supporting information

Aluminum Complexes Containing Bidentate and Symmetrical Tridentate Pincer Type Pyrrolyl Ligands: Synthesis, Reactions and Ring Opening Polymerization

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Homonuclear decoupling of ^{1}H NMR spectra of complex **7** in $CDCl_3$ using 300MHz NMR spectrometer

(1) ^{1}H-^{13}C HSQC 2D NMR spectra of complex **7** in C_6D_6 using 300MHz NMR spectrometer.

(2) ^{1}H-^{1}H NOESY 2D NMR spectrum of complex **7** in C_6D_6 using 300MHz NMR spectrometer

(3) Crystal data and structure refinement for complex **2** (second set of crystal data)

(1)

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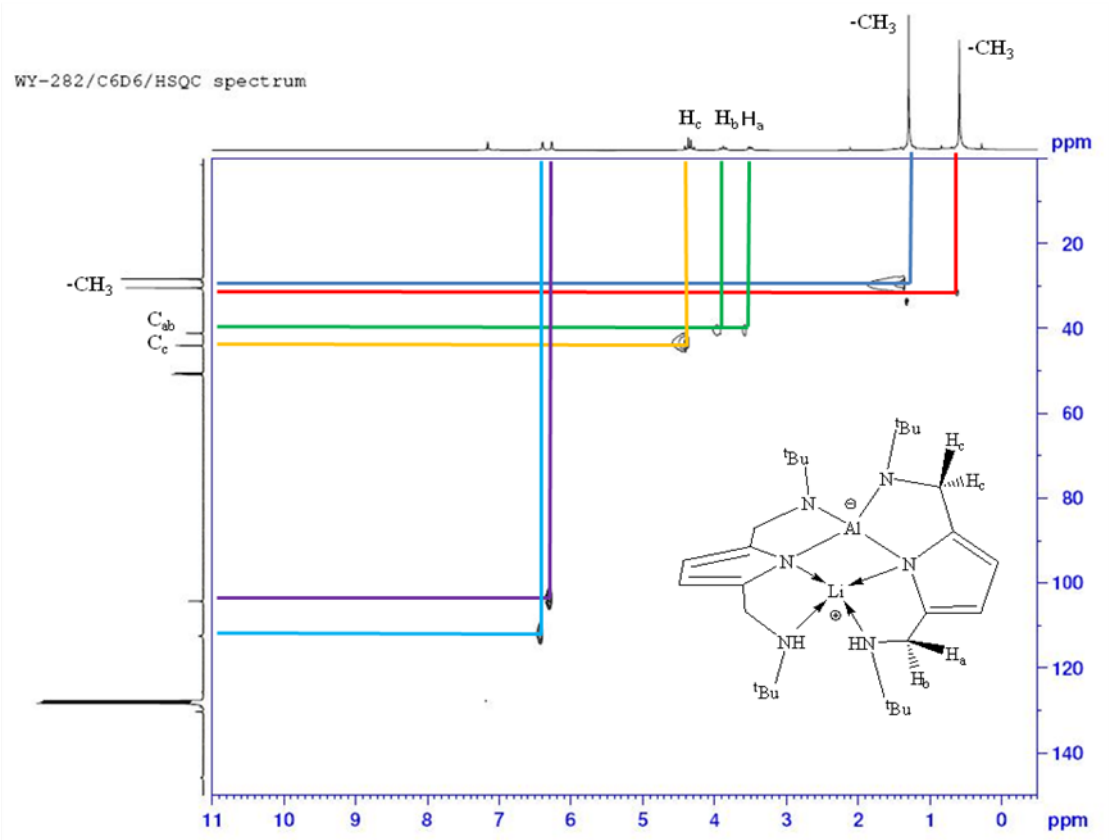
(2)



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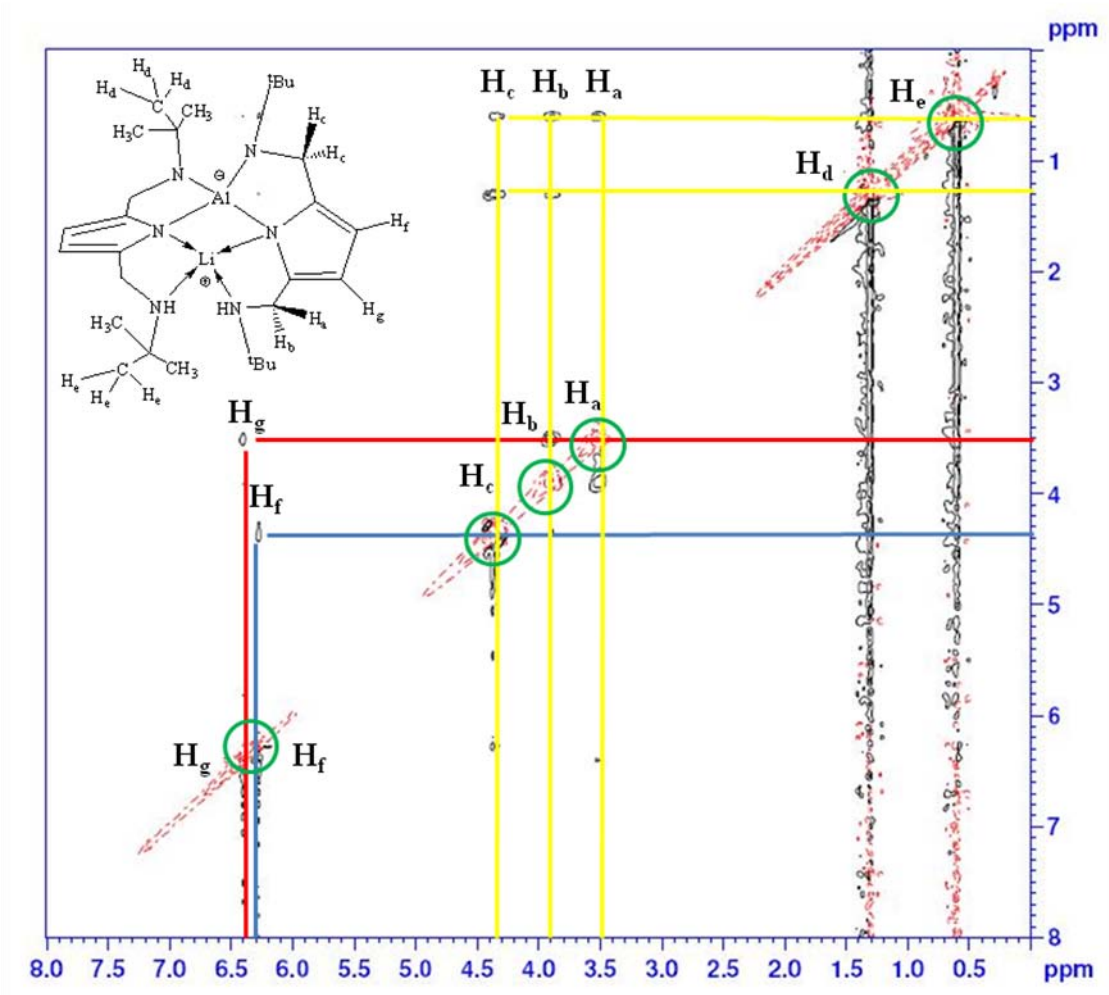
(3)



^{1}H-^{1}H NOESY 2D NMR spectrum of complex **7** in C_6D_6 using 300MHz NMR spectrometer.

(4)

Table 1. Crystal data and structure refinement for complex 2 (second set of crystal data)

Identification code	wy92m	
Empirical formula	C20 H34 Al2 N4	
Formula weight	384.47	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 9.240(4) Å	= 90°.
	b = 14.081(6) Å	= 113.124(18)°.
	c = 18.041(6) Å	= 90°.
Volume	2158.7(15) $Å^3$	
Z	4	
Density (calculated)	1.183 Mg/m^3	
Absorption coefficient	0.146 mm^{-1}	
F(000)	832	
Crystal size	0.17 x 0.15 x 0.11 mm^3	
Theta range for data collection	1.90 to 28.00°.	
Index ranges	-11<=h<=12, -18<=k<=18, -23<=l<=20	
Reflections collected	16742	
Independent reflections	5204 [R(int) = 0.1089]	
Completeness to theta = 28.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9841 and 0.9756	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5204 / 0 / 243	
Goodness-of-fit on F^2	0.924	
Final R indices [I>2sigma(I)]	R1 = 0.0548, wR2 = 0.1194	
R indices (all data)	R1 = 0.1439, wR2 = 0.1479	
Largest diff. peak and hole	0.291 and -0.360 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)
for wy92m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Al(1)	5097(1)	5715(1)	9479(1)	30(1)
Al(2)	-728(1)	5111(1)	5546(1)	38(1)
C(1)	6675(3)	5339(2)	8318(2)	44(1)
C(2)	6656(3)	4590(3)	7854(2)	56(1)
C(3)	5645(3)	3908(2)	7963(2)	46(1)
C(4)	5081(3)	4281(2)	8495(2)	31(1)
C(5)	4007(4)	3908(2)	8867(2)	41(1)
C(6)	1909(3)	4824(2)	9121(2)	30(1)
C(7)	1244(3)	5134(2)	8242(2)	43(1)
C(8)	1093(3)	3927(2)	9229(2)	42(1)
C(9)	1634(3)	5626(2)	9613(2)	35(1)
C(10)	4635(3)	7054(2)	9257(2)	50(1)
C(11)	-845(4)	3465(3)	6590(2)	56(1)
C(12)	194(5)	2780(3)	6960(2)	77(1)
C(13)	1577(5)	2964(2)	6831(2)	61(1)
C(14)	1315(4)	3783(2)	6388(2)	37(1)
C(15)	2308(4)	4336(3)	6071(2)	66(1)
C(16)	2371(3)	6105(2)	5935(2)	42(1)
C(17)	2661(4)	6219(3)	6828(2)	72(1)
C(18)	3929(3)	6075(3)	5827(2)	62(1)
C(19)	1442(3)	6967(2)	5497(2)	42(1)
C(20)	-1949(4)	6055(3)	5843(3)	75(1)
N(1)	5713(2)	5171(2)	8725(1)	33(1)
N(2)	3681(2)	4644(1)	9402(1)	28(1)
N(3)	-189(3)	4096(2)	6229(1)	38(1)
N(4)	1437(2)	5204(2)	5598(1)	37(1)

Table 3. Bond lengths [Å] and angles [°] for wy92m.

Al(1)-N(1)	1.836(2)
Al(1)-C(10)	1.940(3)
Al(1)-N(2)#1	1.955(2)
Al(1)-N(2)	1.965(2)
Al(1)-Al(1)#1	2.8086(18)
Al(2)-N(3)	1.825(3)
Al(2)-C(20)	1.951(3)
Al(2)-N(4)#2	1.954(3)
Al(2)-N(4)	1.970(2)
Al(2)-Al(2)#2	2.8037(19)
C(1)-C(2)	1.342(4)
C(1)-N(1)	1.377(3)
C(1)-H(1)	0.9500
C(2)-C(3)	1.406(4)
C(2)-H(2)	0.9500
C(3)-C(4)	1.364(4)
C(3)-H(3)	0.9500
C(4)-N(1)	1.375(3)
C(4)-C(5)	1.496(4)
C(5)-N(2)	1.524(3)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-C(9)	1.519(4)
C(6)-C(8)	1.522(4)
C(6)-C(7)	1.522(4)
C(6)-N(2)	1.533(3)
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800

C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-C(12)	1.340(5)
C(11)-N(3)	1.375(4)
C(11)-H(11)	0.9500
C(12)-C(13)	1.410(5)
C(12)-H(12)	0.9500
C(13)-C(14)	1.369(4)
C(13)-H(13)	0.9500
C(14)-N(3)	1.376(4)
C(14)-C(15)	1.479(4)
C(15)-N(4)	1.527(4)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(19)	1.517(4)
C(16)-N(4)	1.521(4)
C(16)-C(18)	1.527(4)
C(16)-C(17)	1.535(4)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
N(2)-Al(1)#1	1.954(2)
N(4)-Al(2)#2	1.954(3)

N(1)-Al(1)-C(10)	111.11(13)
N(1)-Al(1)-N(2)#1	115.86(10)
C(10)-Al(1)-N(2)#1	117.08(12)
N(1)-Al(1)-N(2)	91.09(10)
C(10)-Al(1)-N(2)	130.17(12)

N(2)#1-Al(1)-N(2)	88.47(9)
N(1)-Al(1)-Al(1)#1	108.47(9)
C(10)-Al(1)-Al(1)#1	140.19(11)
N(2)#1-Al(1)-Al(1)#1	44.39(6)
N(2)-Al(1)-Al(1)#1	44.08(7)
N(3)-Al(2)-C(20)	112.42(15)
N(3)-Al(2)-N(4)#2	115.13(11)
C(20)-Al(2)-N(4)#2	117.05(15)
N(3)-Al(2)-N(4)	90.99(11)
C(20)-Al(2)-N(4)	128.92(14)
N(4)#2-Al(2)-N(4)	88.80(10)
N(3)-Al(2)-Al(2)#2	107.95(9)
C(20)-Al(2)-Al(2)#2	139.33(14)
N(4)#2-Al(2)-Al(2)#2	44.62(7)
N(4)-Al(2)-Al(2)#2	44.18(7)
C(2)-C(1)-N(1)	110.1(3)
C(2)-C(1)-H(1)	124.9
N(1)-C(1)-H(1)	124.9
C(1)-C(2)-C(3)	107.3(3)
C(1)-C(2)-H(2)	126.4
C(3)-C(2)-H(2)	126.4
C(4)-C(3)-C(2)	107.0(3)
C(4)-C(3)-H(3)	126.5
C(2)-C(3)-H(3)	126.5
C(3)-C(4)-N(1)	109.3(3)
C(3)-C(4)-C(5)	133.2(3)
N(1)-C(4)-C(5)	117.5(2)
C(4)-C(5)-N(2)	112.1(2)
C(4)-C(5)-H(5A)	109.2
N(2)-C(5)-H(5A)	109.2
C(4)-C(5)-H(5B)	109.2
N(2)-C(5)-H(5B)	109.2
H(5A)-C(5)-H(5B)	107.9
C(9)-C(6)-C(8)	109.7(2)
C(9)-C(6)-C(7)	107.6(2)
C(8)-C(6)-C(7)	110.8(2)
C(9)-C(6)-N(2)	109.4(2)
C(8)-C(6)-N(2)	109.8(2)

C(7)-C(6)-N(2)	109.5(2)
C(6)-C(7)-H(7A)	109.5
C(6)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(6)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(6)-C(8)-H(8A)	109.5
C(6)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(6)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(6)-C(9)-H(9A)	109.5
C(6)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(6)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
Al(1)-C(10)-H(10A)	109.5
Al(1)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
Al(1)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(12)-C(11)-N(3)	109.8(3)
C(12)-C(11)-H(11)	125.1
N(3)-C(11)-H(11)	125.1
C(11)-C(12)-C(13)	107.7(3)
C(11)-C(12)-H(12)	126.1
C(13)-C(12)-H(12)	126.1
C(14)-C(13)-C(12)	106.7(3)
C(14)-C(13)-H(13)	126.7
C(12)-C(13)-H(13)	126.7
C(13)-C(14)-N(3)	108.9(3)
C(13)-C(14)-C(15)	132.4(3)
N(3)-C(14)-C(15)	118.7(2)
C(14)-C(15)-N(4)	111.5(2)

C(14)-C(15)-H(15A)	109.3
N(4)-C(15)-H(15A)	109.3
C(14)-C(15)-H(15B)	109.3
N(4)-C(15)-H(15B)	109.3
H(15A)-C(15)-H(15B)	108.0
C(19)-C(16)-N(4)	110.1(2)
C(19)-C(16)-C(18)	109.0(2)
N(4)-C(16)-C(18)	110.0(3)
C(19)-C(16)-C(17)	107.0(3)
N(4)-C(16)-C(17)	110.2(2)
C(18)-C(16)-C(17)	110.6(2)
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(16)-C(19)-H(19A)	109.5
C(16)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(16)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
Al(2)-C(20)-H(20A)	109.5
Al(2)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
Al(2)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(4)-N(1)-C(1)	106.4(2)
C(4)-N(1)-Al(1)	112.66(17)
C(1)-N(1)-Al(1)	140.9(2)

C(5)-N(2)-C(6)	110.7(2)
C(5)-N(2)-Al(1)#1	107.48(17)
C(6)-N(2)-Al(1)#1	119.56(15)
C(5)-N(2)-Al(1)	105.95(15)
C(6)-N(2)-Al(1)	119.44(16)
Al(1)#1-N(2)-Al(1)	91.54(9)
C(11)-N(3)-C(14)	106.9(3)
C(11)-N(3)-Al(2)	140.6(3)
C(14)-N(3)-Al(2)	112.12(17)
C(16)-N(4)-C(15)	110.7(2)
C(16)-N(4)-Al(2)#2	120.93(16)
C(15)-N(4)-Al(2)#2	107.0(2)
C(16)-N(4)-Al(2)	118.72(17)
C(15)-N(4)-Al(2)	106.00(17)
Al(2)#2-N(4)-Al(2)	91.20(10)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for wy92m. 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)	27(1)	24(1)	39(1)	1(1)	14(1)	1(1)
Al(2)	32(1)	29(1)	61(1)	3(1)	26(1)	-1(1)
C(1)	30(2)	71(2)	32(2)	12(2)	13(1)	0(2)
C(2)	36(2)	104(3)	32(2)	1(2)	18(2)	7(2)
C(3)	39(2)	63(2)	36(2)	-8(2)	14(1)	10(2)
C(4)	29(1)	37(2)	26(1)	5(1)	9(1)	13(1)
C(5)	60(2)	26(2)	49(2)	-2(1)	34(2)	6(2)
C(6)	25(1)	36(2)	28(1)	1(1)	9(1)	-4(1)
C(7)	41(2)	48(2)	35(2)	1(2)	10(1)	-9(2)
C(8)	34(2)	45(2)	47(2)	3(2)	17(1)	-8(2)
C(9)	28(2)	42(2)	35(2)	-1(1)	12(1)	6(1)
C(10)	39(2)	33(2)	68(2)	7(2)	10(2)	2(2)
C(11)	75(3)	64(2)	30(2)	-10(2)	22(2)	-45(2)
C(12)	100(3)	61(3)	43(2)	13(2)	0(2)	-51(3)
C(13)	79(3)	36(2)	43(2)	4(2)	-4(2)	-9(2)
C(14)	56(2)	24(2)	26(2)	2(1)	12(1)	-2(2)
C(15)	68(2)	67(2)	78(3)	47(2)	46(2)	32(2)
C(16)	34(2)	58(2)	33(2)	13(2)	11(1)	-11(2)
C(17)	55(2)	118(3)	36(2)	17(2)	9(2)	-27(2)
C(18)	34(2)	88(3)	61(2)	26(2)	16(2)	-11(2)
C(19)	53(2)	35(2)	38(2)	-5(2)	18(2)	-15(2)
C(20)	53(2)	54(2)	128(4)	-19(2)	48(2)	-2(2)
N(1)	27(1)	43(2)	30(1)	11(1)	12(1)	4(1)
N(2)	27(1)	25(1)	35(1)	-7(1)	16(1)	-3(1)
N(3)	52(2)	36(1)	32(1)	-3(1)	22(1)	-13(1)
N(4)	30(1)	35(1)	50(2)	21(1)	18(1)	7(1)