

Supporting Information

Title: Magnesium complexes supported by pyrrolyl ligands: synthesis, characterization, and catalytic activity toward the polymerization of ϵ -caprolactone

Authors:

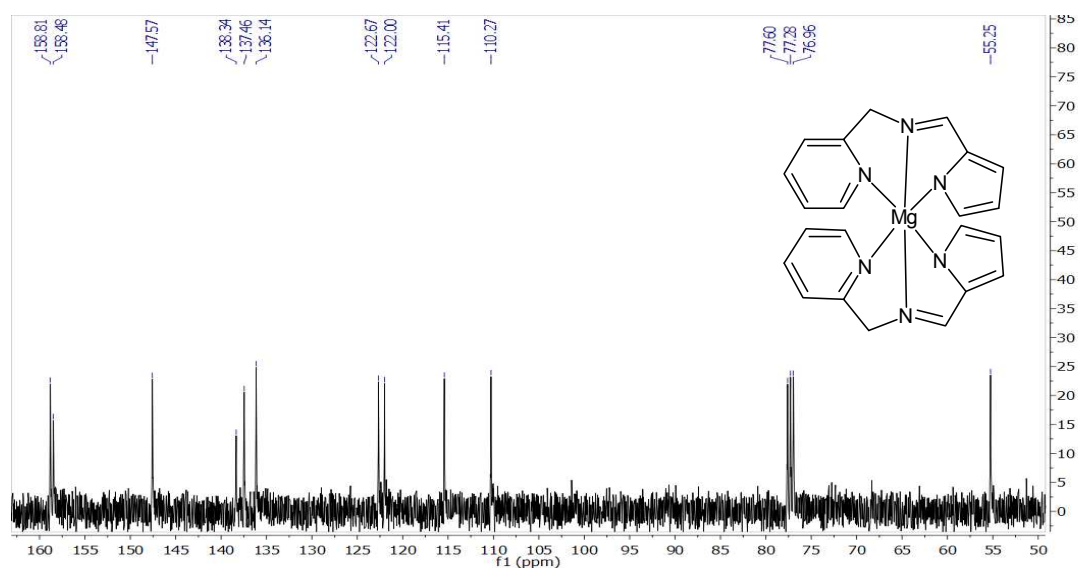
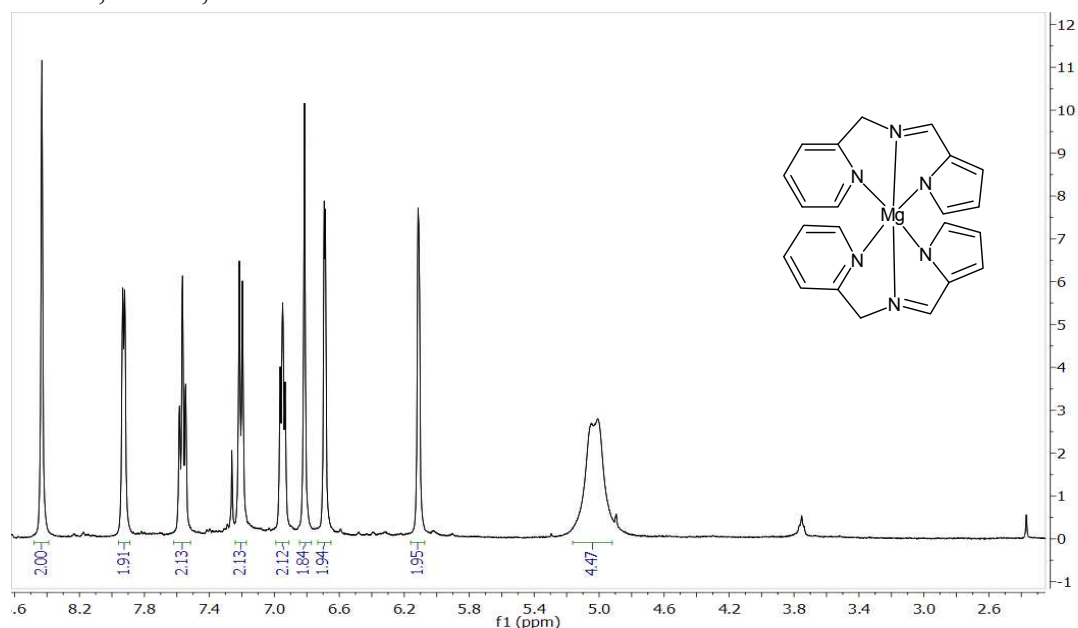
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Xiaoyu Wan, Tao Lei, Yahong Li

1. ^1H and ^{13}C NMR spectra for the complexes **1-5**.
2. Crystallography data for complexes **2-4**.

1. ^1H and ^{13}C NMR spectra for the complexes **1-5**.

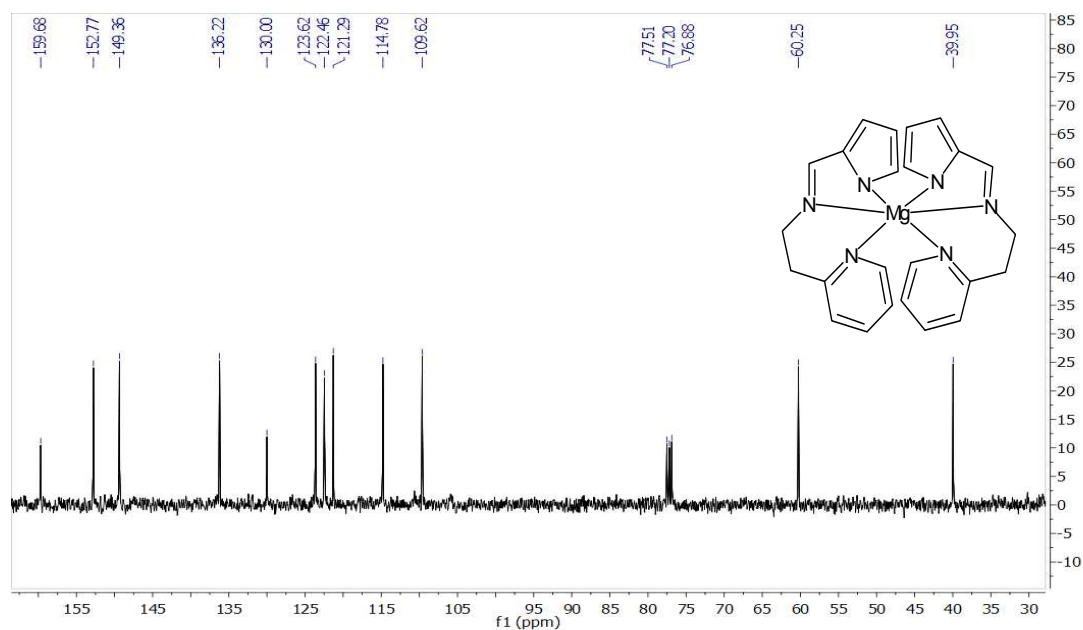
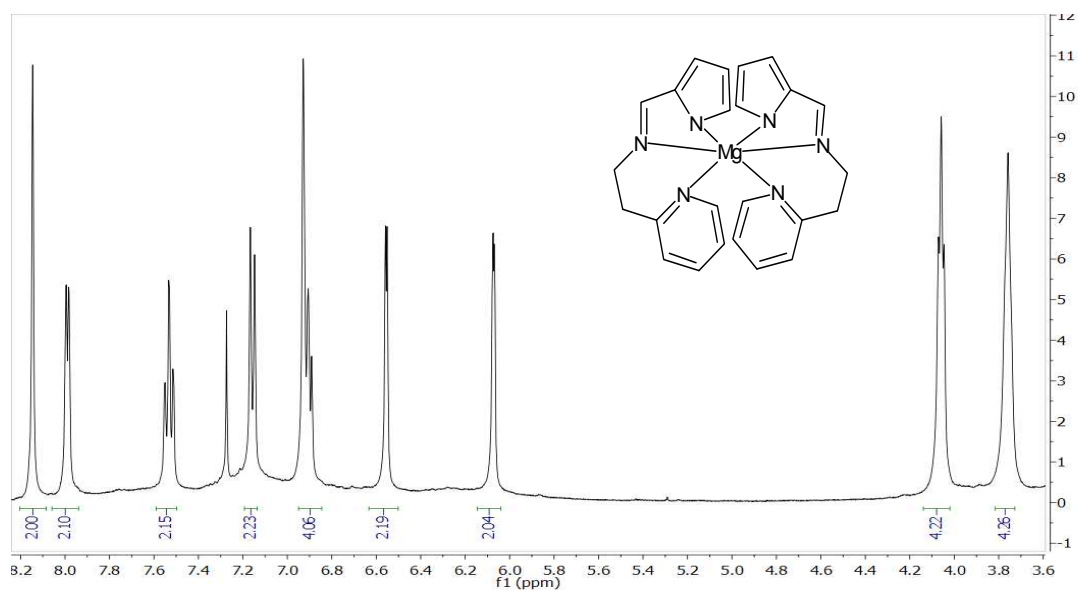
1.1 ^1H and ^{13}C NMR spectra for $\text{Mg}(\text{L1})_2$ (**1**)

^1H NMR (400 MHz, CDCl_3) δ 8.43 (s, 2H, N=CH), 7.93 (d, 2H, $J = 4.7$ Hz, pyridyl-H), 7.56 (t, 2H, $J = 7.5$ Hz, pyridyl-H), 7.21 (d, 2H, $J = 7.8$ Hz, pyridyl-H), 6.99 – 6.91 (m, 2H, pyridyl-H), 6.81 (s, 2H, pyrrole-H), 6.69 (d, $J = 3.0$ Hz, 2H, pyrrole-H), 6.11 (d, $J = 1.8$ Hz, 2H, pyrrole-H), 5.01 (s, 4H, NCH_2). ^{13}C NMR (101 MHz, CDCl_3) δ 158.81, 158.48, 147.57, 138.34, 137.46, 136.14, 122.67, 122.00, 115.41, 110.27, 5.25.



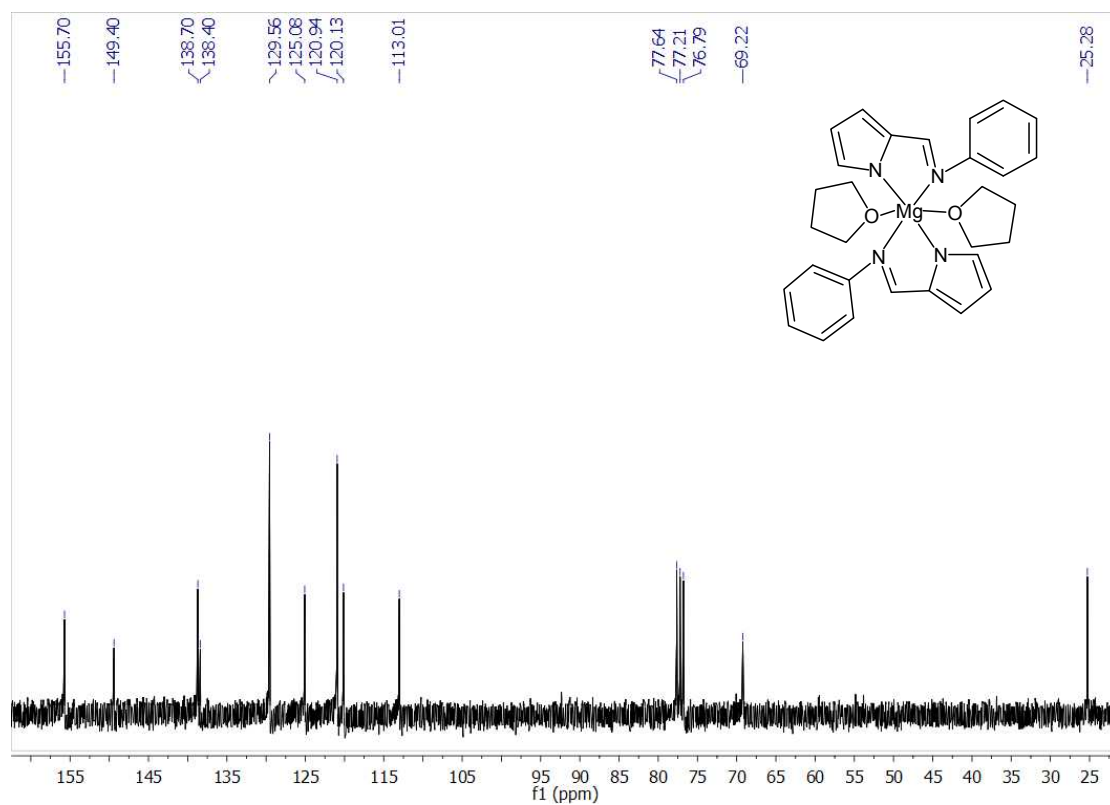
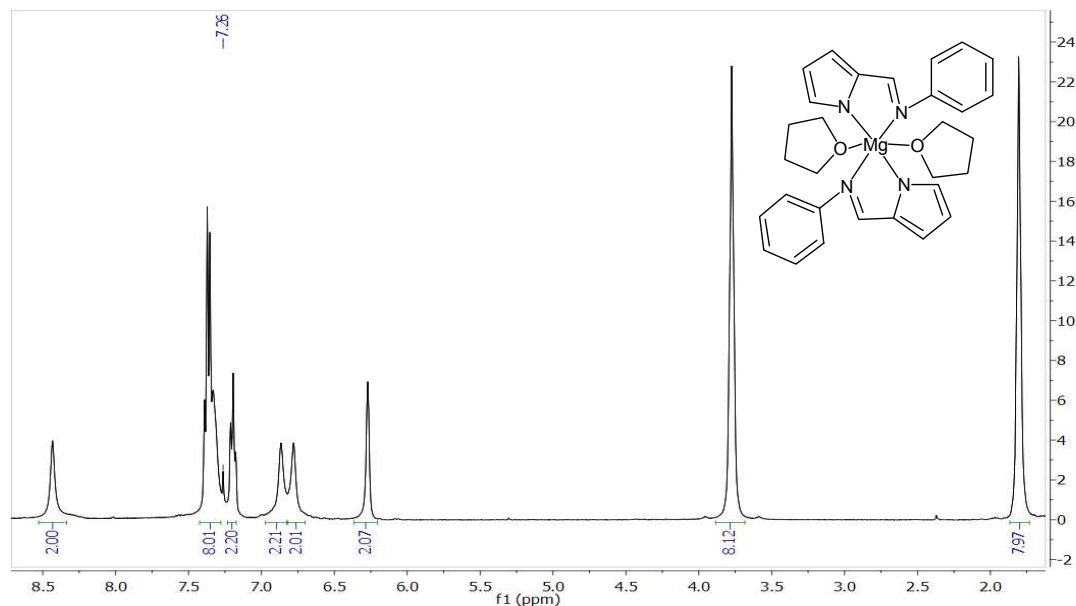
1.2 ^1H and ^{13}C NMR spectra for $\text{Mg}(\text{L}2)_2$ (**2**)

^1H NMR (400 MHz, CDCl_3) δ 8.15 (s, 2H, N=CH), 7.99 (d, 2H, $J = 4.4$ Hz, pyridyl-H), 7.53 (td, $J = 7.6, 1.6$ Hz, 2H, pyridyl-H), 7.16 (d, $J = 7.7$ Hz, 2H, pyridyl-H), 6.95 – 6.84 (m, 4H, pyridyl-H+ pyrrole-H), 6.55 (d, $J = 2.8$ Hz, 2H, pyrrole-H), 6.15 – 6.04 (m, 2H, pyrrole-H), 4.14 – 4.02 (m, 4H, CH_2 -pyridyl), 3.76 (s, 4H, NCH_2). ^{13}C NMR (101 MHz, CDCl_3) δ 159.68, 152.77, 149.36, 136.22, 130.00, 123.62, 122.46, 121.29, 114.78, 109.62, 60.25, 39.95.



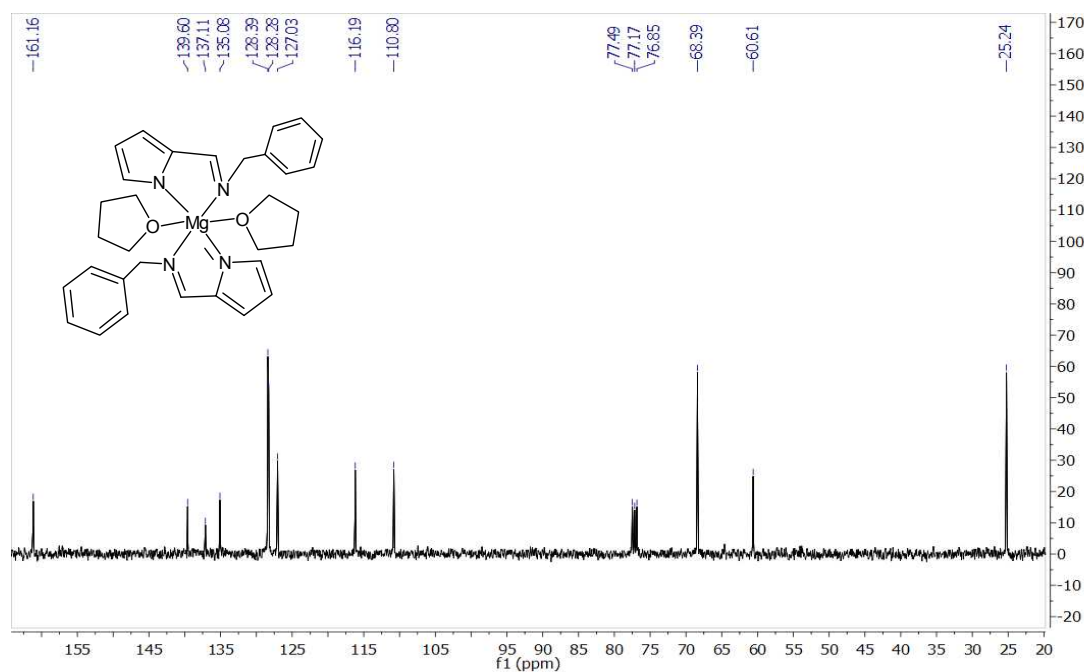
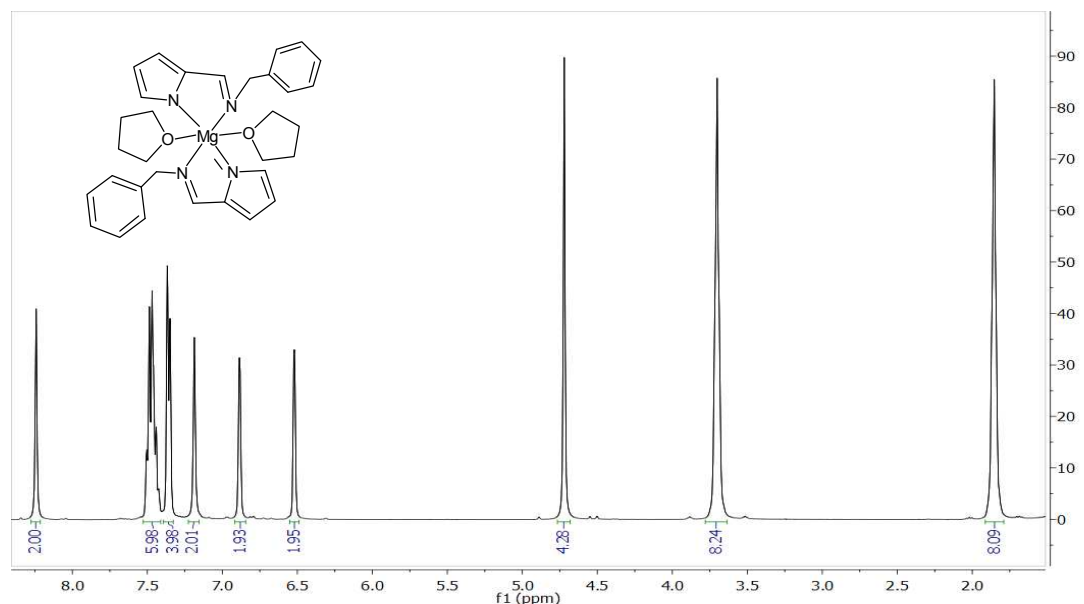
1.3 ^1H and ^{13}C NMR spectra for $\text{Mg}(\text{L3})_2(\text{THF})_2$ (**3**)

^1H NMR (400 MHz, CDCl_3) δ 8.43 (s, 2H, N=CH), 7.36 (dd, $J = 15.5$, 8H, Ar-H), 7.19 (t, $J = 7.0$ Hz, 2H, Ar-H), 6.87 (s, 2H, pyrrole-H), 6.78 (s, 2H, pyrrole-H), 6.27 (s, 2H, pyrrole-H), 3.77 (s, 8H, CH_2O of THF), 1.81 (s, 8H, CH_2 of THF). ^{13}C NMR (75 MHz, CDCl_3) δ 155.70, 149.40, 138.70, 138.40, 129.56, 125.08, 120.94, 120.13, 113.01, 69.22, 25.28.



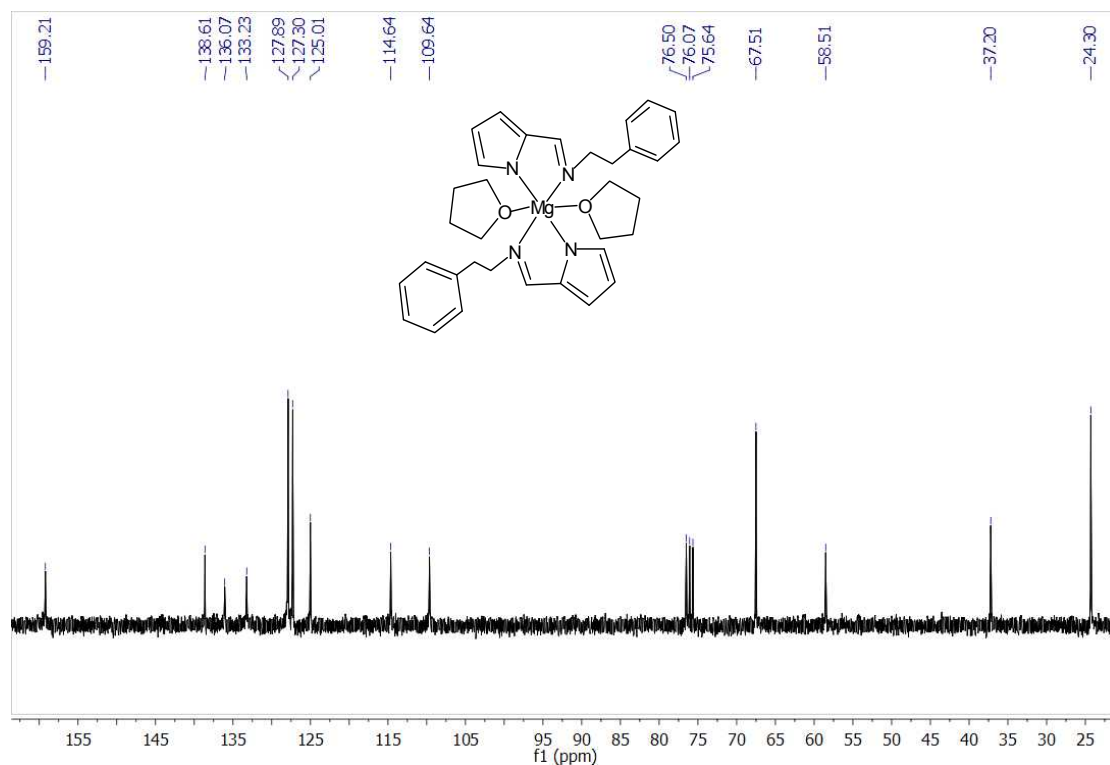
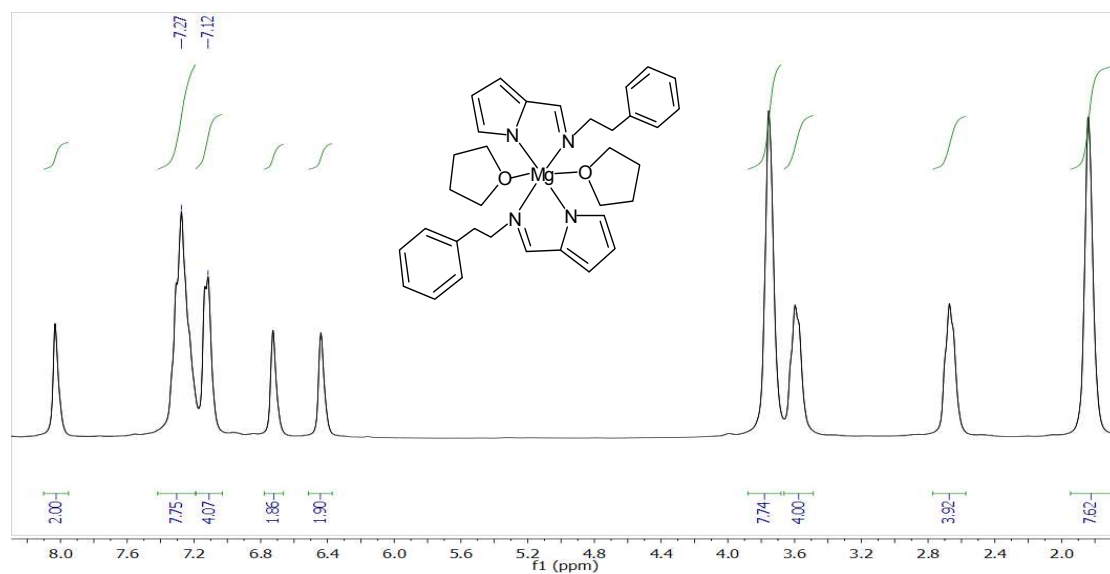
1.4 ^1H and ^{13}C NMR spectra for $\text{Mg}(\text{L4})_2(\text{THF})_2$ (**4**)

^1H NMR (400 MHz, CDCl_3) δ 8.24 (s, 2H, N=CH), 7.53 – 7.41 (m, 6H, Ar-H), 7.36 (d, $J = 7.3$ Hz, 4H, Ar-H), 7.19 (s, 2H, pyrrole-H), 6.89 (s, 2H, pyrrole-H), 6.52 (d, $J = 1.5$ Hz, 2H, pyrrole-H), 4.72 (s, 4H, NCH_2), 3.70 (s, 8H, CH_2O of THF), 1.85 (s, 8H, CH_2 of THF). ^{13}C NMR (100 MHz, CDCl_3) δ 161.16, 139.60, 137.11, 135.08, 128.39, 128.28, 127.03, 116.19, 110.80, 68.39, 60.61, 25.24.



1.5 ^1H and ^{13}C NMR spectra for $\text{Mg}(\text{L5})_2(\text{THF})_2$ (**5**)

^1H NMR (300 MHz, CDCl_3) δ 8.03 (s, 2H, N=CH), 7.37 -7.15(s, 8H, Ar-H), 7.15-7.05 (s, 4H, Ar-H+ pyrrole-H), 6.73 (s, 2H, pyrrole-H), 6.44 (s, 2H, pyrrole-H), 3.70 (s, 8H, CH_2O of THF), 3.60 (s, 4H, $\text{CH}_2\text{-Ar}$, 2.67 (s, 4H, NCH_2), 1.85 (s, 8H, CH_2 of THF). ^{13}C NMR (75 MHz, CDCl_3) δ 160.41, 139.81, 137.27, 134.43, 129.09, 128.50, 126.21, 115.84, 110.84, 68.71, 59.71, 38.40, 25.50.



2. Crystallography data for complexes **2-4**.

2.1 Crystal data for **2-4**

	2	3	4
Formula ^a	C ₂₄ H ₂₄ MgN ₆	C ₃₀ H ₃₄ MgN ₄ O ₂	C ₃₂ H ₃₈ MgN ₄ O ₂
M / g mol ⁻¹ ^a	420.80	506.92	534.97
Temperature/K	293(2)	293(2)	293(2)
Wavelength ^b / Å	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Triclinic
Space group	<i>C</i> 2/ <i>c</i>	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> $\bar{1}$
<i>a</i> / Å	28.215(6)	9.986(2)	10.453(2)
<i>b</i> / Å	16.504(3)	14.269(3)	11.456(2)
<i>c</i> / Å	14.405(3)	19.278(4)	12.516(3)
<i>α</i> / °	90	90	84.02(3)
<i>β</i> / °	98.59(3)	92.42(3)	76.88(3)
<i>γ</i> / °	90	90	89.43(3)
<i>V</i> / Å ³	6633(2)	2744.5(10)	1451.7(5)
<i>Z</i>	12	4	2
<i>ρ</i> / g cm ⁻³	1.264	1.227	1.224
<i>F</i> (000)	2664	1080	572
Crystal size/ mm ³	0.40 x 0.30 x 0.15	0.23 x 0.21 x 0.19	0.25 x 0.20 x 0.17
<i>θ</i> range/ °	3.05 to 25.02°	3.04 to 27.47°	1.68 to 28.36°
Limiting indices	-29 ≤ <i>h</i> ≤ 33 -19 ≤ <i>k</i> ≤ 18 -17 ≤ <i>l</i> ≤ 16	-12 ≤ <i>h</i> ≤ 12 -18 ≤ <i>k</i> ≤ 16 -25 ≤ <i>l</i> ≤ 20	-13 ≤ <i>h</i> ≤ 13 -15 ≤ <i>k</i> ≤ 15 -16 ≤ <i>l</i> ≤ 15
Reflections collected / unique	16422 / 5828	14835 / 6228	26473 / 7247
Data / restraints / parameters	5828 / 0 / 421	6228 / 7 / 334	6228 / 7 / 334
GOF	1.181	1.157	1.066
<i>R</i> ₁ , <i>wR</i> ₂ [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0927	<i>R</i> ₁ = 0.0980	<i>R</i> ₁ = 0.0556

	$wR_2 = 0.1372$	$wR_2 = 0.2011$	$wR_2 = 0.1497$
	$R_1 = 0.1359$	$R_1 = 0.1504$	$R_1 = 0.0685$
$R_1^c, wR_2^{d,e}$ (all data)	$wR_2 = 0.1537$	$wR_2 = 0.2289$	$wR_2 = 0.1597$
Largest diff. peak and hole/ e Å ³	0.284 and -0.254	0.488 and -0.736	0.519 and -0.501

^a Including solvate molecules. ^b Mo K α radiation. ^c $R_1 = \Sigma(|F_o| - |F_c|) / \Sigma(|F_o|)$ for observed reflections. ^d $w = 1 / [\sigma^2(F_o^2) + (aP)^2 + bP]$ and $P = [\max(F_o^2, 0) + 2Fc^2] / 3$. ^e $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{1/2}$ for all data.

2.2 Bond angles and distances for complex 2

Mg(2)-N(7)	2.150(3)
Mg(2)-N(7)#1	2.150(3)
Mg(2)-N(8)	2.188(3)
Mg(2)-N(8)#1	2.188(3)
Mg(2)-N(9)#1	2.301(3)
Mg(2)-N(9)	2.301(3)
N(9)-C(24)	1.342(5)
N(9)-C(11)	1.355(4)
Mg(1)-N(6)	2.156(4)
Mg(1)-N(5)	2.162(3)
Mg(1)-N(3)	2.169(4)
Mg(1)-N(2)	2.176(3)
Mg(1)-N(1)	2.307(4)
Mg(1)-N(4)	2.320(4)

N(7)-C(17)	1.341(5)
N(7)-C(20)	1.379(4)
N(6)-C(23)	1.352(5)
N(6)-C(19)	1.373(5)
N(8)-C(9)	1.281(5)
N(8)-C(13)	1.459(4)
N(2)-C(22)	1.292(5)
N(2)-C(25)	1.460(5)
N(5)-C(29)	1.282(5)
N(5)-C(33)	1.462(5)
N(1)-C(28)	1.349(4)
N(1)-C(31)	1.350(5)
N(4)-C(27)	1.345(5)
N(4)-C(35)	1.354(5)
C(9)-C(20)	1.424(5)
C(9)-H(9)	0.9300
C(10)-C(28)	1.505(5)
C(10)-C(25)	1.516(6)
C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700
C(11)-C(15)	1.373(5)
C(11)-C(16)	1.504(5)

C(12)-C(24)	1.370(6)
C(12)-C(38)	1.377(5)
C(12)-H(12)	0.9300
C(13)-C(16)#1	1.527(5)
C(13)-H(13A)	0.9700
C(13)-H(13B)	0.9700
N(3)-C(40)	1.346(5)
N(3)-C(30)	1.385(5)
C(15)-C(38)	1.367(6)
C(15)-H(15)	0.9300
C(16)-C(13)#1	1.527(5)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(17)-C(34)	1.394(6)
C(17)-H(17)	0.9300
C(18)-C(43)	1.370(6)
C(18)-C(28)	1.381(6)
C(18)-H(18)	0.9300
C(19)-C(44)	1.384(6)
C(19)-C(29)	1.430(5)
C(20)-C(21)	1.384(5)
C(21)-C(34)	1.389(5)

C(21)-H(21)	0.9300
C(22)-C(30)	1.416(6)
C(22)-H(22)	0.9300
C(23)-C(42)	1.389(6)
C(23)-H(23)	0.9300
C(24)-H(24)	0.9300
C(25)-H(25A)	0.9700
C(25)-H(25B)	0.9700
C(26)-C(31)	1.364(6)
C(26)-C(43)	1.369(5)
C(26)-H(26)	0.9300
C(27)-C(41)	1.382(6)
C(27)-C(32)	1.504(6)
C(29)-H(29)	0.9300
C(30)-C(36)	1.387(6)
C(31)-H(31)	0.9300
C(32)-C(33)	1.515(6)
C(32)-H(32A)	0.9700
C(32)-H(32B)	0.9700
C(33)-H(33A)	0.9700
C(33)-H(33B)	0.9700
C(34)-H(34)	0.9300

C(35)-C(37)	1.367(6)
C(35)-H(35)	0.9300
C(36)-C(39)	1.378(6)
C(36)-H(36)	0.9300
C(37)-C(45)	1.377(6)
C(37)-H(37)	0.9300
C(38)-H(38)	0.9300
C(39)-C(40)	1.399(6)
C(39)-H(39)	0.9300
C(40)-H(40)	0.9300
C(41)-C(45)	1.375(7)
C(41)-H(41)	0.9300
C(42)-C(44)	1.389(6)
C(42)-H(42)	0.9300
C(43)-H(43)	0.9300
C(44)-H(44)	0.9300
C(45)-H(45)	0.9300
N(7)-Mg(2)-N(7)#1	93.69(18)
N(7)-Mg(2)-N(8)	77.67(11)
N(7)#1-Mg(2)-N(8)	105.72(12)
N(7)-Mg(2)-N(8)#1	105.72(12)

N(7)#1-Mg(2)-N(8)#1	77.67(11)
N(8)-Mg(2)-N(8)#1	175.18(19)
N(7)-Mg(2)-N(9)#1	160.01(10)
N(7)#1-Mg(2)-N(9)#1	92.52(12)
N(8)-Mg(2)-N(9)#1	82.36(11)
N(8)#1-Mg(2)-N(9)#1	94.16(11)
N(7)-Mg(2)-N(9)	92.52(12)
N(7)#1-Mg(2)-N(9)	160.01(10)
N(8)-Mg(2)-N(9)	94.16(11)
N(8)#1-Mg(2)-N(9)	82.36(11)
N(9)#1-Mg(2)-N(9)	88.04(17)
C(24)-N(9)-C(11)	116.6(3)
C(24)-N(9)-Mg(2)	118.3(2)
C(11)-N(9)-Mg(2)	125.1(3)
N(6)-Mg(1)-N(5)	77.90(13)
N(6)-Mg(1)-N(3)	103.93(14)
N(5)-Mg(1)-N(3)	101.98(13)
N(6)-Mg(1)-N(2)	105.47(13)
N(5)-Mg(1)-N(2)	176.56(15)
N(3)-Mg(1)-N(2)	77.97(13)
N(6)-Mg(1)-N(1)	93.27(13)
N(5)-Mg(1)-N(1)	96.59(13)

N(3)-Mg(1)-N(1)	156.89(14)
N(2)-Mg(1)-N(1)	82.67(13)
N(6)-Mg(1)-N(4)	159.88(13)
N(5)-Mg(1)-N(4)	82.49(13)
N(3)-Mg(1)-N(4)	84.44(13)
N(2)-Mg(1)-N(4)	94.09(13)
N(1)-Mg(1)-N(4)	84.47(12)
C(17)-N(7)-C(20)	105.2(3)
C(17)-N(7)-Mg(2)	143.0(3)
C(20)-N(7)-Mg(2)	111.4(2)
C(23)-N(6)-C(19)	104.9(4)
C(23)-N(6)-Mg(1)	144.0(3)
C(19)-N(6)-Mg(1)	111.0(3)
C(9)-N(8)-C(13)	118.3(3)
C(9)-N(8)-Mg(2)	112.5(2)
C(13)-N(8)-Mg(2)	128.1(2)
C(22)-N(2)-C(25)	117.8(3)
C(22)-N(2)-Mg(1)	112.0(3)
C(25)-N(2)-Mg(1)	130.2(3)
C(29)-N(5)-C(33)	119.2(3)
C(29)-N(5)-Mg(1)	112.9(3)
C(33)-N(5)-Mg(1)	127.6(3)

C(28)-N(1)-C(31)	116.7(3)
C(28)-N(1)-Mg(1)	124.9(3)
C(31)-N(1)-Mg(1)	117.8(3)
C(27)-N(4)-C(35)	116.9(4)
C(27)-N(4)-Mg(1)	125.0(3)
C(35)-N(4)-Mg(1)	116.7(3)
N(8)-C(9)-C(20)	120.2(3)
N(8)-C(9)-H(9)	119.9
C(20)-C(9)-H(9)	119.9
C(28)-C(10)-C(25)	113.8(4)
C(28)-C(10)-H(10A)	108.8
C(25)-C(10)-H(10A)	108.8
C(28)-C(10)-H(10B)	108.8
C(25)-C(10)-H(10B)	108.8
H(10A)-C(10)-H(10B)	107.7
N(9)-C(11)-C(15)	121.8(4)
N(9)-C(11)-C(16)	117.6(3)
C(15)-C(11)-C(16)	120.7(3)
C(24)-C(12)-C(38)	118.5(4)
C(24)-C(12)-H(12)	120.8
C(38)-C(12)-H(12)	120.8
N(8)-C(13)-C(16)#1	107.9(3)

N(8)-C(13)-H(13A)	110.1
C(16)#1-C(13)-H(13A)	110.1
N(8)-C(13)-H(13B)	110.1
C(16)#1-C(13)-H(13B)	110.1
H(13A)-C(13)-H(13B)	108.4
C(40)-N(3)-C(30)	104.7(3)
C(40)-N(3)-Mg(1)	144.1(3)
C(30)-N(3)-Mg(1)	110.0(3)
C(38)-C(15)-C(11)	120.6(4)
C(38)-C(15)-H(15)	119.7
C(11)-C(15)-H(15)	119.7
C(11)-C(16)-C(13)#1	113.1(3)
C(11)-C(16)-H(16A)	109.0
C(13)#1-C(16)-H(16A)	109.0
C(11)-C(16)-H(16B)	109.0
C(13)#1-C(16)-H(16B)	109.0
H(16A)-C(16)-H(16B)	107.8
N(7)-C(17)-C(34)	111.8(4)
N(7)-C(17)-H(17)	124.1
C(34)-C(17)-H(17)	124.1
C(43)-C(18)-C(28)	119.7(4)
C(43)-C(18)-H(18)	120.1

C(28)-C(18)-H(18)	120.1
N(6)-C(19)-C(44)	110.8(4)
N(6)-C(19)-C(29)	117.8(4)
C(44)-C(19)-C(29)	131.3(4)
N(7)-C(20)-C(21)	110.8(3)
N(7)-C(20)-C(9)	118.1(3)
C(21)-C(20)-C(9)	130.8(4)
C(20)-C(21)-C(34)	106.3(4)
C(20)-C(21)-H(21)	126.8
C(34)-C(21)-H(21)	126.8
N(2)-C(22)-C(30)	120.8(4)
N(2)-C(22)-H(22)	119.6
C(30)-C(22)-H(22)	119.6
N(6)-C(23)-C(42)	111.9(4)
N(6)-C(23)-H(23)	124.0
C(42)-C(23)-H(23)	124.0
N(9)-C(24)-C(12)	124.2(4)
N(9)-C(24)-H(24)	117.9
C(12)-C(24)-H(24)	117.9
N(2)-C(25)-C(10)	109.4(3)
N(2)-C(25)-H(25A)	109.8
C(10)-C(25)-H(25A)	109.8

N(2)-C(25)-H(25B)	109.8
C(10)-C(25)-H(25B)	109.8
H(25A)-C(25)-H(25B)	108.2
C(31)-C(26)-C(43)	118.4(4)
C(31)-C(26)-H(26)	120.8
C(43)-C(26)-H(26)	120.8
N(4)-C(27)-C(41)	121.3(4)
N(4)-C(27)-C(32)	118.8(4)
C(41)-C(27)-C(32)	119.9(4)
N(1)-C(28)-C(18)	121.9(4)
N(1)-C(28)-C(10)	117.4(4)
C(18)-C(28)-C(10)	120.7(3)
N(5)-C(29)-C(19)	120.1(4)
N(5)-C(29)-H(29)	120.0
C(19)-C(29)-H(29)	120.0
N(3)-C(30)-C(36)	110.5(4)
N(3)-C(30)-C(22)	118.1(4)
C(36)-C(30)-C(22)	131.4(4)
N(1)-C(31)-C(26)	124.0(4)
N(1)-C(31)-H(31)	118.0
C(26)-C(31)-H(31)	118.0
C(27)-C(32)-C(33)	115.6(4)

C(27)-C(32)-H(32A)	108.4
C(33)-C(32)-H(32A)	108.4
C(27)-C(32)-H(32B)	108.4
C(33)-C(32)-H(32B)	108.4
H(32A)-C(32)-H(32B)	107.5
N(5)-C(33)-C(32)	110.3(3)
N(5)-C(33)-H(33A)	109.6
C(32)-C(33)-H(33A)	109.6
N(5)-C(33)-H(33B)	109.6
C(32)-C(33)-H(33B)	109.6
H(33A)-C(33)-H(33B)	108.1
C(21)-C(34)-C(17)	105.9(4)
C(21)-C(34)-H(34)	127.0
C(17)-C(34)-H(34)	127.0
N(4)-C(35)-C(37)	124.3(4)
N(4)-C(35)-H(35)	117.9
C(37)-C(35)-H(35)	117.9
C(39)-C(36)-C(30)	107.1(4)
C(39)-C(36)-H(36)	126.5
C(30)-C(36)-H(36)	126.5
C(35)-C(37)-C(45)	118.3(5)
C(35)-C(37)-H(37)	120.9

C(45)-C(37)-H(37)	120.9
C(15)-C(38)-C(12)	118.3(4)
C(15)-C(38)-H(38)	120.9
C(12)-C(38)-H(38)	120.9
C(36)-C(39)-C(40)	105.6(4)
C(36)-C(39)-H(39)	127.2
C(40)-C(39)-H(39)	127.2
N(3)-C(40)-C(39)	112.1(4)
N(3)-C(40)-H(40)	124.0
C(39)-C(40)-H(40)	124.0
C(45)-C(41)-C(27)	120.7(4)
C(45)-C(41)-H(41)	119.6
C(27)-C(41)-H(41)	119.6
C(44)-C(42)-C(23)	105.6(4)
C(44)-C(42)-H(42)	127.2
C(23)-C(42)-H(42)	127.2
C(26)-C(43)-C(18)	119.1(4)
C(26)-C(43)-H(43)	120.4
C(18)-C(43)-H(43)	120.4
C(19)-C(44)-C(42)	106.7(4)
C(19)-C(44)-H(44)	126.7
C(42)-C(44)-H(44)	126.7

C(41)-C(45)-C(37)	118.4(4)
C(41)-C(45)-H(45)	120.8
C(37)-C(45)-H(45)	120.8

2.3 Bond angles and distances for complex **3**

Mg(1)-O(1)	2.121(3)
Mg(1)-N(3)	2.125(3)
Mg(1)-O(2)	2.141(3)
Mg(1)-N(1)	2.144(3)
Mg(1)-N(4)	2.257(3)
Mg(1)-N(2)	2.261(3)
N(2)-C(5)	1.301(4)
N(2)-C(6)	1.426(4)
N(4)-C(16)	1.302(4)
N(4)-C(17)	1.423(4)
O(2)-C(27)	1.418(5)
O(2)-C(30)	1.426(5)
N(1)-C(4)	1.340(4)
N(1)-C(1)	1.375(4)
O(1)-C(23)	1.441(4)
O(1)-C(26)	1.443(5)
N(3)-C(15)	1.337(4)
N(3)-C(12)	1.380(4)
C(5)-C(1)	1.413(5)
C(12)-C(16)	1.399(5)
C(12)-C(13)	1.410(5)
C(6)-C(11)	1.388(5)
C(6)-C(7)	1.389(5)
C(1)-C(2)	1.393(5)
C(17)-C(18)	1.390(5)
C(17)-C(22)	1.393(5)
C(2)-C(3)	1.373(5)
C(15)-C(14)	1.388(5)
C(11)-C(10)	1.380(5)
C(18)-C(19)	1.388(5)
C(4)-C(3)	1.391(5)
C(9)-C(10)	1.373(5)

C(9)-C(8)	1.386(5)
C(8)-C(7)	1.379(5)
C(20)-C(21)	1.359(6)
C(20)-C(19)	1.381(6)
C(14)-C(13)	1.373(5)
C(22)-C(21)	1.394(6)
C(26)-C(25)	1.455(6)
C(30)-C(29)	1.468(6)
C(23)-C(24)	1.492(7)
C(29)-C(28)	1.476(7)
C(27)-C(28)	1.465(6)
C(24)-C(25)	1.432(7)
O(1)-Mg(1)-N(3)	90.74(11)
O(1)-Mg(1)-O(2)	177.82(12)
N(3)-Mg(1)-O(2)	89.06(11)
O(1)-Mg(1)-N(1)	92.82(11)
N(3)-Mg(1)-N(1)	175.95(12)
O(2)-Mg(1)-N(1)	87.46(11)
O(1)-Mg(1)-N(4)	89.02(11)
N(3)-Mg(1)-N(4)	78.67(11)
O(2)-Mg(1)-N(4)	88.81(11)
N(1)-Mg(1)-N(4)	103.31(11)
O(1)-Mg(1)-N(2)	90.76(11)
N(3)-Mg(1)-N(2)	99.53(12)
O(2)-Mg(1)-N(2)	91.41(11)
N(1)-Mg(1)-N(2)	78.49(11)
N(4)-Mg(1)-N(2)	178.19(11)
C(5)-N(2)-C(6)	117.0(3)
C(5)-N(2)-Mg(1)	108.5(2)
C(6)-N(2)-Mg(1)	134.1(2)
C(16)-N(4)-C(17)	117.5(3)
C(16)-N(4)-Mg(1)	108.5(2)
C(17)-N(4)-Mg(1)	134.0(2)
C(27)-O(2)-C(30)	109.5(3)
C(27)-O(2)-Mg(1)	123.2(2)
C(30)-O(2)-Mg(1)	126.8(2)
C(4)-N(1)-C(1)	104.9(3)
C(4)-N(1)-Mg(1)	144.4(3)
C(1)-N(1)-Mg(1)	110.4(2)
C(23)-O(1)-C(26)	109.1(3)
C(23)-O(1)-Mg(1)	125.9(2)
C(26)-O(1)-Mg(1)	124.7(2)
C(15)-N(3)-C(12)	105.7(3)

C(15)-N(3)-Mg(1)	142.9(3)
C(12)-N(3)-Mg(1)	110.8(2)
N(2)-C(5)-C(1)	121.6(3)
N(3)-C(12)-C(16)	120.0(3)
N(3)-C(12)-C(13)	109.4(3)
C(16)-C(12)-C(13)	130.5(3)
C(11)-C(6)-C(7)	118.7(3)
C(11)-C(6)-N(2)	119.6(3)
C(7)-C(6)-N(2)	121.7(3)
N(1)-C(1)-C(2)	110.7(3)
N(1)-C(1)-C(5)	120.2(3)
C(2)-C(1)-C(5)	129.1(3)
C(18)-C(17)-C(22)	119.3(3)
C(18)-C(17)-N(4)	118.8(3)
C(22)-C(17)-N(4)	121.9(3)
N(4)-C(16)-C(12)	121.9(3)
C(3)-C(2)-C(1)	106.3(3)
N(3)-C(15)-C(14)	112.0(4)
C(10)-C(11)-C(6)	120.9(3)
C(19)-C(18)-C(17)	120.2(4)
N(1)-C(4)-C(3)	111.9(3)
C(10)-C(9)-C(8)	120.1(3)
C(7)-C(8)-C(9)	119.9(4)
C(8)-C(7)-C(6)	120.5(3)
C(9)-C(10)-C(11)	119.8(3)
C(21)-C(20)-C(19)	120.1(4)
C(13)-C(14)-C(15)	106.4(3)
C(20)-C(19)-C(18)	120.0(4)
C(2)-C(3)-C(4)	106.3(3)
C(17)-C(22)-C(21)	119.3(4)
C(20)-C(21)-C(22)	121.1(4)
O(1)-C(26)-C(25)	106.3(4)
C(14)-C(13)-C(12)	106.5(3)
O(2)-C(30)-C(29)	106.8(3)
O(1)-C(23)-C(24)	105.9(4)
C(30)-C(29)-C(28)	105.4(4)
O(2)-C(27)-C(28)	106.8(4)
C(25)-C(24)-C(23)	105.9(4)
C(27)-C(28)-C(29)	104.5(4)
C(24)-C(25)-C(26)	107.2(4)

2.4 Bond angles and distances for complex 4

Mg(1)-N(1)	2.1393(15)
Mg(1)-O(1)	2.1406(16)
Mg(1)-O(2)	2.1455(15)
Mg(1)-N(3)	2.1480(15)
Mg(1)-N(2)	2.1938(17)
Mg(1)-N(4)	2.2124(16)
N(4)-C(17)	1.284(2)
N(4)-C(18)	1.469(2)
N(2)-C(5)	1.284(2)
N(2)-C(6)	1.463(2)
N(1)-C(1)	1.354(2)
N(1)-C(4)	1.378(2)
O(2)-C(29)	1.424(3)
O(2)-C(32)	1.435(2)
N(3)-C(13)	1.351(2)
N(3)-C(16)	1.378(2)
O(1)-C(25)	1.411(3)
O(1)-C(28)	1.426(3)
C(7)-C(12)	1.384(2)
C(7)-C(8)	1.386(2)
C(7)-C(6)	1.512(2)

C(19)-C(24)	1.385(3)
C(19)-C(20)	1.385(3)
C(19)-C(18)	1.507(3)
C(17)-C(16)	1.432(2)
C(4)-C(3)	1.394(2)
C(4)-C(5)	1.431(3)
C(13)-C(14)	1.388(3)
C(16)-C(15)	1.394(2)
C(15)-C(14)	1.388(3)
C(12)-C(11)	1.386(3)
C(8)-C(9)	1.389(3)
C(3)-C(2)	1.387(3)
C(1)-C(2)	1.389(3)
C(24)-C(23)	1.382(3)
C(9)-C(10)	1.377(3)
C(32)-C(31)	1.502(3)
C(10)-C(11)	1.374(3)
C(20)-C(21)	1.380(3)
C(23)-C(22)	1.375(4)
C(21)-C(22)	1.380(3)
C(25)-C(26)	1.462(4)
C(29)-C(30)	1.391(5)

C(26)-C(27)	1.456(5)
C(28)-C(27)	1.445(5)
C(30)-C(31)	1.463(5)
N(1)-Mg(1)-O(1)	94.63(6)
N(1)-Mg(1)-O(2)	93.07(6)
O(1)-Mg(1)-O(2)	85.23(7)
N(1)-Mg(1)-N(3)	169.32(6)
O(1)-Mg(1)-N(3)	92.66(7)
O(2)-Mg(1)-N(3)	95.30(6)
N(1)-Mg(1)-N(2)	78.65(6)
O(1)-Mg(1)-N(2)	173.25(6)
O(2)-Mg(1)-N(2)	94.34(6)
N(3)-Mg(1)-N(2)	94.09(6)
N(1)-Mg(1)-N(4)	92.95(6)
O(1)-Mg(1)-N(4)	94.17(6)
O(2)-Mg(1)-N(4)	173.98(6)
N(3)-Mg(1)-N(4)	78.74(6)
N(2)-Mg(1)-N(4)	86.95(6)
C(17)-N(4)-C(18)	117.81(15)
C(17)-N(4)-Mg(1)	110.52(11)
C(18)-N(4)-Mg(1)	130.62(11)

C(5)-N(2)-C(6)	118.70(15)
C(5)-N(2)-Mg(1)	110.80(12)
C(6)-N(2)-Mg(1)	129.49(11)
C(1)-N(1)-C(4)	104.80(15)
C(1)-N(1)-Mg(1)	144.26(13)
C(4)-N(1)-Mg(1)	110.22(11)
C(29)-O(2)-C(32)	106.87(17)
C(29)-O(2)-Mg(1)	123.01(14)
C(32)-O(2)-Mg(1)	130.10(12)
C(13)-N(3)-C(16)	104.73(14)
C(13)-N(3)-Mg(1)	144.75(13)
C(16)-N(3)-Mg(1)	110.32(10)
C(25)-O(1)-C(28)	106.89(18)
C(25)-O(1)-Mg(1)	128.31(12)
C(28)-O(1)-Mg(1)	123.32(14)
C(12)-C(7)-C(8)	118.35(17)
C(12)-C(7)-C(6)	120.86(16)
C(8)-C(7)-C(6)	120.76(15)
C(24)-C(19)-C(20)	118.34(19)
C(24)-C(19)-C(18)	121.42(17)
C(20)-C(19)-C(18)	120.22(17)
N(4)-C(17)-C(16)	120.97(16)

N(2)-C(6)-C(7)	112.16(14)
N(1)-C(4)-C(3)	110.91(17)
N(1)-C(4)-C(5)	118.70(15)
C(3)-C(4)-C(5)	130.38(17)
N(2)-C(5)-C(4)	120.50(16)
N(4)-C(18)-C(19)	112.42(15)
N(3)-C(13)-C(14)	112.04(16)
N(3)-C(16)-C(15)	110.94(15)
N(3)-C(16)-C(17)	119.09(14)
C(15)-C(16)-C(17)	129.89(17)
C(14)-C(15)-C(16)	106.09(16)
C(7)-C(12)-C(11)	120.93(19)
C(7)-C(8)-C(9)	120.76(17)
C(2)-C(3)-C(4)	106.18(18)
C(15)-C(14)-C(13)	106.20(15)
N(1)-C(1)-C(2)	111.84(18)
C(23)-C(24)-C(19)	120.8(2)
C(10)-C(9)-C(8)	120.05(19)
O(2)-C(32)-C(31)	106.63(19)
C(3)-C(2)-C(1)	106.27(16)
C(11)-C(10)-C(9)	119.75(18)
C(21)-C(20)-C(19)	121.1(2)

C(10)-C(11)-C(12)	120.15(19)
C(22)-C(23)-C(24)	120.2(2)
C(20)-C(21)-C(22)	119.9(2)
C(23)-C(22)-C(21)	119.7(2)
O(1)-C(25)-C(26)	107.5(2)
C(30)-C(29)-O(2)	108.6(3)
C(27)-C(26)-C(25)	106.1(3)
O(1)-C(28)-C(27)	105.9(3)
C(29)-C(30)-C(31)	108.0(3)
C(28)-C(27)-C(26)	105.6(3)
C(30)-C(31)-C(32)	104.7(2)
