
| C(22)-C(27)-H(27B) | 109.5 |
| H(27A)-C(27)-H(27B) | 109.5 |
| C(22)-C(27)-H(27C) | 109.5 |
| H(27A)-C(27)-H(27C) | 109.5 |
| H(27B)-C(27)-H(27C) | 109.5 |
| C(24)-C(28)-H(28A) | 109.5 |
| C(24)-C(28)-H(28B) | 109.5 |
| H(28A)-C(28)-H(28B) | 109.5 |
| C(24)-C(28)-H(28C) | 109.5 |
| H(28A)-C(28)-H(28C) | 109.5 |
| H(28B)-C(28)-H(28C) | 109.5 |
| C(26)-C(29)-H(29A) | 109.5 |
| C(26)-C(29)-H(29B) | 109.5 |
| H(29A)-C(29)-H(29B) | 109.5 |
| C(26)-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 |
| Si(1)-C(31)-H(31A) | 109.5 |
| Si(1)-C(31)-H(31B) | 109.5 |
| H(31A)-C(31)-H(31B) | 109.5 |
| Si(1)-C(31)-H(31C) | 109.5 |
| H(31A)-C(31)-H(31C) | 109.5 |
| H(31B)-C(31)-H(31C) | 109.5 |
| Si(2)-C(32)-Zr(1) | 130.85(7) |
| Si(2)-C(32)-H(32A) | 104.6 |
| Zr(1)-C(32)-H(32A) | 104.6 |
| Si(2)-C(32)-H(32B) | 104.6 |
| Zr(1)-C(32)-H(32B) | 104.6 |
| H(32A)-C(32)-H(32B) | 105.7 |
| Si(2)-C(33)-H(33A) | 109.5 |
| Si(2)-C(33)-H(33B) | 109.5 |
| H(33A)-C(33)-H(33B) | 109.5 |
| Si(2)-C(33)-H(33C) | 109.5 |
| H(33A)-C(33)-H(33C) | 109.5 |
| H(33B)-C(33)-H(33C) | 109.5 |
| Si(2)-C(34)-H(34A) | 109.5 |
| Si(2)-C(34)-H(34B) | 109.5 |
| H(34A)-C(34)-H(34B) | 109.5 |
| Si(2)-C(34)-H(34C) | 109.5 |
| H(34A)-C(34)-H(34C) | 109.5 |
| H(34B)-C(34)-H(34C) | 109.5 |
| Si(2)-C(35)-H(35A) | 109.5 |
| Si(2)-C(35)-H(35B) | 109.5 |
| H(35A)-C(35)-H(35B) | 109.5 |
| Si(2)-C(35)-H(35C) | 109.5 |
| H(35A)-C(35)-H(35C) | 109.5 |
| H(35B)-C(35)-H(35C) | 109.5 |
| Si(3)-C(36)-Zr(1) | 126.57(7) |
| Si(3)-C(36)-H(36A) | 105.7 |

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|---|---|
| Zr(1)-C(36)-H(36A) | 105.7 |
| Si(3)-C(36)-H(36B) | 105.7 |
| Zr(1)-C(36)-H(36B) | 105.7 |
| H(36A)-C(36)-H(36B) | 106.1 |
| Si(3)-C(37)-H(37A) | 109.5 |
| Si(3)-C(37)-H(37B) | 109.5 |
| H(37A)-C(37)-H(37B) | 109.5 |
| Si(3)-C(37)-H(37C) | 109.5 |
| H(37A)-C(37)-H(37C) | 109.5 |
| H(37B)-C(37)-H(37C) | 109.5 |
| Si(3)-C(38)-H(38A) | 109.5 |
| Si(3)-C(38)-H(38B) | 109.5 |
| H(38A)-C(38)-H(38B) | 109.5 |
| Si(3)-C(38)-H(38C) | 109.5 |
| H(38A)-C(38)-H(38C) | 109.5 |
| H(38B)-C(38)-H(38C) | 109.5 |
| Si(3)-C(39)-H(39A) | 109.5 |
| Si(3)-C(39)-H(39B) | 109.5 |
| H(39A)-C(39)-H(39B) | 109.5 |
| Si(3)-C(39)-H(39C) | 109.5 |
| H(39A)-C(39)-H(39C) | 109.5 |
| H(39B)-C(39)-H(39C) | 109.5 |
| C(44)-C(40)-C(41) | 106.22(11) |
| C(44)-C(40)-Si(1) | 121.44(9) |
| C(41)-C(40)-Si(1) | 125.02(10) |
| C(44)-C(40)-Zr(1) | 73.68(8) |
| C(41)-C(40)-Zr(1) | 75.52(7) |
| Si(1)-C(40)-Zr(1) | 92.13(5) |
| C(42)-C(41)-C(40) | 108.74(12) |
| C(42)-C(41)-C(45) | 123.97(12) |
| C(40)-C(41)-C(45) | 127.17(12) |
| C(42)-C(41)-Zr(1) | 77.42(8) |
| C(40)-C(41)-Zr(1) | 71.09(7) |

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|---|---|
| C(45)-C(41)-Zr(1) | 120.91(9) |
| C(41)-C(42)-C(43) | 108.10(12) |
| C(41)-C(42)-C(46) | 124.68(14) |
| C(43)-C(42)-C(46) | 126.77(13) |
| C(41)-C(42)-Zr(1) | 70.64(7) |
| C(43)-C(42)-Zr(1) | 73.69(8) |
| C(46)-C(42)-Zr(1) | 127.38(10) |
| C(44)-C(43)-C(42) | 107.82(12) |
| C(44)-C(43)-C(47) | 125.08(14) |
| C(42)-C(43)-C(47) | 126.52(14) |
| C(44)-C(43)-Zr(1) | 69.26(8) |
| C(42)-C(43)-Zr(1) | 74.64(8) |
| C(47)-C(43)-Zr(1) | 128.43(10) |
| C(43)-C(44)-C(40) | 109.11(12) |
| C(43)-C(44)-C(48) | 124.59(13) |
| C(40)-C(44)-C(48) | 126.29(13) |
| C(43)-C(44)-Zr(1) | 78.56(8) |
| C(40)-C(44)-Zr(1) | 72.64(7) |
| C(48)-C(44)-Zr(1) | 114.24(10) |
| C(41)-C(45)-H(45A) | 109.5 |
| C(41)-C(45)-H(45B) | 109.5 |
| H(45A)-C(45)-H(45B) | 109.5 |
| C(41)-C(45)-H(45C) | 109.5 |
| H(45A)-C(45)-H(45C) | 109.5 |
| H(45B)-C(45)-H(45C) | 109.5 |
| C(42)-C(46)-H(46A) | 109.5 |
| C(42)-C(46)-H(46B) | 109.5 |
| H(46A)-C(46)-H(46B) | 109.5 |
| C(42)-C(46)-H(46C) | 109.5 |
| H(46A)-C(46)-H(46C) | 109.5 |
| H(46B)-C(46)-H(46C) | 109.5 |
| C(43)-C(47)-H(47A) | 109.5 |
| C(43)-C(47)-H(47B) | 109.5 |

H(47A)-C(47)-H(47B) 109.5

C(43)-C(47)-H(47C) 109.5

H(47A)-C(47)-H(47C) 109.5

H(47B)-C(47)-H(47C) 109.5

C(44)-C(48)-H(48A) 109.5

C(44)-C(48)-H(48B) 109.5

H(48A)-C(48)-H(48B) 109.5

C(44)-C(48)-H(48C) 109.5

H(48A)-C(48)-H(48C) 109.5

H(48B)-C(48)-H(48C) 109.5

C(1X1)-O(1X)-C(1X1)#1 180.0(3)

C(1X1)-O(1X)-C(1X) 68.7(2)

C(1X1)#1-O(1X)-C(1X) 111.3(2)

C(1X1)-O(1X)-C(1X)#1 111.3(2)

C(1X1)#1-O(1X)-C(1X)#1 68.7(2)

C(1X)-O(1X)-C(1X)#1 179.998(2)

O(1X)-C(1X)-C(2X) 106.8(4)

O(1X)-C(1X)-H(1X1) 110.4

C(2X)-C(1X)-H(1X1) 110.4

O(1X)-C(1X)-H(1X2) 110.4

C(2X)-C(1X)-H(1X2) 110.4

H(1X1)-C(1X)-H(1X2) 108.6

O(1X)-C(1X1)-C(2X1) 104.4(4)

O(1X)-C(1X1)-H(1X3) 110.9

C(2X1)-C(1X1)-H(1X3) 110.9

O(1X)-C(1X1)-H(1X4) 110.9

C(2X1)-C(1X1)-H(1X4) 110.9

H(1X3)-C(1X1)-H(1X4) 108.9

C(1X1)-C(2X1)-H(2X4) 109.5

C(1X1)-C(2X1)-H(2X5) 109.5

H(2X4)-C(2X1)-H(2X5) 109.5

C(1X1)-C(2X1)-H(2X6) 109.5

H(2X4)-C(2X1)-H(2X6) 109.5

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|---|---|---|
| H(2X5)-C(2X1)-H(2X6) | 109.5 | |

**Table S16.** Anisotropic displacement parameters ($A^2 \times 10^3$) for **L´Zr($CH_2SiMe_3$)$_2$**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$.

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| Zr(1) | 13(1) | 13(1) | 14(1) | 1(1) | -2(1) | -3(1) |
| Si(1) | 15(1) | 13(1) | 17(1) | -1(1) | 1(1) | -3(1) |
| N(1) | 22(1) | 17(1) | 15(1) | -1(1) | 4(1) | -6(1) |
| C(1) | 13(1) | 16(1) | 14(1) | 0(1) | 0(1) | -1(1) |
| B(1) | 13(1) | 15(1) | 15(1) | 0(1) | -3(1) | -5(1) |
| Si(2) | 17(1) | 15(1) | 20(1) | 1(1) | -4(1) | -2(1) |
| N(2) | 13(1) | 15(1) | 13(1) | 0(1) | -1(1) | -1(1) |
| C(2) | 11(1) | 16(1) | 14(1) | 2(1) | -2(1) | 0(1) |
| Si(3) | 17(1) | 19(1) | 18(1) | 0(1) | -5(1) | -6(1) |
| C(3) | 19(1) | 25(1) | 13(1) | -1(1) | 2(1) | -5(1) |
| C(4) | 21(1) | 26(1) | 15(1) | -6(1) | -1(1) | -6(1) |
| C(5) | 18(1) | 19(1) | 18(1) | -4(1) | -1(1) | -5(1) |
| C(6) | 18(1) | 15(1) | 14(1) | 2(1) | -2(1) | -1(1) |
| C(7) | 17(1) | 15(1) | 16(1) | 3(1) | -1(1) | -4(1) |
| C(8) | 24(1) | 17(1) | 23(1) | 4(1) | 0(1) | -7(1) |
| C(9) | 36(1) | 14(1) | 24(1) | 3(1) | -1(1) | -8(1) |
| C(10) | 36(1) | 14(1) | 23(1) | 0(1) | 2(1) | 1(1) |
| C(11) | 22(1) | 18(1) | 20(1) | 2(1) | 2(1) | 1(1) |
| C(12) | 12(1) | 14(1) | 15(1) | 1(1) | -1(1) | -3(1) |
| C(13) | 12(1) | 17(1) | 16(1) | -1(1) | -1(1) | -2(1) |
| C(14) | 15(1) | 23(1) | 17(1) | 4(1) | -3(1) | -2(1) |
| C(15) | 15(1) | 18(1) | 25(1) | 7(1) | -2(1) | -2(1) |
| C(16) | 21(1) | 14(1) | 25(1) | -1(1) | -2(1) | -4(1) |
| C(17) | 15(1) | 16(1) | 18(1) | -1(1) | -2(1) | -4(1) |
| C(18) | 22(1) | 22(1) | 17(1) | -4(1) | -2(1) | -7(1) |
| C(19) | 31(1) | 22(1) | 34(1) | 12(1) | 1(1) | -2(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(20) | 30(1) | 20(1) | 18(1) | -5(1) | -2(1) | -6(1) |
| C(21) | 15(1) | 16(1) | 16(1) | 0(1) | -1(1) | -5(1) |
| C(22) | 20(1) | 22(1) | 17(1) | 3(1) | -2(1) | -9(1) |
| C(23) | 27(1) | 26(1) | 16(1) | 3(1) | 1(1) | -10(1) |
| C(24) | 26(1) | 23(1) | 22(1) | -4(1) | 8(1) | -11(1) |
| C(25) | 17(1) | 22(1) | 27(1) | -3(1) | 4(1) | -4(1) |
| C(26) | 17(1) | 18(1) | 20(1) | -2(1) | 0(1) | -4(1) |
| C(27) | 23(1) | 42(1) | 21(1) | 11(1) | -7(1) | -8(1) |
| C(28) | 33(1) | 36(1) | 31(1) | 0(1) | 15(1) | -11(1) |
| C(29) | 15(1) | 35(1) | 26(1) | 5(1) | -4(1) | -3(1) |
| C(30) | 27(1) | 17(1) | 34(1) | -5(1) | 3(1) | -1(1) |
| C(31) | 22(1) | 29(1) | 27(1) | -4(1) | -6(1) | -7(1) |
| C(32) | 18(1) | 16(1) | 20(1) | 0(1) | -3(1) | -5(1) |
| C(33) | 20(1) | 24(1) | 34(1) | 8(1) | -6(1) | -6(1) |
| C(34) | 28(1) | 27(1) | 47(1) | 17(1) | -8(1) | -9(1) |
| C(35) | 35(1) | 48(1) | 29(1) | -12(1) | -15(1) | 11(1) |
| C(36) | 17(1) | 20(1) | 21(1) | -2(1) | -3(1) | -4(1) |
| C(37) | 45(1) | 22(1) | 27(1) | 4(1) | -9(1) | -8(1) |
| C(38) | 31(1) | 30(1) | 38(1) | 3(1) | -20(1) | -9(1) |
| C(39) | 29(1) | 39(1) | 36(1) | -17(1) | 3(1) | -13(1) |
| C(40) | 16(1) | 13(1) | 16(1) | 3(1) | -1(1) | -3(1) |
| C(41) | 17(1) | 18(1) | 14(1) | 2(1) | 2(1) | -5(1) |
| C(42) | 28(1) | 22(1) | 13(1) | 1(1) | 1(1) | -9(1) |
| C(43) | 28(1) | 25(1) | 17(1) | 7(1) | -9(1) | -11(1) |
| C(44) | 19(1) | 19(1) | 21(1) | 7(1) | -6(1) | -4(1) |
| C(45) | 16(1) | 20(1) | 28(1) | 2(1) | 5(1) | -3(1) |
| C(46) | 39(1) | 33(1) | 19(1) | -9(1) | 8(1) | -13(1) |
| C(47) | 44(1) | 41(1) | 26(1) | 10(1) | -19(1) | -19(1) |
| C(48) | 20(1) | 22(1) | 44(1) | 8(1) | -11(1) | -1(1) |
| O(1X) | 28(1) | 30(1) | 44(1) | 2(1) | 2(1) | -3(1) |
| C(1X) | 23(2) | 31(2) | 50(2) | -8(2) | 1(1) | -4(1) |
| C(2X) | 34(3) | 30(2) | 57(4) | 2(3) | -15(2) | 5(2) |
| C(1X1) | 29(2) | 27(2) | 64(3) | 1(2) | -2(2) | -6(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(2X1) | 34(3) | 51(4) | 68(5) | -9(3) | 7(3) | -16(3) |

**Table S17.** Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($A^2 \times 10^3$) for **L´Zr($CH_2SiMe_3$)$_2$**.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(3) | 5918 | 3427 | 4272 | 23 |
| H(4) | 6889 | 5068 | 4276 | 25 |
| H(5) | 8027 | 5546 | 3300 | 22 |
| H(8) | 3406 | 912 | 3811 | 25 |
| H(9) | 4614 | -897 | 3359 | 30 |
| H(10) | 6644 | -979 | 2875 | 31 |
| H(11) | 7449 | 763 | 2836 | 25 |
| H(14) | 3784 | 5111 | 1787 | 22 |
| H(16) | 3734 | 7187 | 3392 | 24 |
| H(18A) | 3405 | 3219 | 1862 | 29 |
| H(18B) | 2772 | 2825 | 2557 | 29 |
| H(18C) | 4238 | 2417 | 2362 | 29 |
| H(19A) | 3169 | 8033 | 2183 | 44 |
| H(19B) | 3945 | 7132 | 1606 | 44 |
| H(19C) | 4646 | 7669 | 2136 | 44 |
| H(20A) | 3508 | 6526 | 4448 | 34 |
| H(20B) | 4232 | 5162 | 4539 | 34 |
| H(20C) | 2756 | 5472 | 4570 | 34 |
| H(23) | 2400 | 2055 | 5952 | 27 |
| H(25) | -303 | 3634 | 4886 | 27 |
| H(27A) | 4668 | 2738 | 5361 | 42 |
| H(27B) | 4894 | 1843 | 4732 | 42 |
| H(27C) | 4435 | 1396 | 5452 | 42 |
| H(28A) | -878 | 2979 | 5968 | 51 |

| | | | | |
|---|---|---|---|---|
| H(28B) | 131 | 2821 | 6478 | 51 |
| H(28C) | -27 | 1674 | 6070 | 51 |
| H(29A) | 24 | 4317 | 3857 | 39 |
| H(29B) | 1241 | 3625 | 3401 | 39 |
| H(29C) | 1208 | 4914 | 3728 | 39 |
| H(30A) | 7156 | 6971 | 1988 | 41 |
| H(30B) | 8240 | 7567 | 1634 | 41 |
| H(30C) | 8172 | 7283 | 2411 | 41 |
| H(31A) | 10480 | 5917 | 2449 | 39 |
| H(31B) | 11013 | 5925 | 1679 | 39 |
| H(31C) | 11049 | 4667 | 2054 | 39 |
| H(32A) | 8824 | 713 | 1493 | 22 |
| H(32B) | 9910 | 1122 | 1038 | 22 |
| H(33A) | 12334 | 105 | 1345 | 38 |
| H(33B) | 12667 | 296 | 2077 | 38 |
| H(33C) | 12222 | 1443 | 1629 | 38 |
| H(34A) | 9507 | -915 | 2508 | 50 |
| H(34B) | 10931 | -1228 | 2631 | 50 |
| H(34C) | 10560 | -1422 | 1909 | 50 |
| H(35A) | 10194 | 2442 | 2770 | 59 |
| H(35B) | 10783 | 1275 | 3169 | 59 |
| H(35C) | 9335 | 1573 | 3098 | 59 |
| H(36A) | 5882 | 2699 | 1683 | 23 |
| H(36B) | 5897 | 3411 | 1006 | 23 |
| H(37A) | 6625 | -164 | 1595 | 46 |
| H(37B) | 5689 | -557 | 1145 | 46 |
| H(37C) | 5176 | 428 | 1729 | 46 |
| H(38A) | 3972 | 2157 | 668 | 47 |
| H(38B) | 4509 | 1039 | 164 | 47 |
| H(38C) | 4823 | 2332 | -5 | 47 |
| H(39A) | 7466 | 1177 | -219 | 51 |
| H(39B) | 7261 | -134 | 2 | 51 |
| H(39C) | 8181 | 481 | 358 | 51 |

| | | | | |
|---|---|---|---|---|
| H(45A) | 11498 | 2544 | 579 | 33 |
| H(45B) | 11280 | 3422 | 1215 | 33 |
| H(45C) | 11694 | 3900 | 495 | 33 |
| H(46A) | 10593 | 2472 | -572 | 46 |
| H(46B) | 9320 | 2031 | -559 | 46 |
| H(46C) | 10247 | 1524 | -28 | 46 |
| H(47A) | 6350 | 3759 | -31 | 51 |
| H(47B) | 7469 | 3071 | -553 | 51 |
| H(47C) | 7024 | 4512 | -576 | 51 |
| H(48A) | 6049 | 5637 | 577 | 43 |
| H(48B) | 6803 | 6626 | 745 | 43 |
| H(48C) | 6398 | 5746 | 1313 | 43 |
| H(1X1) | 1359 | 10789 | 4573 | 42 |
| H(1X2) | 1316 | 9545 | 4212 | 42 |
| H(2X1) | 2089 | 9699 | 5510 | 63 |
| H(2X2) | 3002 | 9172 | 4859 | 63 |
| H(2X3) | 1990 | 8453 | 5179 | 63 |
| H(1X3) | 806 | 8499 | 5430 | 49 |
| H(1X4) | 930 | 9727 | 5784 | 49 |
| H(2X4) | 2122 | 8930 | 4470 | 77 |
| H(2X5) | 2845 | 8872 | 5108 | 77 |
| H(2X6) | 2241 | 10154 | 4818 | 77 |

**Table S18**. Torsion angles [º] for **L´Zr($CH_2SiMe_3$)$_2$**.

| | |
|---|---|
| C(32)-Zr(1)-Si(1)-N(1) | -80.88(8) |
| C(36)-Zr(1)-Si(1)-N(1) | 80.83(8) |
| C(40)-Zr(1)-Si(1)-N(1) | 175.60(8) |
| C(44)-Zr(1)-Si(1)-N(1) | 142.93(7) |
| C(41)-Zr(1)-Si(1)-N(1) | -153.74(7) |
| C(43)-Zr(1)-Si(1)-N(1) | 158.52(7) |
| C(42)-Zr(1)-Si(1)-N(1) | -169.81(7) |

| | |
|---|---|
| N(1)-Zr(1)-Si(1)-C(31) | 87.93(9) |
| C(32)-Zr(1)-Si(1)-C(31) | 7.05(7) |
| C(36)-Zr(1)-Si(1)-C(31) | 168.76(8) |
| C(40)-Zr(1)-Si(1)-C(31) | -96.47(8) |
| C(44)-Zr(1)-Si(1)-C(31) | -129.14(7) |
| C(41)-Zr(1)-Si(1)-C(31) | -65.81(7) |
| C(43)-Zr(1)-Si(1)-C(31) | -113.54(7) |
| C(42)-Zr(1)-Si(1)-C(31) | -81.87(7) |
| N(1)-Zr(1)-Si(1)-C(30) | -80.59(9) |
| C(32)-Zr(1)-Si(1)-C(30) | -161.47(8) |
| C(36)-Zr(1)-Si(1)-C(30) | 0.24(9) |
| C(40)-Zr(1)-Si(1)-C(30) | 95.01(8) |
| C(44)-Zr(1)-Si(1)-C(30) | 62.34(8) |
| C(41)-Zr(1)-Si(1)-C(30) | 125.67(8) |
| C(43)-Zr(1)-Si(1)-C(30) | 77.94(7) |
| C(42)-Zr(1)-Si(1)-C(30) | 109.61(7) |
| N(1)-Zr(1)-Si(1)-C(40) | -175.60(8) |
| C(32)-Zr(1)-Si(1)-C(40) | 103.52(6) |
| C(36)-Zr(1)-Si(1)-C(40) | -94.77(7) |
| C(44)-Zr(1)-Si(1)-C(40) | -32.67(6) |
| C(41)-Zr(1)-Si(1)-C(40) | 30.66(6) |
| C(43)-Zr(1)-Si(1)-C(40) | -17.08(6) |
| C(42)-Zr(1)-Si(1)-C(40) | 14.59(6) |
| C(31)-Si(1)-N(1)-C(1) | 80.85(15) |
| C(30)-Si(1)-N(1)-C(1) | -41.59(16) |
| C(40)-Si(1)-N(1)-C(1) | -160.34(14) |
| Zr(1)-Si(1)-N(1)-C(1) | -163.78(18) |
| C(31)-Si(1)-N(1)-Zr(1) | -115.37(7) |
| C(30)-Si(1)-N(1)-Zr(1) | 122.20(7) |
| C(40)-Si(1)-N(1)-Zr(1) | 3.44(6) |
| C(32)-Zr(1)-N(1)-C(1) | -78.02(10) |
| C(36)-Zr(1)-N(1)-C(1) | 45.04(11) |
| C(40)-Zr(1)-N(1)-C(1) | 165.00(11) |

| | |
|---|---|
| C(44)-Zr(1)-N(1)-C(1) | 136.15(10) |
| C(41)-Zr(1)-N(1)-C(1) | -169.36(10) |
| C(43)-Zr(1)-N(1)-C(1) | 143.41(9) |
| C(42)-Zr(1)-N(1)-C(1) | 179.58(9) |
| Si(1)-Zr(1)-N(1)-C(1) | 167.82(14) |
| C(32)-Zr(1)-N(1)-Si(1) | 114.16(6) |
| C(36)-Zr(1)-N(1)-Si(1) | -122.78(6) |
| C(40)-Zr(1)-N(1)-Si(1) | -2.83(5) |
| C(44)-Zr(1)-N(1)-Si(1) | -31.68(6) |
| C(41)-Zr(1)-N(1)-Si(1) | 22.82(6) |
| C(43)-Zr(1)-N(1)-Si(1) | -24.41(8) |
| C(42)-Zr(1)-N(1)-Si(1) | 11.76(8) |
| Si(1)-N(1)-C(1)-N(2) | 167.03(11) |
| Zr(1)-N(1)-C(1)-N(2) | 3.70(14) |
| Si(1)-N(1)-C(1)-C(5) | -12.1(2) |
| Zr(1)-N(1)-C(1)-C(5) | -175.43(10) |
| N(1)-C(1)-N(2)-C(2) | -177.89(11) |
| C(5)-C(1)-N(2)-C(2) | 1.25(18) |
| C(1)-N(2)-C(2)-C(3) | -2.35(18) |
| C(1)-N(2)-C(2)-C(6) | -179.69(11) |
| N(2)-C(2)-C(3)-C(4) | 1.8(2) |
| C(6)-C(2)-C(3)-C(4) | 179.09(12) |
| C(2)-C(3)-C(4)-C(5) | -0.1(2) |
| C(3)-C(4)-C(5)-C(1) | -1.0(2) |
| N(2)-C(1)-C(5)-C(4) | 0.4(2) |
| N(1)-C(1)-C(5)-C(4) | 179.45(13) |
| N(2)-C(2)-C(6)-C(11) | 47.45(17) |
| C(3)-C(2)-C(6)-C(11) | -129.93(14) |
| N(2)-C(2)-C(6)-C(7) | -137.25(12) |
| C(3)-C(2)-C(6)-C(7) | 45.37(18) |
| C(11)-C(6)-C(7)-C(8) | 0.73(19) |
| C(2)-C(6)-C(7)-C(8) | -174.48(12) |
| C(11)-C(6)-C(7)-B(1) | -170.64(12) |

| | |
|---|---|
| C(2)-C(6)-C(7)-B(1) | 14.15(19) |
| C(12)-B(1)-C(7)-C(8) | -132.72(13) |
| C(21)-B(1)-C(7)-C(8) | 41.06(17) |
| C(12)-B(1)-C(7)-C(6) | 38.75(18) |
| C(21)-B(1)-C(7)-C(6) | -147.47(13) |
| C(6)-C(7)-C(8)-C(9) | -1.3(2) |
| B(1)-C(7)-C(8)-C(9) | 170.93(13) |
| C(7)-C(8)-C(9)-C(10) | 1.1(2) |
| C(8)-C(9)-C(10)-C(11) | -0.3(2) |
| C(9)-C(10)-C(11)-C(6) | -0.3(2) |
| C(7)-C(6)-C(11)-C(10) | 0.0(2) |
| C(2)-C(6)-C(11)-C(10) | 175.40(13) |
| C(21)-B(1)-C(12)-C(17) | 55.41(18) |
| C(7)-B(1)-C(12)-C(17) | -131.25(13) |
| C(21)-B(1)-C(12)-C(13) | -126.46(13) |
| C(7)-B(1)-C(12)-C(13) | 46.88(17) |
| C(17)-C(12)-C(13)-C(14) | 3.87(18) |
| B(1)-C(12)-C(13)-C(14) | -174.33(12) |
| C(17)-C(12)-C(13)-C(18) | -171.07(12) |
| B(1)-C(12)-C(13)-C(18) | 10.73(19) |
| C(12)-C(13)-C(14)-C(15) | -0.8(2) |
| C(18)-C(13)-C(14)-C(15) | 174.28(12) |
| C(13)-C(14)-C(15)-C(16) | -2.0(2) |
| C(13)-C(14)-C(15)-C(19) | 179.78(13) |
| C(14)-C(15)-C(16)-C(17) | 1.8(2) |
| C(19)-C(15)-C(16)-C(17) | 179.98(13) |
| C(15)-C(16)-C(17)-C(12) | 1.3(2) |
| C(15)-C(16)-C(17)-C(20) | -178.33(13) |
| C(13)-C(12)-C(17)-C(16) | -4.12(19) |
| B(1)-C(12)-C(17)-C(16) | 174.07(12) |
| C(13)-C(12)-C(17)-C(20) | 175.53(12) |
| B(1)-C(12)-C(17)-C(20) | -6.28(19) |
| C(12)-B(1)-C(21)-C(22) | -139.79(13) |

| | |
|---|---|
| C(7)-B(1)-C(21)-C(22) | 46.84(18) |
| C(12)-B(1)-C(21)-C(26) | 44.62(18) |
| C(7)-B(1)-C(21)-C(26) | -128.75(13) |
| C(26)-C(21)-C(22)-C(23) | 1.1(2) |
| B(1)-C(21)-C(22)-C(23) | -174.67(12) |
| C(26)-C(21)-C(22)-C(27) | -177.10(13) |
| B(1)-C(21)-C(22)-C(27) | 7.2(2) |
| C(21)-C(22)-C(23)-C(24) | 1.6(2) |
| C(27)-C(22)-C(23)-C(24) | 179.87(14) |
| C(22)-C(23)-C(24)-C(25) | -2.6(2) |
| C(22)-C(23)-C(24)-C(28) | 174.87(14) |
| C(23)-C(24)-C(25)-C(26) | 1.0(2) |
| C(28)-C(24)-C(25)-C(26) | -176.44(14) |
| C(24)-C(25)-C(26)-C(21) | 1.6(2) |
| C(24)-C(25)-C(26)-C(29) | 179.66(14) |
| C(22)-C(21)-C(26)-C(25) | -2.59(19) |
| B(1)-C(21)-C(26)-C(25) | 173.22(12) |
| C(22)-C(21)-C(26)-C(29) | 179.44(13) |
| B(1)-C(21)-C(26)-C(29) | -4.7(2) |
| C(35)-Si(2)-C(32)-Zr(1) | 19.36(13) |
| C(33)-Si(2)-C(32)-Zr(1) | -101.41(10) |
| C(34)-Si(2)-C(32)-Zr(1) | 140.13(10) |
| N(1)-Zr(1)-C(32)-Si(2) | 0.84(11) |
| C(36)-Zr(1)-C(32)-Si(2) | -132.53(9) |
| C(40)-Zr(1)-C(32)-Si(2) | 76.97(10) |
| C(44)-Zr(1)-C(32)-Si(2) | 114.25(10) |
| C(41)-Zr(1)-C(32)-Si(2) | 90.97(9) |
| C(43)-Zr(1)-C(32)-Si(2) | 139.90(8) |
| C(42)-Zr(1)-C(32)-Si(2) | 122.86(9) |
| Si(1)-Zr(1)-C(32)-Si(2) | 34.07(11) |
| C(37)-Si(3)-C(36)-Zr(1) | 94.14(10) |
| C(38)-Si(3)-C(36)-Zr(1) | -146.03(9) |
| C(39)-Si(3)-C(36)-Zr(1) | -25.03(12) |

| | |
|---|---|
| N(1)-Zr(1)-C(36)-Si(3) | -159.48(7) |
| C(32)-Zr(1)-C(36)-Si(3) | -32.70(10) |
| C(40)-Zr(1)-C(36)-Si(3) | 116.01(8) |
| C(44)-Zr(1)-C(36)-Si(3) | 113.10(9) |
| C(41)-Zr(1)-C(36)-Si(3) | 72.81(11) |
| C(43)-Zr(1)-C(36)-Si(3) | 82.78(9) |
| C(42)-Zr(1)-C(36)-Si(3) | 60.21(9) |
| Si(1)-Zr(1)-C(36)-Si(3) | 163.39(5) |
| N(1)-Si(1)-C(40)-C(44) | 69.33(11) |
| C(31)-Si(1)-C(40)-C(44) | -172.26(11) |
| C(30)-Si(1)-C(40)-C(44) | -46.86(13) |
| Zr(1)-Si(1)-C(40)-C(44) | 72.13(10) |
| N(1)-Si(1)-C(40)-C(41) | -76.58(12) |
| C(31)-Si(1)-C(40)-C(41) | 41.83(14) |
| C(30)-Si(1)-C(40)-C(41) | 167.24(11) |
| Zr(1)-Si(1)-C(40)-C(41) | -73.77(11) |
| N(1)-Si(1)-C(40)-Zr(1) | -2.81(5) |
| C(31)-Si(1)-C(40)-Zr(1) | 115.60(7) |
| C(30)-Si(1)-C(40)-Zr(1) | -118.99(6) |
| N(1)-Zr(1)-C(40)-C(44) | -119.75(8) |
| C(32)-Zr(1)-C(40)-C(44) | 138.16(8) |
| C(36)-Zr(1)-C(40)-C(44) | -5.24(9) |
| C(41)-Zr(1)-C(40)-C(44) | 112.10(11) |
| C(43)-Zr(1)-C(40)-C(44) | 36.62(8) |
| C(42)-Zr(1)-C(40)-C(44) | 75.89(8) |
| Si(1)-Zr(1)-C(40)-C(44) | -122.21(9) |
| N(1)-Zr(1)-C(40)-C(41) | 128.16(9) |
| C(32)-Zr(1)-C(40)-C(41) | 26.07(9) |
| C(36)-Zr(1)-C(40)-C(41) | -117.34(8) |
| C(44)-Zr(1)-C(40)-C(41) | -112.10(11) |
| C(43)-Zr(1)-C(40)-C(41) | -75.47(8) |
| C(42)-Zr(1)-C(40)-C(41) | -36.21(8) |
| Si(1)-Zr(1)-C(40)-C(41) | 125.70(10) |

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| N(1)-Zr(1)-C(40)-Si(1) | 2.46(5) |
| C(32)-Zr(1)-C(40)-Si(1) | -99.63(6) |
| C(36)-Zr(1)-C(40)-Si(1) | 116.97(6) |
| C(44)-Zr(1)-C(40)-Si(1) | 122.21(9) |
| C(41)-Zr(1)-C(40)-Si(1) | -125.70(10) |
| C(43)-Zr(1)-C(40)-Si(1) | 158.83(7) |
| C(42)-Zr(1)-C(40)-Si(1) | -161.90(7) |
| C(44)-C(40)-C(41)-C(42) | 1.11(14) |
| Si(1)-C(40)-C(41)-C(42) | 151.24(10) |
| Zr(1)-C(40)-C(41)-C(42) | 68.95(9) |
| C(44)-C(40)-C(41)-C(45) | 177.22(13) |
| Si(1)-C(40)-C(41)-C(45) | -32.65(19) |
| Zr(1)-C(40)-C(41)-C(45) | -114.94(13) |
| C(44)-C(40)-C(41)-Zr(1) | -67.83(9) |
| Si(1)-C(40)-C(41)-Zr(1) | 82.30(9) |
| N(1)-Zr(1)-C(41)-C(42) | -161.66(8) |
| C(32)-Zr(1)-C(41)-C(42) | 86.76(9) |
| C(36)-Zr(1)-C(41)-C(42) | -23.55(11) |
| C(40)-Zr(1)-C(41)-C(42) | -115.11(12) |
| C(44)-Zr(1)-C(41)-C(42) | -76.00(9) |
| C(43)-Zr(1)-C(41)-C(42) | -35.91(8) |
| Si(1)-Zr(1)-C(41)-C(42) | -148.46(9) |
| N(1)-Zr(1)-C(41)-C(40) | -46.55(8) |
| C(32)-Zr(1)-C(41)-C(40) | -158.13(8) |
| C(36)-Zr(1)-C(41)-C(40) | 91.55(9) |
| C(44)-Zr(1)-C(41)-C(40) | 39.11(7) |
| C(43)-Zr(1)-C(41)-C(40) | 79.20(8) |
| C(42)-Zr(1)-C(41)-C(40) | 115.11(12) |
| Si(1)-Zr(1)-C(41)-C(40) | -33.36(6) |
| N(1)-Zr(1)-C(41)-C(45) | 76.08(11) |
| C(32)-Zr(1)-C(41)-C(45) | -35.49(11) |
| C(36)-Zr(1)-C(41)-C(45) | -145.81(10) |
| C(40)-Zr(1)-C(41)-C(45) | 122.63(14) |

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| C(44)-Zr(1)-C(41)-C(45) | 161.74(12) |
| C(43)-Zr(1)-C(41)-C(45) | -158.17(12) |
| C(42)-Zr(1)-C(41)-C(45) | -122.26(14) |
| Si(1)-Zr(1)-C(41)-C(45) | 89.28(10) |
| C(40)-C(41)-C(42)-C(43) | -0.11(15) |
| C(45)-C(41)-C(42)-C(43) | -176.37(12) |
| Zr(1)-C(41)-C(42)-C(43) | 64.66(10) |
| C(40)-C(41)-C(42)-C(46) | 172.59(13) |
| C(45)-C(41)-C(42)-C(46) | -3.7(2) |
| Zr(1)-C(41)-C(42)-C(46) | -122.64(14) |
| C(40)-C(41)-C(42)-Zr(1) | -64.77(9) |
| C(45)-C(41)-C(42)-Zr(1) | 118.97(13) |
| N(1)-Zr(1)-C(42)-C(41) | 21.25(10) |
| C(32)-Zr(1)-C(42)-C(41) | -93.48(8) |
| C(36)-Zr(1)-C(42)-C(41) | 162.87(8) |
| C(40)-Zr(1)-C(42)-C(41) | 37.91(8) |
| C(44)-Zr(1)-C(42)-C(41) | 79.98(9) |
| C(43)-Zr(1)-C(42)-C(41) | 116.48(12) |
| Si(1)-Zr(1)-C(42)-C(41) | 27.29(8) |
| N(1)-Zr(1)-C(42)-C(43) | -95.23(9) |
| C(32)-Zr(1)-C(42)-C(43) | 150.04(9) |
| C(36)-Zr(1)-C(42)-C(43) | 46.39(9) |
| C(40)-Zr(1)-C(42)-C(43) | -78.57(9) |
| C(44)-Zr(1)-C(42)-C(43) | -36.49(8) |
| C(41)-Zr(1)-C(42)-C(43) | -116.48(12) |
| Si(1)-Zr(1)-C(42)-C(43) | -89.19(8) |
| N(1)-Zr(1)-C(42)-C(46) | 140.62(13) |
| C(32)-Zr(1)-C(42)-C(46) | 25.89(14) |
| C(36)-Zr(1)-C(42)-C(46) | -77.76(14) |
| C(40)-Zr(1)-C(42)-C(46) | 157.28(15) |
| C(44)-Zr(1)-C(42)-C(46) | -160.65(15) |
| C(41)-Zr(1)-C(42)-C(46) | 119.37(17) |
| C(43)-Zr(1)-C(42)-C(46) | -124.15(17) |

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| Si(1)-Zr(1)-C(42)-C(46) | 146.66(13) |
| C(41)-C(42)-C(43)-C(44) | -0.97(16) |
| C(46)-C(42)-C(43)-C(44) | -173.47(14) |
| Zr(1)-C(42)-C(43)-C(44) | 61.71(10) |
| C(41)-C(42)-C(43)-C(47) | 170.55(14) |
| C(46)-C(42)-C(43)-C(47) | -2.0(2) |
| Zr(1)-C(42)-C(43)-C(47) | -126.78(15) |
| C(41)-C(42)-C(43)-Zr(1) | -62.68(9) |
| C(46)-C(42)-C(43)-Zr(1) | 124.82(15) |
| N(1)-Zr(1)-C(43)-C(44) | -13.71(10) |
| C(32)-Zr(1)-C(43)-C(44) | -150.24(8) |
| C(36)-Zr(1)-C(43)-C(44) | 108.80(9) |
| C(40)-Zr(1)-C(43)-C(44) | -38.40(8) |
| C(41)-Zr(1)-C(43)-C(44) | -80.08(9) |
| C(42)-Zr(1)-C(43)-C(44) | -116.31(12) |
| Si(1)-Zr(1)-C(43)-C(44) | -26.03(8) |
| N(1)-Zr(1)-C(43)-C(42) | 102.60(9) |
| C(32)-Zr(1)-C(43)-C(42) | -33.93(10) |
| C(36)-Zr(1)-C(43)-C(42) | -134.89(9) |
| C(40)-Zr(1)-C(43)-C(42) | 77.91(9) |
| C(44)-Zr(1)-C(43)-C(42) | 116.31(12) |
| C(41)-Zr(1)-C(43)-C(42) | 36.23(8) |
| Si(1)-Zr(1)-C(43)-C(42) | 90.29(8) |
| N(1)-Zr(1)-C(43)-C(47) | -132.66(14) |
| C(32)-Zr(1)-C(43)-C(47) | 90.80(15) |
| C(36)-Zr(1)-C(43)-C(47) | -10.15(14) |
| C(40)-Zr(1)-C(43)-C(47) | -157.36(16) |
| C(44)-Zr(1)-C(43)-C(47) | -118.95(18) |
| C(41)-Zr(1)-C(43)-C(47) | 160.97(16) |
| C(42)-Zr(1)-C(43)-C(47) | 124.74(18) |
| Si(1)-Zr(1)-C(43)-C(47) | -144.98(14) |
| C(42)-C(43)-C(44)-C(40) | 1.68(16) |
| C(47)-C(43)-C(44)-C(40) | -169.98(14) |

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| Zr(1)-C(43)-C(44)-C(40) | 66.90(9) |
| C(42)-C(43)-C(44)-C(48) | -176.89(13) |
| C(47)-C(43)-C(44)-C(48) | 11.4(2) |
| Zr(1)-C(43)-C(44)-C(48) | -111.67(14) |
| C(42)-C(43)-C(44)-Zr(1) | -65.22(10) |
| C(47)-C(43)-C(44)-Zr(1) | 123.11(14) |
| C(41)-C(40)-C(44)-C(43) | -1.72(15) |
| Si(1)-C(40)-C(44)-C(43) | -153.16(10) |
| Zr(1)-C(40)-C(44)-C(43) | -70.84(10) |
| C(41)-C(40)-C(44)-C(48) | 176.82(13) |
| Si(1)-C(40)-C(44)-C(48) | 25.38(19) |
| Zr(1)-C(40)-C(44)-C(48) | 107.70(14) |
| C(41)-C(40)-C(44)-Zr(1) | 69.12(9) |
| Si(1)-C(40)-C(44)-Zr(1) | -82.33(9) |
| N(1)-Zr(1)-C(44)-C(43) | 167.85(9) |
| C(32)-Zr(1)-C(44)-C(43) | 46.64(12) |
| C(36)-Zr(1)-C(44)-C(43) | -69.81(9) |
| C(40)-Zr(1)-C(44)-C(43) | 114.40(12) |
| C(41)-Zr(1)-C(44)-C(43) | 75.65(9) |
| C(42)-Zr(1)-C(44)-C(43) | 35.89(8) |
| Si(1)-Zr(1)-C(44)-C(43) | 149.69(9) |
| N(1)-Zr(1)-C(44)-C(40) | 53.45(8) |
| C(32)-Zr(1)-C(44)-C(40) | -67.77(11) |
| C(36)-Zr(1)-C(44)-C(40) | 175.78(8) |
| C(41)-Zr(1)-C(44)-C(40) | -38.75(7) |
| C(43)-Zr(1)-C(44)-C(40) | -114.40(12) |
| C(42)-Zr(1)-C(44)-C(40) | -78.51(8) |
| Si(1)-Zr(1)-C(44)-C(40) | 35.28(6) |
| N(1)-Zr(1)-C(44)-C(48) | -69.18(11) |
| C(32)-Zr(1)-C(44)-C(48) | 169.60(10) |
| C(36)-Zr(1)-C(44)-C(48) | 53.15(11) |
| C(40)-Zr(1)-C(44)-C(48) | -122.63(14) |
| C(41)-Zr(1)-C(44)-C(48) | -161.38(12) |

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| C(43)-Zr(1)-C(44)-C(48) | 122.97(15) |
| C(42)-Zr(1)-C(44)-C(48) | 158.86(13) |
| Si(1)-Zr(1)-C(44)-C(48) | -87.35(10) |
| C(1X1)-O(1X)-C(1X)-C(2X) | -2.3(5) |
| C(1X1)#1-O(1X)-C(1X)-C(2X) | 177.7(5) |
| C(1X)#1-O(1X)-C(1X)-C(2X) | -16(37) |
| C(1X1)#1-O(1X)-C(1X1)-C(2X1) | 94(32) |
| C(1X)-O(1X)-C(1X1)-C(2X1) | -3.1(5) |
| C(1X)#1-O(1X)-C(1X1)-C(2X1) | 176.9(5) |