Synthesis of *Lewis* Acidic, Aromatic Aminotroponiminate Zinc Complexes for the Ring-Opening Polymerization of Cyclic Esters

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1. Different reaction conditions for the complexation of pro-ligand **1b** with $Zn(NTMS_2)_2$

Table S1. Varying temperature for the complexation of ligand **1b**. All reactions were performed in 20 mL toluene under argon atmosphere.

entry	eq. $Zn(NTMS_2)_2$	temp. [°C]	time [h]	amount heteroleptic complex **I** [%]	amount homoleptic complex **I'** [%]
S1[a]	1.2	0 °C	24	51	49
S2	1.2	25 °C	24	50	50
S3	1.2	100 °C	72	41	59
S4[b]	1.2	25 °C	3	55	45

[a]Performing the reaction at 0 °C lead to a lower conversion to the complexes **I** and **I'** with 26% remaining ligand **1b.** [b]The order of addition was changed; in this experiment a solution of ligand **1b** in toluene was added to a solution of $Zn(NTMS_2)_2$ in toluene (92% remaining ligand **1b**).

2. *In situ* IR monitoring of ROP of BBL at different temperatures: Plot of the carbonyl stretching bond of PHB (ν = 1750 cm^{-1}) against time

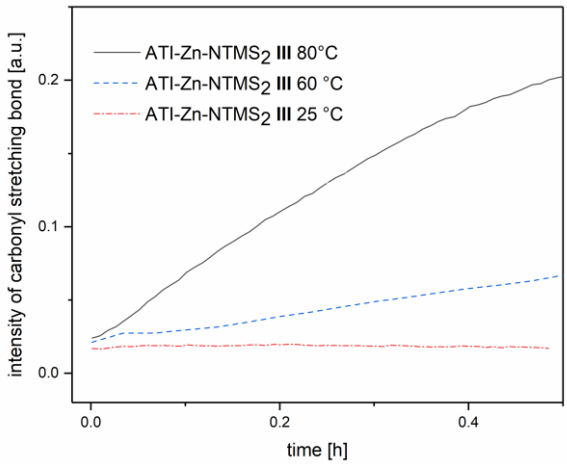


Figure S1. Polymerization of BBL with catalyst **III** under the same conditions with varying temperature monitored by *in situ* IR spectroscopy ($\nu_{C=O, PHB}$ = 1750 cm^{-1}). The plot shows the slope of the carbonyl stretching bond within the first 30 minutes reaction time. All polymerizations were performed in the same autoclave.

3. Behavior of catalyst **III** towards 1.0 eq. 2-propanol

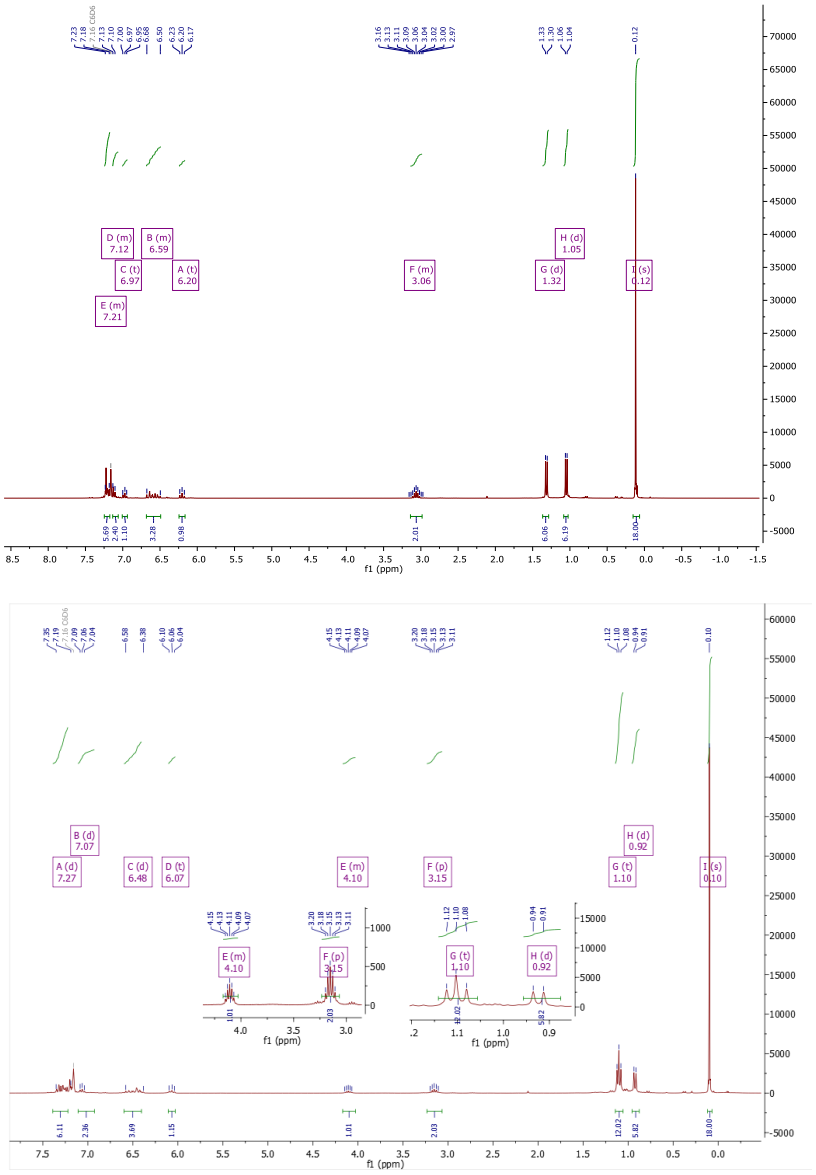


Figure S2. ^{1}H NMR spectrum of complex **III** in C_6D_6 (top) and complex **III** 10 minutes after the addition of 1.0 equiv. *i*PrOH (bottom).

4. *In situ* IR monitoring of ROP of BBL with the addition of 1.0 eq. *i*PrOH: Plot of the carbonyl stretching bond of PHB (ν = 1750 cm^{-1}) against time

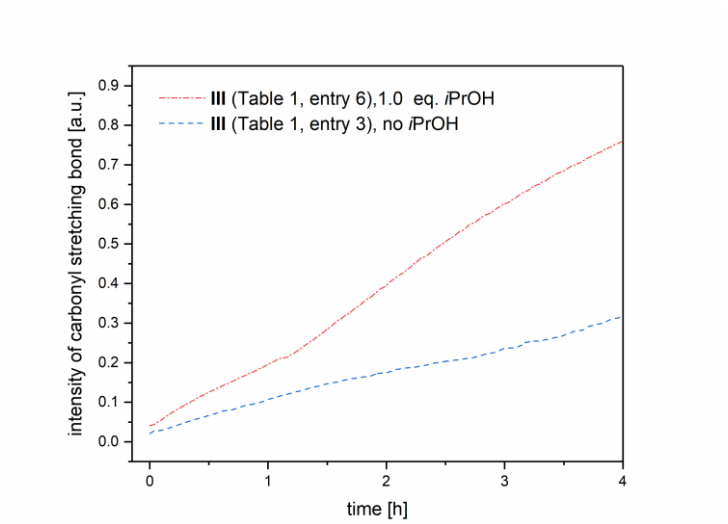


Figure S3. Polymerization of BBL with catalyst **III** under the same conditions at 60 °C with and without the presence of 1.0 eq. *i*PrOH monitored by *in situ* IR spectroscopy ($\nu_{C=O,\ PHB}$ = 1750 cm^{-1}). The plot shows the slope of the carbonyl stretching bond within four hours reaction time.

5. *In situ* IR monitoring of ROP of BBL with catalysts **I**–**IV**: Plot of the carbonyl stretching bond of PHB (ν = 1750 cm^{-1}) against time

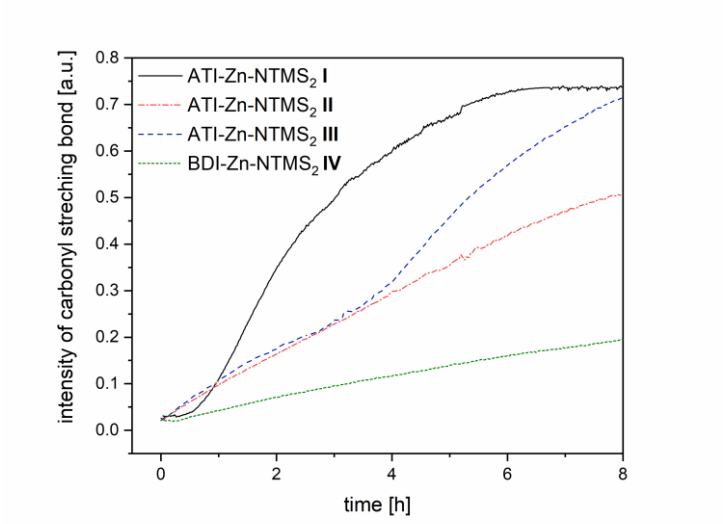


Figure S4. Polymerization of BBL with catalysts **I-IV** under the same conditions monitored by *in situ* IR spectroscopy ($\nu_{C=O,\ PHB}$ = 1750 cm^{-1}).

6. Carbonyl region of ^{13}C-NMR spectra of PHB (Table 1)

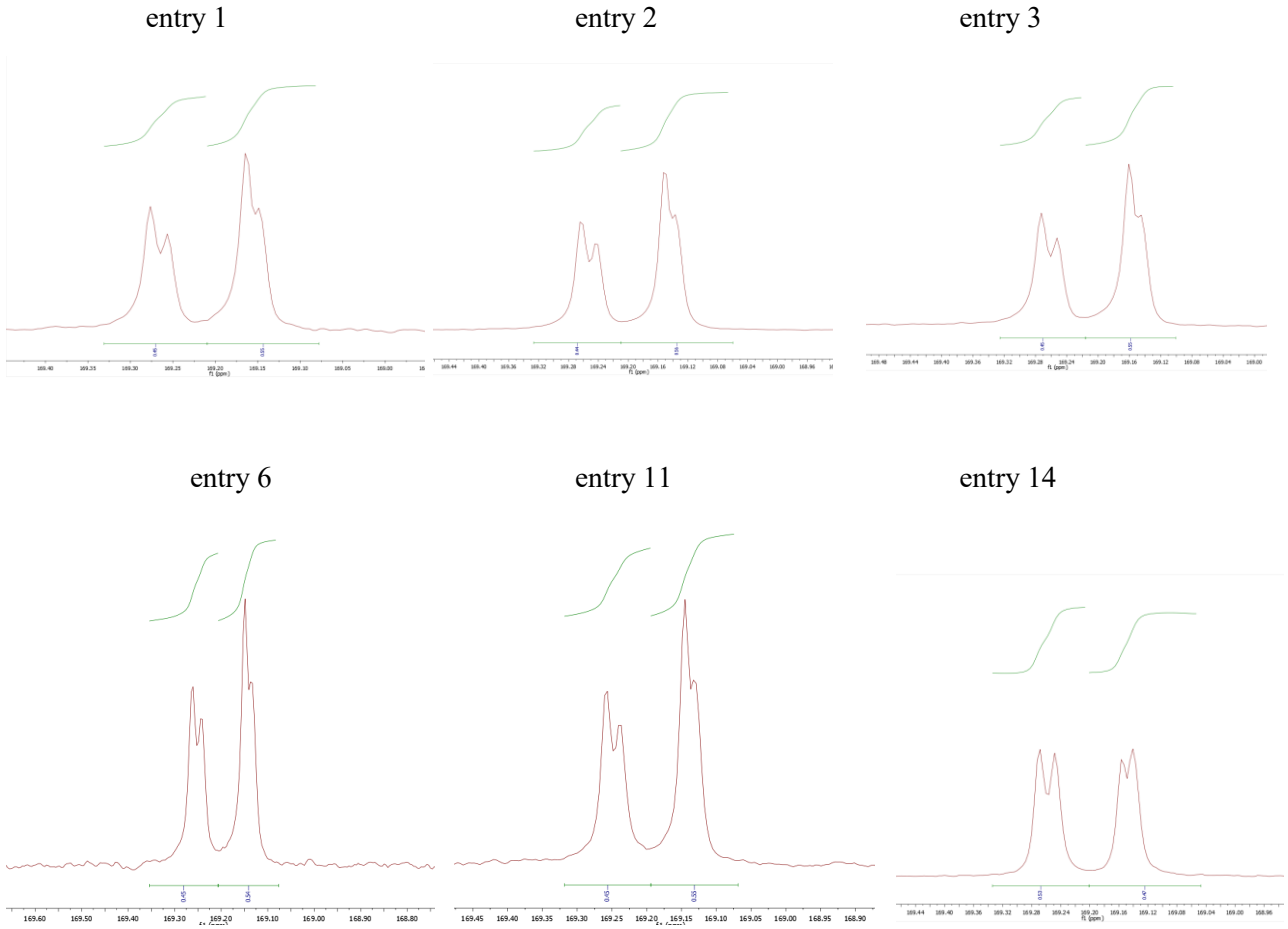


Figure S5. Microstructure determination. ^{13}C-NMR spectra of PHB produced with catalyst **I**–**IV**.

7. Microstructure determination of poly(lactide) (Table 2)

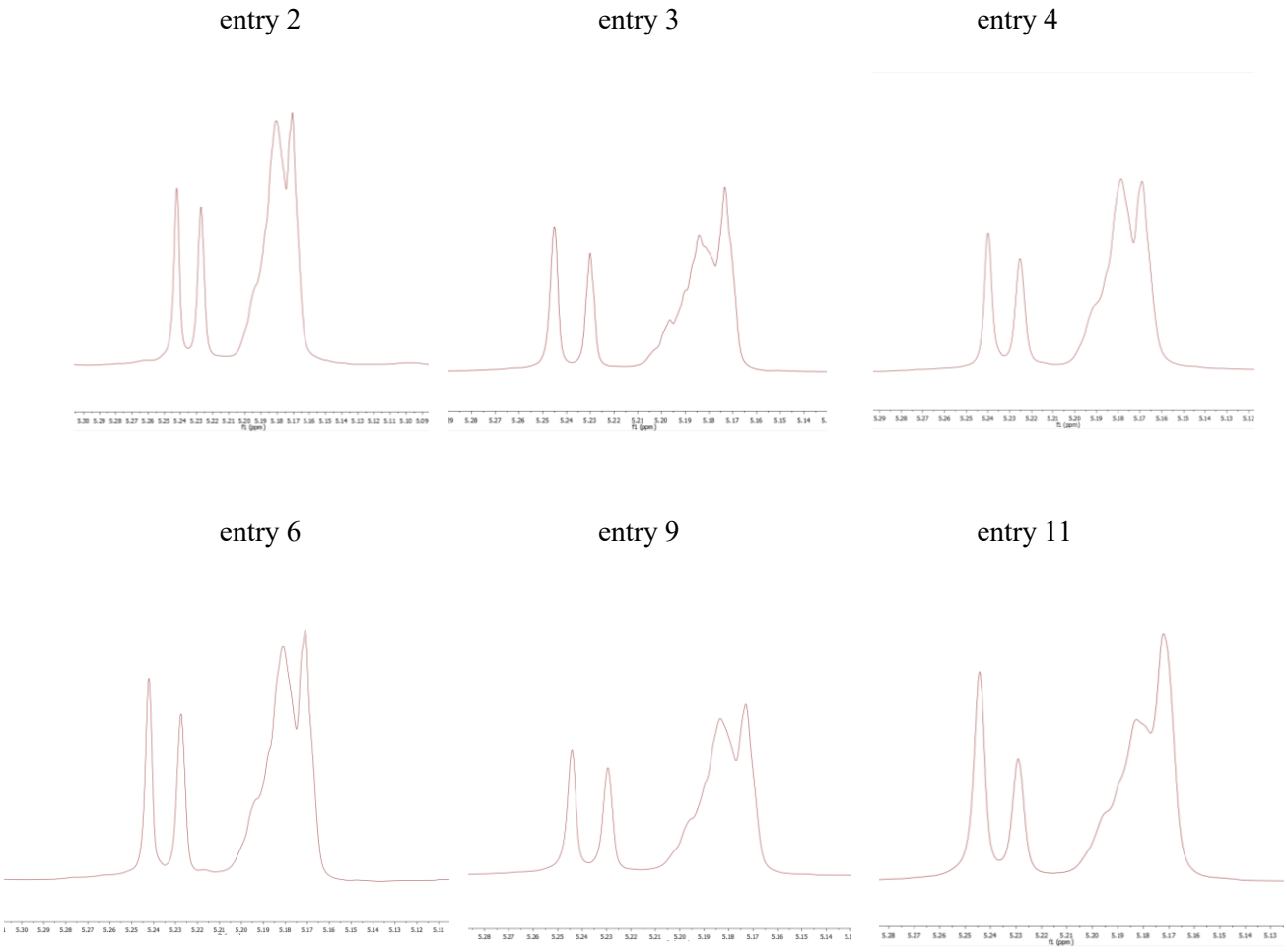


Figure S6. Microstructure determination. Homodecoupled ^{1}H-NMR spectra of polylactide produced with catalyst **II**–**IV**.

8. Proof of living-type polymerization of *rac*–LA with catalyst **III**

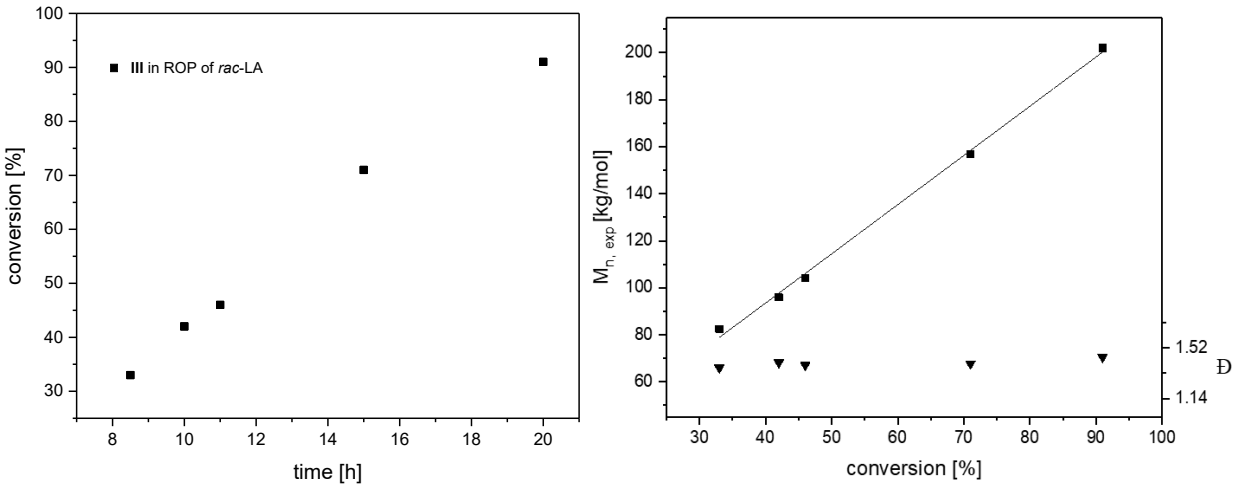


Figure S7. Polymerization of *rac*–LA with catalyst **III**. Plot of PLA conversion [%] vs. time [h] (left) until a conversion of 95% was reached. PLA molecular weight ■ ($M_{n,exp}$ vs. polystyrene standard in THF) and polydispersity index ▼ as a function of conversion (right).

9. Stability of complex **I** in toluene-d_8 and dichloromethane-d_2.

Toluene-d_8.

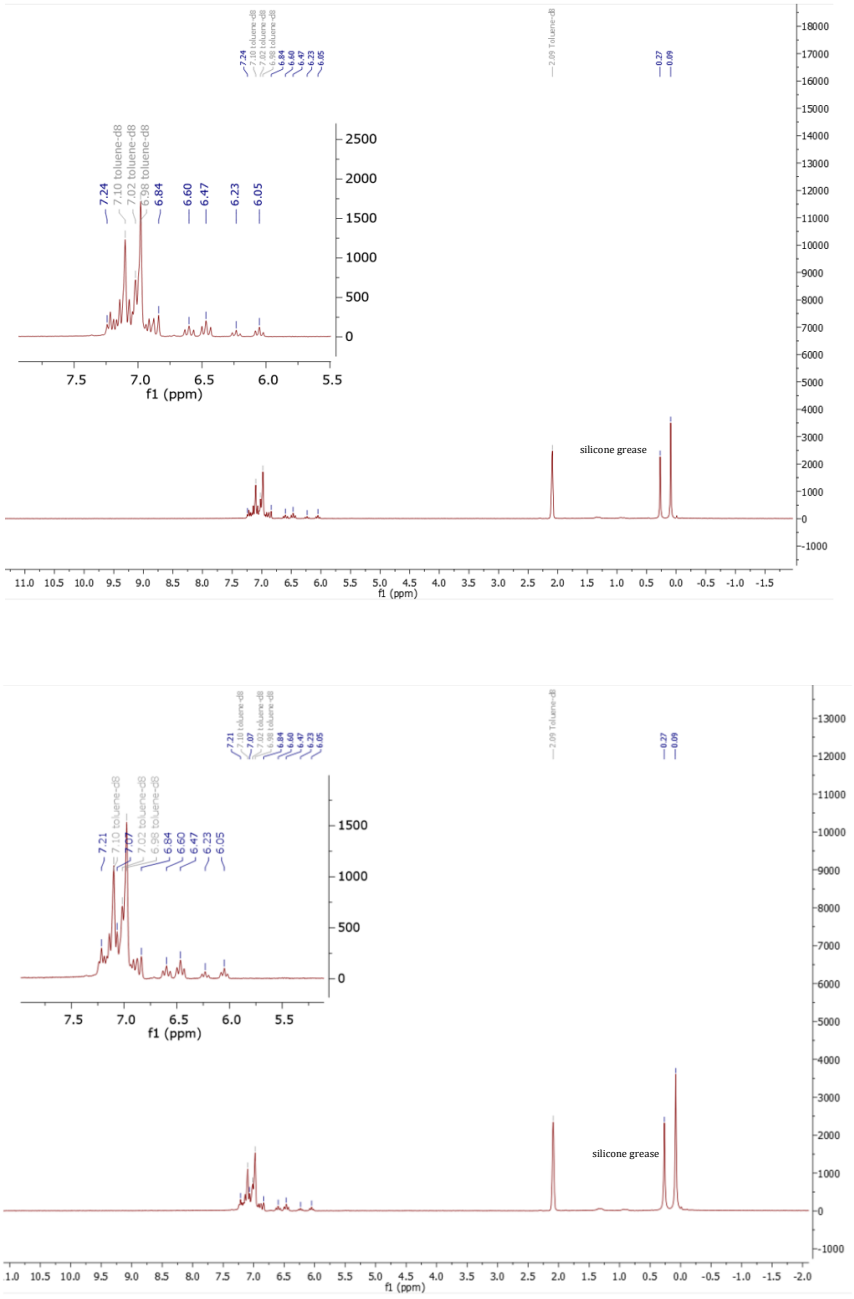


Figure S8. ^{1}H NMR spectrum of complex **I** in toluene-d_8 after 15 min (top) and 12 h (bottom).

Dichloromethane-d_2.

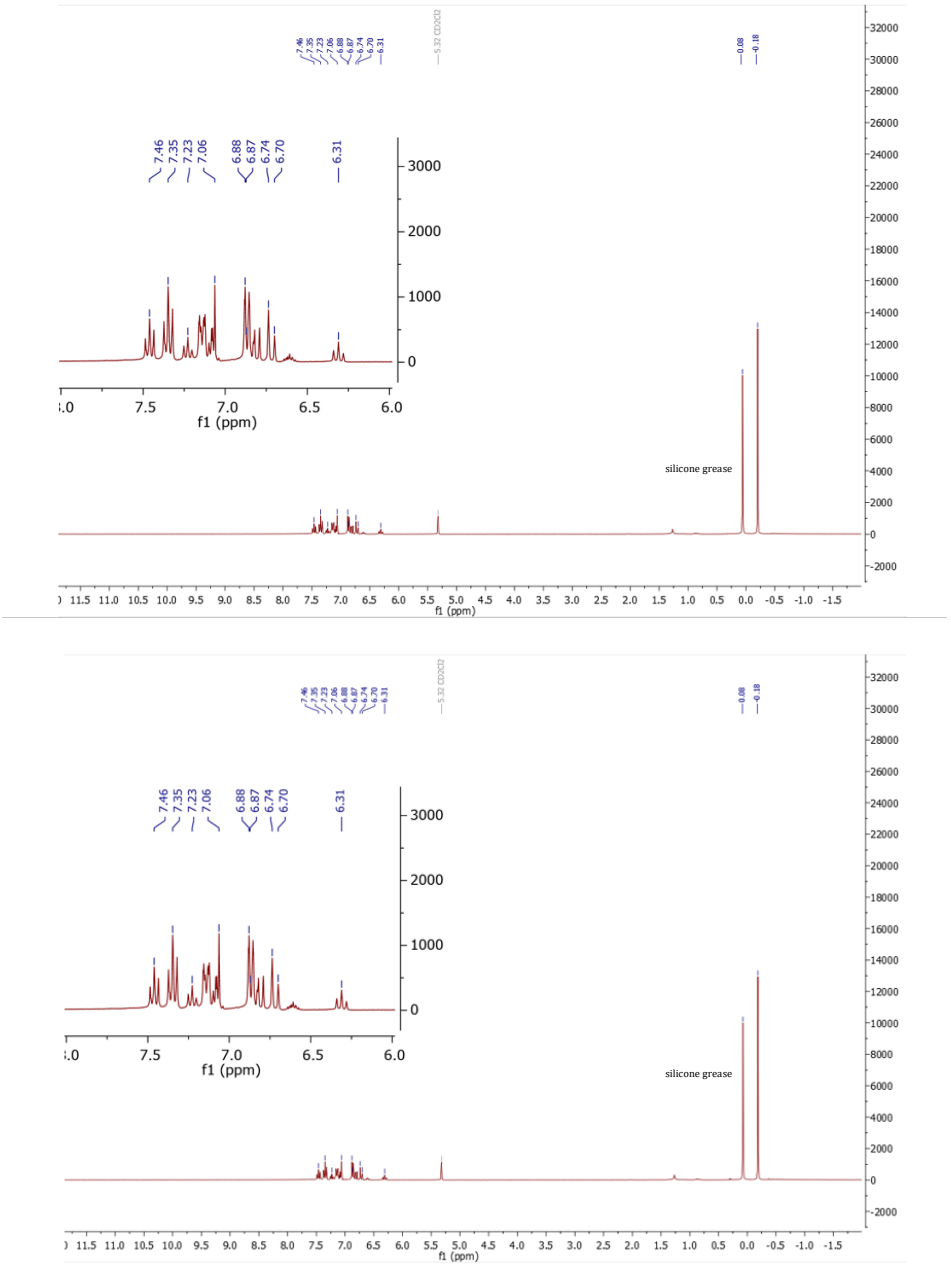


Figure S9. ^{1}H NMR spectrum of complex **I** in dichloromethane-d_2 after 15 min (top) and 12 h (bottom).

10. ^{1}H DOSY NMR experiments

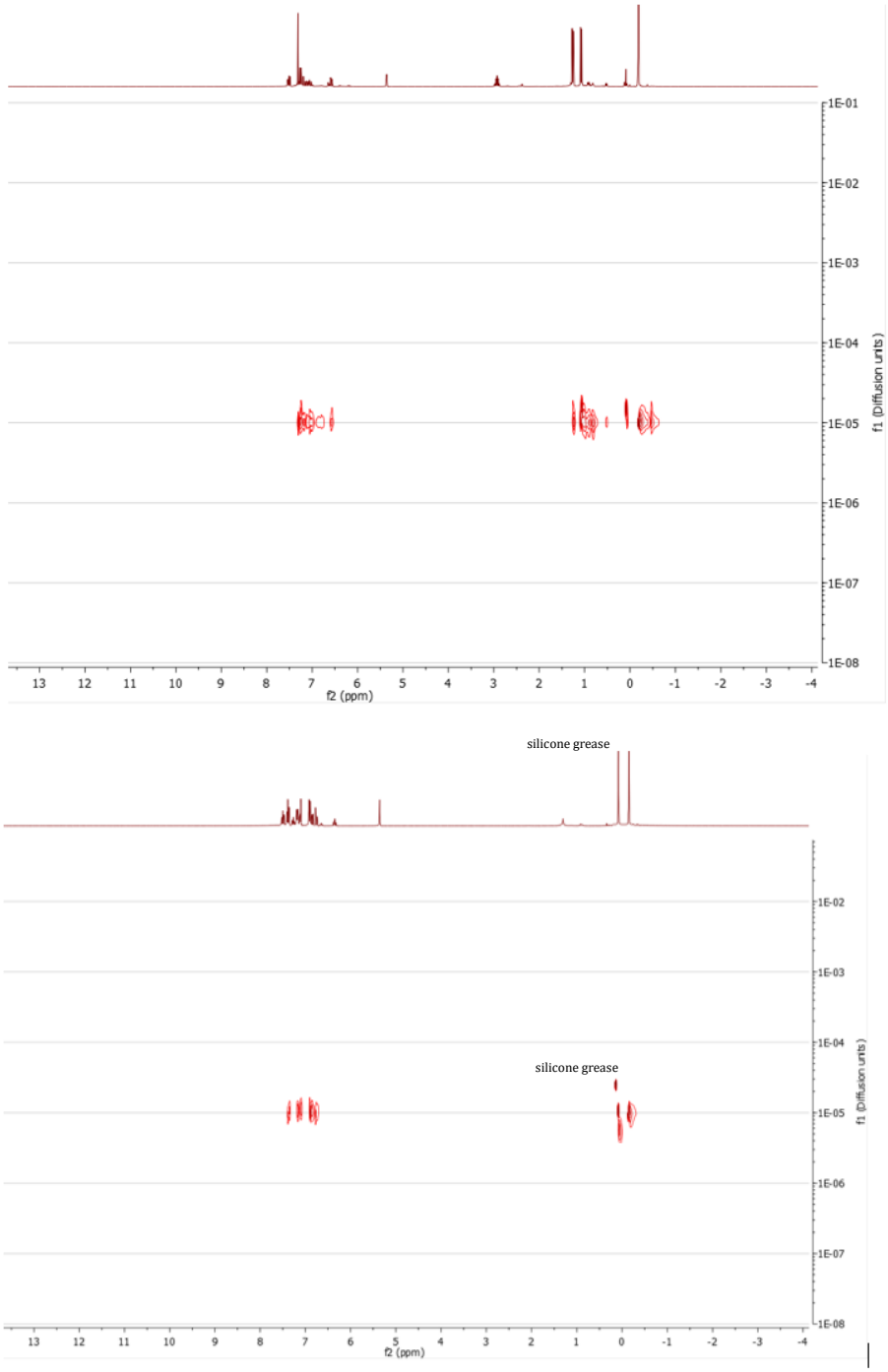
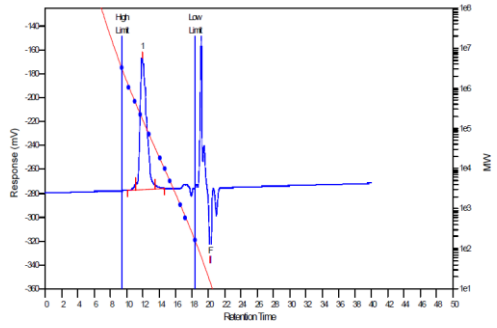


Figure S10. ^{1}H DOSY NMR spectrum of complex **III** in dichloromethane-d_2 (top) and of complex **I** (bottom).

11. GPC results of Table 1 and Table 2

Table 1: PHB. GPC traces exemplarily for all polymerization shown in Figure 5.

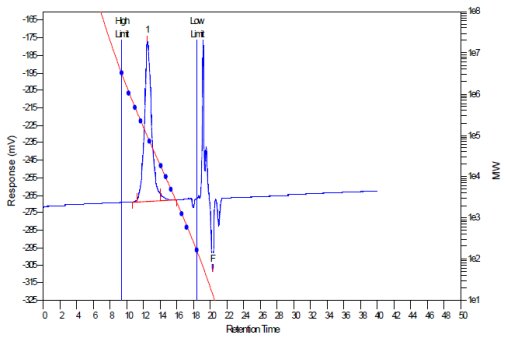
entry 1



MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	179095	129314	157570	184710	211261	153529	1.21851
2	0	0	0	0	0	0	0

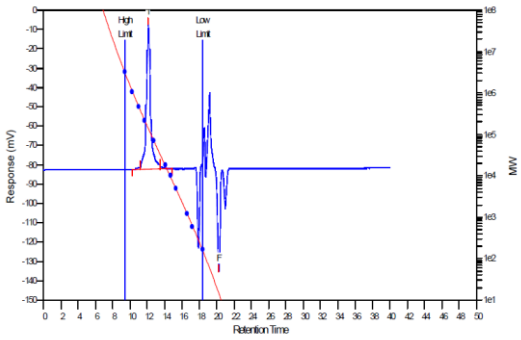
entry 2



MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	95519	75235	96405	120868	149995	93107	1.28138
2	0	0	0	0	0	0	0

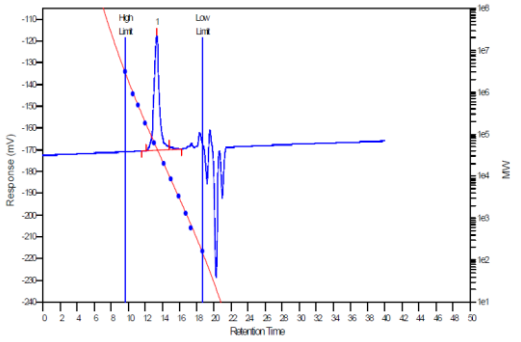
entry 3



MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	141594	122376	142554	162416	185115	139709	1.16489
2	0	0	0	0	0	0	0

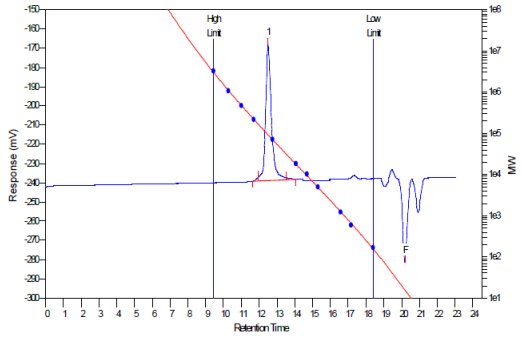
entry 12



MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	47099	49230	52768	57594	64406	52149	1.07187

entry 14

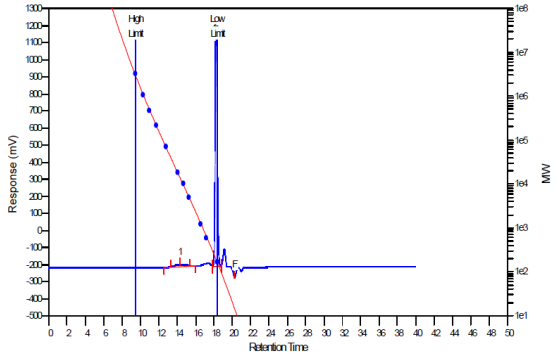


MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	92182	84163	88721	92663	96385	88107	1.05416
2	0	0	0	0	0	0	0

Table 2: PLA. GPC traces exemplarily shown for catalysts **I-IV** and **II** under different conditions (40 °C, addition of 1.0 eq. *i*PrOH)

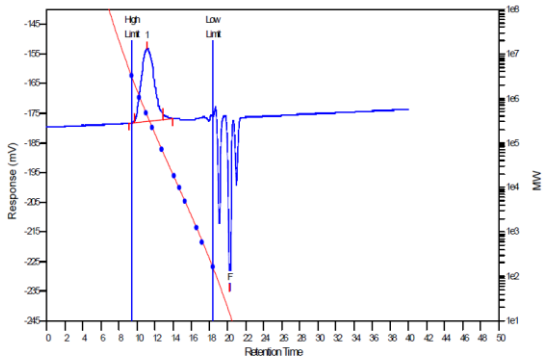
entry 1



MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	15766	12771	16446	20446	24118	15868	1.28776
2	210	186	190	193	196	189	1.02151
3	0	0	0	0	0	0	0

entry 2

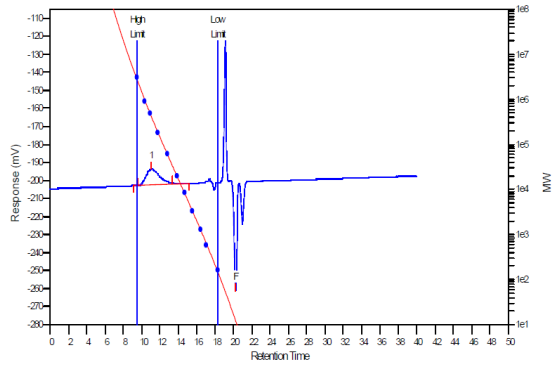


MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	426318	289472	471389	704943	945543	440647	1.62844
2	0	0	0	0	0	0	0

entry 1. unprecipitated polymer (M_n = 186 g/mol corresponds to lactide)

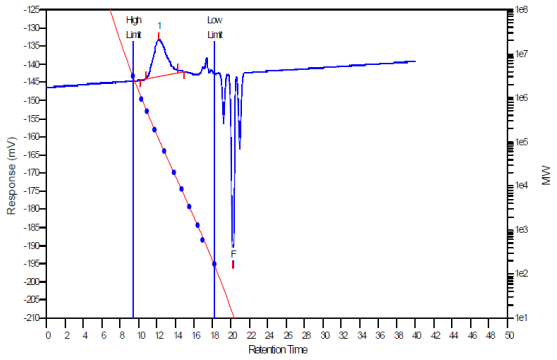
entry 3



MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	430331	216335	408012	632276	849402	377416	1.88602
2	0	0	0	0	0	0	0

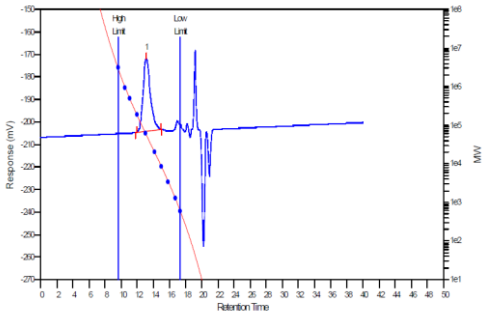
entry 4



MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	110961	71049	120603	182270	245445	112417	1.69746
2	0	0	0	0	0	0	0

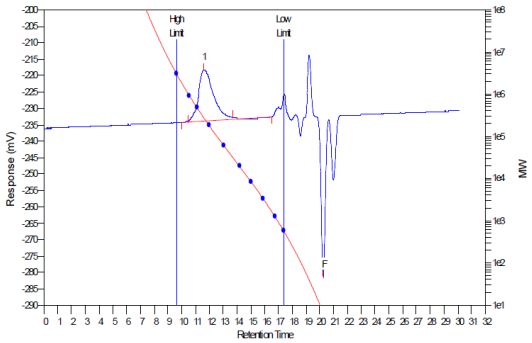
entry 5



MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	56138	44997	55694	66443	77438	54131	1.23773

entry 11



MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	271037	174044	248182	328428	413803	236924	1.42597
2	0	0	0	0	0	0	0

12. Single-crystal XRD (SC-XRD) data

12.1 General information

The X-ray intensity data were collected on an X-ray single crystal diffractometer equipped with a CMOS detector (Bruker Photon-100), a rotating anode (Bruker TXS) with MoK_α radiation ($\lambda = 0.71073$ Å) and a Helios mirror optic by using the APEX III software package[1] or an X-ray single crystal diffractometer equipped with a CMOS detector (Bruker Photon-100), an IMS microsource with MoK_α radiation ($\lambda = 0.71073$ Å) and a Helios mirror optic by using the APEX III software package.[1] The measurement was performed on single crystals coated with perfluorinated ether. The crystal was fixed on the top of a microsampler, transferred to the diffractometer and frozen under a stream of cold nitrogen. A matrix scan was used to determine the initial lattice parameters. Reflections were merged and corrected for Lorenz and polarization effects, scan speed, and background using SAINT.[2] Absorption corrections, including odd and even ordered spherical harmonics were performed using SADABS.[2] Space group assignments were based upon systematic absences, E statistics, and successful refinement of the structures. Structures were solved by direct methods with the aid of successive difference Fourier maps, and were refined against all data using the APEX III software[1] in conjunction with SHELXL-2014[3] and SHELXLE[4]. Methyl hydrogen atoms were refined as part of rigid rotating groups, with a C–H distance of 0.98 Å and $U_{iso(H)} = 1.5 \cdot U_{eq(C)}$. Other H atoms were placed in calculated positions and refined using a riding model, with methylene and aromatic C–H distances of 0.99 and 0.95 Å, respectively, and $U_{iso(H)} = 1.2 \cdot U_{eq(C)}$. If not mentioned otherwise, non-hydrogen atoms were refined with anisotropic displacement parameters. Full-matrix least-squares refinements were carried out by minimizing $\Delta w(F_o^2-F_c^2)^2$ with SHELXL-97[5] weighting scheme. Neutral atom scattering factors for all atoms and anomalous dispersion corrections for the non-hydrogen atoms were taken from International Tables for Crystallography.[6] Images of the crystal structures were generated by PLATON.[7]

12.2 ***I = [(Ph$_2$)ATI]Zn–N(SiMe$_3$)$_2$***

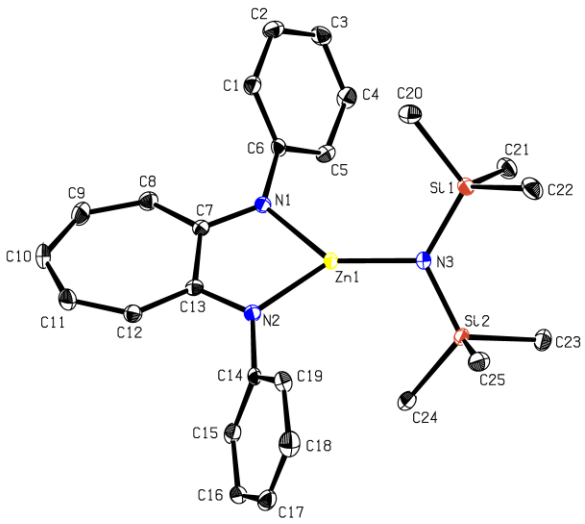


Figure S11: Crystal structure of **I**. ADPs are given at the 50% probability level.

A clear yellow fragment-like specimen of $C_{25}H_{33}N_3Si_2Zn$, approximate dimensions 0.278 mm x 0.342 mm x 0.416 mm, was used for the X-ray crystallographic analysis.

A total of 1542 frames were collected. The total exposure time was 1.94 hours. The frames were integrated with the Bruker SAINT software package[2] using a narrow-frame algorithm. The integration of the data using a triclinic unit cell yielded a total of 51463 reflections to a maximum θ angle of 25.03° (0.84 Å resolution), of which 8875 were independent (average redundancy 5.799, completeness = 99.6%, R_{int} = 4.76%, R_{sig} = 3.31%) and 7463 (84.09%) were greater than $2\sigma(F^2)$. The final cell constants of a = 11.3195(6) Å, b =11.6627(7) Å, c = 20.7273(11) Å, α = 78.134(2)°, β = 85.315(2)°,γ = 70.541(2), volume = 2524.6(2) Å^3, are based upon the refinement of the XYZ-centroids of 124 reflections above 20 σ(I) with 8.570° < 2θ <47.31°. Data were corrected for absorption effects using the multi-scan method (SADABS).[6] The ratio of minimum to maximum apparent transmission was 0.901. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.6724 and 0.7459.

The final anisotropic full-matrix least-squares refinement on F^2 with 571 variables converged at R1 = 2.91%, for the observed data and wR2 = 6.16% for all data. The goodness-of-fit was 1.018. The largest peak in the final difference electron density synthesis was 0.299 e$^-$/Å^3 and the largest hole was -0.284 e$^-$/Å^3 with an RMS deviation of 0.057 e$^-$/Å^3. On the basis of the final model, the calculated density was 1.308 g/cm^3 and F(000), 1048 e$^-$.

Table S2: Sample and crystal data for **I**.

Identification code	KerSe6	
Chemical formula	$C_{25}H_{33}N_3Si_2Zn$	
Formula weight	497.09	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.278 mm x 0.342 mm x 0.416 mm	
Crystal habit	clear yellow fragment	
Crystal system	triclinic	
Space group	*P* -1	
Unit cell dimensions	a = 11.3195(6) Å	α = 78.134(2)°
	b = 11.6627(7) Å	β = 85.315(2)°
	c = 20.7273(11) Å	γ = 70.541(2)°
Volume	2524.6(2) $Å^3$	
Z	4	
Density (calculated)	1.308 g/cm^3	
Absorption coefficient	1.085 mm^{-1}	
F(000)	1048	

Table S3: Data collection and structure refinement for **I**.

Diffractometer	Bruker D8 Venture, CMOS detector (Bruker Photon-100)	
Radiation source	IMS microsource, Mo	
Theta range for data collection	2.21 to 25.03°	
Index ranges	-13<=h<=13, -13<=k<=13, -24<=l<=24	
Reflections collected	51463	
Independent reflections	8875 [R(int) = 0.0476]	
Coverage of independent reflections	99.6%	
Absorption correction	multi-scan	
Max. and min. transmission	0.6724 and 0.7459	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	8875 / 0 / 571	
Goodness-of-fit on F^2	1.018	
Δ/σ_{max}	0.001	
Final R indices	7463 data; I>2σ(I)	R1 = 0.0291, wR2 = 0.0580
	all data	R1 = 0.0414, wR2 = 0.0616
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0212P)^2+2.2146P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.299 and -0.284 $eÅ^{-3}$	
R.M.S. deviation from mean	0.057 $eÅ^{-3}$	

12.3 ***II = [(C$_6$H$_3$-2,6-C$_2$H$_5$/Ph)ATI]Zn–N(SiMe$_3$)$_2$***

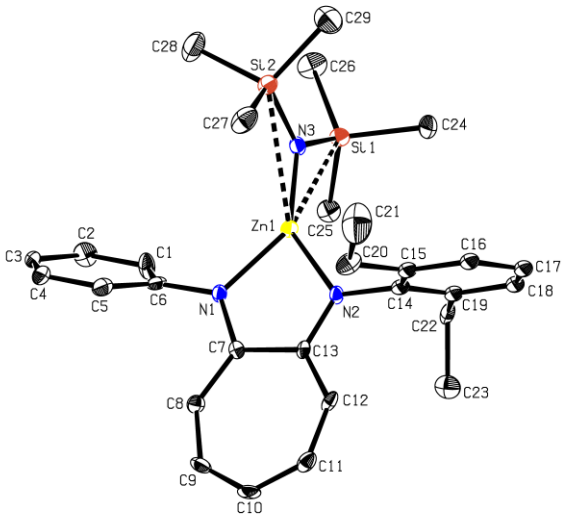


Figure S12: Crystal structure of **II**. ADPs are given at the 50% probability level.

A clear yellow fragment-like specimen of $C_{29}H_{41}N_3Si_2Zn$, approximate dimensions 0.064 mm x 0.132 mm x 0.216 mm, was used for the X-ray crystallographic analysis.

A total of 1612 frames were collected. The total exposure time was 2.04 hours. The frames were integrated with the Bruker SAINT software package[2] using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 68514 reflections to a maximum θ angle of 25.03° (0.84 Å resolution), of which 15610 were independent (average redundancy 4.389, completeness = 99.9%, R_{int} = 10.70%, R_{sig} = 11.09%) and 10289 (65.91%) were greater than $2\sigma(F^2)$. The final cell constants of a = 26.284(7) Å, b =11.002(3) Å, c = 30.934(9) Å, β = 97.989(10)°, volume = 8859(4) Å^3, are based upon the refinement of the XYZ-centroids of 136 reflections above 20 σ(I) with 4.693° < 2θ < 31.54°. Data were corrected for absorption effects using the multi-scan method (SADABS).[6] The ratio of minimum to maximum apparent transmission was 0.717. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.5614 and 0.7453.

The final anisotropic full-matrix least-squares refinement on F^2 with 970 variables converged at R1 = 6.73%, for the observed data and wR2 = 12.89% for all data. The goodness-of-fit was 1.038. The largest peak in the final difference electron density synthesis was 0.842 e$^-$/Å^3 and the largest hole was -0.718 e$^-$/Å^3 with an RMS deviation of 0.104 e$^-$/Å^3. On the basis of the final model, the calculated density was 1.244 g/cm^3 and F(000), 3528 e$^-$.

Table S4: Sample and crystal data for **II**.

Identification code	KerSe5	
Chemical formula	$C_{29}H_{41}N_3Si_2Zn$	
Formula weight	442.56	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.064 mm x 0.132 mm x 0.216 mm	
Crystal habit	clear yellow fragment	
Crystal system	monoclinic	
Space group	*P* 21/n	
Unit cell dimensions	a = 26.284(7) Å	α = 90°
	b = 11.002(3) Å	β = 97.989(10)°
	c = 30.934(9) Å	γ = 90°
Volume	8859(4) $Å^3$	
Z	12	
Density (calculated)	1.244 g/cm^3	
Absorption coefficient	0.934 mm^{-1}	
F(000)	3528	

Table S5: Data collection and structure refinement for **II**.

Diffractometer	Bruker D8 Venture, CMOS detector (Bruker Photon-100)
Radiation source	TXS rotating anode, Mo
Theta range for data collection	2.01 to 25.03°
Index ranges	-31<=h<=31, -10<=k<=10, -36<=l<=360
Reflections collected	68514
Independent reflections	15610 [R(int) = 0.1070]
Coverage of independent reflections	99.9%
Absorption correction	multi-scan
Max. and min. transmission	0.5614 and 0.7453
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	15610 / 186 / 970
Goodness-of-fit on F^2	1.038
Δ/σ_{max}	0.001
Final R indices	102892 data; I>2σ(I) R1 = 0.0673, wR2 = 0.1126
	all data R1 = 0.1211, wR2 = 0.1289
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0386P)^2+18.5456P]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	0.842 and -0.718 $eÅ^{-3}$
R.M.S. deviation from mean	0.104 $eÅ^{-3}$

*12.4 **III = [C$_6$H$_3$-2,6-CH(CH$_3$)$_2$/Ph)ATI]Zn–N(SiMe$_3$)$_2$)***

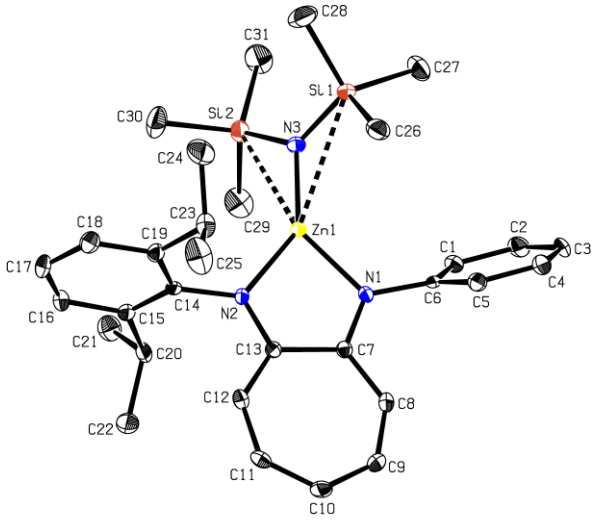


Figure S13: Crystal structure of **III**. ADPs are given at the 50% probability level.

A clear yellow fragment-like specimen of $C_{31}H_{45}N_3Si_2Zn$, approximate dimensions 0.136 mm x 0.179 mm x 0.232 mm, was used for the X-ray crystallographic analysis.

A total of 1106 frames were collected. The total exposure time was 7.87 hours. The frames were integrated with the Bruker SAINT software package[2] using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 48290 reflections to a maximum θ angle of 25.68° (0.82 Å resolution), of which 6097 were independent (average redundancy 7.920, completeness = 100%, R_{int} = 8.35%, R_{sig} = 4.14%) and 4888 (80.17%) were greater than 2σ(F^2). The final cell constants of a = 15.3484(12) Å, b = 11.2145(9) Å, c = 18.6812(15) Å, β = 94.874(3)° , volume = 3203.9(4) Å^3, are based upon the refinement of the XYZ-centroids of 9955 reflections above 20 σ(I) with 4.907° < 2θ < 51.98°. Data were corrected for absorption effects using the multi-scan method (SADABS).[6] The ratio of minimum to maximum apparent transmission was 0.914. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.6813 and 0.7453.

The final anisotropic full-matrix least-squares refinement on F^2 with 2397 variables converged at R1 = 3.57%, for the observed data and wR2 = 6.87% for all data. The goodness-of-fit was 1.065. The largest peak in the final difference electron density synthesis was 0.342 e$^-$/Å^3 and the largest hole was -0.312 e$^-$/Å^3 with an RMS deviation of 0.060 e$^-$/Å^3. On the basis of the final model, the calculated density was 1.205 g/cm^3 and F(000), 1240 e$^-$.

Table S6: Sample and crystal data for **III**.

Identification code	KerSe4	
Chemical formula	$C_{31}H_{45}N_3Si_2Zn$	
Formula weight	581.25	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.136 mm x 0.179 mm x 0.232 mm	
Crystal habit	clear yellow fragment	
Crystal system	monoclinic	
Space group	*P* 21/c	
Unit cell dimensions	a = 15.3484(12) Å	α = 90°
	b = 11.2145(9) Å	β = 94.874(3)°
	c = 18.6812(15) Å	γ = 90°
Volume	3203.9(4) $Å^3$	
Z	4	
Density (calculated)	1.205 g/cm^3	
Absorption coefficient	0.864 mm^{-1}	
F(000)	1240	

Table S7: Data collection and structure refinement for **III**.

Diffractometer	Bruker D8 Venture, CMOS detector (Bruker Photon-100)	
Radiation source	IMS microsource, Mo	
Theta range for data collection	2.25 to 25.68°	
Index ranges	-18<=h<=18, -13<=k<=13, -22<=l<=22	
Reflections collected	48290	
Independent reflections	6097 [R(int) = 0.0835]	
Coverage of independent reflections	100%	
Absorption correction	multi-scan	
Max. and min. transmission	0.6813 and 0.7453	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	6097 / 0 / 344	
Goodness-of-fit on F^2	1.065	
Δ/σ_{max}	0.001	
Final R indices	4888 data; I>2σ(I)	R1 = 0.0357, wR2 = 0.0636
	all data	R1 = 0.0549, wR2 = 0.0687
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0146P)^2+2.9741P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.342 and –0.312 $eÅ^{-3}$	
R.M.S. deviation from mean	0.060 $eÅ^{-3}$	

12.5 IV = [CH(CMeNPh)$_2$]Zn–N(SiMe$_3$)$_2$

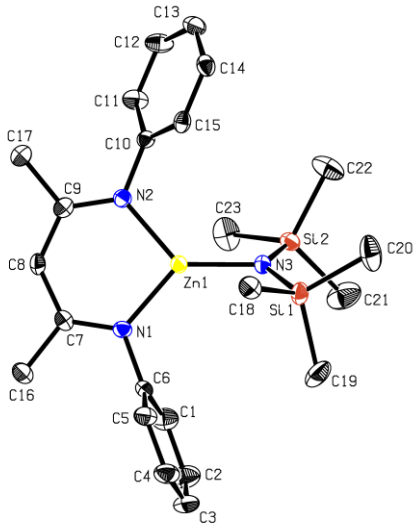


Figure S14: Crystal structure of **IV**. ADPs are given at the 50% probability level.

A clear colorless fragment-like specimen of $C_{23}H_{35}N_3Si_2Zn$, approximate dimensions 0.206 mm x 0.285 mm x 0.286 mm, was used for the X-ray crystallographic analysis.

A total of 2738 frames were collected. The total exposure time was 7.16 hours. The frames were integrated with the Bruker SAINT software package[2] using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 85482 reflections to a maximum θ angle of 26.02° (0.81 Å resolution), of which 5128 were independent (average redundancy 16.670, completeness = 99.9%, R_{int} = 6.91%, R_{sig} = 2.65%) and 4313 (84.11%) were greater than $2\sigma(F^2)$. The final cell constants of a = 10.5205(6) Å, b =10.7363(6) Å, c = 23.0345(13) Å, β = 90.624(2)°, volume = 2601.6(3) Å^3, are based upon the refinement of the XYZ-centroids of 122 reflections above 20 σ(I) with 4.239° < 2θ < 43.45°. Data were corrected for absorption effects using the multi-scan method (SADABS).[6] The ratio of minimum to maximum apparent transmission was 0.889. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.6632 and 0.7458.

The final anisotropic full-matrix least-squares refinement on F^2 with 270 variables converged at R1 = 3.30%, for the observed data and wR2 = 6.39% for all data. The goodness-of-fit was 1.078. The largest peak in the final difference electron density synthesis was 0.290 e$^-$/Å^3 and the largest hole was -0.365 e$^-$/Å^3 with an RMS deviation of 0.059 e$^-$/Å^3. On the basis of the final model, the calculated density was 1.213 g/cm^3 and F(000), 1008 e$^-$.

Table S8: Sample and crystal data for **IV**.

Identification code	KerSe8	
Chemical formula	$C_{23}H_{35}N_3Si_2Zn$	
Formula weight	475.09	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.206 mm x 0.285 mm x 0.286 mm	
Crystal habit	clear colorless fragment	
Crystal system	monoclinic	
Space group	*P* 21/c	
Unit cell dimensions	a = 10.5205(6) Å	α = 90°
	b = 10.7363(6) Å	β = 90.624(2)°
	c = 23.0345(13) Å	γ = 90°
Volume	2601.6(3) $Å^3$	
Z	4	
Density (calculated)	1.213 g/cm^3	
Absorption coefficient	1.049 mm^{-1}	
F(000)	1008	

Table S9: Data collection and structure refinement for **IV**.

Diffractometer	Bruker D8 Venture, CMOS detector (Bruker Photon-100)	
Radiation source	IMS microsource, Mo	
Theta range for data collection	2.59 to 26.02°	
Index ranges	-12<=h<=12, -13<=k<=13, -28<=l<=28	
Reflections collected	85482	
Independent reflections	5128 [R(int) = 0.0691]	
Coverage of independent reflections	99.9%	
Absorption correction	multi-scan	
Max. and min. transmission	0.6632 and 0.7458	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	5128 / 0 / 270	
Goodness-of-fit on F^2	1.078	
Δ/σ_{max}	0.001	
Final R indices	4313 data; I>2σ(I)	R1 = 0.0330, wR2 = 0.0605
	all data	R1 = 0.0457, wR2 = 0.0639
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0170P)^2+2.4987P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.290 and -0.365 $eÅ^{-3}$	
R.M.S. deviation from mean	0.059 $eÅ^{-3}$	

13. References

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