ELECTRONIC SUPPORTING INFORMATION

For

Synthesis, Structural Characterization and Catalytic Evaluation of the Ring-Opening Polymerization of Discrete Five-Coordinate Alkyl Aluminium Complexes

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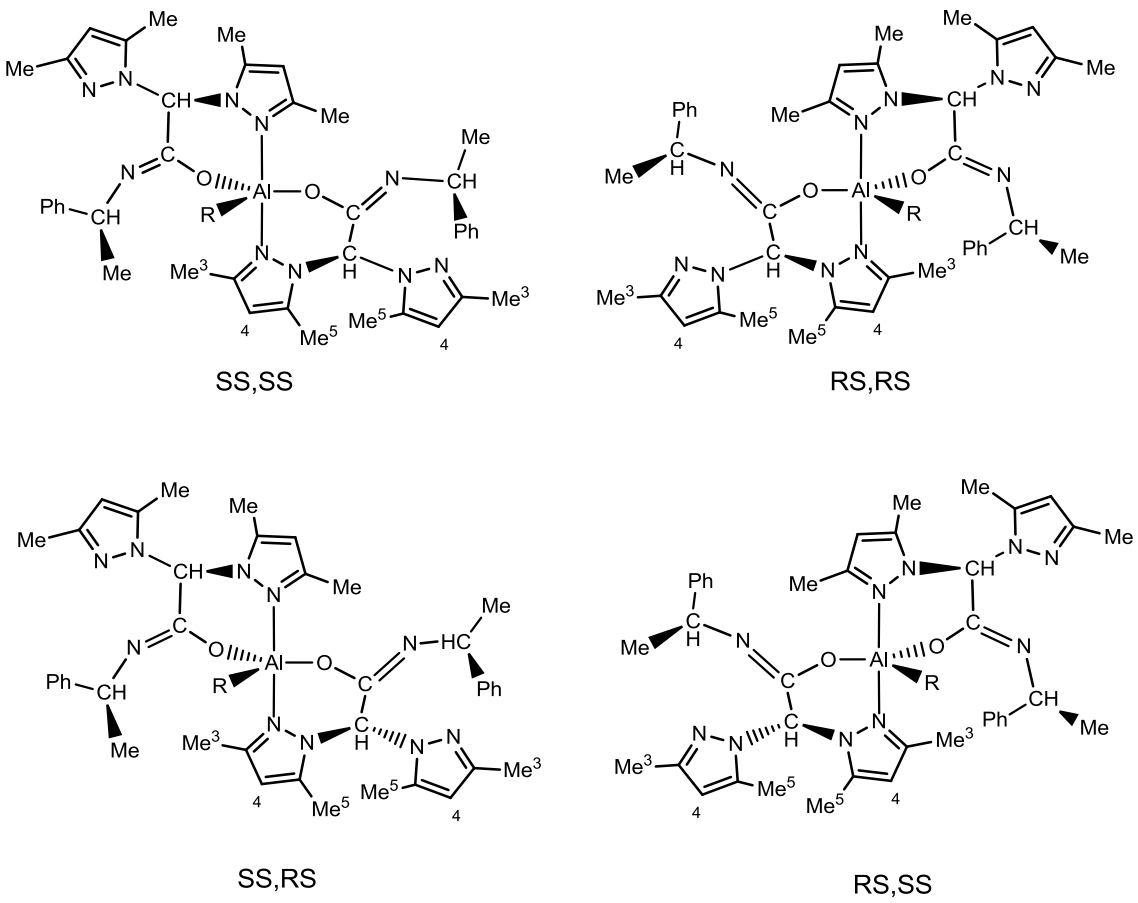

Figure S1. Proposed structures for the possible stereoisomers of complexes **5** and **6**

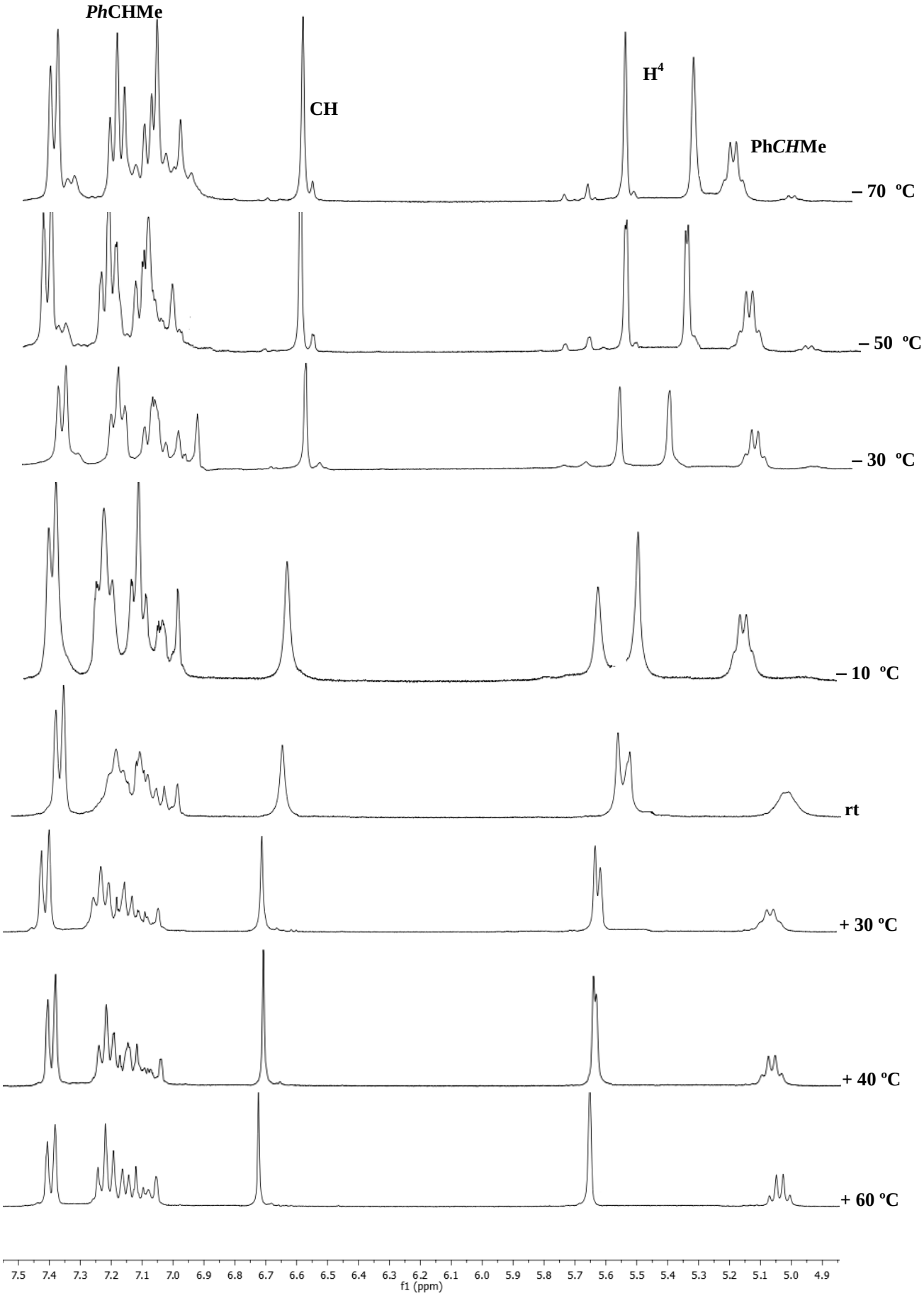

Figure S2. Variable-temperature ^{1}H NMR spectra in the region from 4.9 ppm to 7.6 ppm of complex **5**

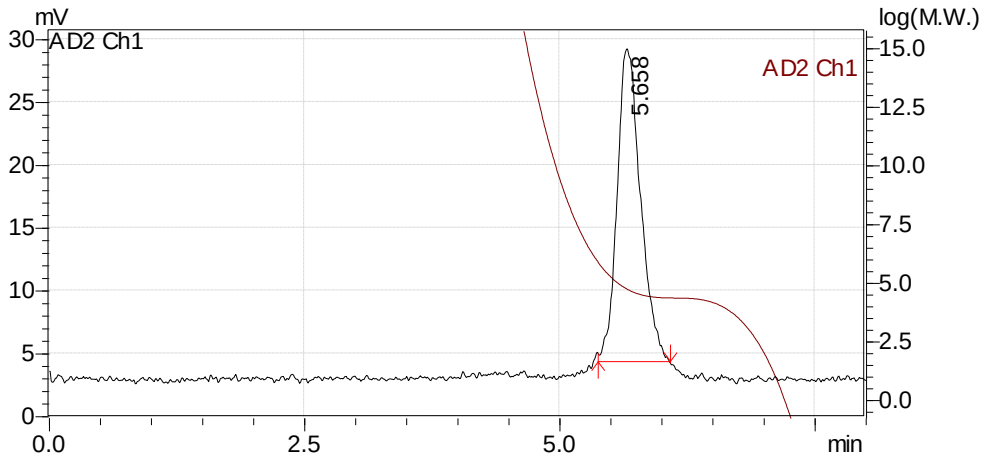

Figure S3 – GPC profile of PLA with M_n = 27220 Da and M_w/M_n = 1.18 (entry 1 in Table 1).

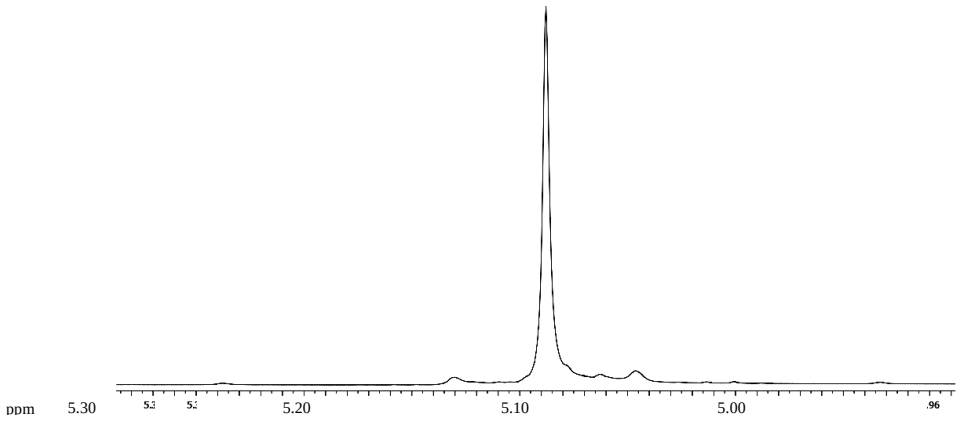

Figure S4. ^{1}H-NMR spectrum (500 MHz, 298 K, $CDCl_3$,) of the homodecoupled CH resonance of poly(L-lactide) prepared with complex **5** as initiator

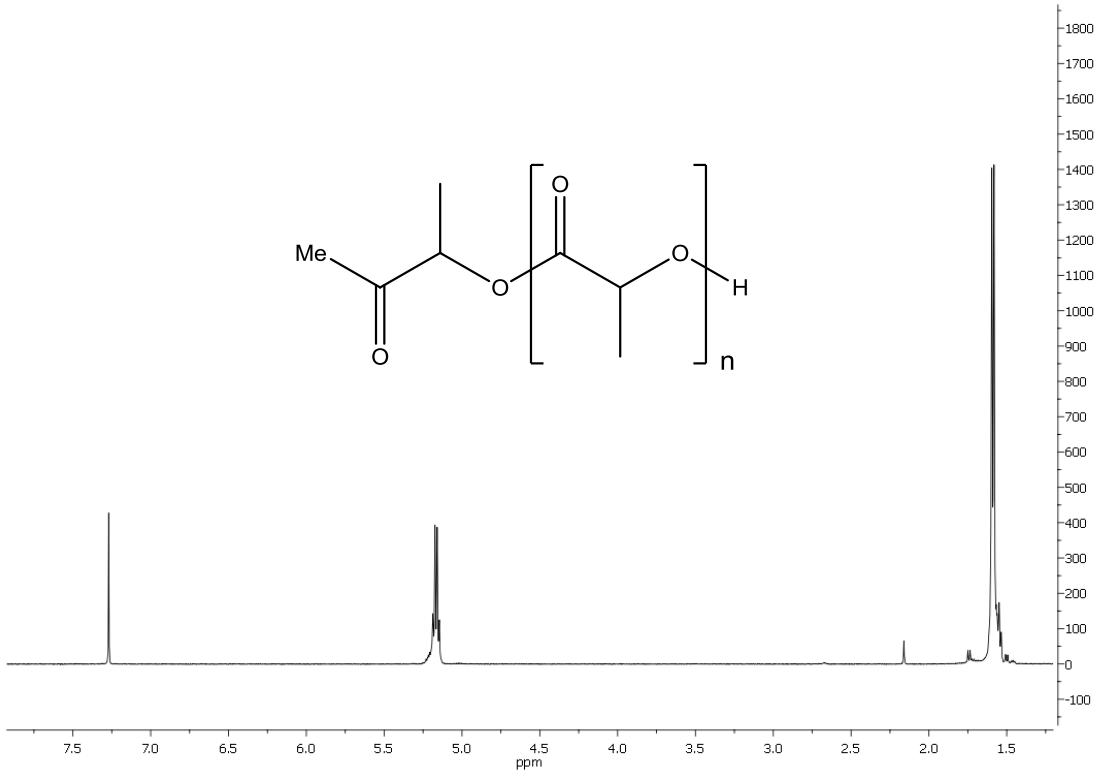

Figure S5. Representative ^{1}H NMR spectrum of low molecular weight PLA obtained by **5** (M_w = 1848 Da $[M+Na]^+$); LA/**5** = 15/1)

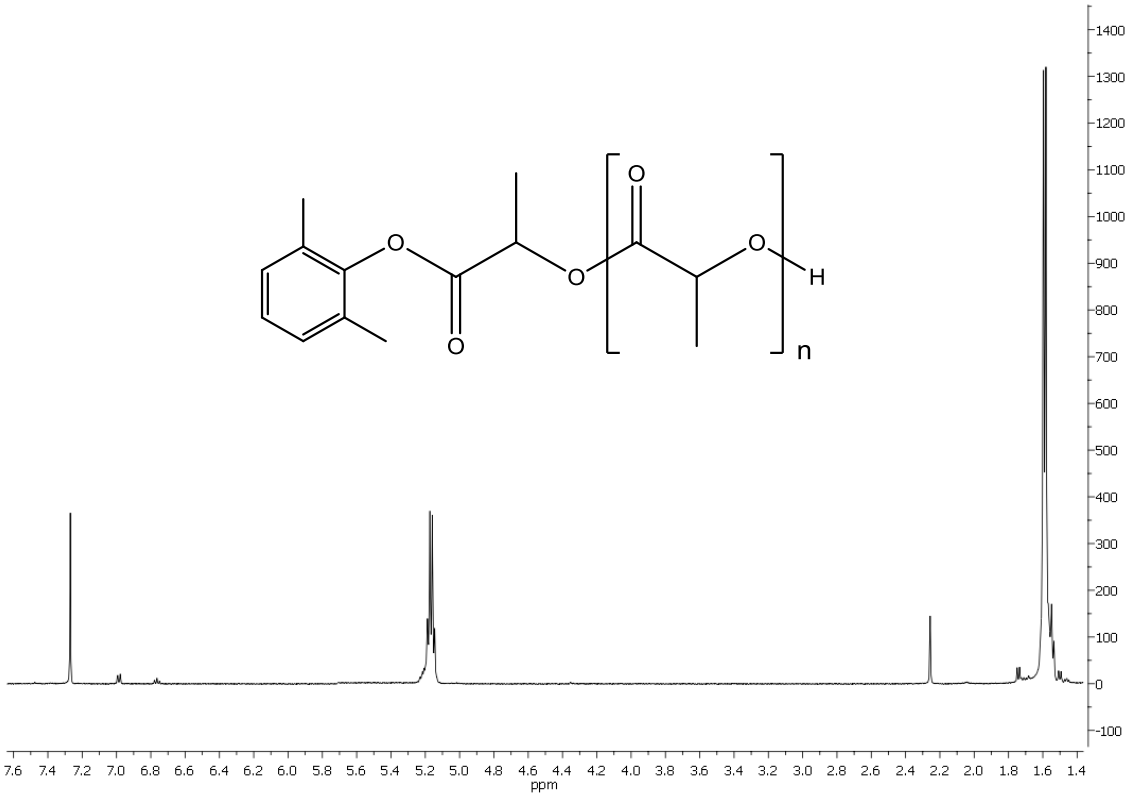

Figure S6. Representative ^{1}H NMR spectrum of low molecular weight PLA obtained by **5/co-initiator** (M_w = 1801.54 $[M+Na]^+$) Da; LA/**5** = 15/1)

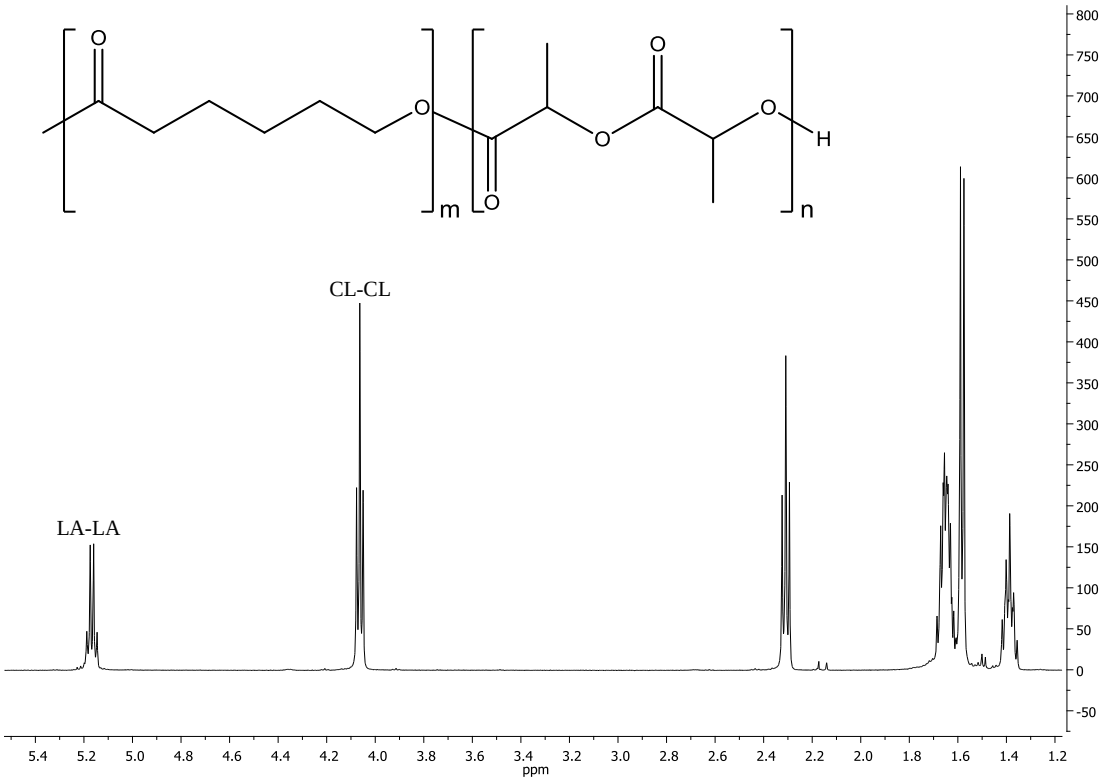

Figure S7. ^{1}H-NMR spectrum (500 MHz, 298 K, $CDCl_3$,) of block copolymer PCL-PLA 100:100 prepared with complex **5** as initiator

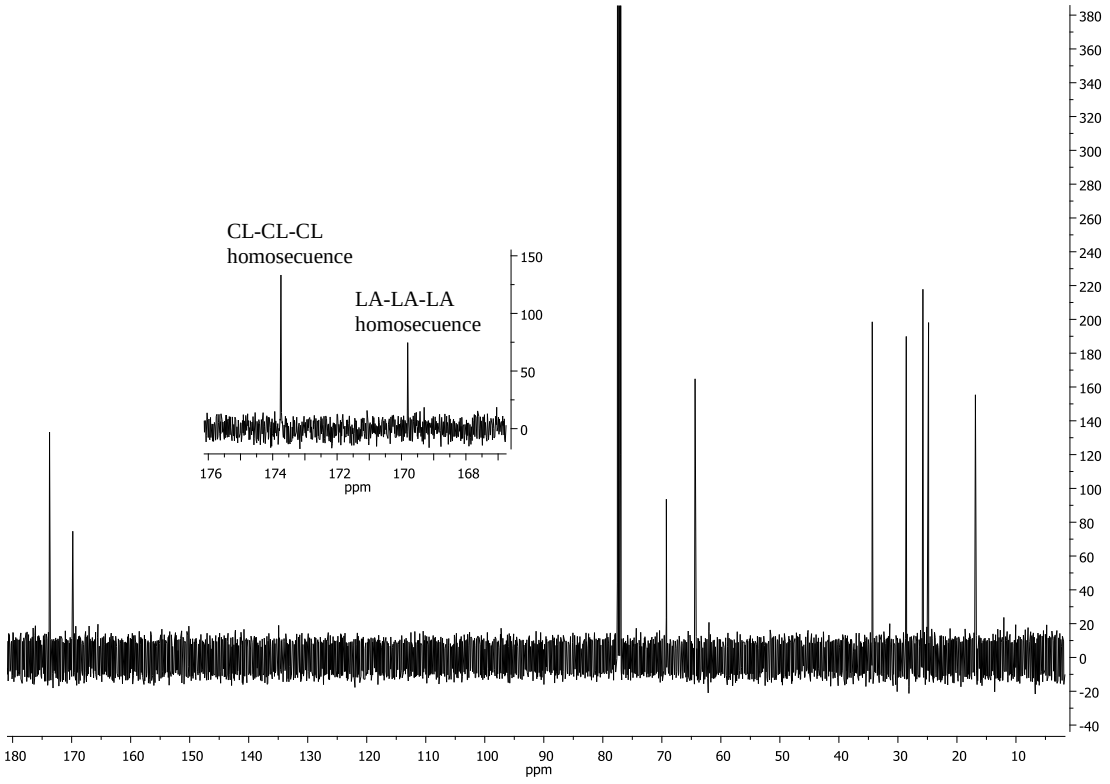

Figure S8. ^{13}C-NMR spectrum (500 MHz, 298 K, $CDCl_3$,) of block copolymer PCL-PLA 100:100 prepared with complex **5** as initiator

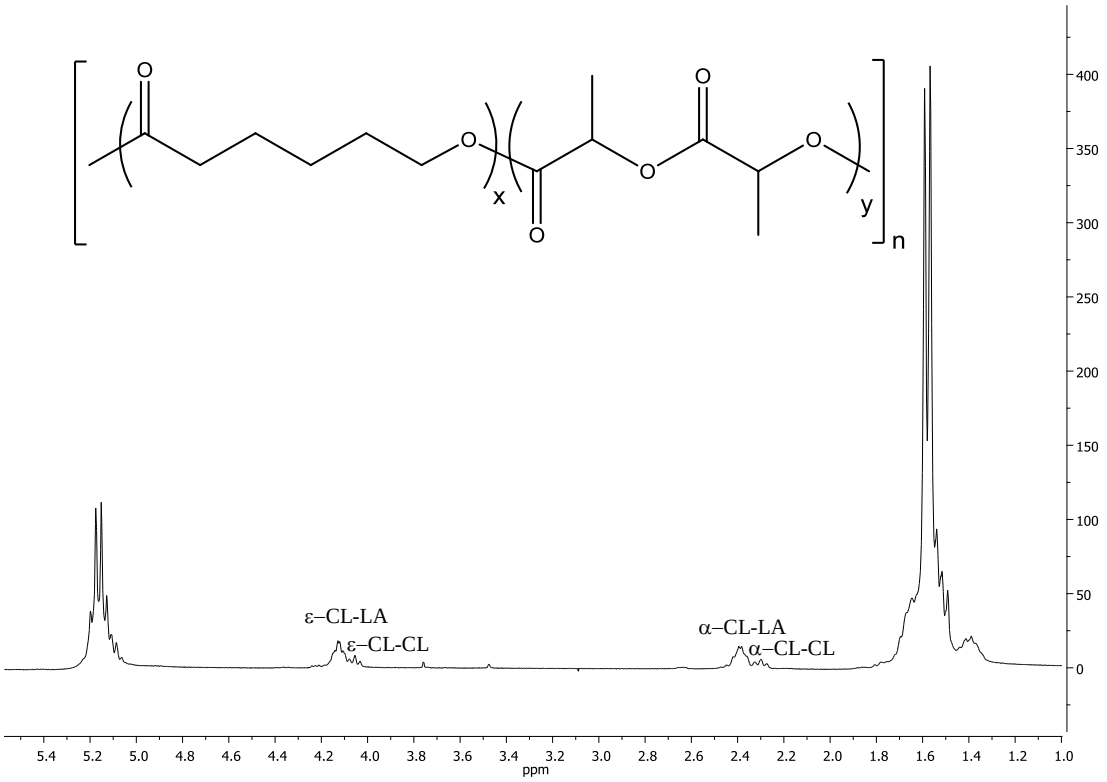

Figure S9. ^{1}H-NMR spectrum (500 MHz, 298 K, $CDCl_3$,) of random copolymer PCL-PLA 100:100 prepared with complex **5** as initiator

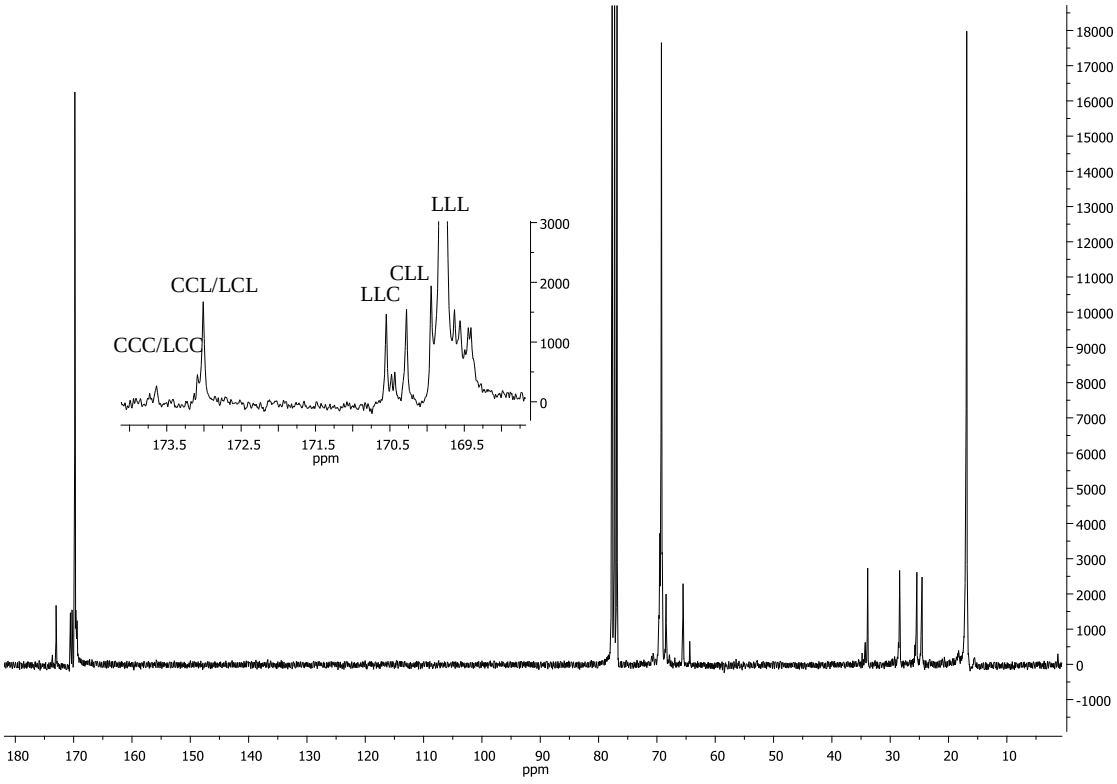

Figure S10. ^{13}C-NMR spectrum (500 MHz, 298 K, $CDCl_3$,) of random copolymer PCL-PLA 100:100 prepared with complex **5** as initiator.

Determination of Reactivity Ratios.

The reactivity ratios were calculated using the Fineman-Ross method. To determine the reactivity ratios, the copolymerizations of the monomer with different compositions (LA:CL of 16:84, 40:60, 60:40 and 80:20) were performed, and the monomer composition in the obtained oligomer was examined at a low converision (< 10%).

$$F - \left(\frac{F}{f}\right) = -r_2 + r_1\left(\frac{F^2}{f}\right)$$

$[LA]_0$	$[CL]_0$	F	LA in copolymer	CL in copolymer	*f*
80	20	4.00	89	11	8.09
60	40	1.50	66	34	1.94
40	60	0.67	38	62	0.61
16	84	0.19	12	88	0.14

Crystal Data and Structure Refinement for 2, 6 and 7

Table S1. Crystal data and structure refinement for **2**.

Identification code	2	
Empirical formula	C_{38} H_{45} Al N_{10} O_2	
Formula weight	700.82	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	Pī	
Unit cell dimensions	a = 11.3249(13) Å	α= 76.246(4)°.
	b = 12.5257(15) Å	β= 85.353(5)°.
	c = 14.309(2) Å	γ = 74.044(4)°.
Volume	1895.4(4) $Å^3$	
Z	2	
Density (calculated)	1.228 Mg/m^3	
Absorption coefficient	0.101 mm^{-1}	
F(000)	744	
Crystal size	0.16 x 0.10 x 0.05 mm^3	
Theta range for data collection	2.19 to 25.00°.	
Index ranges	-13≤h≤11, -14≤k≤14, -16≤l≤17	
Reflections collected	15785	
Independent reflections	6588 [R(int) = 0.0758]	
Completeness to theta = 25.00°	98.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7454 and 0.6789	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6588 / 0 / 469
Goodness-of-fit on F^2	0.930
Final R indices [I>2sigma(I)]	R1 = 0.0611, wR2 = 0.1206
R indices (all data)	R1 = 0.1710, wR2 = 0.1621
Largest diff. peak and hole	0.222 and -0.282 e.Å^{-3}

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Al(1)	2152(1)	3859(1)	7367(1)	38(1)
O(1)	2922(2)	2447(2)	7239(2)	39(1)
O(2)	3191(2)	4423(2)	7829(2)	39(1)
N(1)	2832(3)	4435(2)	5993(2)	35(1)
N(2)	3411(3)	5304(2)	5771(2)	36(1)
N(3)	2069(3)	6960(3)	6735(3)	53(1)
N(4)	3323(3)	6703(3)	6657(2)	42(1)
N(5)	5256(3)	4380(3)	7782(2)	41(1)
N(6)	1804(3)	3135(3)	8836(3)	43(1)
N(7)	1743(3)	2023(3)	9119(3)	42(1)
N(8)	688(3)	1720(3)	7868(3)	45(1)
N(9)	831(3)	1546(3)	6952(3)	52(1)
N(10)	3741(3)	494(3)	7801(2)	42(1)
C(1)	3425(3)	5753(3)	4811(3)	39(1)
C(2)	2844(3)	5164(3)	4398(3)	43(1)
C(3)	2492(3)	4362(3)	5140(3)	40(1)
C(4)	3966(3)	6725(3)	4400(3)	49(1)
C(5)	1824(4)	3509(3)	5065(3)	55(1)
C(6)	3788(4)	7529(3)	6835(3)	46(1)
C(7)	2796(5)	8358(4)	7020(3)	61(1)
C(8)	1765(4)	7976(4)	6956(3)	60(1)
C(9)	5132(4)	7416(4)	6816(4)	68(1)
C(10)	443(4)	8540(4)	7098(4)	103(2)
C(11)	4001(3)	5600(3)	6495(3)	37(1)
C(12)	4186(4)	4704(3)	7436(3)	38(1)
C(13)	5422(3)	3589(3)	8690(3)	42(1)
C(14)	5826(4)	3894(4)	9442(3)	51(1)
C(15)	6019(4)	3151(4)	10323(4)	65(1)
C(16)	5834(4)	2094(4)	10461(4)	65(1)
C(17)	5458(4)	1767(4)	9723(4)	66(1)
C(18)	5254(4)	2514(3)	8826(3)	53(1)
C(19)	1696(4)	1683(4)	10093(3)	51(1)
C(20)	1705(4)	2603(4)	10443(3)	60(1)
C(21)	1774(4)	3490(4)	9654(4)	53(1)
C(22)	1624(4)	515(4)	10599(3)	69(1)

C(23)	1836(4)	4670(4)	9656(3)	77(2)
C(24)	-310(4)	1794(4)	6643(4)	58(1)
C(25)	-1162(4)	2088(4)	7353(4)	66(2)
C(26)	-515(4)	2032(3)	8132(4)	52(1)
C(27)	-503(4)	1733(4)	5632(4)	83(2)
C(28)	-979(4)	2301(4)	9076(4)	73(2)
C(29)	1804(3)	1354(3)	8420(3)	41(1)
C(30)	2911(4)	1424(3)	7756(3)	36(1)
C(31)	4800(4)	426(3)	7201(3)	43(1)
C(32)	5923(4)	-145(4)	7604(4)	66(1)
C(33)	6939(4)	-346(5)	7020(5)	88(2)
C(34)	6894(5)	-5(4)	6049(4)	68(2)
C(35)	5784(5)	557(4)	5646(4)	66(1)
C(36)	4740(4)	784(3)	6222(4)	54(1)
C(37)	456(3)	4666(3)	7026(3)	52(1)
C(38)	-387(4)	5295(4)	7704(4)	95(2)

Table S3. Bond lengths [Å] and angles [°] for **2**.

Al(1)-O(2)	1.769(3)
Al(1)-O(1)	1.790(3)
Al(1)-C(37)	1.949(4)
Al(1)-N(1)	2.090(3)
Al(1)-N(6)	2.133(4)
O(1)-C(30)	1.321(4)
O(2)-C(12)	1.315(4)
N(1)-C(3)	1.339(5)
N(1)-N(2)	1.382(3)
N(2)-C(1)	1.355(5)
N(2)-C(11)	1.445(4)
N(3)-C(8)	1.330(5)
N(3)-N(4)	1.368(4)
N(4)-C(6)	1.364(4)
N(4)-C(11)	1.447(4)
N(5)-C(12)	1.269(4)
N(5)-C(13)	1.424(5)
N(6)-C(21)	1.342(5)
N(6)-N(7)	1.374(4)
N(7)-C(19)	1.357(5)
N(7)-C(29)	1.437(5)
N(8)-C(26)	1.358(5)
N(8)-N(9)	1.369(4)
N(8)-C(29)	1.450(5)
N(9)-C(24)	1.330(5)
N(10)-C(30)	1.272(4)
N(10)-C(31)	1.412(5)
C(1)-C(2)	1.366(5)
C(1)-C(4)	1.487(5)
C(2)-C(3)	1.394(5)
C(3)-C(5)	1.496(5)
C(6)-C(7)	1.361(5)
C(6)-C(9)	1.487(5)
C(7)-C(8)	1.396(6)
C(8)-C(10)	1.489(6)
C(11)-C(12)	1.521(5)
C(13)-C(14)	1.372(5)
C(13)-C(18)	1.378(5)

C(14)-C(15)	1.371(6)
C(15)-C(16)	1.364(6)
C(16)-C(17)	1.356(6)
C(17)-C(18)	1.391(6)
C(19)-C(20)	1.365(6)
C(19)-C(22)	1.492(5)
C(20)-C(21)	1.397(6)
C(21)-C(23)	1.500(5)
C(24)-C(25)	1.387(6)
C(24)-C(27)	1.503(6)
C(25)-C(26)	1.361(6)
C(26)-C(28)	1.490(6)
C(29)-C(30)	1.520(5)
C(31)-C(36)	1.368(5)
C(31)-C(32)	1.372(5)
C(32)-C(33)	1.368(6)
C(33)-C(34)	1.353(7)
C(34)-C(35)	1.359(6)
C(35)-C(36)	1.388(5)
C(37)-C(38)	1.508(6)

O(2)-Al(1)-O(1)	108.92(13)
O(2)-Al(1)-C(37)	125.23(16)
O(1)-Al(1)-C(37)	125.84(16)
O(2)-Al(1)-N(1)	87.88(12)
O(1)-Al(1)-N(1)	86.94(12)
C(37)-Al(1)-N(1)	93.36(16)
O(2)-Al(1)-N(6)	85.35(12)
O(1)-Al(1)-N(6)	87.62(13)
C(37)-Al(1)-N(6)	97.15(16)
N(1)-Al(1)-N(6)	169.46(13)
C(30)-O(1)-Al(1)	133.1(3)
C(12)-O(2)-Al(1)	130.2(3)
C(3)-N(1)-N(2)	104.4(3)
C(3)-N(1)-Al(1)	128.9(2)
N(2)-N(1)-Al(1)	123.4(2)
C(1)-N(2)-N(1)	111.7(3)
C(1)-N(2)-C(11)	126.2(3)
N(1)-N(2)-C(11)	121.9(3)
C(8)-N(3)-N(4)	103.5(3)

C(6)-N(4)-N(3)	112.8(3)
C(6)-N(4)-C(11)	127.5(3)
N(3)-N(4)-C(11)	119.5(3)
C(12)-N(5)-C(13)	116.8(3)
C(21)-N(6)-N(7)	105.4(3)
C(21)-N(6)-Al(1)	133.2(3)
N(7)-N(6)-Al(1)	120.8(3)
C(19)-N(7)-N(6)	111.3(3)
C(19)-N(7)-C(29)	127.9(3)
N(6)-N(7)-C(29)	120.6(3)
C(26)-N(8)-N(9)	111.9(4)
C(26)-N(8)-C(29)	131.7(4)
N(9)-N(8)-C(29)	115.3(3)
C(24)-N(9)-N(8)	104.3(4)
C(30)-N(10)-C(31)	121.7(3)
N(2)-C(1)-C(2)	106.2(3)
N(2)-C(1)-C(4)	121.6(4)
C(2)-C(1)-C(4)	132.1(4)
C(1)-C(2)-C(3)	106.9(4)
N(1)-C(3)-C(2)	110.7(3)
N(1)-C(3)-C(5)	121.4(3)
C(2)-C(3)-C(5)	127.9(4)
C(7)-C(6)-N(4)	105.5(4)
C(7)-C(6)-C(9)	132.4(4)
N(4)-C(6)-C(9)	122.0(4)
C(6)-C(7)-C(8)	106.4(4)
N(3)-C(8)-C(7)	111.8(4)
N(3)-C(8)-C(10)	119.0(4)
C(7)-C(8)-C(10)	129.2(4)
N(2)-C(11)-N(4)	110.3(3)
N(2)-C(11)-C(12)	113.3(3)
N(4)-C(11)-C(12)	110.9(3)
N(5)-C(12)-O(2)	127.8(4)
N(5)-C(12)-C(11)	116.4(3)
O(2)-C(12)-C(11)	115.6(3)
C(14)-C(13)-C(18)	119.1(4)
C(14)-C(13)-N(5)	118.4(4)
C(18)-C(13)-N(5)	122.4(4)
C(15)-C(14)-C(13)	120.3(4)
C(16)-C(15)-C(14)	120.6(5)

C(17)-C(16)-C(15)	120.1(5)
C(16)-C(17)-C(18)	120.0(4)
C(13)-C(18)-C(17)	120.0(4)
N(7)-C(19)-C(20)	106.3(4)
N(7)-C(19)-C(22)	122.8(4)
C(20)-C(19)-C(22)	130.9(4)
C(19)-C(20)-C(21)	107.3(4)
N(6)-C(21)-C(20)	109.7(4)
N(6)-C(21)-C(23)	122.1(4)
C(20)-C(21)-C(23)	128.2(4)
N(9)-C(24)-C(25)	111.1(5)
N(9)-C(24)-C(27)	119.0(5)
C(25)-C(24)-C(27)	129.9(4)
C(26)-C(25)-C(24)	106.8(4)
N(8)-C(26)-C(25)	105.8(4)
N(8)-C(26)-C(28)	125.2(4)
C(25)-C(26)-C(28)	128.9(4)
N(7)-C(29)-N(8)	111.6(3)
N(7)-C(29)-C(30)	109.7(3)
N(8)-C(29)-C(30)	110.4(3)
N(10)-C(30)-O(1)	127.9(3)
N(10)-C(30)-C(29)	115.6(3)
O(1)-C(30)-C(29)	116.4(3)
C(36)-C(31)-C(32)	118.4(4)
C(36)-C(31)-N(10)	122.5(4)
C(32)-C(31)-N(10)	118.6(4)
C(33)-C(32)-C(31)	119.4(5)
C(34)-C(33)-C(32)	122.9(5)
C(33)-C(34)-C(35)	117.9(5)
C(34)-C(35)-C(36)	120.4(5)
C(31)-C(36)-C(35)	120.9(4)
C(38)-C(37)-Al(1)	120.8(3)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Al(1)	36(1)	34(1)	45(1)	-9(1)	2(1)	-10(1)
O(1)	40(2)	29(2)	43(2)	-6(1)	5(1)	-7(1)
O(2)	39(2)	39(2)	40(2)	-7(1)	3(1)	-15(1)
N(1)	38(2)	32(2)	39(2)	-7(2)	-1(2)	-14(2)
N(2)	40(2)	33(2)	37(2)	-9(2)	-5(2)	-13(2)
N(3)	43(2)	39(2)	74(3)	-14(2)	5(2)	-6(2)
N(4)	44(2)	30(2)	53(3)	-10(2)	3(2)	-9(2)
N(5)	37(2)	38(2)	43(2)	-1(2)	-4(2)	-9(2)
N(6)	46(2)	41(2)	46(3)	-12(2)	8(2)	-19(2)
N(7)	42(2)	41(2)	43(3)	-6(2)	3(2)	-15(2)
N(8)	35(2)	46(2)	55(3)	-11(2)	-3(2)	-12(2)
N(9)	52(3)	54(2)	54(3)	-15(2)	-7(2)	-18(2)
N(10)	38(2)	34(2)	50(3)	-7(2)	2(2)	-4(2)
C(1)	41(2)	35(2)	34(3)	0(2)	0(2)	-6(2)
C(2)	51(3)	42(3)	35(3)	-8(2)	-4(2)	-8(2)
C(3)	44(3)	42(3)	36(3)	-6(2)	-4(2)	-13(2)
C(4)	53(3)	42(3)	47(3)	-4(2)	0(2)	-9(2)
C(5)	68(3)	53(3)	50(3)	-11(2)	-7(2)	-24(2)
C(6)	59(3)	35(3)	46(3)	-7(2)	1(2)	-18(2)
C(7)	87(4)	37(3)	61(4)	-16(2)	1(3)	-14(3)
C(8)	69(3)	36(3)	70(4)	-14(3)	7(3)	-4(3)
C(9)	68(3)	61(3)	86(4)	-23(3)	-5(3)	-29(3)
C(10)	69(4)	68(4)	164(7)	-45(4)	28(4)	3(3)
C(11)	35(2)	33(2)	44(3)	-11(2)	3(2)	-8(2)
C(12)	45(3)	30(2)	39(3)	-6(2)	1(2)	-13(2)
C(13)	37(2)	41(3)	42(3)	-6(2)	-1(2)	-6(2)
C(14)	57(3)	47(3)	42(3)	-2(3)	-7(2)	-9(2)
C(15)	74(4)	66(4)	49(4)	-15(3)	-6(3)	-6(3)
C(16)	69(3)	58(3)	50(4)	6(3)	0(3)	-3(3)
C(17)	69(3)	46(3)	75(4)	2(3)	-6(3)	-18(3)
C(18)	61(3)	43(3)	50(3)	-1(3)	-11(2)	-10(2)
C(19)	55(3)	59(3)	38(3)	-8(3)	3(2)	-18(2)
C(20)	75(3)	77(4)	34(3)	-10(3)	2(3)	-31(3)
C(21)	58(3)	63(3)	52(3)	-27(3)	14(3)	-29(2)
C(22)	89(4)	60(3)	48(3)	2(3)	8(3)	-17(3)

C(23)	100(4)	82(4)	71(4)	-42(3)	32(3)	-52(3)
C(24)	43(3)	60(3)	77(4)	-11(3)	-13(3)	-22(2)
C(25)	41(3)	72(3)	84(4)	-5(3)	-9(3)	-22(3)
C(26)	40(3)	48(3)	67(4)	-12(3)	8(3)	-15(2)
C(27)	77(4)	101(4)	80(5)	-21(4)	-25(3)	-32(3)
C(28)	44(3)	78(4)	95(5)	-24(3)	15(3)	-14(3)
C(29)	41(3)	34(2)	47(3)	-5(2)	-1(2)	-11(2)
C(30)	40(2)	39(3)	33(3)	-7(2)	-4(2)	-16(2)
C(31)	44(3)	35(2)	51(3)	-13(2)	5(2)	-11(2)
C(32)	42(3)	93(4)	58(4)	-22(3)	-10(3)	-5(3)
C(33)	36(3)	137(5)	96(5)	-53(4)	1(3)	-9(3)
C(34)	54(4)	77(4)	81(5)	-34(3)	17(3)	-22(3)
C(35)	78(4)	51(3)	67(4)	-13(3)	14(3)	-18(3)
C(36)	53(3)	47(3)	53(4)	-4(3)	6(3)	-5(2)
C(37)	42(3)	48(3)	62(3)	-8(2)	0(2)	-11(2)
C(38)	66(4)	107(5)	88(5)	-29(4)	15(3)	18(3)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **2**

	x	y	z	U(eq)
H(2)	2710	5276	3745	52
H(4A)	3460	7400	4577	73
H(4B)	4010	6843	3711	73
H(4C)	4776	6557	4645	73
H(5A)	2074	2843	5574	83
H(5B)	2015	3302	4455	83
H(5C)	955	3835	5117	83
H(7)	2804	9043	7162	74
H(9A)	5522	6761	7295	102
H(9B)	5273	8087	6949	102
H(9C)	5467	7329	6193	102
H(10A)	210	9247	6630	155
H(10B)	315	8685	7733	155
H(10C)	-47	8051	7024	155
H(11)	4815	5663	6242	45
H(14)	5970	4608	9353	61
H(15)	6278	3371	10831	78
H(16)	5965	1596	11062	78
H(17)	5336	1044	9816	79
H(18)	5004	2288	8317	64
H(20)	1671	2634	11088	73
H(22A)	907	369	10396	103
H(22B)	1575	458	11281	103
H(22C)	2344	-35	10445	103
H(23A)	2679	4679	9673	115
H(23B)	1403	4898	10211	115
H(23C)	1466	5189	9083	115
H(25)	-2013	2286	7306	79
H(27A)	275	1436	5341	124
H(27B)	-882	2483	5265	124
H(27C)	-1025	1242	5644	124
H(28A)	-1860	2480	9095	109
H(28B)	-722	2943	9156	109
H(28C)	-655	1654	9585	109
H(29)	1908	557	8761	49

H(32)	5992	-393	8269	79
H(33)	7694	-734	7302	106
H(34)	7601	-150	5670	82
H(35)	5724	791	4980	79
H(36)	3989	1185	5937	65
H(37A)	478	5213	6423	62
H(37B)	69	4114	6899	62
H(38A)	-380	4794	8327	142
H(38B)	-1207	5555	7461	142
H(38C)	-110	5937	7756	142

Table S6. Crystal data and structure refinement for **6**.

Identification code	6	
Empirical formula	C_{42} H_{53} Al N_{10} O_2	
Formula weight	756.92	
Temperature	230(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 12.3440(4) Å	α= 90°.
	b = 14.5660(6) Å	β= 90°.
	c = 23.8390(9) Å	γ = 90°.
Volume	4286.3(3) $Å^3$	
Z	4	
Density (calculated)	1.173 Mg/m^3	
Absorption coefficient	0.094 mm^{-1}	
F(000)	1616	
Crystal size	0.23 x 0.21 x 0.18 mm^3	
Theta range for data collection	1.64 to 25.00°.	
Index ranges	-14≤h≤14, -15≤k≤17, -26≤l≤28	
Reflections collected	18884	
Independent reflections	7408 [R(int) = 0.1147]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9833 and 0.9787	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7408 / 0 / 528	
Goodness-of-fit on F^2	0.940	
Final R indices [I>2sigma(I)]	R1 = 0.0767, wR2 = 0.1560	
R indices (all data)	R1 = 0.2126, wR2 = 0.2306	
Absolute structure parameter	0.3(5)	
Extinction coefficient	0.0071(9)	
Largest diff. peak and hole	0.389 and -0.344 $e.Å^{-3}$	

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **6**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Al(1)	748(2)	5146(2)	3427(1)	55(1)
O(1)	1541(3)	5801(3)	3905(2)	53(1)
O(2)	-146(3)	4388(3)	3792(2)	53(1)
N(1)	1917(5)	4087(5)	3506(3)	58(2)
N(2)	2953(5)	4218(5)	3703(2)	57(2)
N(3)	3857(6)	5150(6)	2878(3)	81(2)
N(4)	3640(5)	5626(5)	3353(3)	64(2)
N(5)	2565(4)	5711(4)	4714(3)	50(2)
N(6)	-444(4)	6176(5)	3509(2)	57(2)
N(7)	-1526(4)	6000(4)	3579(2)	50(2)
N(8)	-2098(5)	5146(5)	2651(3)	76(2)
N(9)	-2079(5)	4639(5)	3127(3)	58(2)
N(10)	-1374(4)	4375(4)	4526(3)	51(2)
C(1)	3573(7)	3468(7)	3626(3)	71(2)
C(2)	2907(7)	2821(6)	3406(4)	76(3)
C(3)	1893(7)	3216(6)	3329(3)	66(2)
C(4)	4756(6)	3444(6)	3754(4)	94(3)
C(5)	900(7)	2777(6)	3111(3)	85(3)
C(6)	3872(6)	6535(7)	3304(4)	66(2)
C(7)	4230(7)	6639(8)	2767(4)	84(3)
C(8)	4228(8)	5795(9)	2527(4)	92(3)
C(9)	3753(7)	7226(6)	3752(3)	81(3)
C(10)	4527(10)	5499(9)	1957(4)	161(5)
C(11)	3314(6)	5117(6)	3854(3)	59(2)
C(12)	2402(5)	5581(5)	4188(3)	50(2)
C(13)	1631(6)	6060(5)	5028(3)	56(2)
C(14)	1752(7)	5780(6)	5642(3)	84(3)
C(15)	1571(6)	7112(5)	4984(3)	53(2)
C(16)	2454(7)	7656(6)	5049(3)	68(2)
C(17)	2388(9)	8605(7)	5015(3)	80(3)
C(18)	1415(10)	9021(7)	4918(4)	95(3)
C(19)	532(9)	8490(8)	4842(4)	105(3)
C(20)	591(7)	7532(6)	4881(3)	70(2)
C(21)	-2147(6)	6767(6)	3504(3)	58(2)
C(22)	-1434(7)	7464(6)	3410(3)	64(2)

C(23)	-391(6)	7081(7)	3417(3)	67(2)
C(24)	-3350(6)	6743(6)	3516(3)	75(2)
C(25)	654(7)	7572(6)	3324(4)	97(3)
C(26)	-2314(6)	3737(6)	3024(4)	61(2)
C(27)	-2499(7)	3687(7)	2466(4)	80(3)
C(28)	-2334(8)	4565(8)	2248(4)	87(3)
C(29)	-2350(6)	3010(6)	3464(4)	82(3)
C(30)	-2366(9)	4903(7)	1660(3)	134(4)
C(31)	-1904(6)	5063(5)	3664(3)	56(2)
C(32)	-1091(5)	4571(5)	4030(3)	49(2)
C(33)	-554(6)	3930(5)	4897(3)	58(2)
C(34)	-776(8)	4206(6)	5497(3)	90(3)
C(35)	-594(7)	2917(6)	4803(3)	58(2)
C(36)	292(8)	2438(6)	4619(4)	82(3)
C(37)	240(11)	1500(9)	4518(5)	120(4)
C(38)	-704(13)	1050(7)	4628(5)	116(4)
C(39)	-1597(10)	1495(8)	4825(4)	102(3)
C(40)	-1531(8)	2426(7)	4902(3)	76(3)
C(41)	720(20)	4990(20)	2631(13)	70(8)
C(42)	800(30)	5780(20)	2237(11)	82(18)
C(41A)	970(20)	5440(20)	2615(13)	72(10)
C(42A)	1350(20)	4891(16)	2214(8)	76(8)

Table S8. Bond lengths [Å] and angles [°] for **6**.

Al(1)-O(1)	1.779(5)
Al(1)-O(2)	1.786(5)
Al(1)-C(41)	1.91(3)
Al(1)-C(41A)	2.00(3)
Al(1)-N(6)	2.110(6)
Al(1)-N(1)	2.120(7)
O(1)-C(12)	1.300(7)
O(2)-C(32)	1.324(8)
N(1)-C(3)	1.337(9)
N(1)-N(2)	1.376(7)
N(2)-C(1)	1.347(9)
N(2)-C(11)	1.429(9)
N(3)-C(8)	1.340(11)
N(3)-N(4)	1.354(8)
N(4)-C(6)	1.359(10)
N(4)-C(11)	1.463(9)
N(5)-C(12)	1.284(8)
N(5)-C(13)	1.466(8)
N(6)-C(23)	1.338(9)
N(6)-N(7)	1.371(7)
N(7)-C(21)	1.366(8)
N(7)-C(31)	1.456(9)
N(8)-C(28)	1.314(11)
N(8)-N(9)	1.353(8)
N(9)-C(26)	1.368(9)
N(9)-C(31)	1.438(9)
N(10)-C(32)	1.265(8)
N(10)-C(33)	1.493(8)
C(1)-C(2)	1.355(11)
C(1)-C(4)	1.493(11)
C(2)-C(3)	1.389(11)
C(3)-C(5)	1.477(10)
C(6)-C(7)	1.362(11)
C(6)-C(9)	1.475(11)
C(7)-C(8)	1.357(12)
C(8)-C(10)	1.472(12)
C(11)-C(12)	1.535(9)
C(13)-C(14)	1.526(9)

C(13)-C(15)	1.538(10)
C(15)-C(16)	1.357(10)
C(15)-C(20)	1.378(10)
C(16)-C(17)	1.386(11)
C(17)-C(18)	1.365(12)
C(18)-C(19)	1.348(13)
C(19)-C(20)	1.400(12)
C(21)-C(22)	1.363(10)
C(21)-C(24)	1.486(10)
C(22)-C(23)	1.404(10)
C(23)-C(25)	1.493(10)
C(26)-C(27)	1.350(10)
C(26)-C(29)	1.492(10)
C(27)-C(28)	1.396(12)
C(28)-C(30)	1.485(12)
C(31)-C(32)	1.510(9)
C(33)-C(35)	1.492(10)
C(33)-C(34)	1.511(9)
C(35)-C(36)	1.369(11)
C(35)-C(40)	1.381(11)
C(36)-C(37)	1.388(13)
C(37)-C(38)	1.363(14)
C(38)-C(39)	1.363(14)
C(39)-C(40)	1.371(13)
C(41)-C(42)	1.49(3)
C(41A)-C(42A)	1.33(4)

O(1)-Al(1)-O(2)	111.1(2)
O(1)-Al(1)-C(41)	135.3(7)
O(2)-Al(1)-C(41)	113.4(7)
O(1)-Al(1)-C(41A)	115.3(8)
O(2)-Al(1)-C(41A)	133.6(8)
C(41)-Al(1)-C(41A)	21.4(10)
O(1)-Al(1)-N(6)	86.7(2)
O(2)-Al(1)-N(6)	87.9(2)
C(41)-Al(1)-N(6)	99.3(11)
C(41A)-Al(1)-N(6)	91.9(11)
O(1)-Al(1)-N(1)	87.6(2)
O(2)-Al(1)-N(1)	85.9(2)
C(41)-Al(1)-N(1)	90.9(11)

C(41A)-Al(1)-N(1)	98.4(11)
N(6)-Al(1)-N(1)	169.6(2)
C(12)-O(1)-Al(1)	130.6(5)
C(32)-O(2)-Al(1)	129.0(5)
C(3)-N(1)-N(2)	105.1(6)
C(3)-N(1)-Al(1)	130.3(6)
N(2)-N(1)-Al(1)	124.2(5)
C(1)-N(2)-N(1)	111.7(7)
C(1)-N(2)-C(11)	127.0(7)
N(1)-N(2)-C(11)	120.2(6)
C(8)-N(3)-N(4)	103.3(8)
N(3)-N(4)-C(6)	112.7(7)
N(3)-N(4)-C(11)	118.5(7)
C(6)-N(4)-C(11)	128.4(8)
C(12)-N(5)-C(13)	115.3(6)
C(23)-N(6)-N(7)	104.6(6)
C(23)-N(6)-Al(1)	130.7(5)
N(7)-N(6)-Al(1)	123.9(5)
C(21)-N(7)-N(6)	112.2(6)
C(21)-N(7)-C(31)	127.2(6)
N(6)-N(7)-C(31)	120.3(6)
C(28)-N(8)-N(9)	105.5(8)
N(8)-N(9)-C(26)	111.7(7)
N(8)-N(9)-C(31)	121.0(7)
C(26)-N(9)-C(31)	127.2(8)
C(32)-N(10)-C(33)	117.6(6)
N(2)-C(1)-C(2)	105.8(7)
N(2)-C(1)-C(4)	123.1(9)
C(2)-C(1)-C(4)	131.1(9)
C(1)-C(2)-C(3)	108.1(8)
N(1)-C(3)-C(2)	109.3(8)
N(1)-C(3)-C(5)	122.7(8)
C(2)-C(3)-C(5)	128.0(9)
N(4)-C(6)-C(7)	104.9(8)
N(4)-C(6)-C(9)	125.5(8)
C(7)-C(6)-C(9)	129.5(10)
C(8)-C(7)-C(6)	107.2(9)
N(3)-C(8)-C(7)	111.8(8)
N(3)-C(8)-C(10)	117.3(11)
C(7)-C(8)-C(10)	130.9(11)

N(2)-C(11)-N(4)	110.1(6)
N(2)-C(11)-C(12)	107.8(6)
N(4)-C(11)-C(12)	113.7(7)
N(5)-C(12)-O(1)	126.9(7)
N(5)-C(12)-C(11)	117.1(6)
O(1)-C(12)-C(11)	116.0(6)
N(5)-C(13)-C(14)	108.7(6)
N(5)-C(13)-C(15)	110.4(6)
C(14)-C(13)-C(15)	109.7(6)
C(16)-C(15)-C(20)	117.8(7)
C(16)-C(15)-C(13)	122.4(8)
C(20)-C(15)-C(13)	119.8(8)
C(15)-C(16)-C(17)	121.9(9)
C(18)-C(17)-C(16)	120.3(9)
C(19)-C(18)-C(17)	118.7(10)
C(18)-C(19)-C(20)	121.4(9)
C(15)-C(20)-C(19)	120.0(8)
C(22)-C(21)-N(7)	105.7(6)
C(22)-C(21)-C(24)	131.7(8)
N(7)-C(21)-C(24)	122.6(8)
C(21)-C(22)-C(23)	107.0(7)
N(6)-C(23)-C(22)	110.5(7)
N(6)-C(23)-C(25)	122.6(8)
C(22)-C(23)-C(25)	126.9(8)
C(27)-C(26)-N(9)	105.4(8)
C(27)-C(26)-C(29)	130.4(9)
N(9)-C(26)-C(29)	124.2(8)
C(26)-C(27)-C(28)	107.0(8)
N(8)-C(28)-C(27)	110.4(8)
N(8)-C(28)-C(30)	118.9(11)
C(27)-C(28)-C(30)	130.7(10)
N(9)-C(31)-N(7)	109.0(6)
N(9)-C(31)-C(32)	114.3(6)
N(7)-C(31)-C(32)	108.2(6)
N(10)-C(32)-O(2)	126.8(7)
N(10)-C(32)-C(31)	117.6(6)
O(2)-C(32)-C(31)	115.6(6)
C(35)-C(33)-N(10)	108.5(6)
C(35)-C(33)-C(34)	113.6(6)
N(10)-C(33)-C(34)	108.8(6)

C(36)-C(35)-C(40)	117.4(8)
C(36)-C(35)-C(33)	121.7(8)
C(40)-C(35)-C(33)	120.9(8)
C(35)-C(36)-C(37)	121.3(10)
C(38)-C(37)-C(36)	118.7(11)
C(37)-C(38)-C(39)	121.9(11)
C(38)-C(39)-C(40)	118.0(11)
C(39)-C(40)-C(35)	122.6(10)
C(42)-C(41)-Al(1)	122(2)
C(42A)-C(41A)-Al(1)	128(3)

Symmetry transformations used to generate equivalent atoms:

Table S9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **6**. 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}
Al(1)	48(1)	74(2)	44(1)	0(1)	1(1)	5(1)
O(1)	46(3)	60(4)	55(3)	-3(3)	-5(2)	6(3)
O(2)	45(3)	57(3)	55(3)	-3(3)	5(2)	3(3)
N(1)	51(4)	69(5)	55(4)	-10(4)	11(3)	4(3)
N(2)	51(4)	54(5)	65(4)	-9(4)	6(3)	-3(4)
N(3)	91(5)	101(7)	50(5)	-13(5)	16(4)	13(5)
N(4)	56(4)	74(6)	61(5)	4(4)	3(3)	1(4)
N(5)	49(3)	46(4)	55(4)	4(3)	-4(3)	1(3)
N(6)	46(4)	67(5)	58(4)	21(4)	-8(3)	-3(3)
N(7)	40(3)	59(5)	52(4)	2(3)	-1(3)	-4(3)
N(8)	81(5)	79(6)	68(5)	-10(5)	-14(4)	20(4)
N(9)	58(4)	62(5)	52(5)	-18(4)	-11(3)	12(4)
N(10)	57(4)	37(4)	58(4)	-3(3)	3(3)	-6(3)
C(1)	68(6)	66(6)	78(6)	-4(5)	5(5)	19(5)
C(2)	87(6)	53(6)	88(6)	-13(5)	17(6)	18(5)
C(3)	75(6)	67(7)	55(5)	-14(5)	22(4)	6(5)
C(4)	65(6)	94(7)	125(8)	-12(6)	3(5)	33(5)
C(5)	90(6)	84(7)	81(6)	-34(5)	7(5)	-2(6)
C(6)	47(4)	80(8)	71(7)	-11(6)	-5(4)	-1(5)
C(7)	75(6)	116(10)	60(6)	17(6)	8(5)	-1(7)
C(8)	106(7)	125(10)	45(6)	-7(7)	17(5)	2(8)
C(9)	78(6)	83(7)	83(6)	15(6)	-5(5)	-17(5)
C(10)	230(14)	176(12)	76(8)	-11(8)	62(9)	-24(11)
C(11)	44(4)	81(7)	51(5)	-11(5)	-7(4)	10(5)
C(12)	42(4)	54(5)	53(5)	6(4)	-7(4)	2(4)
C(13)	58(5)	50(6)	59(5)	-8(4)	14(4)	-1(4)
C(14)	120(7)	73(7)	60(6)	1(5)	17(5)	6(6)
C(15)	55(5)	49(6)	56(5)	-3(4)	5(4)	8(4)
C(16)	61(5)	59(6)	84(6)	-9(5)	-1(5)	-6(5)
C(17)	111(8)	62(7)	67(6)	-13(5)	13(6)	-23(6)
C(18)	126(9)	69(8)	90(8)	-3(6)	-16(7)	11(8)
C(19)	101(8)	69(8)	145(10)	-14(7)	-34(7)	23(7)
C(20)	67(5)	67(6)	77(6)	-2(5)	-12(5)	-3(5)
C(21)	65(5)	61(6)	48(5)	-7(4)	-4(4)	14(5)
C(22)	81(6)	51(5)	59(5)	7(5)	-11(5)	11(5)

C(23)	65(6)	80(7)	57(5)	20(5)	-7(4)	-2(5)
C(24)	64(5)	78(6)	83(6)	-7(5)	-16(5)	25(5)
C(25)	81(6)	84(7)	125(8)	27(6)	-6(6)	-16(6)
C(26)	54(5)	61(7)	68(6)	-11(5)	-1(4)	0(5)
C(27)	80(6)	83(8)	75(7)	-28(6)	-25(5)	15(6)
C(28)	104(7)	94(9)	62(6)	-23(7)	-17(5)	37(7)
C(29)	75(6)	75(7)	97(7)	-18(6)	-2(6)	-21(5)
C(30)	225(12)	122(9)	54(6)	-24(7)	-40(7)	52(9)
C(31)	47(4)	55(6)	65(5)	9(5)	4(4)	-2(4)
C(32)	48(4)	46(5)	52(5)	-5(4)	6(4)	6(4)
C(33)	69(5)	45(5)	59(5)	1(4)	-13(4)	-5(4)
C(34)	138(8)	92(7)	41(5)	3(5)	-7(5)	4(7)
C(35)	71(5)	55(6)	49(5)	14(4)	2(4)	-3(5)
C(36)	90(7)	52(6)	104(7)	13(5)	18(6)	12(5)
C(37)	144(11)	72(9)	144(11)	25(8)	28(9)	39(8)
C(38)	172(12)	51(7)	124(10)	-3(7)	-3(9)	2(9)
C(39)	123(9)	58(8)	124(9)	19(7)	7(8)	-9(7)
C(40)	76(6)	61(7)	91(7)	5(5)	7(5)	2(5)
C(41)	78(17)	71(3)	62(15)	15(17)	25(12)	-20(14)
C(42)	98(5)	86(3)	62(17)	49(18)	30(20)	30(30)
C(41A)	69(15)	97(3)	50(14)	30(20)	18(11)	-24(16)
C(42A)	95(2)	97(19)	36(11)	16(12)	2(13)	30(18)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **6**.

	x	y	z	U(eq)
H(2)	3096	2219	3321	91
H(4A)	5135	3844	3502	142
H(4B)	5022	2829	3711	142
H(4C)	4873	3644	4133	142
H(5A)	578	2408	3400	127
H(5B)	1080	2396	2796	127
H(5C)	397	3242	2995	127
H(7)	4437	7187	2597	100
H(9A)	3000	7301	3840	122
H(9B)	4046	7801	3627	122
H(9C)	4137	7025	4080	122
H(10A)	4298	4876	1899	241
H(10B)	5298	5540	1912	241
H(10C)	4178	5890	1687	241
H(11)	3946	5055	4100	70
H(13)	965	5792	4876	67
H(14A)	1846	5127	5666	126
H(14B)	1114	5955	5846	126
H(14C)	2372	6081	5801	126
H(16)	3124	7385	5117	82
H(17)	3008	8959	5060	96
H(18)	1362	9657	4903	114
H(19)	-130	8765	4763	126
H(20)	-31	7179	4837	84
H(22)	-1607	8079	3353	76
H(24A)	-3606	6301	3248	112
H(24B)	-3629	7339	3422	112
H(24C)	-3592	6573	3884	112
H(25A)	929	7790	3676	145
H(25B)	538	8083	3076	145
H(25C)	1170	7159	3158	145
H(27)	-2698	3165	2266	95
H(29A)	-2756	2494	3327	123
H(29B)	-2693	3249	3795	123
H(29C)	-1626	2819	3553	123

H(30A)	-2566	5539	1657	200
H(30B)	-2888	4555	1451	200
H(30C)	-1664	4832	1492	200
H(31)	-2597	5085	3864	67
H(33)	167	4153	4792	69
H(34A)	-1446	3937	5619	136
H(34B)	-825	4862	5521	136
H(34C)	-197	3994	5733	136
H(36)	941	2747	4560	99
H(37)	838	1186	4379	144
H(38)	-740	420	4566	139
H(39)	-2232	1177	4905	122
H(40)	-2142	2739	5027	91
H(41A)	1299	4571	2537	84
H(41B)	45	4674	2544	84
H(42A)	222	6203	2311	123
H(42B)	741	5558	1858	123
H(42C)	1483	6078	2287	123
H(41C)	276	5656	2481	86
H(41D)	1448	5972	2612	86
H(42D)	2020	4624	2332	114
H(42E)	1461	5240	1877	114
H(42F)	830	4413	2143	114

Table S11. Crystal data and structure refinement for **7**.

Identification code	7	
Empirical formula	$C_{40}\ H_{57}\ Al\ N_{10}\ O_3$	
Formula weight	752.94	
Temperature	230(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 18.826(3) Å	α= 90°.
	b = 14.547(4) Å	β= 112.58(2)°.
	c = 16.447(3) Å	γ = 90°.
Volume	4158.9(15) $Å^3$	
Z	4	
Density (calculated)	1.203 Mg/m^3	
Absorption coefficient	0.098 mm^{-1}	
F(000)	1616	
Crystal size	0.18 x 0.12 x 0.06 mm^3	
Theta range for data collection	2.68 to 22.49°.	
Index ranges	-20≤h≤20, -15≤k≤15, -17≤l≤17	
Reflections collected	8930	
Independent reflections	2705 [R(int) = 0.2158]	
Completeness to theta = 22.49°	99.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9941 and 0.9726	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2705 / 0 / 247	
Goodness-of-fit on F^2	0.794	
Final R indices [I>2sigma(I)]	R1 = 0.0690, wR2 = 0.1382	
R indices (all data)	R1 = 0.2310, wR2 = 0.2233	
Largest diff. peak and hole	0.147 and -0.162 $e.Å^{-3}$	

Table S12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 7. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Al(1)	0	3581(2)	2500	64(1)
N(1)	1002(4)	3543(4)	3607(4)	65(2)
N(2)	1066(3)	3168(4)	4394(4)	65(2)
N(3)	837(3)	1473(4)	3408(3)	60(2)
N(4)	767(3)	1584(4)	4206(3)	59(2)
N(5)	-776(4)	2430(4)	4240(3)	73(2)
O(1)	-490(2)	3096(3)	3123(3)	62(1)
O(2)	0	4752(5)	2500	89(2)
C(1)	1739(4)	3394(6)	5066(5)	79(2)
C(2)	2092(5)	3949(6)	4684(6)	90(3)
C(3)	1653(5)	4044(5)	3796(6)	75(2)
C(4)	1971(4)	3068(5)	5976(4)	104(3)
C(5)	1798(5)	4565(5)	3083(5)	105(3)
C(6)	837(4)	764(6)	4645(4)	69(2)
C(7)	962(4)	124(5)	4104(5)	74(2)
C(8)	958(4)	583(6)	3350(5)	71(2)
C(9)	784(4)	681(5)	5522(4)	90(2)
C(10)	1090(4)	231(5)	2579(4)	93(3)
C(12)	515(4)	2472(5)	4435(4)	66(2)
C(13)	-321(4)	2673(5)	3877(5)	58(2)
C(14)	-1580(5)	2613(5)	3768(5)	83(2)
C(15)	-1753(15)	3415(15)	4286(14)	123(10)
C(16)	-2021(12)	1927(14)	4054(15)	102(8)
C(17)	-2959(9)	2142(11)	3477(10)	120(6)
C(15A)	-1777(11)	3573(13)	3970(13)	82(6)
C(16A)	-2086(14)	1738(14)	3732(14)	122(10)
C(17A)	-2627(14)	3592(14)	3659(14)	194(9)
C(18)	0	5691(8)	2500	76(3)
C(19)	9(4)	6143(5)	3243(5)	70(2)
C(20)	18(4)	7076(6)	3225(5)	92(3)
C(21)	0	7602(9)	2500	114(4)
C(22)	-16(5)	5594(5)	4017(4)	108(3)

Table S13. Bond lengths [Å] and angles [°] for **7**.

Al(1)-O(2)	1.704(8)
Al(1)-O(1)#1	1.768(4)
Al(1)-O(1)	1.768(4)
Al(1)-N(1)	2.058(6)
Al(1)-N(1)#1	2.058(6)
N(1)-C(3)	1.356(8)
N(1)-N(2)	1.368(6)
N(2)-C(1)	1.363(8)
N(2)-C(12)	1.470(8)
N(3)-C(8)	1.325(8)
N(3)-N(4)	1.377(6)
N(4)-C(6)	1.374(8)
N(4)-C(12)	1.475(7)
N(5)-C(13)	1.268(7)
N(5)-C(14)	1.436(8)
O(1)-C(13)	1.309(7)
O(2)-C(18)	1.366(11)
C(1)-C(2)	1.346(9)
C(1)-C(4)	1.467(9)
C(2)-C(3)	1.381(8)
C(3)-C(5)	1.506(9)
C(6)-C(7)	1.369(8)
C(6)-C(9)	1.488(7)
C(7)-C(8)	1.407(8)
C(8)-C(10)	1.474(8)
C(12)-C(13)	1.515(8)
C(14)-C(16)	1.49(2)
C(14)-C(15A)	1.514(19)
C(14)-C(15)	1.55(2)
C(14)-C(16A)	1.58(2)
C(16)-C(17)	1.68(3)
C(15A)-C(17A)	1.48(3)
C(18)-C(19)	1.382(8)
C(18)-C(19)#1	1.382(8)
C(19)-C(20)	1.357(9)
C(19)-C(22)	1.519(8)
C(20)-C(21)	1.406(9)
C(21)-C(20)#1	1.406(9)

O(2)-Al(1)-O(1)#1	113.51(15)
O(2)-Al(1)-O(1)	113.51(15)
O(1)#1-Al(1)-O(1)	133.0(3)
O(2)-Al(1)-N(1)	91.52(17)
O(1)#1-Al(1)-N(1)	89.8(2)
O(1)-Al(1)-N(1)	89.0(2)
O(2)-Al(1)-N(1)#1	91.52(17)
O(1)#1-Al(1)-N(1)#1	89.0(2)
O(1)-Al(1)-N(1)#1	89.8(2)
N(1)-Al(1)-N(1)#1	177.0(3)
C(3)-N(1)-N(2)	104.7(6)
C(3)-N(1)-Al(1)	129.0(6)
N(2)-N(1)-Al(1)	124.5(5)
C(1)-N(2)-N(1)	112.9(7)
C(1)-N(2)-C(12)	125.6(7)
N(1)-N(2)-C(12)	120.7(6)
C(8)-N(3)-N(4)	105.4(5)
N(3)-N(4)-C(6)	112.0(6)
N(3)-N(4)-C(12)	120.2(5)
C(6)-N(4)-C(12)	127.0(6)
C(13)-N(5)-C(14)	117.1(6)
C(13)-O(1)-Al(1)	138.2(5)
C(18)-O(2)-Al(1)	180.000(2)
C(2)-C(1)-N(2)	103.7(8)
C(2)-C(1)-C(4)	131.6(8)
N(2)-C(1)-C(4)	124.7(8)
C(1)-C(2)-C(3)	110.6(7)
N(1)-C(3)-C(2)	108.1(7)
N(1)-C(3)-C(5)	120.6(8)
C(2)-C(3)-C(5)	131.3(8)
N(4)-C(6)-C(7)	104.7(6)
N(4)-C(6)-C(9)	123.5(7)
C(7)-C(6)-C(9)	131.8(7)
C(6)-C(7)-C(8)	107.8(7)
N(3)-C(8)-C(7)	110.0(6)
N(3)-C(8)-C(10)	119.5(7)
C(7)-C(8)-C(10)	130.4(8)
N(2)-C(12)-N(4)	106.9(5)
N(2)-C(12)-C(13)	115.3(6)

N(4)-C(12)-C(13)	112.1(5)
N(5)-C(13)-O(1)	128.0(6)
N(5)-C(13)-C(12)	113.1(7)
O(1)-C(13)-C(12)	118.8(7)
N(5)-C(14)-C(16)	107.8(10)
N(5)-C(14)-C(15A)	110.4(9)
C(16)-C(14)-C(15A)	109.7(13)
N(5)-C(14)-C(15)	104.0(11)
C(16)-C(14)-C(15)	94.0(12)
C(15A)-C(14)-C(15)	20.8(12)
N(5)-C(14)-C(16A)	111.6(10)
C(16)-C(14)-C(16A)	21.1(13)
C(15A)-C(14)-C(16A)	123.8(14)
C(15)-C(14)-C(16A)	112.1(13)
C(14)-C(16)-C(17)	106.8(13)
C(17A)-C(15A)-C(14)	105.4(15)
O(2)-C(18)-C(19)	118.4(5)
O(2)-C(18)-C(19)#1	118.4(5)
C(19)-C(18)-C(19)#1	123.1(11)
C(20)-C(19)-C(18)	116.9(8)
C(20)-C(19)-C(22)	123.3(7)
C(18)-C(19)-C(22)	119.8(7)
C(19)-C(20)-C(21)	124.5(9)
C(20)#1-C(21)-C(20)	114.0(11)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+1/2

Table S14. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 7. 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}
Al(1)	64(2)	61(2)	73(2)	0	32(2)	0
N(1)	67(5)	59(4)	64(4)	-6(3)	19(4)	-15(4)
N(2)	44(4)	85(5)	56(4)	2(3)	6(4)	7(4)
N(3)	61(4)	65(4)	57(4)	-7(3)	26(3)	-10(3)
N(4)	67(4)	63(4)	51(4)	2(3)	28(3)	-4(3)
N(5)	48(5)	103(5)	72(4)	13(3)	26(4)	10(4)
O(1)	54(3)	68(3)	61(3)	10(2)	18(3)	2(2)
O(2)	105(6)	73(6)	86(5)	0	34(4)	0
C(1)	23(5)	124(7)	73(7)	-23(5)	0(5)	-7(5)
C(2)	46(6)	110(7)	96(8)	-52(5)	9(6)	-25(5)
C(3)	53(6)	76(6)	94(7)	-17(5)	25(6)	-7(5)
C(4)	52(6)	156(8)	63(6)	-15(5)	-22(4)	-14(5)
C(5)	105(7)	89(6)	140(7)	-13(5)	66(6)	-31(5)
C(6)	68(6)	68(6)	60(5)	-2(4)	13(4)	-18(4)
C(7)	75(6)	71(5)	68(5)	7(5)	16(5)	5(4)
C(8)	57(5)	77(6)	79(6)	-16(5)	25(5)	-7(5)
C(9)	108(7)	120(6)	44(5)	13(4)	30(5)	0(5)
C(10)	100(7)	103(6)	82(5)	-30(4)	44(5)	-4(5)
C(12)	58(6)	78(6)	61(5)	-15(4)	22(4)	-13(5)
C(13)	28(5)	77(5)	61(5)	-2(4)	10(5)	2(4)
C(14)	59(6)	103(7)	85(5)	14(5)	26(5)	-13(5)
C(18)	51(7)	70(9)	98(10)	0	19(7)	0
C(19)	68(6)	69(6)	76(6)	-14(5)	31(4)	-3(5)
C(20)	87(7)	82(7)	122(8)	-26(6)	57(6)	-5(6)
C(21)	123(12)	72(10)	175(14)	0	88(11)	0
C(22)	147(9)	132(7)	59(5)	-6(5)	57(5)	19(6)

Table S15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for 7.

	x	y	z	U(eq)
H(2)	2566	4230	4977	108
H(4A)	2112	2431	6006	155
H(4B)	1550	3140	6163	155
H(4C)	2403	3420	6353	155
H(5A)	2340	4675	3263	158
H(5B)	1530	5141	2982	158
H(5C)	1618	4210	2550	158
H(7)	1036	-503	4216	89
H(9A)	854	50	5707	135
H(9B)	287	888	5481	135
H(9C)	1176	1051	5943	135
H(10A)	836	-351	2406	139
H(10B)	1632	154	2729	139
H(10C)	888	659	2101	139
H(12)	563	2432	5048	79
H(14)	-1746	2702	3131	99
H(15A)	-1518	3968	4191	185
H(15B)	-1550	3271	4903	185
H(15C)	-2299	3502	4085	185
H(16A)	-1901	1985	4680	123
H(16B)	-1893	1308	3936	123
H(17A)	-3265	1724	3657	180
H(17B)	-3072	2064	2860	180
H(17C)	-3074	2762	3586	180
H(15D)	-1543	3695	4597	99
H(15E)	-1598	4029	3662	99
H(16C)	-2002	1283	3356	182
H(16D)	-2620	1908	3503	182
H(16E)	-1946	1490	4314	182
H(17D)	-2778	4042	3989	291
H(17E)	-2810	2997	3742	291
H(17F)	-2843	3749	3045	291
H(20)	37	7388	3726	111
H(21)	0	8241	2500	137
H(22A)	-33	4949	3885	161

H(22B)	-465	5761	4124	161
H(22C)	436	5724	4531	161