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Four-fold increase in epoxide polymerization rate with change of alkyl-substitution on mono-μ-oxo-dialuminum initiators

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Table of Figures

Table of Tables

Table S 1. Crystal data and structure refinement for **Me-TAxEDA**.

Empirical formula	C21 H33 Al2 N O	
Formula weight	369.44	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 12.5747(19) Å	α= 90°.
	b = 7.0541(12) Å	β= 90.098(8)°.
	c = 24.349(4) Å	γ = 90°.
Volume	2159.8(6) $Å^3$	
Z	4	
Density (calculated)	1.136 Mg/m^3	
Absorption coefficient	0.143 mm^{-1}	
F(000)	800	
Crystal size	0.330 x 0.050 x 0.030 mm^3	
Theta range for data collection	1.619 to 25.348°.	
Index ranges	-15<=h<=15, -8<=k<=8, 0<=l<=29	
Reflections collected	3916	
Independent reflections	3916 [R(int) = ?]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00 and 0.700	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3916 / 150 / 232	
Goodness-of-fit on F^2	0.990	
Final R indices [I>2sigma(I)]	R1 = 0.0585, wR2 = 0.1084	
R indices (all data)	R1 = 0.1208, wR2 = 0.1273	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.386 and -0.429 $e.Å^{-3}$	

Table S 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **Me-TAxEDA**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C1	3702(4)	1128(6)	4567(2)	21(1)
C2	3849(3)	2301(6)	4056(2)	19(1)
C3	2355(3)	822(6)	3530(2)	19(1)
C4	2984(4)	-88(5)	3080(1)	18(1)
C5	3908(4)	-1144(6)	3194(2)	24(1)
C6	4465(4)	-1998(6)	2780(2)	29(1)
C7	4136(4)	-1819(6)	2239(2)	30(1)
C8	3219(4)	-811(6)	2119(2)	27(1)
C9	2657(3)	67(6)	2538(2)	23(1)
C10	3002(4)	4095(6)	3336(1)	21(1)
C11	2058(4)	4794(6)	3009(1)	19(1)
C12	1182(4)	5653(6)	3249(2)	26(1)
C13	402(4)	6472(6)	2933(2)	29(1)
C14	477(4)	6476(6)	2367(2)	30(1)
C15	1333(4)	5629(6)	2116(2)	26(1)
C16	2108(4)	4776(6)	2440(2)	22(1)
C17	1629(4)	3113(7)	5878(2)	40(2)
C18	3236(4)	-617(6)	5868(2)	32(1)
C19	4254(4)	3661(7)	5744(2)	34(1)
C20	510(3)	2345(7)	4406(2)	32(1)
C21	2230(4)	6056(6)	4592(2)	31(1)
O1	2822(2)	1927(4)	4868(1)	19(1)
N1	2794(3)	2613(4)	3778(1)	16(1)
Al1	2987(1)	2018(2)	5637(1)	25(1)
Al2	1931(1)	3395(2)	4451(1)	22(1)

Table S 3. Bond lengths [Å] and angles [°] for **Me-TAxEDA**.

C1-O1	1.442(5)	C13-C14	1.382(6)
C1-C2	1.507(5)	C13-H13	0.95
C1-H1A	0.99	C14-C15	1.376(6)
C1-H1B	0.99	C14-H14	0.95
C2-N1	1.505(5)	C15-C16	1.389(6)
C2-H2A	0.99	C15-H15	0.95
C2-H2B	0.99	C16-H16	0.95
C3-C4	1.498(5)	C17-Al1	1.966(5)
C3-N1	1.504(5)	C17-H17A	0.98
C3-H3A	0.99	C17-H17B	0.98
C3-H3B	0.99	C17-H17C	0.98
C4-C9	1.383(5)	C18-Al1	1.967(4)
C4-C5	1.408(6)	C18-H18A	0.98
C5-C6	1.370(6)	C18-H18B	0.98
C5-H5	0.95	C18-H18C	0.98
C6-C7	1.385(6)	C19-Al1	1.987(5)
C6-H6	0.95	C19-H19A	0.98
C7-C8	1.386(6)	C19-H19B	0.98
C7-H7	0.95	C19-H19C	0.98
C8-C9	1.389(5)	C20-Al2	1.938(5)
C8-H8	0.95	C20-H20A	0.98
C9-H9	0.95	C20-H20B	0.98
C10-C11	1.511(6)	C20-H20C	0.98
C10-N1	1.522(5)	C21-Al2	1.945(4)
C10-H10A	0.99	C21-H21A	0.98
C10-H10B	0.99	C21-H21B	0.98
C11-C12	1.388(6)	C21-H21C	0.98
C11-C16	1.389(5)	O1-Al2	1.831(3)
C12-C13	1.373(6)	O1-Al1	1.884(2)
C12-H12	0.95	N1-Al2	2.044(3)
O1-C1-C2	107.5(3)	O1-C1-H1A	110.2

C2-C1-H1A	110.2	N1-C10-H10A	107.9
O1-C1-H1B	110.2	C11-C10-H10B	107.9
C2-C1-H1B	110.2	N1-C10-H10B	107.9
H1A-C1-H1B	108.5	H10A-C10-H10B	107.2
N1-C2-C1	110.0(4)	C12-C11-C16	117.5(4)
N1-C2-H2A	109.7	C12-C11-C10	123.0(3)
C1-C2-H2A	109.7	C16-C11-C10	119.2(4)
N1-C2-H2B	109.7	C13-C12-C11	120.9(4)
C1-C2-H2B	109.7	C13-C12-H12	119.5
H2A-C2-H2B	108.2	C11-C12-H12	119.5
C4-C3-N1	117.4(3)	C12-C13-C14	120.8(5)
C4-C3-H3A	108.0	C12-C13-H13	119.6
N1-C3-H3A	108.0	C14-C13-H13	119.6
C4-C3-H3B	108.0	C15-C14-C13	119.7(4)
N1-C3-H3B	108.0	C15-C14-H14	120.1
H3A-C3-H3B	107.2	C13-C14-H14	120.1
C9-C4-C5	118.3(4)	C14-C15-C16	119.0(4)
C9-C4-C3	120.5(4)	C14-C15-H15	120.5
C5-C4-C3	121.2(4)	C16-C15-H15	120.5
C6-C5-C4	120.6(4)	C11-C16-C15	122.1(4)
C6-C5-H5	119.7	C11-C16-H16	119.0
C4-C5-H5	119.7	C15-C16-H16	119.0
C5-C6-C7	120.5(5)	Al1-C17-H17A	109.5
C5-C6-H6	119.7	Al1-C17-H17B	109.5
C7-C6-H6	119.7	H17A-C17-H17B	109.5
C6-C7-C8	119.7(4)	Al1-C17-H17C	109.5
C6-C7-H7	120.2	H17A-C17-H17C	109.5
C8-C7-H7	120.2	H17B-C17-H17C	109.5
C7-C8-C9	119.8(4)	Al1-C18-H18A	109.5
C7-C8-H8	120.1	Al1-C18-H18B	109.5
C9-C8-H8	120.1	H18A-C18-H18B	109.5
C4-C9-C8	121.0(4)	Al1-C18-H18C	109.5
C4-C9-H9	119.5	H18A-C18-H18C	109.5
C8-C9-H9	119.5	H18B-C18-H18C	109.5
C11-C10-N1	117.4(4)	Al1-C19-H19A	109.5
C11-C10-H10A	107.9	Al1-C19-H19B	109.5

H19A-C19-H19B	109.5	C3-N1-C2	112.3(3)
Al1-C19-H19C	109.5	C3-N1-C10	110.9(3)
H19A-C19-H19C	109.5	C2-N1-C10	105.4(3)
H19B-C19-H19C	109.5	C3-N1-Al2	110.7(2)
Al2-C20-H20A	109.5	C2-N1-Al2	98.5(2)
Al2-C20-H20B	109.5	C10-N1-Al2	118.3(2)
H20A-C20-H20B	109.5	O1-Al1-C17	102.52(17)
Al2-C20-H20C	109.5	O1-Al1-C18	105.61(15)
H20A-C20-H20C	109.5	C17-Al1-C18	115.0(2)
H20B-C20-H20C	109.5	O1-Al1-C19	103.73(17)
Al2-C21-H21A	109.5	C17-Al1-C19	115.4(2)
Al2-C21-H21B	109.5	C18-Al1-C19	112.8(2)
H21A-C21-H21B	109.5	O1-Al2-C20	112.28(17)
Al2-C21-H21C	109.5	O1-Al2-C21	109.32(18)
H21A-C21-H21C	109.5	C20-Al2-C21	123.9(2)
H21B-C21-H21C	109.5	O1-Al2-N1	88.11(13)
C1-O1-Al2	114.1(2)	C20-Al2-N1	109.96(17)
C1-O1-Al1	115.7(2)	C21-Al2-N1	107.39(17)
Al2-O1-Al1	126.69(16)		

Table S 4. Anisotropic displacement parameters ($Å^2$x 10^3) for **Me-TAxEDA**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C1	31(3)	20(3)	11(2)	0(2)	0(2)	6(2)
C2	23(3)	19(3)	15(2)	0(2)	1(2)	2(2)
C3	28(3)	16(2)	14(2)	-4(2)	3(2)	2(2)
C4	23(3)	15(2)	15(2)	-3(2)	3(2)	-3(2)
C5	25(3)	22(3)	23(2)	-1(2)	0(2)	4(2)
C6	32(3)	19(3)	38(3)	-3(2)	4(2)	-1(2)
C7	35(3)	29(3)	25(2)	-9(2)	12(2)	0(3)
C8	38(3)	27(3)	16(2)	-6(2)	-1(2)	-9(3)
C9	31(3)	15(3)	24(2)	-3(2)	-2(2)	0(2)
C10	33(3)	16(2)	14(2)	3(2)	1(2)	6(3)
C11	24(3)	17(2)	18(2)	0(2)	-5(2)	1(2)
C12	28(3)	31(3)	20(2)	4(2)	1(2)	8(2)
C13	29(3)	30(3)	28(2)	4(2)	0(2)	4(2)
C14	31(3)	27(3)	33(2)	10(2)	-6(2)	-1(3)
C15	37(3)	26(3)	16(2)	2(2)	1(2)	-1(3)
C16	27(3)	20(2)	20(2)	2(2)	1(2)	0(2)
C17	55(4)	39(3)	25(2)	3(2)	8(2)	2(3)
C18	45(4)	36(3)	17(2)	7(2)	-1(2)	2(3)
C19	42(3)	31(3)	29(3)	-8(2)	-3(2)	1(3)
C20	31(3)	37(3)	28(2)	1(2)	6(2)	7(2)
C21	51(4)	24(3)	18(2)	-4(2)	1(2)	7(3)
O1	21(2)	23(2)	13(1)	2(1)	4(1)	8(2)
N1	19(2)	12(2)	15(2)	1(1)	-3(2)	0(2)
Al1	34(1)	27(1)	13(1)	1(1)	-2(1)	2(1)
Al2	27(1)	23(1)	15(1)	-1(1)	-1(1)	5(1)

Table S 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10 ^{3}) for **Me-TAxEDA**.

	x	y	z	U(eq)
H1A	3548	-206	4469	25
H1B	4356	1159	4794	25
H2A	4169	3538	4153	23
H2B	4338	1641	3801	23
H3A	2271	-118	3829	23
H3B	1636	1103	3386	23
H5	4147	-1266	3563	28
H6	5083	-2720	2863	35
H7	4538	-2384	1952	36
H8	2975	-720	1750	33
H9	2040	785	2453	28
H10A	3339	5205	3514	25
H10B	3526	3563	3076	25
H12	1120	5675	3638	31
H13	-195	7042	3105	35
H14	-62	7061	2151	36
H15	1394	5627	1727	31
H16	2689	4162	2266	27
H17A	1567	4413	5740	59
H17B	1603	3123	6281	59
H17C	1040	2348	5735	59
H18A	2593	-1368	5801	48
H18B	3410	-646	6260	48
H18C	3828	-1150	5657	48
H19A	4859	3127	5544	51
H19B	4426	3730	6136	51
H19C	4101	4937	5605	51
H20A	547	960	4431	48
H20B	186	2705	4055	48

H20C	78	2838	4708	48
H21A	2500	6205	4967	46
H21B	1576	6797	4548	46
H21C	2765	6509	4331	46

Table S 6. Torsion angles [°] for **Me-TAxEDA**.

O1-C1-C2-N1	-47.2(4)	C2-C1-O1-Al1	-140.0(3)
N1-C3-C4-C9	-104.3(5)	C4-C3-N1-C2	-62.9(4)
N1-C3-C4-C5	76.7(5)	C4-C3-N1-C10	54.7(5)
C9-C4-C5-C6	-0.2(6)	C4-C3-N1-Al2	-171.9(3)
C3-C4-C5-C6	178.8(4)	C1-C2-N1-C3	-69.5(4)
C4-C5-C6-C7	0.8(6)	C1-C2-N1-C10	169.7(3)
C5-C6-C7-C8	-1.8(7)	C1-C2-N1-Al2	47.1(3)
C6-C7-C8-C9	2.2(7)	C11-C10-N1-C3	62.0(4)
C5-C4-C9-C8	0.6(6)	C11-C10-N1-C2	-176.2(3)
C3-C4-C9-C8	-178.4(4)	C11-C10-N1-Al2	-67.4(4)
C7-C8-C9-C4	-1.7(6)	C1-O1-Al1-C17	-178.6(3)
N1-C10-C11-C12	58.8(5)	Al2-O1-Al1-C17	23.7(3)
N1-C10-C11-C16	-128.5(4)	C1-O1-Al1-C18	-57.8(3)
C16-C11-C12-C13	-0.8(7)	Al2-O1-Al1-C18	144.5(2)
C10-C11-C12-C13	172.0(4)	C1-O1-Al1-C19	61.0(3)
C11-C12-C13-C14	-0.6(7)	Al2-O1-Al1-C19	-96.7(2)
C12-C13-C14-C15	0.9(7)	C1-O1-Al2-C20	116.3(3)
C13-C14-C15-C16	0.3(7)	Al1-O1-Al2-C20	-85.6(2)
C12-C11-C16-C15	1.9(6)	C1-O1-Al2-C21	-102.3(3)
C10-C11-C16-C15	-171.2(4)	Al1-O1-Al2-C21	55.8(3)
C14-C15-C16-C11	-1.7(7)	C1-O1-Al2-N1	5.5(3)
C2-C1-O1-Al2	20.5(4)	Al1-O1-Al2-N1	163.5(2)

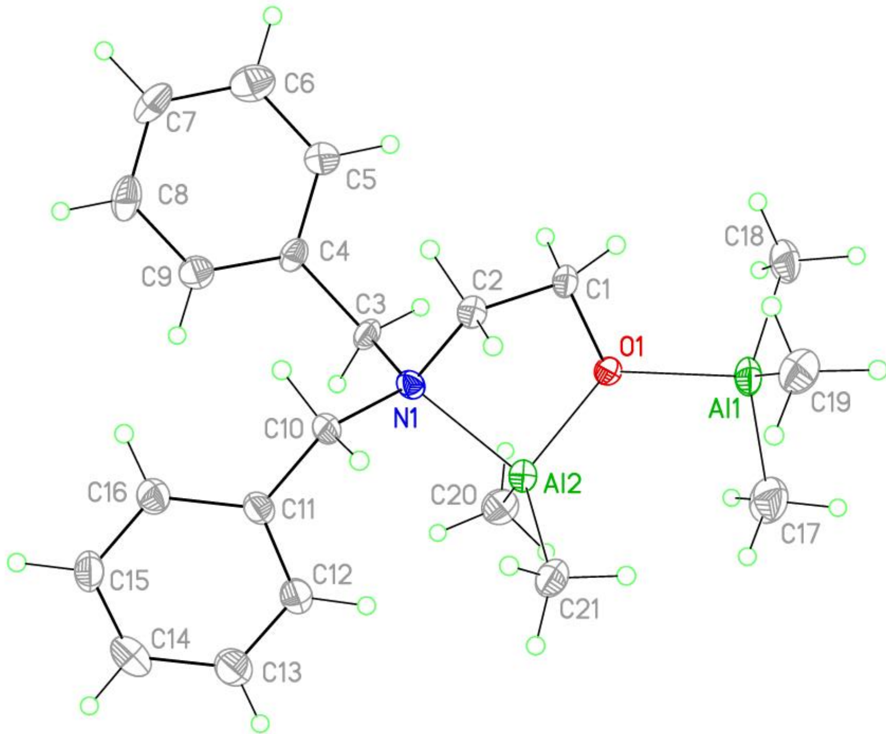

Figure S 1. View of **Me-TAxEDA** showing the atom labeling scheme. Displacement ellipsoids are scaled to the 50% probability level.

Table S 7. Crystal data and structure refinement for **iBu-TAxEDA**.

Empirical formula	C72 H126 Al4 N2 O2	
Formula weight	1159.66	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 21.170(4) Å	α= 90°.
	b = 13.038(3) Å	β= 110.776(4)°.
	c = 28.359(6) Å	γ = 90°.
Volume	7318(3) $Å^3$	
Z	4	
Density (calculated)	1.052 Mg/m^3	
Absorption coefficient	0.105 mm^{-1}	
F(000)	2560	
Crystal size	0.410 x 0.210 x 0.100 mm^3	
Theta range for data collection	2.191 to 25.121°.	
Index ranges	-25<=h<=25, -15<=k<=15, -33<=l<=33	
Reflections collected	58991	
Independent reflections	13049 [R(int) = 0.0972]	
Completeness to theta = 25.121°	99.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13049 / 480 / 741	
Goodness-of-fit on F^2	1.085	
Final R indices [I>2sigma(I)]	R1 = 0.0928, wR2 = 0.2097	
R indices (all data)	R1 = 0.1319, wR2 = 0.2279	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.106 and -0.480 e.$Å^{-3}$	

Table S 8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **iBu-TAxEDA**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C1	2244(2)	3277(3)	1907(2)	16(1)
C2	1604(2)	2696(3)	1860(2)	15(1)
C3	1120(2)	2805(3)	922(2)	13(1)
C4	1248(2)	1699(3)	837(1)	15(1)
C5	1905(2)	1332(4)	955(2)	20(1)
C6	2024(2)	313(4)	868(2)	26(1)
C7	1489(3)	-344(4)	663(2)	29(1)
C8	839(2)	8(4)	536(2)	28(1)
C9	720(2)	1022(3)	620(2)	20(1)
C10	409(2)	2563(3)	1453(2)	16(1)
C11	-256(2)	2842(3)	1047(2)	17(1)
C12	-706(2)	2072(4)	812(2)	26(1)
C13	-1336(2)	2294(4)	456(2)	30(1)
C14	-1517(2)	3300(4)	333(2)	33(1)
C15	-1078(2)	4083(4)	568(2)	28(1)
C16	-454(2)	3850(4)	926(2)	22(1)
C17	809(2)	4891(4)	2097(2)	22(1)
C18	1270(2)	5134(4)	2628(2)	27(1)
C19	881(3)	5191(5)	2993(2)	42(1)
C20	1668(3)	6102(4)	2671(2)	34(1)
C21	889(2)	5441(3)	936(2)	16(1)
C22	387(2)	6330(4)	885(2)	25(1)
C23	62(3)	6667(5)	332(2)	46(2)
C24	690(3)	7222(4)	1209(2)	38(1)
C25	2654(2)	4597(3)	940(2)	18(1)
C26	3247(2)	4548(4)	753(2)	27(1)
C27	3023(3)	4580(6)	177(2)	60(2)
C28	3670(3)	3601(5)	938(2)	51(2)
C29	3672(2)	4530(3)	2148(2)	17(1)

C30	3904(2)	4946(4)	2689(2)	22(1)
C31	4627(2)	4615(4)	3001(2)	32(1)
C32	3435(2)	4642(4)	2964(2)	30(1)
C33	2627(2)	6503(3)	1758(2)	19(1)
C34	2919(2)	7377(4)	1533(2)	28(1)
C35	3692(2)	7320(4)	1728(2)	34(1)
C36	2639(3)	7360(4)	958(2)	33(1)
C37	7258(2)	9621(3)	1880(2)	19(1)
C38	6615(2)	10222(3)	1813(2)	17(1)
C39	5414(2)	10318(3)	1424(2)	19(1)
C40	4741(2)	10092(4)	1024(2)	20(1)
C41	4516(2)	9097(4)	885(2)	22(1)
C42	3871(2)	8928(4)	540(2)	30(1)
C43	3441(2)	9743(4)	334(2)	29(1)
C44	3662(2)	10730(4)	473(2)	33(1)
C45	4308(2)	10911(4)	818(2)	25(1)
C46	6093(2)	9939(3)	879(2)	17(1)
C47	6213(2)	11031(3)	748(2)	19(1)
C48	6869(2)	11402(4)	854(2)	22(1)
C49	6976(2)	12386(4)	723(2)	29(1)
C50	6438(3)	13021(4)	489(2)	33(1)
C51	5782(3)	12668(4)	375(2)	32(1)
C52	5673(2)	11672(3)	503(2)	24(1)
C53	5938(2)	7330(3)	1006(2)	16(1)
C54	5694(2)	6257(3)	1088(2)	18(1)
C55	5744(3)	5493(4)	702(2)	33(1)
C56	4972(2)	6281(4)	1090(2)	26(1)
C57	5846(2)	8107(3)	2144(2)	19(1)
C58	5958(2)	7112(4)	2444(2)	25(1)
C59	5584(3)	7135(5)	2817(2)	40(1)
C60	6692(3)	6899(5)	2723(2)	46(2)
C61	7688(2)	6369(4)	1801(2)	29(1)
C62	8056(3)	5651(5)	1536(3)	50(2)
C63	7840(3)	4595(5)	1496(3)	72(2)
C64	8819(2)	5740(4)	1798(2)	40(1)
C65	8685(2)	8395(4)	2216(2)	19(1)

C66	8909(2)	7994(4)	2760(2)	24(1)
C67	8443(3)	8347(5)	3026(2)	40(1)
C68	9642(3)	8292(5)	3075(2)	41(1)
C69	7742(2)	8153(4)	987(2)	25(1)
C70	8383(2)	8351(4)	868(2)	29(1)
C71	8290(3)	8134(6)	318(2)	51(2)
C72	8635(3)	9435(5)	1007(2)	54(2)
N1	1025(2)	3070(3)	1413(1)	13(1)
N2	6028(2)	9785(3)	1390(1)	16(1)
O1	2085(1)	4341(2)	1781(1)	14(1)
O2	7100(1)	8551(2)	1793(1)	16(1)
Al1	1181(1)	4621(1)	1563(1)	12(1)
Al2	2808(1)	5039(1)	1646(1)	14(1)
Al3	6195(1)	8267(1)	1589(1)	14(1)
Al4	7844(1)	7835(1)	1703(1)	17(1)

Table S 9. Bond lengths [Å] and angles [°] for **iBu-TAxEDA**.

C1-O1	1.443(5)	C14-C15	1.383(7)
C1-C2	1.517(5)	C14-H14	0.95
C1-H1A	0.99	C15-C16	1.384(6)
C1-H1B	0.99	C15-H15	0.95
C2-N1	1.499(5)	C16-H16	0.95
C2-H2A	0.99	C17-C18	1.510(6)
C2-H2B	0.99	C17-Al1	1.972(4)
C3-C4	1.502(6)	C17-H17A	0.99
C3-N1	1.516(5)	C17-H17B	0.99
C3-H3A	0.99	C18-C20	1.499(7)
C3-H3B	0.99	C18-C19	1.536(6)
C4-C9	1.385(6)	C18-H18	1.00
C4-C5	1.396(6)	C19-H19A	0.98
C5-C6	1.390(6)	C19-H19B	0.98
C5-H5	0.95	C19-H19C	0.98
C6-C7	1.373(7)	C20-H20A	0.98
C6-H6	0.95	C20-H20B	0.98
C7-C8	1.372(7)	C20-H20C	0.98
C7-H7	0.95	C21-C22	1.545(6)
C8-C9	1.382(6)	C21-Al1	1.976(4)
C8-H8	0.95	C21-H21A	0.99
C9-H9	0.95	C21-H21B	0.99
C10-N1	1.503(5)	C22-C24	1.479(7)
C10-C11	1.513(6)	C22-C23	1.537(7)
C10-H10A	0.99	C22-H22	1.00
C10-H10B	0.99	C23-H23A	0.98
C11-C12	1.382(6)	C23-H23B	0.98
C11-C16	1.385(6)	C23-H23C	0.98
C12-C13	1.389(6)	C24-H24A	0.98
C12-H12	0.95	C24-H24B	0.98
C13-C14	1.376(7)	C24-H24C	0.98
C13-H13	0.95	C25-C26	1.527(6)

C25-Al2	1.998(4)	C36-H36B	0.98
C25-H25A	0.99	C36-H36C	0.98
C25-H25B	0.99	C37-O2	1.436(5)
C26-C28	1.505(7)	C37-C38	1.524(6)
C26-C27	1.532(7)	C37-H37A	0.99
C26-H26	1.00	C37-H37B	0.99
C27-H27A	0.98	C38-N2	1.499(5)
C27-H27B	0.98	C38-H38A	0.99
C27-H27C	0.98	C38-H38B	0.99
C28-H28A	0.98	C39-C40	1.502(6)
C28-H28B	0.98	C39-N2	1.507(5)
C28-H28C	0.98	C39-H39A	0.99
C29-C30	1.535(6)	C39-H39B	0.99
C29-Al2	1.991(4)	C40-C41	1.390(6)
C29-H29A	0.99	C40-C45	1.394(6)
C29-H29B	0.99	C41-C42	1.387(6)
C30-C32	1.515(6)	C41-H41	0.95
C30-C31	1.533(6)	C42-C43	1.386(7)
C30-H30	1.00	C42-H42	0.95
C31-H31A	0.98	C43-C44	1.379(7)
C31-H31B	0.98	C43-H43	0.95
C31-H31C	0.98	C44-C45	1.391(7)
C32-H32A	0.98	C44-H44	0.95
C32-H32B	0.98	C45-H45	0.95
C32-H32C	0.98	C46-C47	1.516(6)
C33-C34	1.540(6)	C46-N2	1.516(5)
C33-Al2	1.995(5)	C46-H46A	0.99
C33-H33A	0.99	C46-H46B	0.99
C33-H33B	0.99	C47-C52	1.387(6)
C34-C36	1.525(7)	C47-C48	1.398(6)
C34-C35	1.532(6)	C48-C49	1.377(7)
C34-H34	1.00	C48-H48	0.95
C35-H35A	0.98	C49-C50	1.375(7)
C35-H35B	0.98	C49-H49	0.95
C35-H35C	0.98	C50-C51	1.389(7)
C36-H36A	0.98	C50-H50	0.95

C51-C52	1.390(7)	C63-H63A	0.98
C51-H51	0.95	C63-H63B	0.98
C52-H52	0.95	C63-H63C	0.98
C53-C54	1.538(6)	C64-H64A	0.98
C53-Al3	1.969(4)	C64-H64B	0.98
C53-H53A	0.99	C64-H64C	0.98
C53-H53B	0.99	C65-C66	1.537(6)
C54-C55	1.512(6)	C65-Al4	1.995(4)
C54-C56	1.531(6)	C65-H65A	0.99
C54-H54	1.00	C65-H65B	0.99
C55-H55A	0.98	C66-C67	1.510(7)
C55-H55B	0.98	C66-C68	1.539(6)
C55-H55C	0.98	C66-H66	1.00
C56-H56A	0.98	C67-H67A	0.98
C56-H56B	0.98	C67-H67B	0.98
C56-H56C	0.98	C67-H67C	0.98
C57-C58	1.522(6)	C68-H68A	0.98
C57-Al3	1.975(4)	C68-H68B	0.98
C57-H57A	0.99	C68-H68C	0.98
C57-H57B	0.99	C69-C70	1.532(6)
C58-C60	1.499(7)	C69-Al4	2.010(5)
C58-C59	1.531(6)	C69-H69A	0.99
C58-H58	1.00	C69-H69B	0.99
C59-H59A	0.98	C70-C72	1.513(8)
C59-H59B	0.98	C70-C71	1.527(7)
C59-H59C	0.98	C70-H70	1.00
C60-H60A	0.98	C71-H71A	0.98
C60-H60B	0.98	C71-H71B	0.98
C60-H60C	0.98	C71-H71C	0.98
C61-C62	1.570(7)	C72-H72A	0.98
C61-Al4	1.976(5)	C72-H72B	0.98
C61-H61A	0.99	C72-H72C	0.98
C61-H61B	0.99	N1-Al1	2.069(4)
C62-C63	1.442(9)	N2-Al3	2.054(4)
C62-C64	1.525(7)	O1-Al1	1.827(3)
C62-H62	1.00	O1-Al2	1.932(3)

O2-Al3	1.831(3)	O2-Al4	1.924(3)
O1-C1-C2	109.6(3)	C8-C9-H9	119.4
O1-C1-H1A	109.7	C4-C9-H9	119.4
C2-C1-H1A	109.7	N1-C10-C11	115.8(3)
O1-C1-H1B	109.7	N1-C10-H10A	108.3
C2-C1-H1B	109.7	C11-C10-H10A	108.3
H1A-C1-H1B	108.2	N1-C10-H10B	108.3
N1-C2-C1	110.4(3)	C11-C10-H10B	108.3
N1-C2-H2A	109.6	H10A-C10-H10B	107.4
C1-C2-H2A	109.6	C12-C11-C16	118.2(4)
N1-C2-H2B	109.6	C12-C11-C10	119.2(4)
C1-C2-H2B	109.6	C16-C11-C10	122.3(4)
H2A-C2-H2B	108.1	C11-C12-C13	121.3(5)
C4-C3-N1	117.1(3)	C11-C12-H12	119.4
C4-C3-H3A	108.0	C13-C12-H12	119.4
N1-C3-H3A	108.0	C14-C13-C12	119.5(5)
C4-C3-H3B	108.0	C14-C13-H13	120.2
N1-C3-H3B	108.0	C12-C13-H13	120.2
H3A-C3-H3B	107.3	C13-C14-C15	120.2(4)
C9-C4-C5	117.8(4)	C13-C14-H14	119.9
C9-C4-C3	121.3(4)	C15-C14-H14	119.9
C5-C4-C3	120.8(4)	C14-C15-C16	119.7(5)
C6-C5-C4	120.8(4)	C14-C15-H15	120.2
C6-C5-H5	119.6	C16-C15-H15	120.2
C4-C5-H5	119.6	C15-C16-C11	121.1(4)
C7-C6-C5	119.9(4)	C15-C16-H16	119.4
C7-C6-H6	120.1	C11-C16-H16	119.4
C5-C6-H6	120.1	C18-C17-Al1	120.7(3)
C8-C7-C6	120.1(4)	C18-C17-H17A	107.2
C8-C7-H7	120.0	Al1-C17-H17A	107.2
C6-C7-H7	120.0	C18-C17-H17B	107.2
C7-C8-C9	120.1(4)	Al1-C17-H17B	107.2
C7-C8-H8	119.9	H17A-C17-H17B	106.8
C9-C8-H8	119.9	C20-C18-C17	113.8(4)
C8-C9-C4	121.2(4)	C20-C18-C19	109.0(4)

C17-C18-C19	111.7(4)	H24A-C24-H24B	109.5
C20-C18-H18	107.4	C22-C24-H24C	109.5
C17-C18-H18	107.4	H24A-C24-H24C	109.5
C19-C18-H18	107.4	H24B-C24-H24C	109.5
C18-C19-H19A	109.5	C26-C25-Al2	119.9(3)
C18-C19-H19B	109.5	C26-C25-H25A	107.3
H19A-C19-H19B	109.5	Al2-C25-H25A	107.3
C18-C19-H19C	109.5	C26-C25-H25B	107.3
H19A-C19-H19C	109.5	Al2-C25-H25B	107.3
H19B-C19-H19C	109.5	H25A-C25-H25B	106.9
C18-C20-H20A	109.5	C28-C26-C25	111.9(4)
C18-C20-H20B	109.5	C28-C26-C27	108.4(4)
H20A-C20-H20B	109.5	C25-C26-C27	112.8(4)
C18-C20-H20C	109.5	C28-C26-H26	107.8
H20A-C20-H20C	109.5	C25-C26-H26	107.8
H20B-C20-H20C	109.5	C27-C26-H26	107.8
C22-C21-Al1	118.3(3)	C26-C27-H27A	109.5
C22-C21-H21A	107.7	C26-C27-H27B	109.5
Al1-C21-H21A	107.7	H27A-C27-H27B	109.5
C22-C21-H21B	107.7	C26-C27-H27C	109.5
Al1-C21-H21B	107.7	H27A-C27-H27C	109.5
H21A-C21-H21B	107.1	H27B-C27-H27C	109.5
C24-C22-C23	110.3(4)	C26-C28-H28A	109.5
C24-C22-C21	113.6(4)	C26-C28-H28B	109.5
C23-C22-C21	110.7(4)	H28A-C28-H28B	109.5
C24-C22-H22	107.3	C26-C28-H28C	109.5
C23-C22-H22	107.3	H28A-C28-H28C	109.5
C21-C22-H22	107.3	H28B-C28-H28C	109.5
C22-C23-H23A	109.5	C30-C29-Al2	119.0(3)
C22-C23-H23B	109.5	C30-C29-H29A	107.6
H23A-C23-H23B	109.5	Al2-C29-H29A	107.6
C22-C23-H23C	109.5	C30-C29-H29B	107.6
H23A-C23-H23C	109.5	Al2-C29-H29B	107.6
H23B-C23-H23C	109.5	H29A-C29-H29B	107.0
C22-C24-H24A	109.5	C32-C30-C31	109.4(4)
C22-C24-H24B	109.5	C32-C30-C29	112.7(4)

C31-C30-C29	112.1(4)	H36A-C36-H36B	109.5
C32-C30-H30	107.5	C34-C36-H36C	109.5
C31-C30-H30	107.5	H36A-C36-H36C	109.5
C29-C30-H30	107.5	H36B-C36-H36C	109.5
C30-C31-H31A	109.5	O2-C37-C38	109.6(3)
C30-C31-H31B	109.5	O2-C37-H37A	109.8
H31A-C31-H31B	109.5	C38-C37-H37A	109.8
C30-C31-H31C	109.5	O2-C37-H37B	109.8
H31A-C31-H31C	109.5	C38-C37-H37B	109.8
H31B-C31-H31C	109.5	H37A-C37-H37B	108.2
C30-C32-H32A	109.5	N2-C38-C37	110.7(3)
C30-C32-H32B	109.5	N2-C38-H38A	109.5
H32A-C32-H32B	109.5	C37-C38-H38A	109.5
C30-C32-H32C	109.5	N2-C38-H38B	109.5
H32A-C32-H32C	109.5	C37-C38-H38B	109.5
H32B-C32-H32C	109.5	H38A-C38-H38B	108.1
C34-C33-Al2	120.9(3)	C40-C39-N2	118.0(3)
C34-C33-H33A	107.1	C40-C39-H39A	107.8
Al2-C33-H33A	107.1	N2-C39-H39A	107.8
C34-C33-H33B	107.1	C40-C39-H39B	107.8
Al2-C33-H33B	107.1	N2-C39-H39B	107.8
H33A-C33-H33B	106.8	H39A-C39-H39B	107.1
C36-C34-C35	110.2(4)	C41-C40-C45	119.2(4)
C36-C34-C33	111.9(4)	C41-C40-C39	122.4(4)
C35-C34-C33	110.4(4)	C45-C40-C39	118.2(4)
C36-C34-H34	108.1	C42-C41-C40	120.1(4)
C35-C34-H34	108.1	C42-C41-H41	119.9
C33-C34-H34	108.1	C40-C41-H41	119.9
C34-C35-H35A	109.5	C43-C42-C41	120.7(5)
C34-C35-H35B	109.5	C43-C42-H42	119.6
H35A-C35-H35B	109.5	C41-C42-H42	119.6
C34-C35-H35C	109.5	C44-C43-C42	119.3(4)
H35A-C35-H35C	109.5	C44-C43-H43	120.3
H35B-C35-H35C	109.5	C42-C43-H43	120.3
C34-C36-H36A	109.5	C43-C44-C45	120.6(5)
C34-C36-H36B	109.5	C43-C44-H44	119.7

C45-C44-H44	119.7	C56-C54-C53	111.8(3)
C44-C45-C40	120.1(5)	C55-C54-H54	107.6
C44-C45-H45	119.9	C56-C54-H54	107.6
C40-C45-H45	119.9	C53-C54-H54	107.6
C47-C46-N2	116.0(3)	C54-C55-H55A	109.5
C47-C46-H46A	108.3	C54-C55-H55B	109.5
N2-C46-H46A	108.3	H55A-C55-H55B	109.5
C47-C46-H46B	108.3	C54-C55-H55C	109.5
N2-C46-H46B	108.3	H55A-C55-H55C	109.5
H46A-C46-H46B	107.4	H55B-C55-H55C	109.5
C52-C47-C48	118.6(4)	C54-C56-H56A	109.5
C52-C47-C46	120.5(4)	C54-C56-H56B	109.5
C48-C47-C46	120.8(4)	H56A-C56-H56B	109.5
C49-C48-C47	120.7(4)	C54-C56-H56C	109.5
C49-C48-H48	119.7	H56A-C56-H56C	109.5
C47-C48-H48	119.7	H56B-C56-H56C	109.5
C50-C49-C48	120.3(5)	C58-C57-Al3	120.4(3)
C50-C49-H49	119.9	C58-C57-H57A	107.2
C48-C49-H49	119.9	Al3-C57-H57A	107.2
C49-C50-C51	120.1(5)	C58-C57-H57B	107.2
C49-C50-H50	120.0	Al3-C57-H57B	107.2
C51-C50-H50	120.0	H57A-C57-H57B	106.8
C50-C51-C52	119.6(5)	C60-C58-C57	112.3(4)
C50-C51-H51	120.2	C60-C58-C59	109.3(4)
C52-C51-H51	120.2	C57-C58-C59	110.7(4)
C47-C52-C51	120.6(4)	C60-C58-H58	108.1
C47-C52-H52	119.7	C57-C58-H58	108.1
C51-C52-H52	119.7	C59-C58-H58	108.1
C54-C53-Al3	116.4(3)	C58-C59-H59A	109.5
C54-C53-H53A	108.2	C58-C59-H59B	109.5
Al3-C53-H53A	108.2	H59A-C59-H59B	109.5
C54-C53-H53B	108.2	C58-C59-H59C	109.5
Al3-C53-H53B	108.2	H59A-C59-H59C	109.5
H53A-C53-H53B	107.3	H59B-C59-H59C	109.5
C55-C54-C56	110.1(4)	C58-C60-H60A	109.5
C55-C54-C53	112.1(4)	C58-C60-H60B	109.5

H60A-C60-H60B	109.5	C65-C66-C68	112.7(4)
C58-C60-H60C	109.5	C67-C66-H66	107.4
H60A-C60-H60C	109.5	C65-C66-H66	107.4
H60B-C60-H60C	109.5	C68-C66-H66	107.4
C62-C61-Al4	111.9(4)	C66-C67-H67A	109.5
C62-C61-H61A	109.2	C66-C67-H67B	109.5
Al4-C61-H61A	109.2	H67A-C67-H67B	109.5
C62-C61-H61B	109.2	C66-C67-H67C	109.5
Al4-C61-H61B	109.2	H67A-C67-H67C	109.5
H61A-C61-H61B	107.9	H67B-C67-H67C	109.5
C63-C62-C64	111.2(5)	C66-C68-H68A	109.5
C63-C62-C61	114.2(5)	C66-C68-H68B	109.5
C64-C62-C61	109.8(4)	H68A-C68-H68B	109.5
C63-C62-H62	107.1	C66-C68-H68C	109.5
C64-C62-H62	107.1	H68A-C68-H68C	109.5
C61-C62-H62	107.1	H68B-C68-H68C	109.5
C62-C63-H63A	109.5	C70-C69-Al4	118.2(3)
C62-C63-H63B	109.5	C70-C69-H69A	107.8
H63A-C63-H63B	109.5	Al4-C69-H69A	107.8
C62-C63-H63C	109.5	C70-C69-H69B	107.8
H63A-C63-H63C	109.5	Al4-C69-H69B	107.8
H63B-C63-H63C	109.5	H69A-C69-H69B	107.1
C62-C64-H64A	109.5	C72-C70-C71	110.2(5)
C62-C64-H64B	109.5	C72-C70-C69	110.9(4)
H64A-C64-H64B	109.5	C71-C70-C69	113.0(4)
C62-C64-H64C	109.5	C72-C70-H70	107.5
H64A-C64-H64C	109.5	C71-C70-H70	107.5
H64B-C64-H64C	109.5	C69-C70-H70	107.5
C66-C65-Al4	119.0(3)	C70-C71-H71A	109.5
C66-C65-H65A	107.6	C70-C71-H71B	109.5
Al4-C65-H65A	107.6	H71A-C71-H71B	109.5
C66-C65-H65B	107.6	C70-C71-H71C	109.5
Al4-C65-H65B	107.6	H71A-C71-H71C	109.5
H65A-C65-H65B	107.0	H71B-C71-H71C	109.5
C67-C66-C65	112.0(4)	C70-C72-H72A	109.5
C67-C66-C68	109.6(4)	C70-C72-H72B	109.5

H72A-C72-H72B	109.5	O1-Al1-C21	111.64(15)
C70-C72-H72C	109.5	C17-Al1-C21	120.83(19)
H72A-C72-H72C	109.5	O1-Al1-N1	86.88(13)
H72B-C72-H72C	109.5	C17-Al1-N1	104.71(17)
C2-N1-C10	105.3(3)	C21-Al1-N1	111.54(16)
C2-N1-C3	111.7(3)	O1-Al2-C29	107.04(16)
C10-N1-C3	111.7(3)	O1-Al2-C33	102.01(15)
C2-N1-Al1	97.0(2)	C29-Al2-C33	112.62(18)
C10-N1-Al1	119.6(3)	O1-Al2-C25	101.79(15)
C3-N1-Al1	110.4(2)	C29-Al2-C25	113.76(18)
C38-N2-C39	105.2(3)	C33-Al2-C25	117.63(19)
C38-N2-C46	112.6(3)	O2-Al3-C53	109.69(16)
C39-N2-C46	111.9(3)	O2-Al3-C57	114.51(16)
C38-N2-Al3	97.7(2)	C53-Al3-C57	122.26(19)
C39-N2-Al3	119.7(3)	O2-Al3-N2	87.18(14)
C46-N2-Al3	108.9(2)	C53-Al3-N2	113.49(17)
C1-O1-Al1	113.6(2)	C57-Al3-N2	104.09(17)
C1-O1-Al2	111.7(2)	O2-Al4-C61	105.38(16)
Al1-O1-Al2	130.30(16)	O2-Al4-C65	106.71(16)
C37-O2-Al3	113.9(2)	C61-Al4-C65	113.7(2)
C37-O2-Al4	110.0(2)	O2-Al4-C69	103.55(17)
Al3-O2-Al4	132.39(16)	C61-Al4-C69	112.2(2)
O1-Al1-C17	115.56(16)	C65-Al4-C69	114.17(19)

Table S 10. Anisotropic displacement parameters ($Å^2$x 10^3) for **iBu-TAxEDA**. The anisotropic displacement factor exponent takes the form: $-2\pi^2$[h^2 $a^{*2}U^{11}$ + ... + 2 h k a* b* U^{12}]

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C1	13(2)	12(2)	22(2)	3(2)	4(2)	0(2)
C2	18(2)	11(2)	13(2)	4(2)	1(2)	-2(2)
C3	16(2)	10(2)	15(2)	2(2)	7(2)	-1(2)
C4	22(2)	13(2)	11(2)	1(2)	7(2)	0(2)
C5	20(2)	21(2)	19(2)	-2(2)	7(2)	1(2)
C6	27(2)	23(3)	29(2)	-5(2)	13(2)	7(2)
C7	42(3)	16(2)	29(2)	0(2)	15(2)	8(2)
C8	33(3)	16(2)	32(3)	-7(2)	7(2)	-6(2)
C9	21(2)	11(2)	27(2)	-2(2)	7(2)	2(2)
C10	15(2)	13(2)	21(2)	4(2)	9(2)	-1(2)
C11	13(2)	19(2)	19(2)	-2(2)	8(2)	-1(2)
C12	18(2)	28(3)	32(3)	-4(2)	9(2)	-4(2)
C13	18(2)	38(3)	34(3)	-12(2)	8(2)	-7(2)
C14	15(2)	49(3)	31(3)	-6(2)	4(2)	4(2)
C15	21(2)	28(3)	34(3)	1(2)	9(2)	4(2)
C16	17(2)	17(2)	31(2)	-4(2)	8(2)	0(2)
C17	16(2)	23(2)	30(2)	-6(2)	12(2)	-3(2)
C18	28(2)	29(3)	28(2)	1(2)	14(2)	0(2)
C19	52(3)	49(4)	35(3)	-9(3)	27(3)	-16(3)
C20	32(3)	38(3)	37(3)	-16(2)	17(2)	-11(2)
C21	12(2)	12(2)	22(2)	1(2)	6(2)	3(2)
C22	31(2)	16(2)	30(2)	5(2)	13(2)	10(2)
C23	53(4)	43(4)	32(3)	4(3)	4(3)	26(3)
C24	39(3)	31(3)	40(3)	6(2)	9(2)	9(2)
C25	15(2)	18(2)	23(2)	2(2)	8(2)	-4(2)
C26	21(2)	19(2)	46(3)	-11(2)	20(2)	-4(2)
C27	72(4)	76(5)	55(4)	30(3)	52(4)	38(4)
C28	51(4)	67(4)	32(3)	-7(3)	9(3)	37(3)
C29	11(2)	17(2)	24(2)	-3(2)	6(2)	0(2)

C30	12(2)	27(3)	26(2)	-6(2)	4(2)	4(2)
C31	20(2)	37(3)	30(3)	-3(2)	-3(2)	4(2)
C32	24(2)	41(3)	23(2)	-7(2)	8(2)	1(2)
C33	14(2)	18(2)	25(2)	-3(2)	6(2)	-2(2)
C34	25(2)	17(2)	42(3)	-2(2)	12(2)	-5(2)
C35	23(2)	38(3)	42(3)	0(2)	12(2)	-12(2)
C36	36(3)	22(3)	43(3)	12(2)	16(2)	2(2)
C37	16(2)	15(2)	25(2)	-4(2)	6(2)	-2(2)
C38	18(2)	13(2)	20(2)	-5(2)	6(2)	-2(2)
C39	18(2)	17(2)	26(2)	-4(2)	10(2)	5(2)
C40	17(2)	25(2)	23(2)	0(2)	13(2)	6(2)
C41	18(2)	25(3)	24(2)	-4(2)	7(2)	5(2)
C42	21(2)	36(3)	33(3)	-12(2)	10(2)	0(2)
C43	20(2)	43(3)	26(2)	-7(2)	8(2)	7(2)
C44	22(2)	40(3)	35(3)	6(2)	8(2)	12(2)
C45	22(2)	23(3)	36(3)	0(2)	17(2)	6(2)
C46	19(2)	14(2)	21(2)	-1(2)	11(2)	7(2)
C47	22(2)	17(2)	20(2)	-1(2)	11(2)	1(2)
C48	23(2)	21(2)	26(2)	-1(2)	12(2)	0(2)
C49	31(3)	27(3)	35(3)	-7(2)	18(2)	-8(2)
C50	53(3)	17(2)	37(3)	-2(2)	26(2)	-1(2)
C51	45(3)	24(3)	35(3)	4(2)	25(2)	9(2)
C52	26(2)	17(2)	33(3)	4(2)	16(2)	5(2)
C53	17(2)	14(2)	20(2)	-4(2)	9(2)	2(2)
C54	14(2)	15(2)	22(2)	2(2)	5(2)	4(2)
C55	41(3)	14(2)	45(3)	-11(2)	17(2)	1(2)
C56	21(2)	17(2)	38(3)	0(2)	10(2)	-7(2)
C57	16(2)	23(2)	21(2)	-4(2)	9(2)	0(2)
C58	30(2)	21(2)	28(2)	-3(2)	16(2)	-2(2)
C59	28(3)	57(4)	40(3)	13(3)	18(2)	-1(3)
C60	36(3)	48(4)	66(4)	31(3)	34(3)	22(3)
C61	15(2)	20(3)	51(3)	-8(2)	9(2)	2(2)
C62	32(3)	34(3)	80(4)	-19(3)	16(3)	7(2)
C63	45(4)	54(4)	126(6)	-51(4)	42(4)	-11(3)
C64	24(3)	30(3)	69(4)	-14(3)	21(3)	6(2)
C65	13(2)	22(2)	24(2)	-6(2)	9(2)	-4(2)

C66	20(2)	26(3)	24(2)	1(2)	6(2)	-6(2)
C67	41(3)	57(4)	27(3)	3(3)	15(2)	-7(3)
C68	32(3)	46(4)	34(3)	6(3)	-1(2)	-9(3)
C69	20(2)	36(3)	21(2)	-4(2)	9(2)	2(2)
C70	20(2)	45(3)	23(2)	9(2)	10(2)	4(2)
C71	38(3)	94(5)	29(3)	1(3)	21(3)	5(3)
C72	46(3)	63(4)	47(3)	18(3)	10(3)	-20(3)
N1	10(2)	12(2)	14(2)	3(1)	2(1)	-4(1)
N2	14(2)	14(2)	21(2)	0(2)	7(1)	0(2)
O1	12(1)	11(2)	17(1)	1(1)	4(1)	0(1)
O2	14(1)	11(2)	23(2)	-3(1)	9(1)	0(1)
Al1	11(1)	10(1)	16(1)	-2(1)	5(1)	0(1)
Al2	10(1)	13(1)	19(1)	-2(1)	5(1)	0(1)
Al3	12(1)	13(1)	18(1)	-2(1)	8(1)	-1(1)
Al4	12(1)	19(1)	21(1)	-2(1)	8(1)	1(1)

Table S 11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **iBu-TAxEDA**.

	x	y	z	U(eq)
H1A	2572	3221	2257	20
H1B	2453	2976	1677	20
H2A	1674	1954	1823	18
H2B	1498	2794	2171	18
H3A	710	3027	641	16
H3B	1503	3214	901	16
H5	2277	1784	1096	24
H6	2474	71	951	31
H7	1570	-1044	608	34
H8	470	-446	390	34
H9	268	1258	527	24
H10A	381	2741	1785	19
H10B	469	1811	1447	19
H12	-582	1377	896	31
H13	-1641	1756	299	36
H14	-1944	3457	85	39
H15	-1203	4777	485	34
H16	-157	4390	1091	26
H17A	488	5470	1982	27
H17B	539	4282	2117	27
H18	1601	4557	2743	33
H19A	1200	5286	3338	64
H19B	629	4552	2974	64
H19C	566	5770	2900	64
H20A	1903	6084	2429	51
H20B	1999	6164	3014	51
H20C	1361	6692	2598	51
H21A	1299	5731	895	19
H21B	683	4965	650	19
H22	17	6063	993	30

H23A	-286	7182	303	69
H23B	-143	6071	123	69
H23C	409	6962	218	69
H24A	893	6997	1560	57
H24B	338	7732	1180	57
H24C	1038	7527	1100	57
H25A	2448	3905	895	22
H25B	2313	5065	712	22
H26	3541	5158	890	32
H27A	3422	4557	78	90
H27B	2773	5216	51	90
H27C	2733	3990	33	90
H28A	3826	3576	1307	77
H28B	4061	3621	830	77
H28C	3398	2991	797	77
H29A	3637	3775	2167	21
H29B	4035	4676	2014	21
H30	3901	5712	2668	27
H31A	4757	4904	3341	48
H31B	4936	4864	2839	48
H31C	4649	3865	3022	48
H32A	2976	4879	2772	45
H32B	3591	4957	3300	45
H32C	3435	3894	2998	45
H33A	2130	6592	1631	23
H33B	2787	6613	2127	23
H34	2787	8043	1647	34
H35A	3833	6654	1638	52
H35B	3868	7398	2095	52
H35C	3870	7870	1575	52
H36A	2761	7998	829	50
H36B	2146	7297	838	50
H36C	2829	6775	837	50
H37A	7465	9873	1639	22
H37B	7587	9721	2226	22
H38A	6518	10198	2130	21

H38B	6680	10949	1740	21
H39A	5383	10145	1755	23
H39B	5492	11067	1423	23
H41	4805	8532	1027	27
H42	3722	8246	444	36
H43	2999	9622	99	35
H44	3370	11292	333	40
H45	4455	11594	913	30
H46A	6471	9508	864	21
H46B	5674	9685	617	21
H48	7244	10970	1019	27
H49	7424	12627	795	35
H50	6515	13704	404	40
H51	5409	13104	210	38
H52	5224	11427	422	28
H53A	5575	7661	724	20
H53B	6333	7248	900	20
H54	5996	6012	1428	21
H55A	5600	4816	775	49
H55B	6213	5456	716	49
H55C	5452	5713	364	49
H56A	4663	6518	762	38
H56B	4950	6750	1354	38
H56C	4841	5590	1157	38
H57A	6042	8668	2388	23
H57B	5352	8227	2001	23
H58	5769	6537	2202	30
H59A	5665	6491	3008	60
H59B	5098	7217	2632	60
H59C	5749	7711	3051	60
H60A	6936	6916	2487	69
H60B	6742	6221	2881	69
H60C	6878	7422	2985	69
H61A	7854	6215	2167	35
H61B	7197	6228	1664	35
H62	7945	5913	1184	60

H63A	8073	4203	1312	108
H63B	7351	4559	1316	108
H63C	7950	4306	1835	108
H64A	8938	5613	2160	60
H64B	8965	6431	1747	60
H64C	9044	5234	1656	60
H65A	9060	8270	2091	23
H65B	8630	9147	2227	23
H66	8887	7228	2744	28
H67A	8453	9098	3047	61
H67B	8593	8056	3366	61
H67C	7982	8118	2836	61
H68A	9689	9040	3077	61
H68B	9950	7980	2927	61
H68C	9753	8046	3422	61
H69A	7498	7574	774	30
H69B	7449	8765	880	30
H70	8741	7875	1082	34
H71A	7934	8578	97	77
H71B	8163	7414	240	77
H71C	8715	8270	264	77
H72A	9080	9512	977	81
H72B	8671	9577	1354	81
H72C	8317	9919	778	81

Table S 12. Torsion angles [°] for **iBu-TAxEDA**.

O1-C1-C2-N1	38.8(4)	N2-C39-C40-C41	49.6(6)
N1-C3-C4-C9	87.6(5)	N2-C39-C40-C45	-135.8(4)
N1-C3-C4-C5	-95.2(5)	C45-C40-C41-C42	0.8(6)
C9-C4-C5-C6	-1.6(6)	C39-C40-C41-C42	175.3(4)
C3-C4-C5-C6	-178.8(4)	C40-C41-C42-C43	-0.7(7)
C4-C5-C6-C7	0.2(7)	C41-C42-C43-C44	0.3(7)
C5-C6-C7-C8	1.0(7)	C42-C43-C44-C45	-0.2(7)
C6-C7-C8-C9	-0.8(7)	C43-C44-C45-C40	0.3(7)
C7-C8-C9-C4	-0.7(7)	C41-C40-C45-C44	-0.6(6)
C5-C4-C9-C8	1.8(6)	C39-C40-C45-C44	-175.4(4)
C3-C4-C9-C8	179.1(4)	N2-C46-C47-C52	-89.9(5)
N1-C10-C11-C12	133.4(4)	N2-C46-C47-C48	92.6(5)
N1-C10-C11-C16	-51.4(5)	C52-C47-C48-C49	0.7(7)
C16-C11-C12-C13	1.2(7)	C46-C47-C48-C49	178.3(4)
C10-C11-C12-C13	176.7(4)	C47-C48-C49-C50	0.5(7)
C11-C12-C13-C14	0.2(7)	C48-C49-C50-C51	-1.1(7)
C12-C13-C14-C15	-1.1(7)	C49-C50-C51-C52	0.5(7)
C13-C14-C15-C16	0.4(7)	C48-C47-C52-C51	-1.3(7)
C14-C15-C16-C11	1.1(7)	C46-C47-C52-C51	-178.9(4)
C12-C11-C16-C15	-1.9(7)	C50-C51-C52-C47	0.7(7)
C10-C11-C16-C15	-177.2(4)	Al3-C53-C54-C55	-160.0(3)
Al1-C17-C18-C20	62.8(5)	Al3-C53-C54-C56	75.9(4)
Al1-C17-C18-C19	-173.3(4)	Al3-C57-C58-C60	63.0(5)
Al1-C21-C22-C24	71.8(5)	Al3-C57-C58-C59	-174.5(3)
Al1-C21-C22-C23	-163.5(4)	Al4-C61-C62-C63	-166.7(5)
Al2-C25-C26-C28	78.2(5)	Al4-C61-C62-C64	67.6(6)
Al2-C25-C26-C27	-159.3(4)	Al4-C65-C66-C67	-69.9(5)
Al2-C29-C30-C32	65.4(5)	Al4-C65-C66-C68	166.0(4)
Al2-C29-C30-C31	-170.6(3)	Al4-C69-C70-C72	-80.1(5)
Al2-C33-C34-C36	63.8(5)	Al4-C69-C70-C71	155.6(4)
Al2-C33-C34-C35	-59.3(5)	C1-C2-N1-C10	-171.4(3)
O2-C37-C38-N2	-37.2(5)	C1-C2-N1-C3	67.1(4)

C1-C2-N1-Al1	-48.2(3)	C2-C1-O1-Al1	-4.5(4)
C11-C10-N1-C2	178.4(3)	C2-C1-O1-Al2	-163.6(3)
C11-C10-N1-C3	-60.2(5)	C38-C37-O2-Al3	4.3(4)
C11-C10-N1-Al1	70.9(4)	C38-C37-O2-Al4	165.2(3)
C4-C3-N1-C2	54.1(4)	C1-O1-Al1-C17	85.1(3)
C4-C3-N1-C10	-63.6(4)	Al2-O1-Al1-C17	-120.6(2)
C4-C3-N1-Al1	160.7(3)	C1-O1-Al1-C21	-131.6(3)
C37-C38-N2-C39	170.3(3)	Al2-O1-Al1-C21	22.6(3)
C37-C38-N2-C46	-67.6(4)	C1-O1-Al1-N1	-19.7(3)
C37-C38-N2-Al3	46.6(4)	Al2-O1-Al1-N1	134.6(2)
C40-C39-N2-C38	176.0(4)	C37-O2-Al3-C53	133.1(3)
C40-C39-N2-C46	53.5(5)	Al4-O2-Al3-C53	-22.4(3)
C40-C39-N2-Al3	-75.6(4)	C37-O2-Al3-C57	-85.0(3)
C47-C46-N2-C38	-53.6(5)	Al4-O2-Al3-C57	119.4(2)
C47-C46-N2-C39	64.7(5)	C37-O2-Al3-N2	19.2(3)
C47-C46-N2-Al3	-160.8(3)	Al4-O2-Al3-N2	-136.3(2)

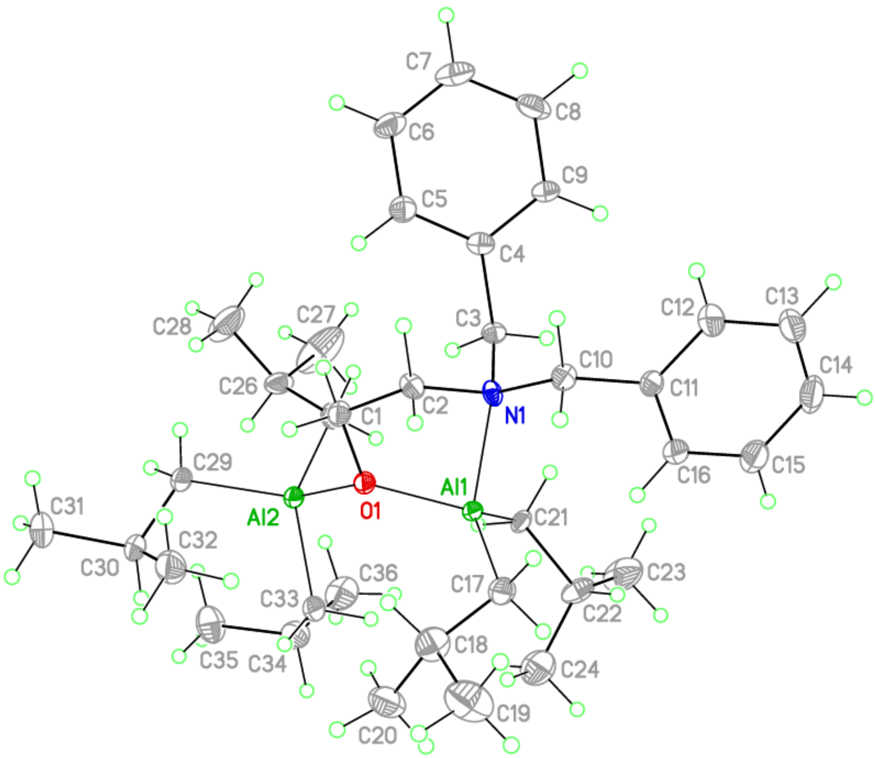

Figure S 2. View of **iBu-TAxEDA** showing the atom labeling scheme. Displacement ellipsoids are scaled to the 50% probability level.

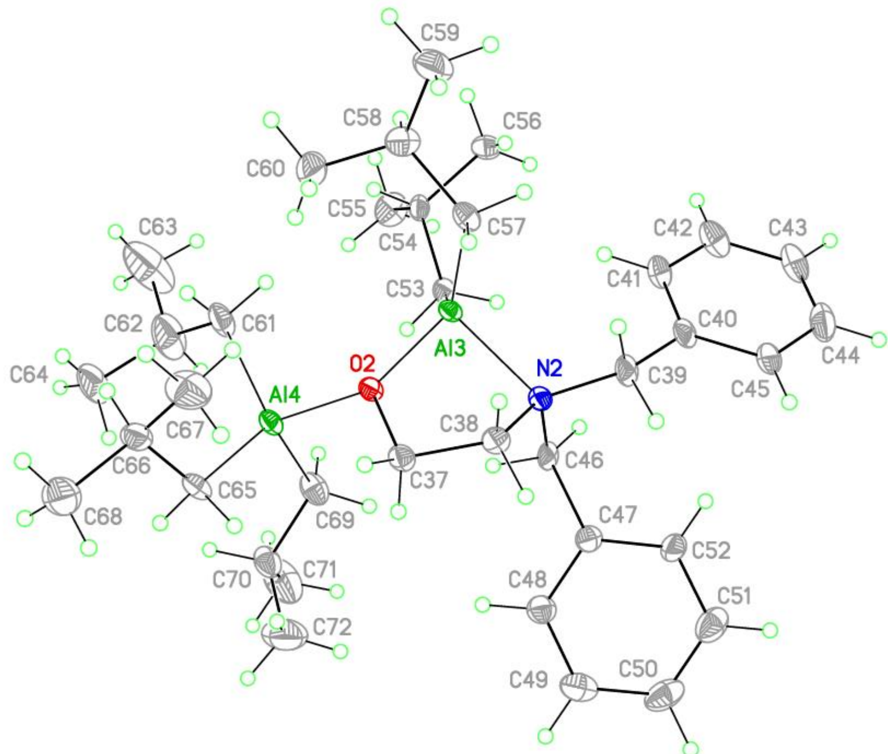

Figure S 3. View of **iBu-TAxEDA** showing the atom labeling scheme. Displacement ellipsoids are scaled to the 50% probability level.

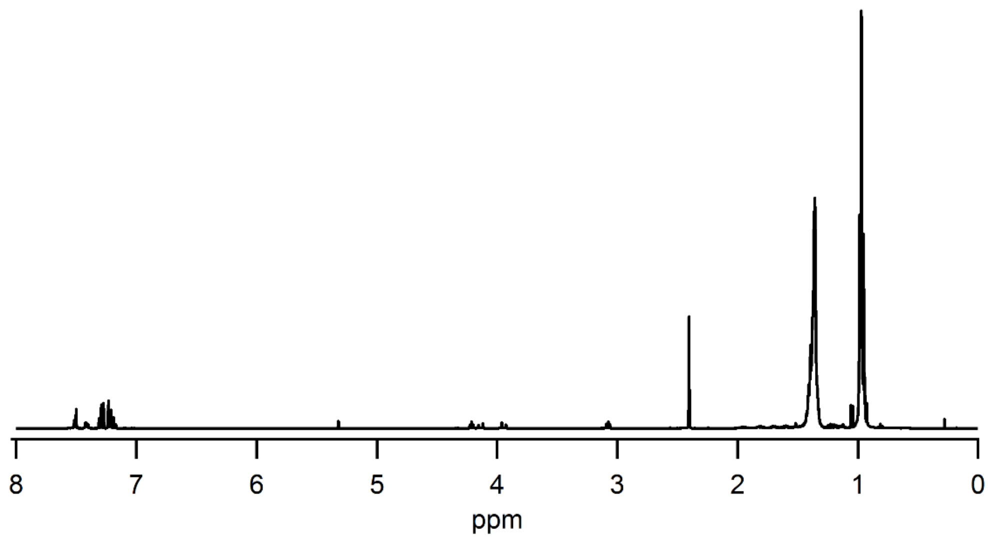

Figure S 4. [1]H NMR spectrum of Me-TAxEDA. [1]H NMR (CD2Cl2, 400 MHz) δ –0.94 (s, –Al–(CH3)3), –0.56 (s, –Al–(CH3)2), 3.05 (t, –N–CH2–CH2–O–), 3.90/4.07 (d, –Ph–CH2–N–), 4.14 (t, –N–CH2–CH2–O–), 7.32/7.48 (m, –Ph–CH2–N–).

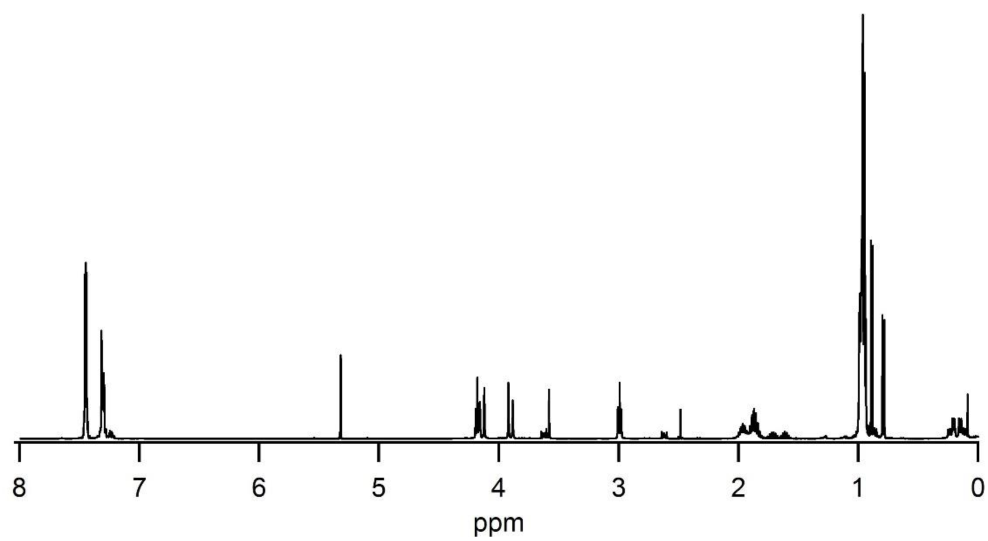

Figure S 5. [1]H NMR spectrum of iBu-TAxEDA. [1]H NMR (CD2Cl2, 400 MHz) δ –0.03 (d, –Al–CH2–CH–(CH3)3), 0.12 (m, –O–Al[CH2–CH–(CH3)2]3, 0.22 (m, N–Al[CH2-CH-(CH3)2]2, 0.79 (d, Al–CH2–CH–(CH3)2), 0.91 (m, Al–CH2–CH–(CH3)2), 0.96 (m Al–CH2–CH–(CH3)2), 1.90 (m, Al–CH2–CH–(CH3)2), 2.99 (t, N–CH2–CH2–O), 3.90 (d, N–CH2–Ph), 4.16 (m, N–CH2–CH2–O), 7.29/7.45 (m, –Ph–CH2–N–).

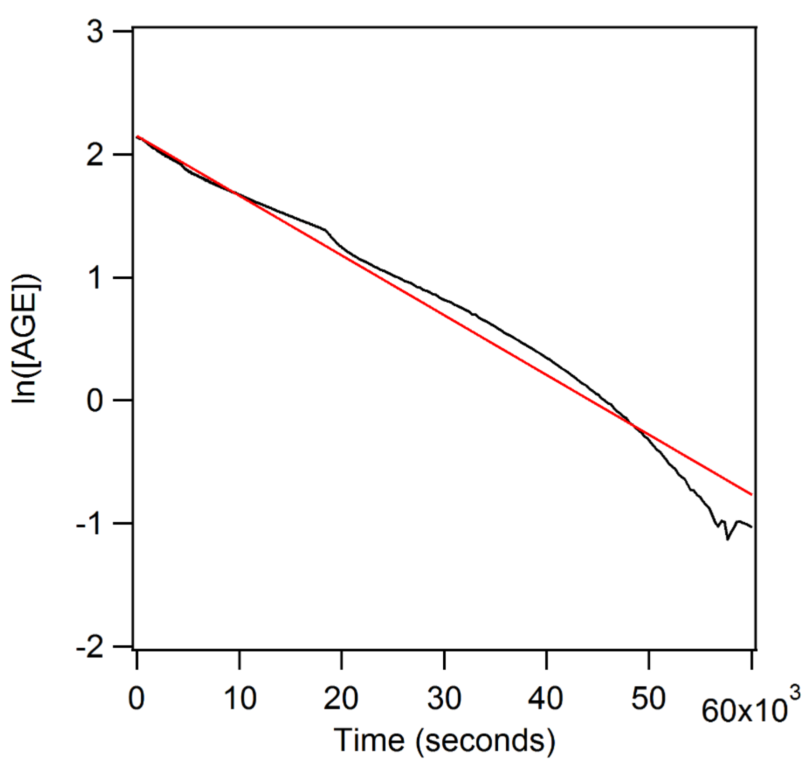

Figure S 6. Plot of ln([AGE]) as a function of time for the polymerization of PAGE with Me-TAxEDA. The data are roughly linear, consistent with first order kinetics. The slope of the fit line (in red) is $-4.85 \times 10^{-5} \pm 6.3 \times 10^{-7}$. The k_p can be calculated by dividing the slope by the initiator concentration ([I]) which in this case is 0.097 M. Therefore, the k_p^{Me} is $0.500 \pm 0.011 \times 10^{-3}$ M^{-1} s^{-1}.

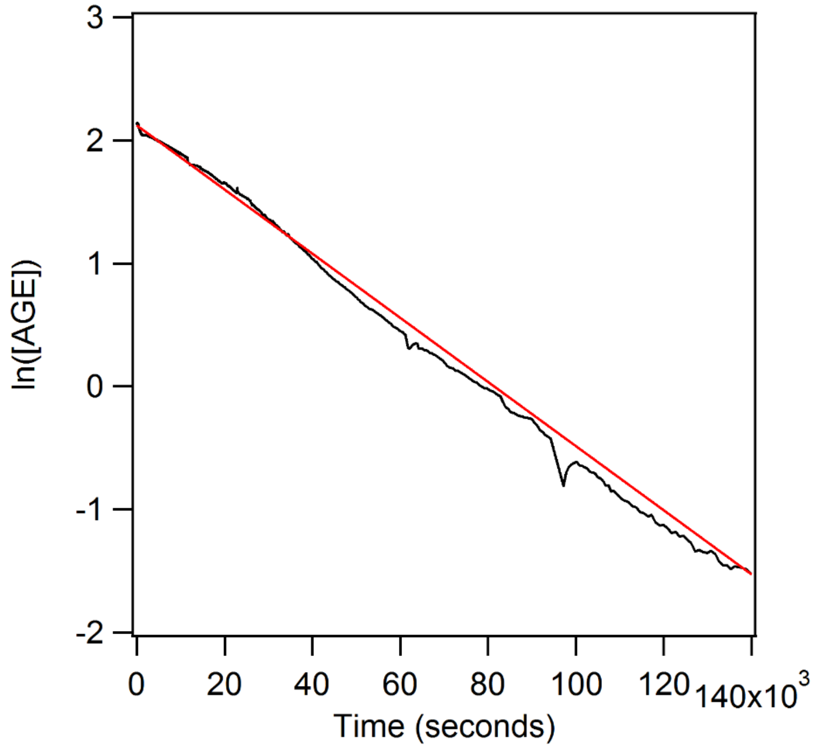

Figure S 7. Plot of ln([AGE]) as a function of time for the polymerization of PAGE with Et-TAxEDA. The data are roughly linear, consistent with first order kinetics. The slope of the fit line (in red) is $-2.67 \times 10^{-5} \pm 2.4 \times 10^{-7}$. The k_p can be calculated by dividing the slope by the initiator concentration ([I]) which in this case is 0.098 M. Therefore, the k_p^{Et} is $0.270 \pm 0.003 \times 10^{-3}$ M^{-1} s^{-1}.

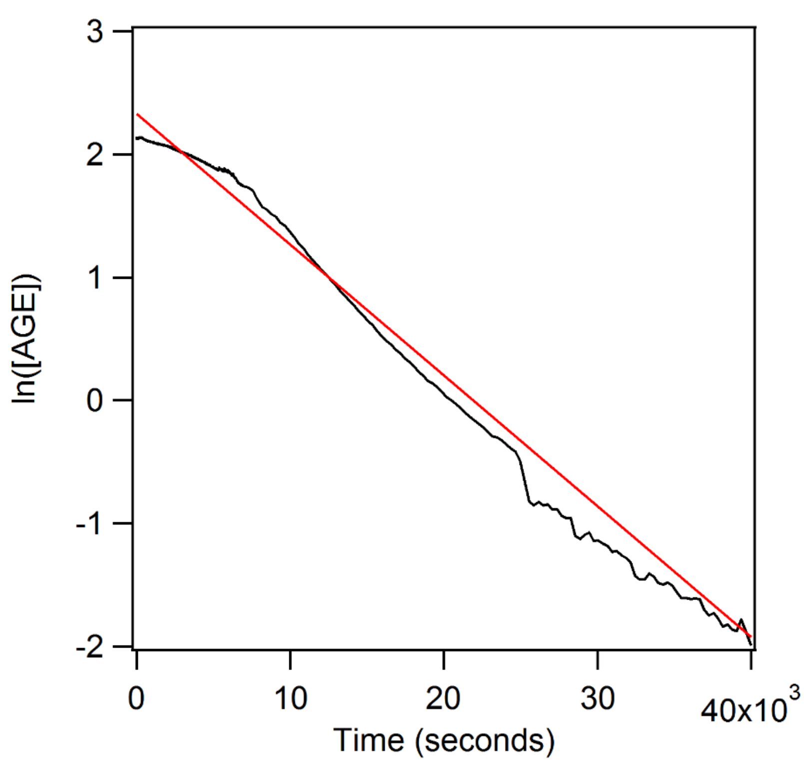

Figure S 8. Plot of ln([AGE]) as a function of time for the polymerization of PAGE with iBu-TAxEDA. The data are roughly linear, consistent with first order kinetics. The slope of the fit line (in red) is $-1.063 \times 10^{-4} \pm 1.7 \times 10^{-6}$. The k_p can be calculated by dividing the slope by the initiator concentration ([I]) which in this case is 0.096 M. Therefore, the k_p^{iBu} is $1.100 \pm 0.022 \times 10^{-3}$ M^{-1} s^{-1}.

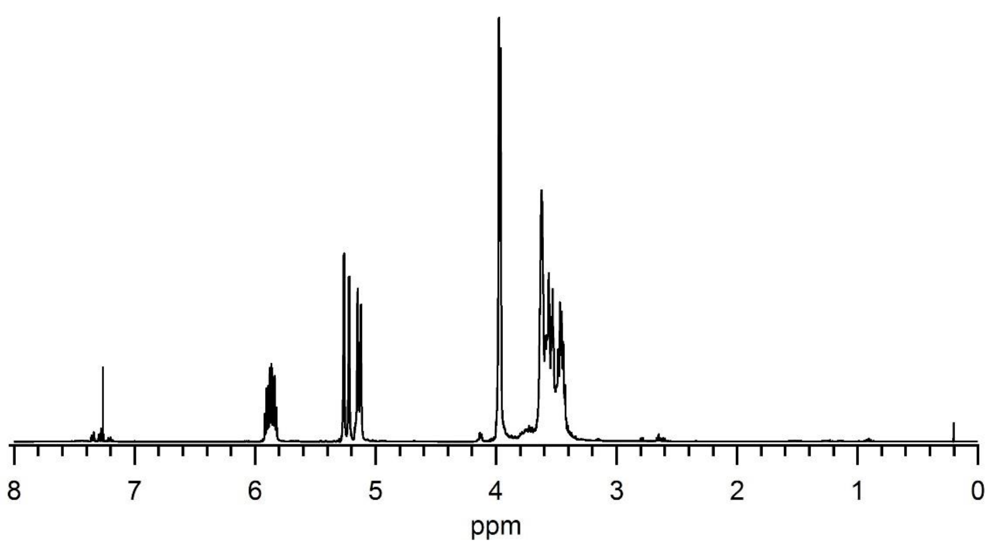

Figure S 9. Me-TAxEDA 10 kg/mol PAGE crude.

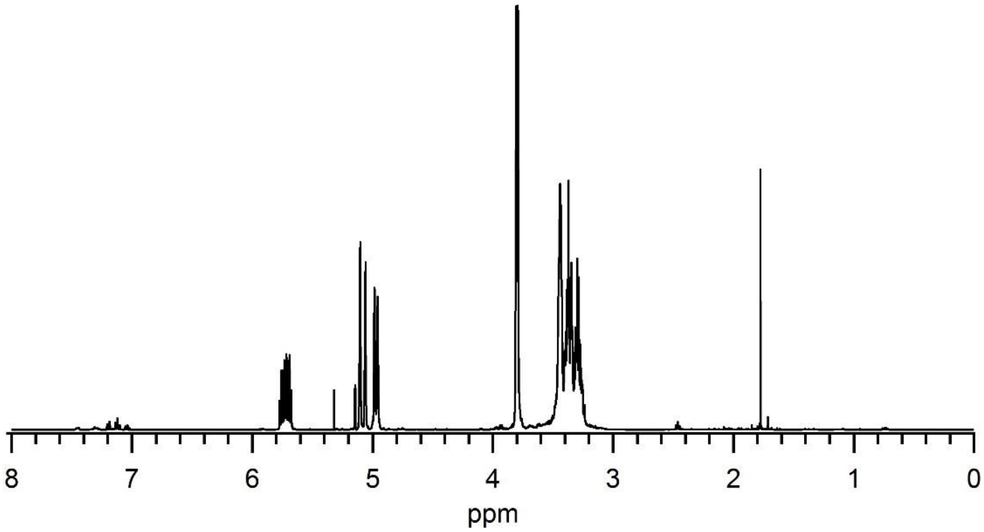

Figure S 10 [1]H NMR spectrum of PAGE synthesized with Me-TAxEDA after purification. [1]H NMR (CD_2Cl_2, 400 MHz) δ 3.38–3.71 (broad m, –O–C<u>H</u>$_2$–C<u>H</u>(C<u>H</u>$_2$–O–CH_2–CH=CH_2)–O–), 3.99 (d, –O–C<u>H</u>$_2$–CH=CH_2), 5.16/5.27 (doublet of doublets, –O–CH_2–CH=C<u>H</u>$_2$), 5.91 (m, –O–CH_2–C<u>H</u>=CH_2), 7.19–7.68 (broad m, –<u>Ph</u>–CH_2–N–).

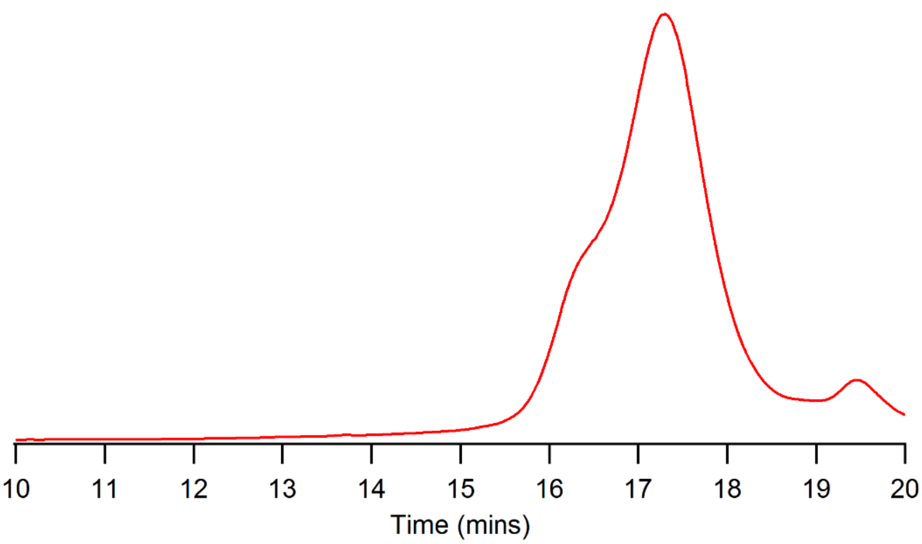

Figure S 11. SEC trace of the differential refractometry signal for PAGE synthesized with Me-TAxEDA

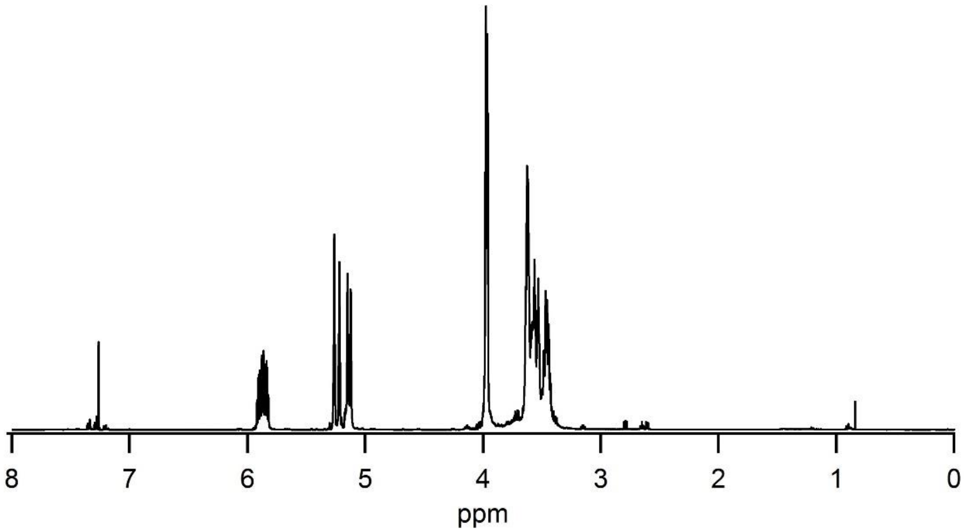

Figure S 12. Crude ^{1}H NMR spectrum of PAGE synthesized with Et-TAxEDA.

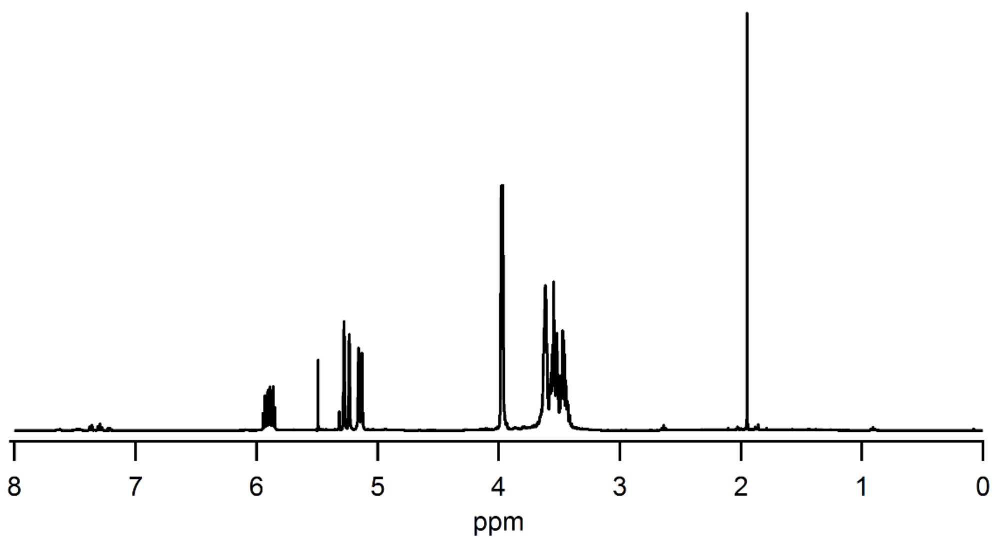

Figure S 13. ^{1}H NMR spectrum of PAGE synthesized with Et-TAxEDA after purification. ^{1}H NMR (CD_2Cl_2, 400 MHz) δ 3.38–3.71 (broad m, –O–C$\underline{H}_2$–C$\underline{H}$(C$\underline{H}_2$–O–CH_2–CH=CH_2)–O–), 3.99 (d, –O–C$\underline{H}_2$–CH=CH_2), 5.16/5.27 (doublet of doublets, –O–CH_2–CH=C$\underline{H}_2$), 5.91 (m, –O–CH_2–C$\underline{H}$=CH_2), 7.19–7.68 (broad m, –$\underline{Ph}$–CH_2–N–).

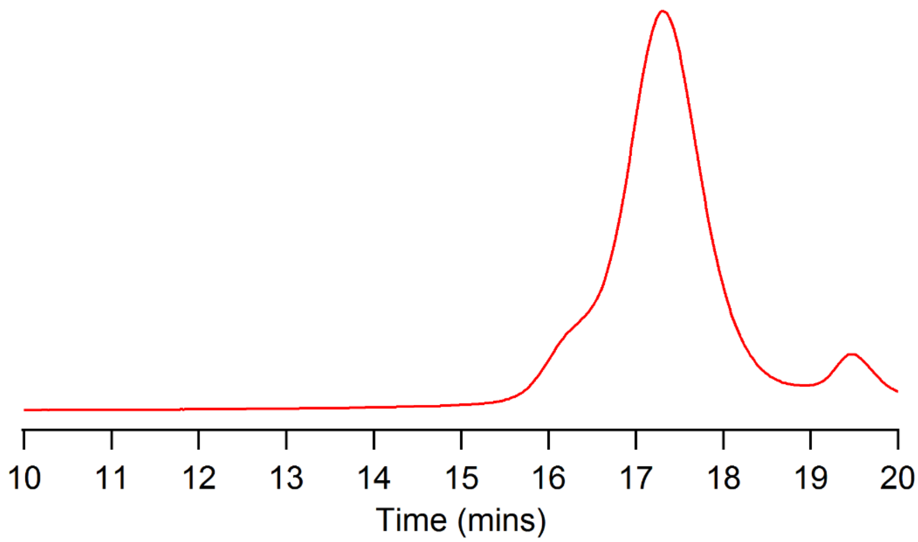

Figure S 14. SEC trace of the differential refractometry signal for PAGE synthesized with Et-TAxEDA

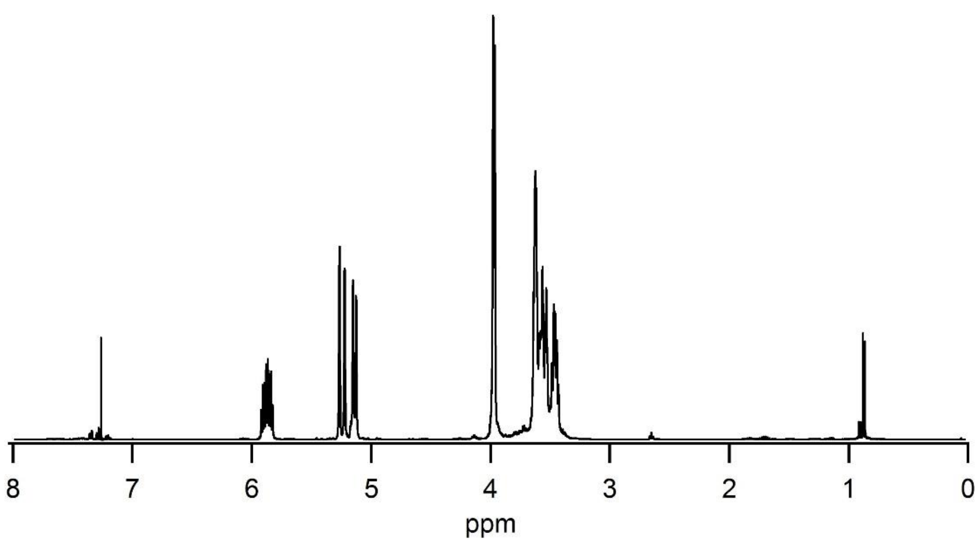

Figure S 15. Crude ^{1}H NMR spectrum of PAGE synthesized with iBu-TAxEDA.

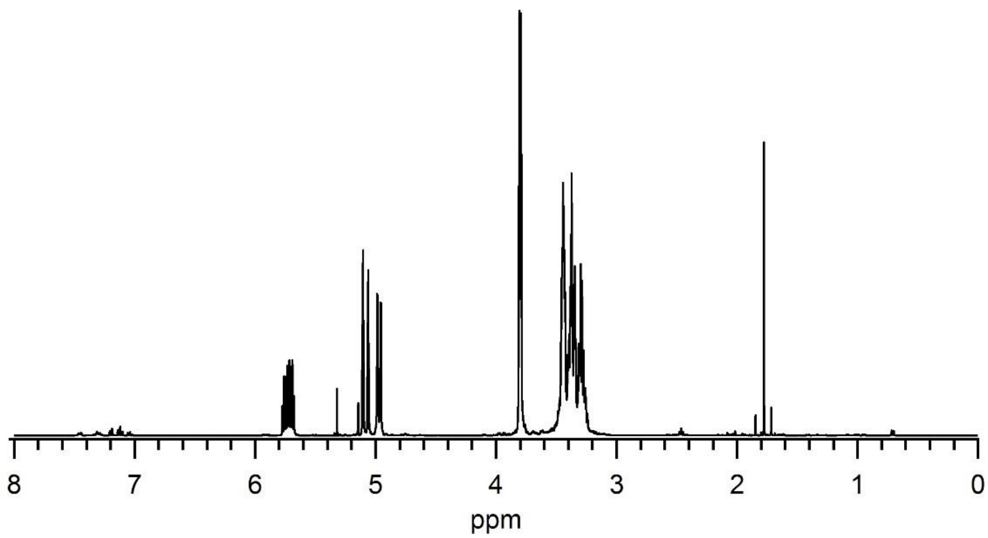

Figure S 16. [1]H NMR spectrum of PAGE synthesized with iBu-TAxEDA after purification. [1]H NMR (CD_2Cl_2, 400 MHz) δ 3.38–3.71 (broad m, –O–C$\underline{H}_2$–C$\underline{H}$(C$\underline{H}_2$–O–CH_2–CH=CH_2)–O–), 3.99 (d, –O–C$\underline{H}_2$–CH=CH_2), 5.16/5.27 (doublet of doublets, –O–CH_2–CH=C$\underline{H}_2$), 5.91 (m, –O–CH_2–C$\underline{H}$=CH_2), 7.19–7.68 (broad m, –$\underline{Ph}$–CH_2–N–).

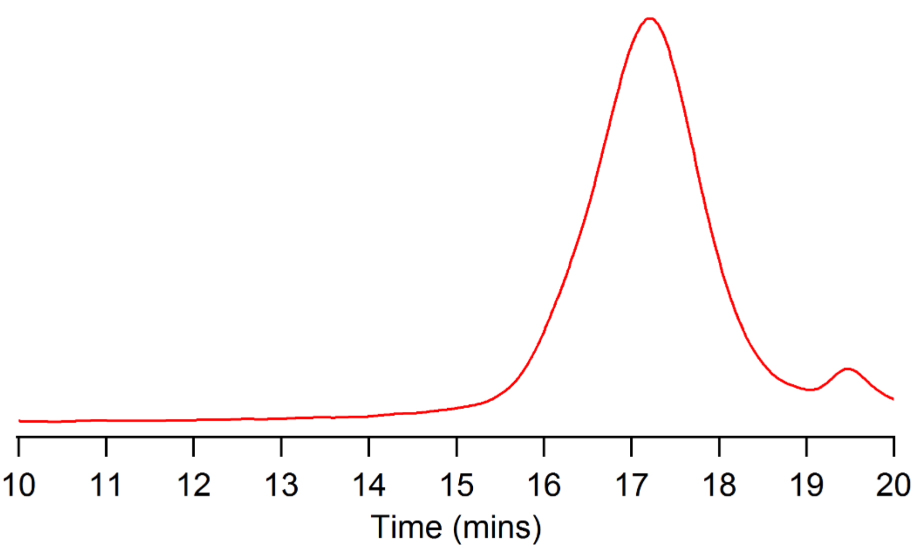

Figure S 17. SEC trace of the differential refractometry signal for PAGE synthesized with iBu-TAxEDA

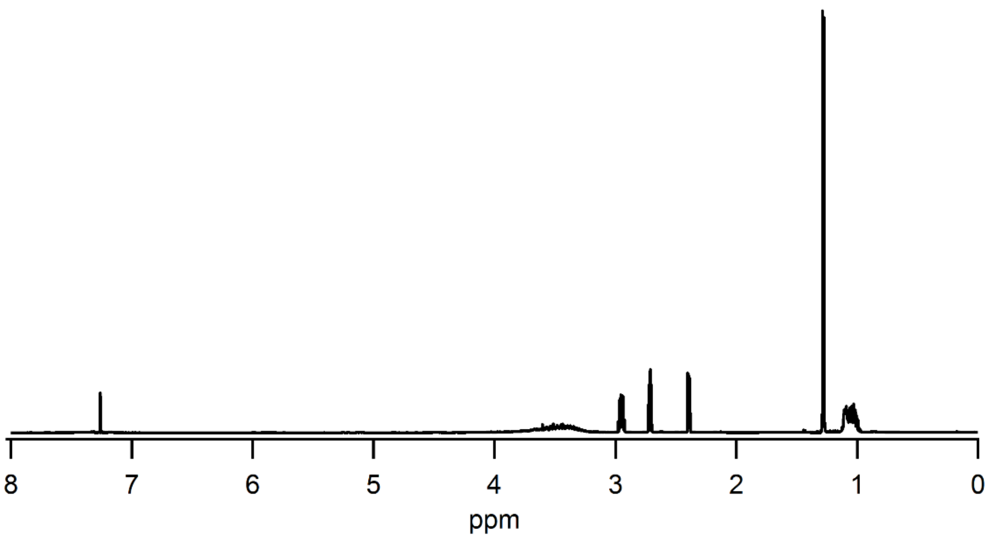

Figure S 18. Crude [1]H NMR spectrum of PPO synthesized with iBu-TAxEDA

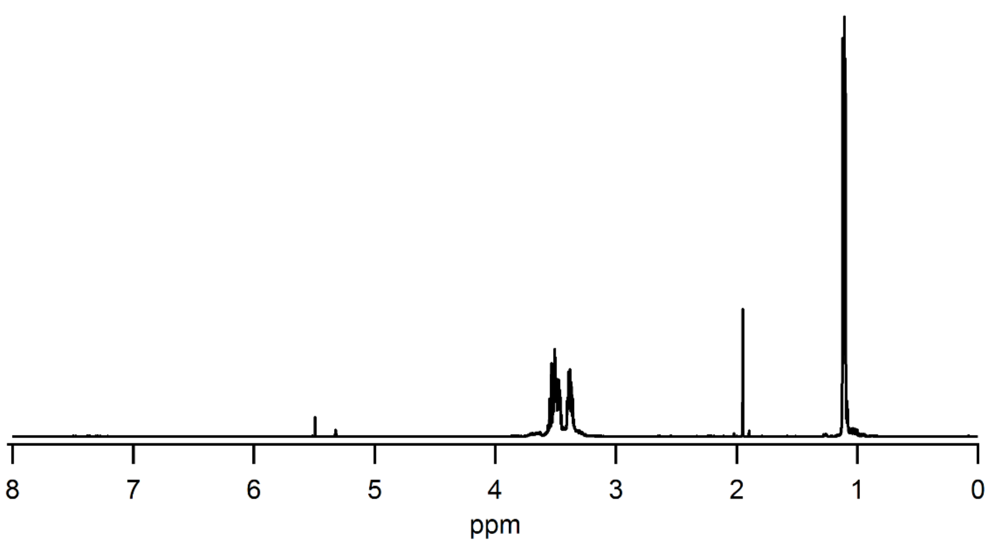

Figure S 19. [1]H NMR spectrum of PPO synthesized with iBu-TAxEDA after purification. [1]H NMR (CD_2Cl_2, 400 MHz) δ 1.12 (m, –C<u>H</u>$_3$), 3.32-3.60 (broad m, –O–C<u>H</u>$_2$–C<u>H</u>(CH_3)–O–), 7.17–7.65 (broad m, –<u>Ph</u>–CH_2–N–).

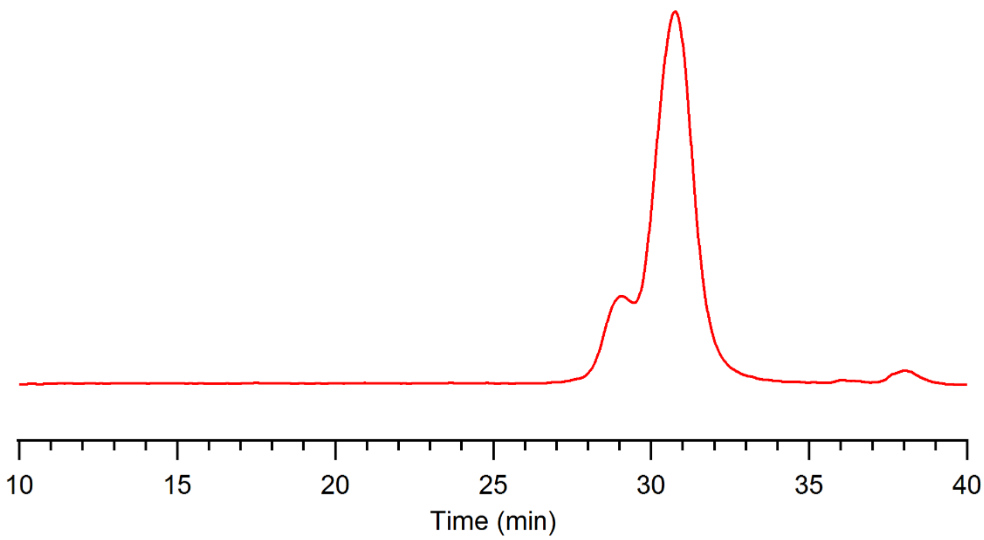

Figure S 20. SEC trace of the differential refractometry signal for PPO synthesized with iBu-TAxEDA.

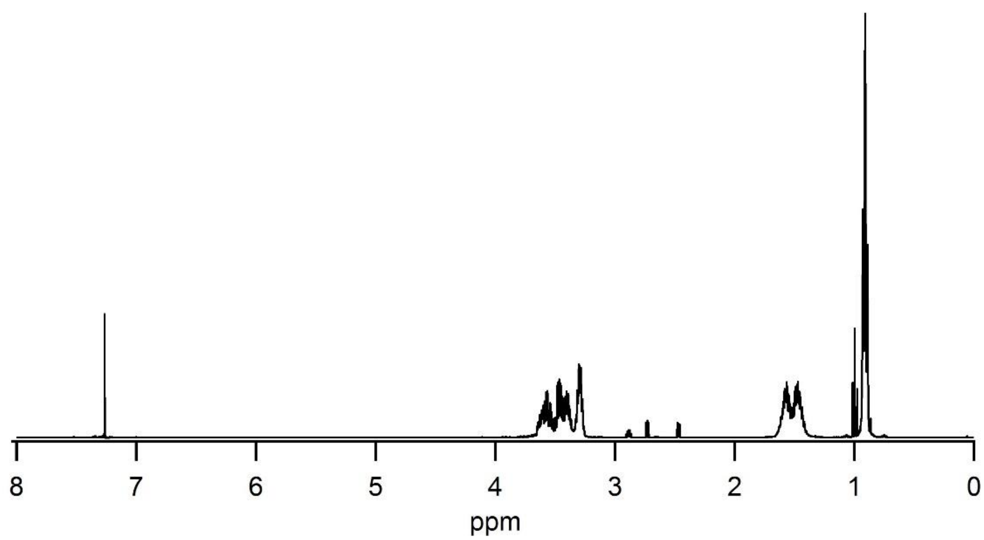

Figure S 21. Crude ^{1}H NMR spectrum of PBO synthesized with iBu-TAxEDA.

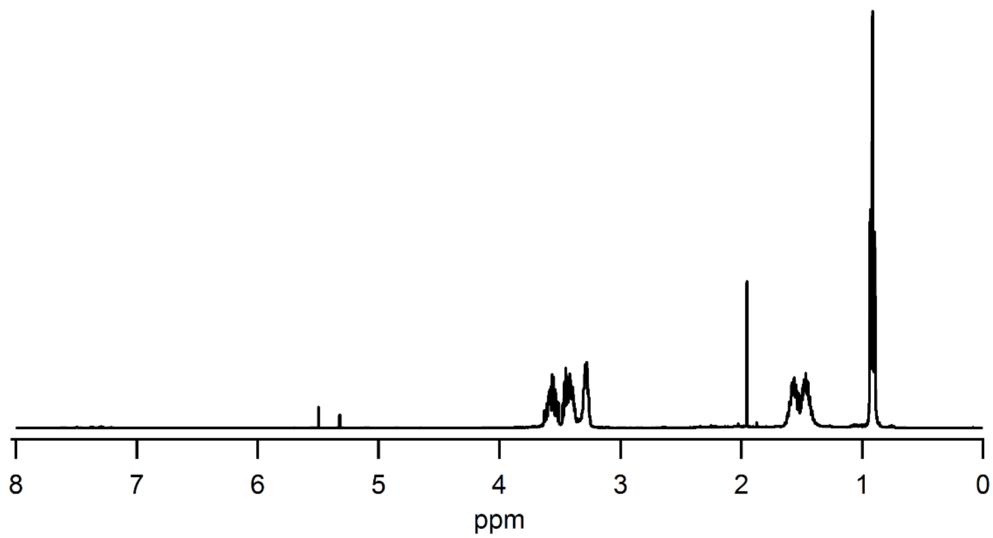

Figure S 22. [1]H NMR spectrum of PBO synthesized with iBu-TAxEDA after purification. [1]H NMR (CD_2Cl_2, 400 MHz) δ 0.92 (t, –CH_2–C<u>H</u>$_3$), 1.50 (m, –C<u>H</u>$_2$–CH_3), 3.26-3.68 (broad m, –O–C<u>H</u>$_2$–C<u>H</u>(C<u>H</u>$_2$–CH_3)–O–), 7.20–7.65 (broad m, –<u>Ph</u>–CH_2–N–).

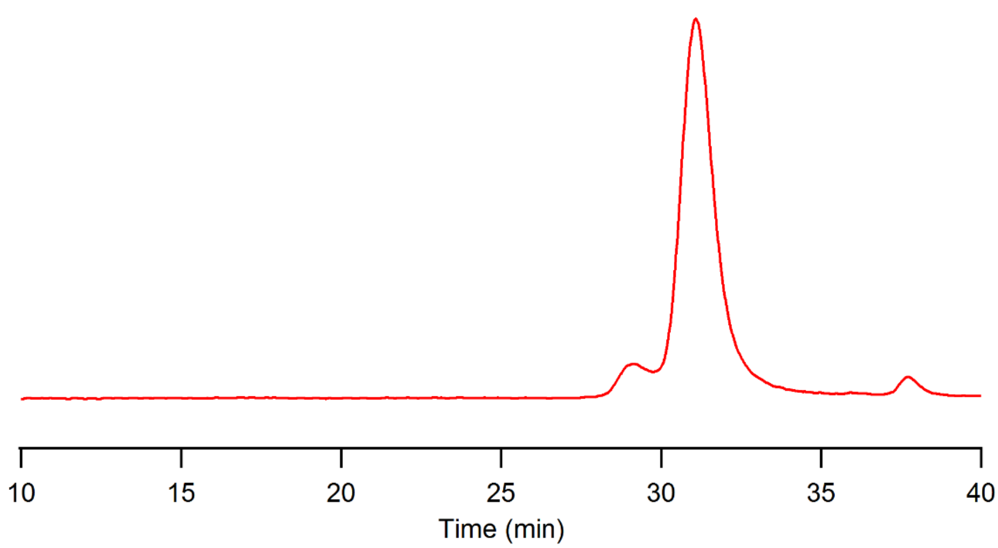

Figure S 23. SEC trace of the differential refractometry signal for PBO synthesized with iBu-TAxEDA.

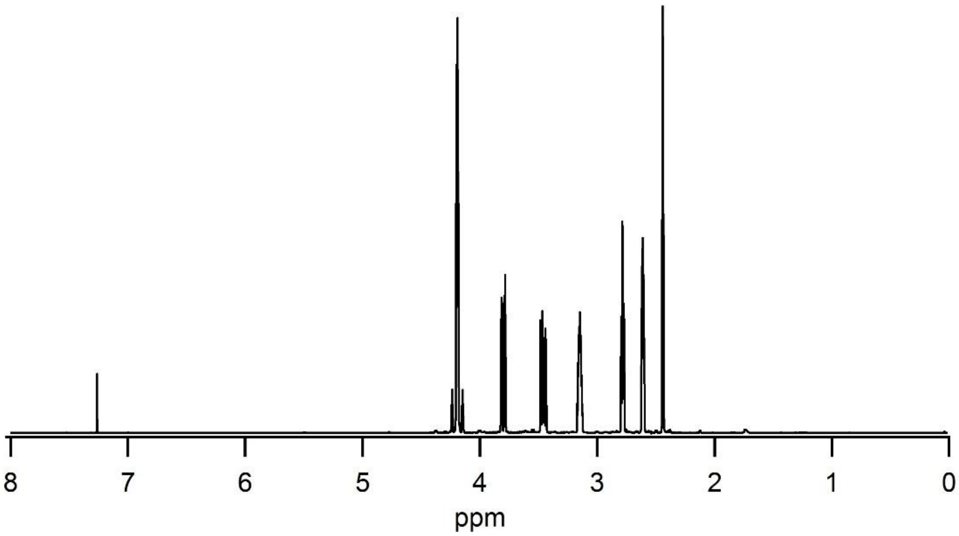

Figure S 24. ^{1}H NMR spectrum of PGE monomer. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 4.19 (m, $HC{\equiv}CCH_2O$–), 3.80 (m, –OCH_2CH–), 3.46 (m, –OCH_2CH–), 3.15 (m, $HC{\equiv}CCH_2$–), 2.78 (m, epoxide CH_2–O–CH–), 2.61 (m, epoxide CH_2–O–CH–), 2.44 (m, epoxide CH_2–O–CH–).

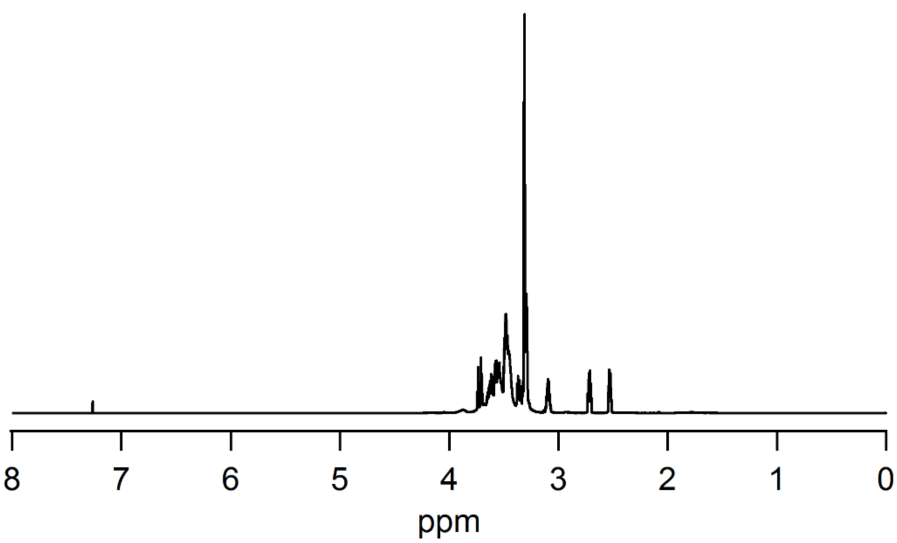

Figure S 25. ^{1}H NMR spectrum of EGMGE monomer. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.78 (dd, $H_3COCH_2CH_2OC\underline{H_2}$–), 3.72-3.60 (m, $H_3COC\underline{H_2}CH_2OCH_2$–), 3.55 (m, $H_3COCH_2C\underline{H_2}OCH_2$–), 3.42 (dd, $H_3COCH_2CH_2OC\underline{H_2}$–), 3.38 (s, $\underline{H_3}COCH_2CH_2OCH_2$–), 3.16 (m, epoxide CH_2–O–C$\underline{H}$–), 2.78 (m, epoxide C$\underline{H_2}$–O–CH–), 2.60 (m, epoxide C$\underline{H_2}$–O–CH–).

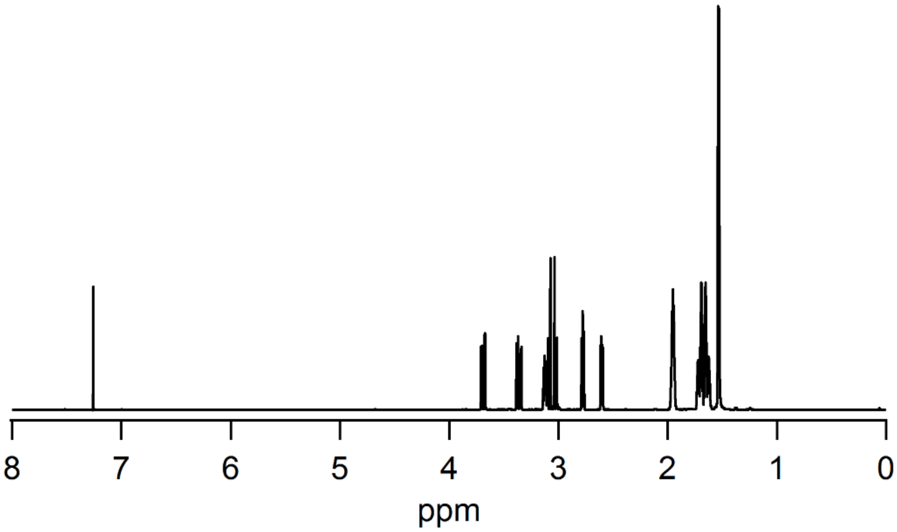

Figure S 26. ^{1}H NMR spectrum of AMGE monomer. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.53 (d, adamantyl –C–C$\underline{H}_2$–CH–), 1.59–1.75 (m, adamantyl –CH–C$\underline{H}_2$–CH–), 1.92–1.98 (m, adamantyl –CH–), 2.60 (dd, epoxide C$\underline{H}_2$–O–CH–), 2.78 (dd, epoxide C$\underline{H}_2$–O–CH–), 3.03 (d, –O–C$\underline{H}_2$–C–), 3.09 (d, –O–C$\underline{H}_2$–C–), 3.10–3.15 (m, epoxide CH_2–O–C$\underline{H}$–), 3.37 (dd, –O–C$\underline{H}_2$–CH–), 3.69 (dd, –O–C$\underline{H}_2$–CH–).

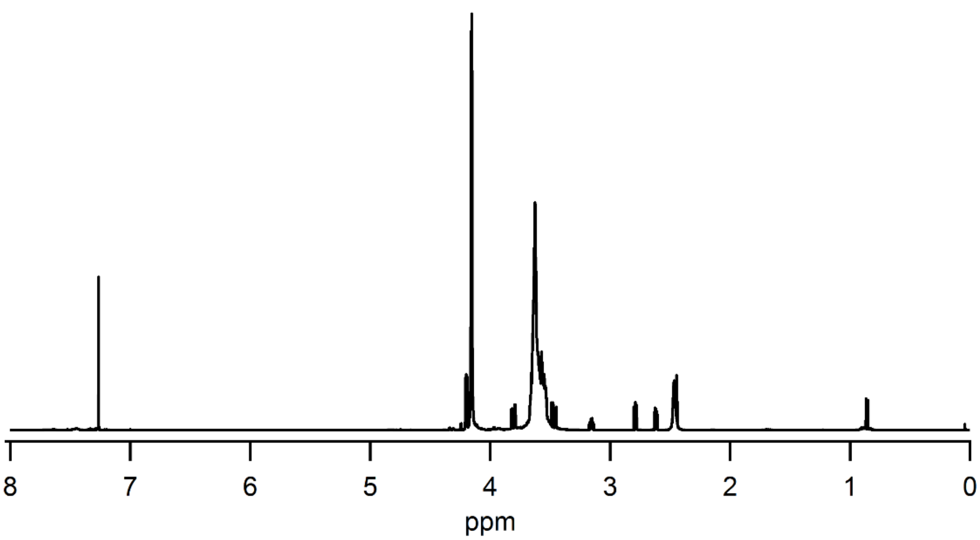

Figure S 27. Crude ^{1}H NMR spectrum of PPGE synthesized with iBu-TAxEDA.

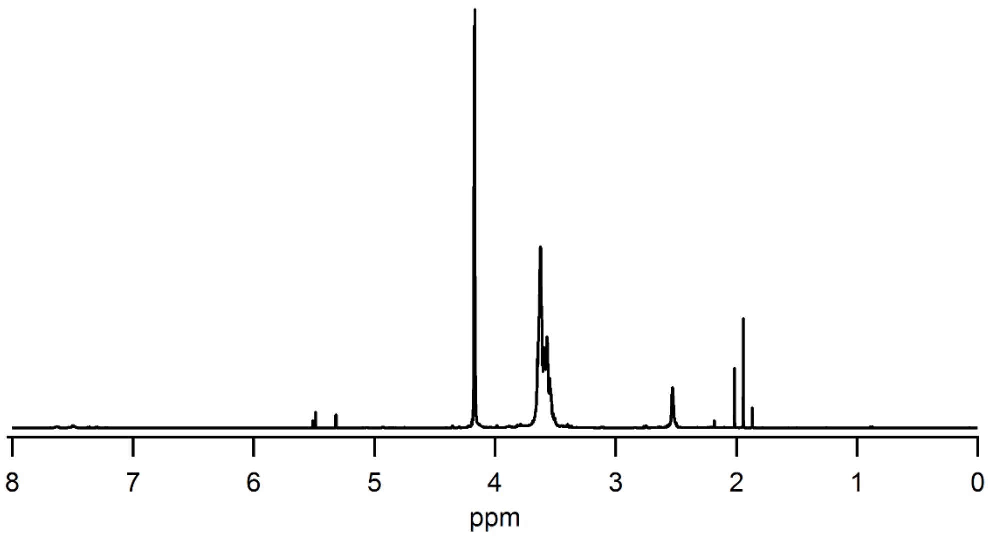

Figure S 28.^{1}H NMR spectrum of PPGE synthesized with iBu-TAxEDA after purification. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.48 (s, –O–CH_2–C≡C$\underline{H}$), 3.54–3.70 (broad m, –O–C$\underline{H}_2$–C$\underline{H}$(C$\underline{H}_2$–O–CH_2–C≡CH)–O–), 4.17 (s, –O–C$\underline{H}_2$–C≡CH), 7.20–7.75 (broad m, –$\underline{Ph}$–CH_2–N–).

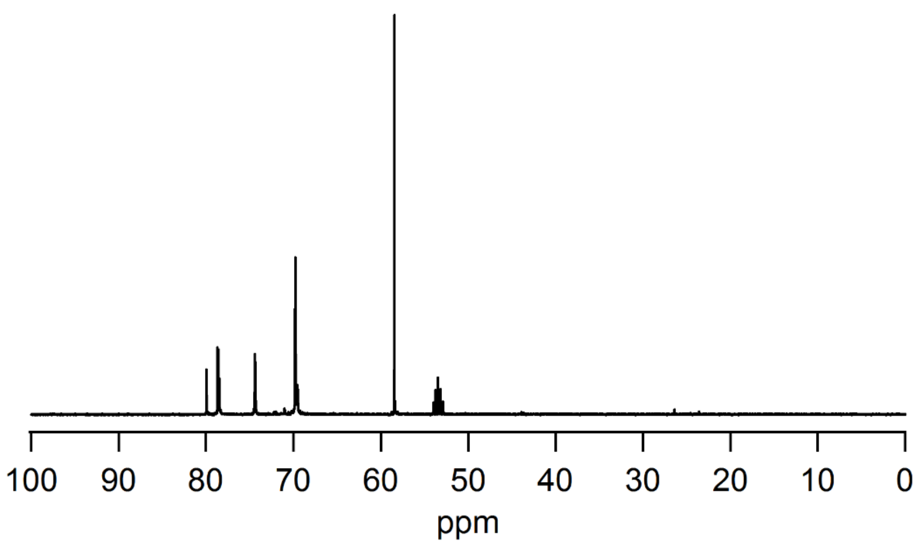

Figure S 29. ^{13}C NMR spectrum of PPGE synthesized with iBu-TAxEDA. ^{13}C NMR (CD_2Cl_2, 400 MHz) δ 58.49 (–O–$\underline{C}H_2$–C≡CH), 69.26–70.35 (–O–$\underline{C}H_2$–CH($\underline{C}H_2$–O–CH_2–C≡CH)–O–, rrm, mrr, or m), 74.39 (–O–CH_2–C≡$\underline{C}$H), 78.56 (–O–CH_2–$\underline{C}$H(CH_2–O–CH_2–C≡CH)–O–), 79.95 (–O–CH_2–$\underline{C}$≡CH), 128.2/133.9 (–$\underline{Ph}$–CH_2–N–).

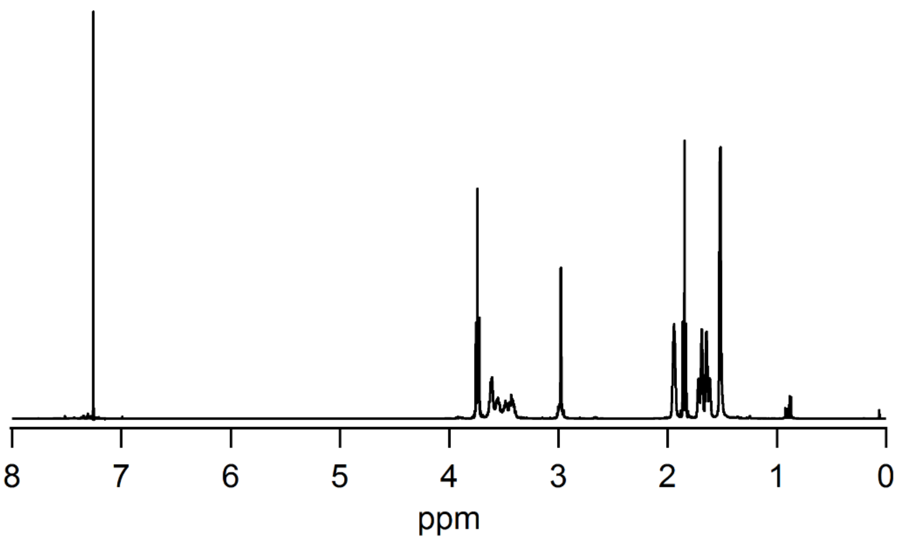

Figure S 30. Crude [1]H NMR spectrum of PAMGE synthesized with iBu-TAxEDA.

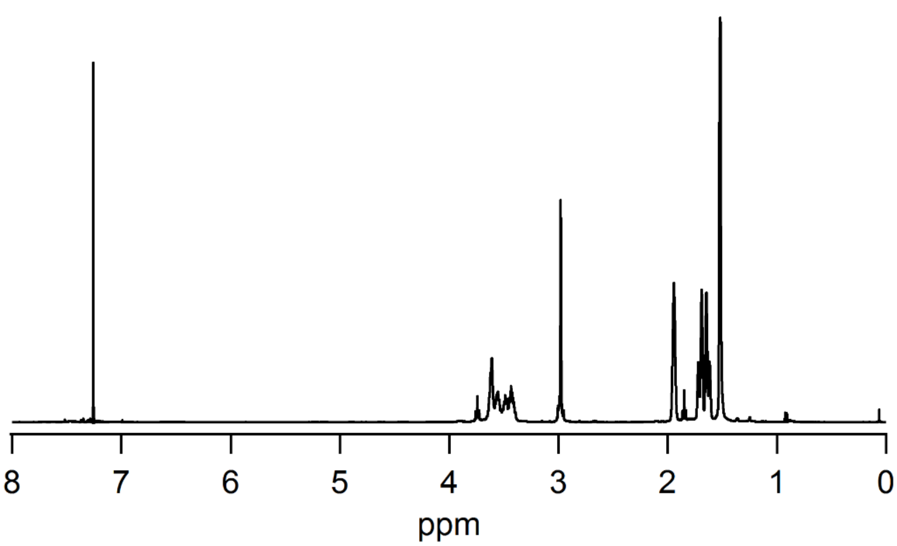

Figure S 31. [1]H NMR spectrum of PAMGE synthesized with iBu-TAxEDA. [1]H NMR ($CDCl_3$, 400 MHz) δ 1.48–1.55 (d, adamantyl –C–C<u>H</u>$_2$–CH–), 1.59–1.75 (m, adamantyl –CH–C<u>H</u>$_2$–CH–), 1.91–1.98 (m, adamantyl –CH–), 2.95–3.01 (m, –O–C<u>H</u>$_2$–C–) 3.37–3.68 (broad m, –O–C<u>H</u>$_2$–C<u>H</u>(C<u>H</u>$_2$)–O–), 7.17–7.74 (broad m, –<u>Ph</u>–CH_2–N–).

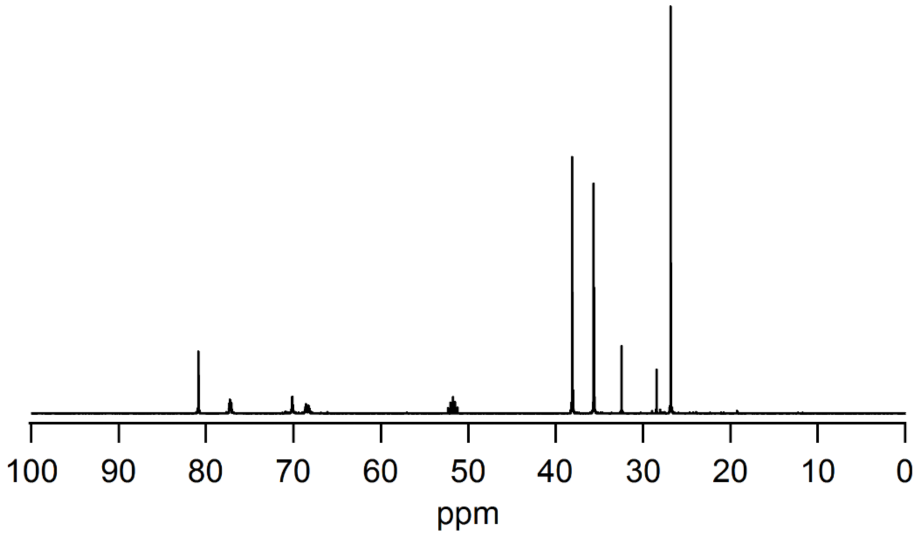

Figure S 32. ^{13}C NMR spectrum of PAMGE synthesized with iBu-TAxEDA. ^{13}C NMR (CD_2Cl_2, 400 MHz) δ 29.1 (adamantyl –CH–), 34.7 (–O–CH$_2$–$\underline{C}$–), 37.9 (adamantyl –CH–$\underline{C}$H$_2$–CH–), 40.3 (adamantyl –C–$\underline{C}$H$_2$–CH–), 70.5 (–O–$\underline{CH_2}$–CH(C$\underline{H_2}$)–O–, rrm or mrr), 70.8 (–O–$\underline{CH_2}$–CH($\underline{CH_2}$)–O–, m), 79.5 (–O–C$\underline{H_2}$–$\underline{C}$H(C$\underline{H_2}$)–O–), 83.1 (–O–$\underline{C}$H$_2$–C–), 128.9/136.4 (broad m, –$\underline{Ph}$–CH$_2$–N–).

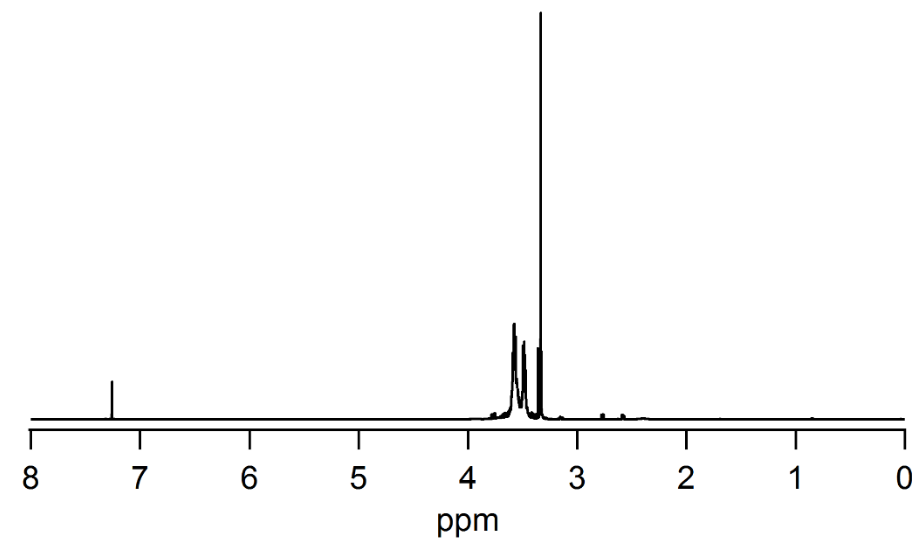

Figure S 33. Crude ^{1}H NMR spectrum of PEGMGE synthesized with iBu-TAxEDA

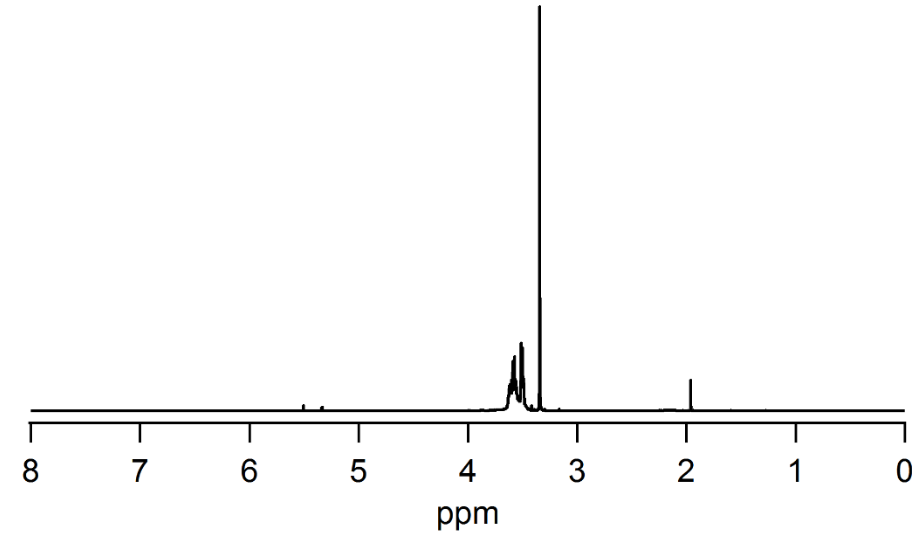

Figure S 34. ^{1}H NMR spectrum of PEGMGE synthesized with iBu-TAxEDA. ^{1}H NMR (CD_2Cl_2, 400 MHz) δ 3.34 (CH_2–O–CH_2–CH_2–O–C<u>H</u>$_3$) 3.46–3.65 (broad m, –O–C<u>H</u>$_2$–C<u>H</u>(C<u>H</u>$_2$–O–C<u>H</u>$_2$–C<u>H</u>$_2$–O–CH_3)–O–), 7.19–7.67 (broad m, –<u>Ph</u>–CH_2–N–).

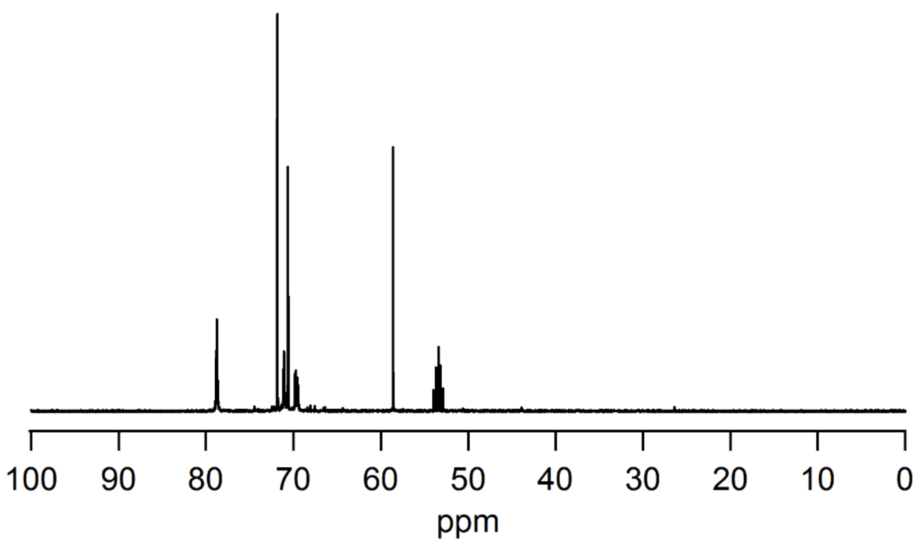

Figure S 35. ^{13}C NMR spectrum of PEGMGE synthesized with iBu-TAxEDA. ^{13}C NMR (CD_2Cl_2, 400 MHz) δ 58.6 (CH_2–O–CH_2–CH_2–O–<u>C</u>H_3), 69.5 (–<u>C</u>H_2–O–CH_2–CH_2–O–CH_3), 69.8 (–<u>C</u>H_2–O–CH_2–CH_2–O–CH_3), 70.6 (–O–<u>C</u>H_2–CH(CH_2–O–CH_2–CH_2–O–CH_3)–O–), 71.1 (–O–<u>C</u>H_2–CH_2–O–CH_3) 71.9 (–O–CH_2–<u>C</u>H_2–O–CH_3), 78.6–78.9 (–O–CH_2–<u>C</u>H(CH_2–O–CH_2–CH_2–O–CH_3)–O–), 128.1/128.7 (–<u>Ph</u>–CH_2–N–).

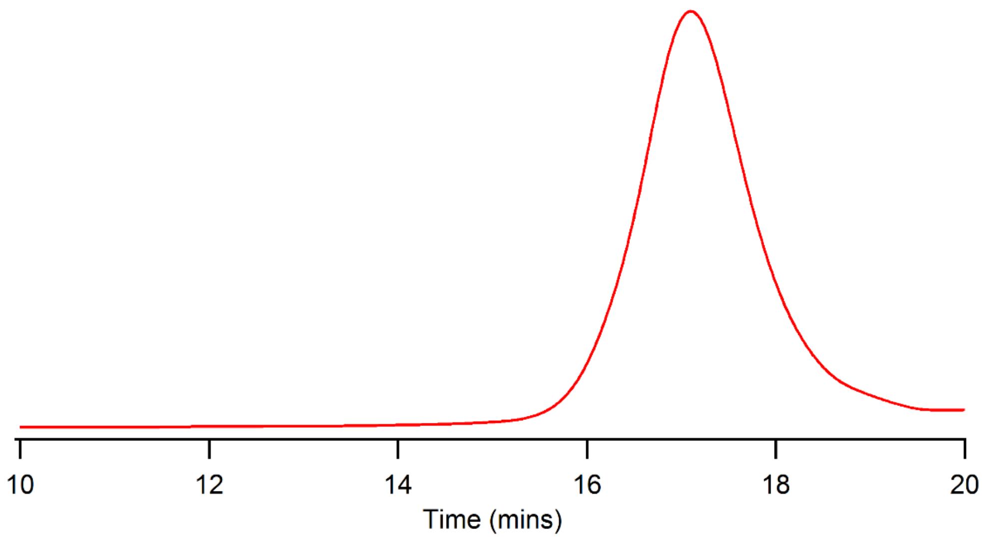

Figure S 36. SEC trace of the differential refractometry signal for PPGE synthesized with iBu-TAxEDA

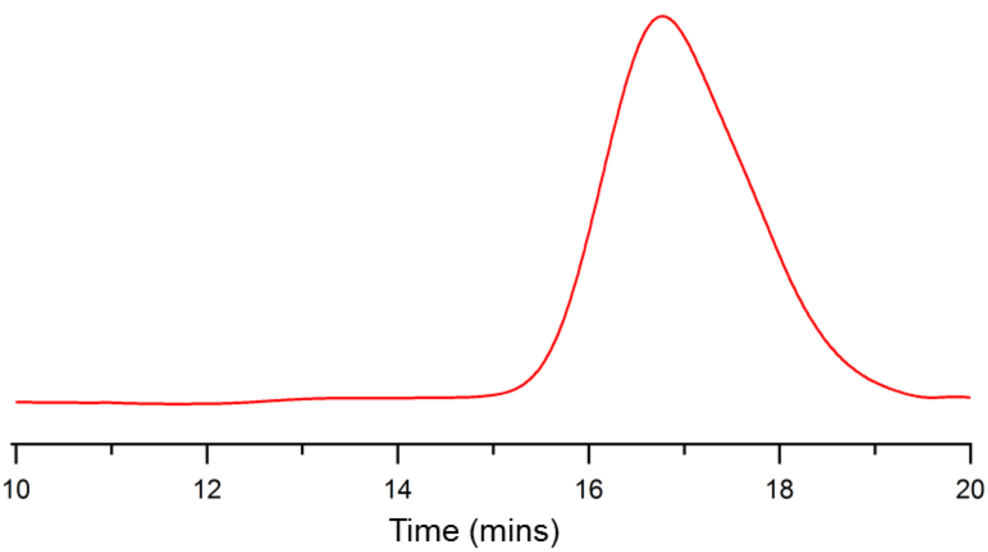

Figure S 37. SEC trace of the differential refractometry signal for PAMGE synthesized wtih iBu-TAxEDA

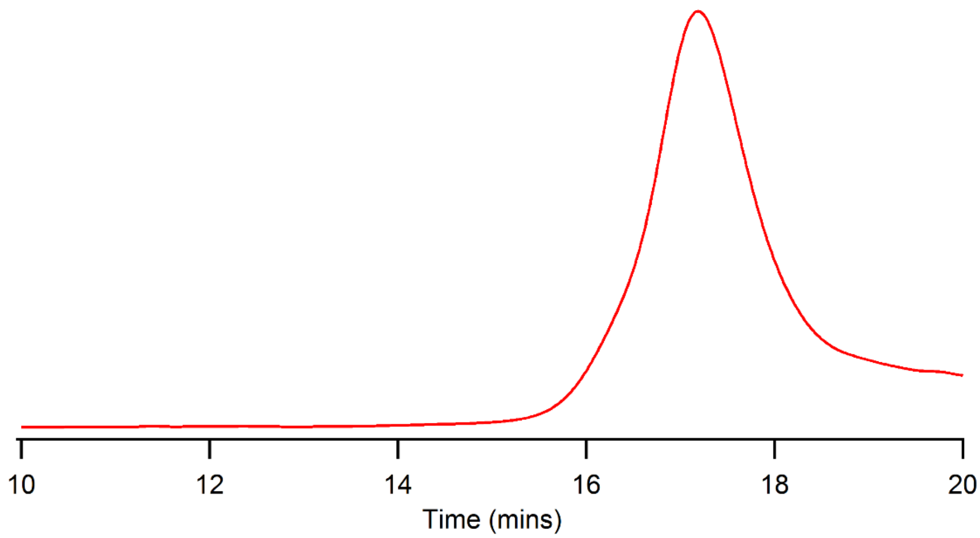

Figure S 38. SEC trace of the differential refractometry signal for PEGMGE synthesized with iBu-TAxEDA

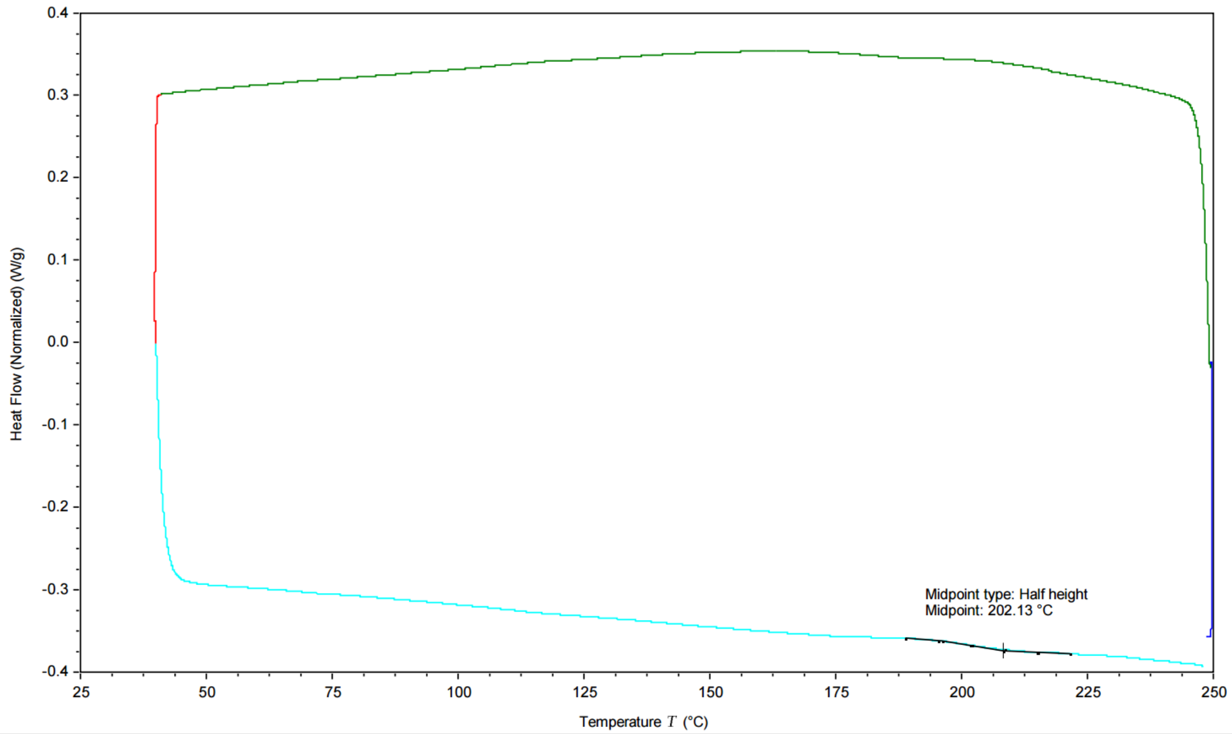

Figure S 39. DSC trace for PAMGE. The T_g was found to be 202 °C.