Supporting Information: Synthesis and Computational Studies of Mg Complexes Supported by 2,2':6,2''-Terpyridine Ligands

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X-Ray Crystallography

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Table S1. Crystal data and structure refinement for **5a**

Empirical Formula	$Br_2MgN_3C_{25}H_{23}Cl_2$
Formula Weight	620.50
Crystal Color, Habit	colorless, block
Crystal Dimensions	0.20 X 0.15 X 0.15 mm
Crystal System	monoclinic
Lattice Type	C-centered
Lattice Parameters	a = 20.815(3) Å b = 15.326(3) Å c = 16.421(3) Å β = 100.713(7) ° V = 5147.3(15) Å^3
Space Group	C2/c (#15)
Z value	8
D_{calc}	1.601 g/cm^3
F_{000}	2480.00
μ(MoKα)	34.099 cm^{-1}
Data Images	350 exposures
ω oscillation Range (χ=54.0, ϕ=0.0)	-120.0 - 60.0°
Exposure Rate	90.0 sec./°
Detector Swing Angle	-28.40°
ω oscillation Range (χ=54.0, ϕ=120.0)	-120.0 - 50.0°
Exposure Rate	90.0 sec./°
Detector Swing Angle	-28.40°
Detector Position	49.90 mm
Pixel Size	0.146 mm
$2\theta_{max}$	55.0°
No. of Reflections Measured	Total: 17018 Unique: 5888 (R_{int} = 0.0660)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.417 - 0.600)
Structure Solution	Direct Methods
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w $(Fo^2 - Fc^2)^2$
Least Squares Weights	w = 1/ [$\sigma^2(Fo^2)$ + $(0.0499 \cdot P)^2$ + 13.7902 • P] where P = $(Max(Fo^2,0) + 2Fc^2)/3$
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	5888
No. Variables	298
Reflection/Parameter Ratio	19.76
Residuals: R1 (I>2.00σ(I))	0.0613
Residuals: R (All reflections)	0.1232
Residuals: wR2 (All reflections)	0.1390
Goodness of Fit Indicator	1.039
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	0.52 e$^-$/Å^3
Minimum peak in Final Diff. Map	-0.55 e$^-$/Å^3

Table S2. Atomic coordinates and Biso/Beq for **5a**

atom	x	y	z	Beq
Br(1)	0.37979(3)	0.47003(4)	0.03419(3)	4.251(15)
Br(2)	0.21975(3)	0.56219(4)	0.12415(4)	5.195(17)
Cl(1)	0.21160(12)	0.35873(15)	0.32362(14)	8.74(6)
Cl(2)	0.15628(13)	0.51521(14)	0.37126(18)	9.80(7)
Mg(1)	0.31798(8)	0.47145(10)	0.14851(9)	2.95(3)
N(1)	0.37946(19)	0.5578(3)	0.2359(2)	3.11(8)
N(2)	0.36302(18)	0.3927(2)	0.2473(2)	2.59(7)
N(3)	0.26983(18)	0.3455(3)	0.1299(2)	2.88(7)
C(1)	0.3819(3)	0.6433(3)	0.2286(3)	3.89(11)
C(2)	0.4226(3)	0.6938(4)	0.2829(4)	4.27(11)
C(3)	0.4628(3)	0.6557(4)	0.3476(4)	4.36(12)
C(4)	0.4608(2)	0.5673(3)	0.3559(3)	3.57(10)
C(5)	0.4184(2)	0.5201(3)	0.2999(3)	2.82(8)
C(6)	0.4094(2)	0.4252(3)	0.3067(3)	2.63(8)
C(7)	0.4411(2)	0.3738(3)	0.3692(3)	2.90(9)
C(8)	0.4252(2)	0.2870(3)	0.3727(3)	2.83(9)
C(9)	0.3764(2)	0.2545(3)	0.3114(3)	2.76(8)
C(10)	0.3467(2)	0.3086(3)	0.2497(3)	2.57(8)
C(11)	0.2920(2)	0.2830(3)	0.1835(3)	2.65(8)
C(12)	0.2642(2)	0.2016(3)	0.1800(3)	3.20(9)
C(13)	0.2120(3)	0.1851(4)	0.1187(3)	3.64(10)
C(14)	0.1886(3)	0.2489(4)	0.0636(3)	3.93(11)
C(15)	0.2184(2)	0.3277(4)	0.0716(3)	3.83(11)
C(16)	0.4555(2)	0.2297(3)	0.4411(3)	2.92(9)
C(17)	0.5144(3)	0.1898(3)	0.4392(3)	3.67(10)
C(18)	0.5396(3)	0.1324(4)	0.5018(3)	4.22(11)
C(19)	0.5077(3)	0.1151(4)	0.5654(3)	4.19(12)
C(20)	0.4502(3)	0.1564(3)	0.5663(3)	4.12(11)
C(21)	0.4223(3)	0.2133(3)	0.5045(3)	3.44(10)
C(22)	0.5505(3)	0.2084(5)	0.3719(4)	5.56(14)
C(23)	0.5362(4)	0.0533(4)	0.6332(4)	6.31(17)
C(24)	0.3589(3)	0.2574(4)	0.5074(4)	4.65(12)
C(25)	0.2185(5)	0.4419(6)	0.3936(6)	9.8(3)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)2 + U_{22}(bb^*)2 + U_{33}(cc^*)2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table S3. Anisotropic displacement parameters for **5a**

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Br(1)	0.0564(4)	0.0640(4)	0.0426(3)	-0.0135(3)	0.0132(2)	-0.0111(3)
Br(2)	0.0647(4)	0.0607(4)	0.0668(4)	0.0229(3)	-0.0011(3)	-0.0099(3)
Cl(1)	0.1292(18)	0.1109(16)	0.1097(17)	-0.0000(14)	0.0682(14)	-0.0230(13)
Cl(2)	0.142(2)	0.0714(13)	0.178(3)	-0.0021(14)	0.0767(19)	0.0021(14)
Mg(1)	0.0448(9)	0.0340(8)	0.0308(8)	0.0007(8)	0.0010(7)	-0.0016(7)
N(1)	0.052(3)	0.031(2)	0.034(2)	-0.0044(20)	0.0064(19)	-0.0014(17)
N(2)	0.035(2)	0.033(2)	0.0300(20)	-0.0029(18)	0.0072(16)	0.0006(16)
N(3)	0.036(2)	0.041(2)	0.030(2)	-0.0015(19)	-0.0022(17)	0.0004(17)
C(1)	0.062(4)	0.040(3)	0.044(3)	0.001(3)	0.004(3)	0.004(2)
C(2)	0.065(4)	0.035(3)	0.063(4)	-0.011(3)	0.013(3)	0.003(3)
C(3)	0.061(4)	0.042(3)	0.058(4)	-0.016(3)	-0.002(3)	-0.008(3)
C(4)	0.044(3)	0.042(3)	0.046(3)	-0.004(3)	0.001(2)	-0.003(2)
C(5)	0.039(3)	0.035(3)	0.032(2)	-0.005(2)	0.004(2)	-0.003(2)
C(6)	0.038(3)	0.031(3)	0.031(2)	-0.007(2)	0.008(2)	-0.0015(20)
C(7)	0.042(3)	0.036(3)	0.029(2)	-0.004(2)	-0.001(2)	-0.001(2)

C(8)	0.036(3)	0.042(3)	0.029(2)	-0.001(2)	0.0051(20)	0.001(2)
C(9)	0.040(3)	0.029(2)	0.036(3)	0.000(2)	0.007(2)	0.003(2)
C(10)	0.033(2)	0.033(3)	0.032(2)	-0.002(2)	0.0081(19)	-0.0039(20)
C(11)	0.037(3)	0.035(3)	0.029(2)	0.001(2)	0.0064(20)	-0.0064(20)
C(12)	0.045(3)	0.038(3)	0.035(3)	-0.002(2)	-0.001(2)	0.000(2)
C(13)	0.048(3)	0.046(3)	0.044(3)	-0.011(3)	0.009(2)	-0.011(3)
C(14)	0.045(3)	0.054(4)	0.045(3)	-0.009(3)	-0.005(2)	-0.011(3)
C(15)	0.048(3)	0.052(3)	0.039(3)	0.001(3)	-0.006(2)	0.001(2)
C(16)	0.041(3)	0.034(3)	0.031(3)	-0.011(2)	-0.005(2)	0.0022(20)
C(17)	0.046(3)	0.047(3)	0.043(3)	-0.003(3)	-0.000(2)	0.008(2)
C(18)	0.043(3)	0.056(4)	0.056(4)	-0.004(3)	-0.005(3)	0.006(3)
C(19)	0.061(4)	0.044(3)	0.046(3)	-0.015(3)	-0.012(3)	0.009(3)
C(20)	0.071(4)	0.047(3)	0.036(3)	-0.024(3)	0.004(3)	0.006(2)
C(21)	0.055(3)	0.038(3)	0.033(3)	-0.017(3)	-0.004(2)	-0.001(2)
C(22)	0.057(4)	0.095(5)	0.061(4)	0.018(4)	0.015(3)	0.015(4)
C(23)	0.102(5)	0.062(4)	0.063(4)	-0.009(4)	-0.017(4)	0.026(3)
C(24)	0.069(4)	0.059(4)	0.054(4)	-0.006(3)	0.025(3)	-0.001(3)
C(25)	0.118(7)	0.104(7)	0.132(8)	-0.023(6)	-0.019(6)	-0.036(6)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S4. Bond lengths (Å) for **5a**

atom	atom	distance	atom	atom	distance
Br(1)	Mg(1)	2.4653(18)	Br(2)	Mg(1)	2.4435(17)
Cl(1)	C(25)	1.704(9)	Cl(2)	C(25)	1.701(9)
Mg(1)	N(1)	2.183(4)	Mg(1)	N(2)	2.098(4)
Mg(1)	N(3)	2.170(4)	N(1)	C(1)	1.317(6)
N(1)	C(5)	1.333(5)	N(2)	C(6)	1.335(5)
N(2)	C(10)	1.335(6)	N(3)	C(11)	1.325(6)
N(3)	C(15)	1.325(6)	C(1)	C(2)	1.354(7)
C(2)	C(3)	1.356(8)	C(3)	C(4)	1.364(7)
C(4)	C(5)	1.359(6)	C(5)	C(6)	1.474(6)
C(6)	C(7)	1.363(6)	C(7)	C(8)	1.374(7)
C(8)	C(9)	1.382(6)	C(8)	C(16)	1.472(6)
C(9)	C(10)	1.366(6)	C(10)	C(11)	1.473(6)
C(11)	C(12)	1.372(7)	C(12)	C(13)	1.361(6)
C(13)	C(14)	1.360(7)	C(14)	C(15)	1.352(8)
C(16)	C(17)	1.375(7)	C(16)	C(21)	1.376(7)
C(17)	C(18)	1.381(7)	C(17)	C(22)	1.475(9)
C(18)	C(19)	1.364(9)	C(19)	C(20)	1.357(9)
C(19)	C(23)	1.497(8)	C(20)	C(21)	1.382(7)
C(21)	C(24)	1.491(8)			

Table S5. Bond angles (°) for **5a**

atom	atom	atom	angle	atom	atom	atom	angle
Br(1)	Mg(1)	Br(2)	114.81(6)	Br(1)	Mg(1)	N(1)	100.41(13)
Br(1)	Mg(1)	N(2)	111.22(13)	Br(1)	Mg(1)	N(3)	100.23(12)
Br(2)	Mg(1)	N(1)	97.65(12)	Br(2)	Mg(1)	N(2)	133.96(14)
Br(2)	Mg(1)	N(3)	97.62(12)	N(1)	Mg(1)	N(2)	73.60(15)
N(1)	Mg(1)	N(3)	146.18(15)	N(2)	Mg(1)	N(3)	74.06(14)
Mg(1)	N(1)	C(1)	124.8(3)	Mg(1)	N(1)	C(5)	116.8(3)
C(1)	N(1)	C(5)	118.3(4)	Mg(1)	N(2)	C(6)	120.6(3)
Mg(1)	N(2)	C(10)	119.9(3)	C(6)	N(2)	C(10)	119.4(4)
Mg(1)	N(3)	C(11)	117.1(3)	Mg(1)	N(3)	C(15)	125.1(3)

C(11)	N(3)	C(15)	117.8(4)	N(1)	C(1)	C(2)	122.6(5)
C(1)	C(2)	C(3)	119.4(5)	C(2)	C(3)	C(4)	118.7(5)
C(3)	C(4)	C(5)	119.3(5)	N(1)	C(5)	C(4)	121.7(4)
N(1)	C(5)	C(6)	114.9(4)	C(4)	C(5)	C(6)	123.4(4)
N(2)	C(6)	C(5)	113.4(4)	N(2)	C(6)	C(7)	121.2(4)
C(5)	C(6)	C(7)	125.3(4)	C(6)	C(7)	C(8)	120.3(4)
C(7)	C(8)	C(9)	118.0(4)	C(7)	C(8)	C(16)	122.4(4)
C(9)	C(8)	C(16)	119.5(4)	C(8)	C(9)	C(10)	119.4(4)
N(2)	C(10)	C(9)	121.7(4)	N(2)	C(10)	C(11)	113.7(4)
C(9)	C(10)	C(11)	124.5(4)	N(3)	C(11)	C(10)	115.0(4)
N(3)	C(11)	C(12)	122.5(4)	C(10)	C(11)	C(12)	122.4(4)
C(11)	C(12)	C(13)	118.2(4)	C(12)	C(13)	C(14)	119.7(5)
C(13)	C(14)	C(15)	118.5(5)	N(3)	C(15)	C(14)	123.3(5)
C(8)	C(16)	C(17)	120.4(4)	C(8)	C(16)	C(21)	118.8(4)
C(17)	C(16)	C(21)	120.7(4)	C(16)	C(17)	C(18)	118.9(5)
C(16)	C(17)	C(22)	120.8(5)	C(18)	C(17)	C(22)	120.3(5)
C(17)	C(18)	C(19)	121.5(5)	C(18)	C(19)	C(20)	118.3(5)
C(18)	C(19)	C(23)	120.7(6)	C(20)	C(19)	C(23)	121.0(6)
C(19)	C(20)	C(21)	122.5(5)	C(16)	C(21)	C(20)	118.0(5)
C(16)	C(21)	C(24)	120.9(4)	C(20)	C(21)	C(24)	121.1(5)
Cl(1)	C(25)	Cl(2)	112.6(5)				

X-Ray Data for 5b

Table S6. Crystal data and structure refinement for **5b**

Empirical Formula	$Br_2MgN_3C_{27}H_{35}$
Formula Weight	585.71
Crystal Color, Habit	colorless, prism
Crystal Dimensions	0.20 X 0.20 X 0.20 mm
Crystal System	trigonal
Lattice Type	Primitive
Lattice Parameters	a = 12.5029(20) Å c = 15.991(3) Å V = 2164.9(6) Å^3
Space Group	$P3_221$ (#154)
Z value	3
Dcalc	1.348 g/cm^3
F_{000}	900.00
μ(MoKα)	28.569 cm^{-1}
Data Images	540 exposures
ω oscillation Range (χ=54.0, ϕ=0.0)	-120.0 - 60.0°
Exposure Rate	40.0 sec./°
Detector Swing Angle	-28.40°
ω oscillation Range (χ=54.0, ϕ=120.0)	-120.0 - 60.0°
Exposure Rate	40.0 sec./°
Detector Swing Angle	-28.40°
ω oscillation Range (χ=54.0, ϕ=240.0)	-120.0 - 60.0°
Exposure Rate	40.0 sec./°
Detector Swing Angle	-28.40°
Detector Position	49.90 mm
Pixel Size	0.146 mm
$2\theta_{max}$	48.8°
No. of Reflections Measured	Total: 13546 Unique: 2392 (R_{int} = 0.0590) Friedel pairs: 1019

Corrections	Lorentz-polarization Absorption (trans. factors: 0.420 - 0.565)
Structure Solution	Direct Methods
Refinement	Full-matrix least-squares on F2
Function Minimized	Σ w (Fo2 - Fc2)2
Least Squares Weights	w = 1/ [σ2(Fo2) + (0.0278 • P)2 + 0.0000 • P] where P = (Max(Fo2,0) + 2Fc2)/3
2θmax cutoff	53.5°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	2392
No. Variables	171
Reflection/Parameter Ratio	13.99
Residuals: R1 (I>2.00σ(I))	0.0424
Residuals: R (All reflections)	0.0510
Residuals: wR2 (All reflections)	0.0931
Goodness of Fit Indicator	1.088
Flack Parameter	0.038(16)
Max Shift/Error in Final Cycle	0.002
Maximum peak in Final Diff. Map	0.41 e^- /Å^3
Minimum peak in Final Diff. Map	-0.33 e^- /Å^3

Table S7. Atomic coordinates and Biso/Beq for **5b**

atom	x	y	z	Beq	occ
Br(1)	0.26164(6)	0.17783(5)	1.21309(3)	4.821(17)	
Mg(2)	0.27942(17)	0.0000	1.1667	2.46(3)	1/2
N(1)	0.4482(3)	0.0000	1.1667	2.42(8)	1/2
N(2)	0.3634(3)	0.0716(4)	1.0467(2)	2.79(6)	
C(1)	0.5192(4)	0.0335(4)	1.0980(2)	2.51(7)	
C(2)	0.6280(4)	0.0298(4)	1.0951(3)	2.90(8)	
C(3)	0.6696(5)	0.0000	1.1667	3.17(11)	1/2
C(4)	0.4688(4)	0.0727(4)	1.0275(3)	2.55(8)	
C(5)	0.5259(4)	0.1158(5)	0.9525(3)	3.07(8)	
C(6)	0.4790(4)	0.1618(5)	0.8929(3)	3.62(9)	
C(7)	0.3720(5)	0.1608(5)	0.9141(3)	3.67(9)	
C(8)	0.3177(4)	0.1155(5)	0.9901(3)	3.75(9)	
C(9)	0.7928(6)	0.0000	1.1667	4.19(16)	1/2
C(10)	0.7754(17)	-0.1018(18)	1.1003(10)	7.3(4)	1/2
C(11)	0.8503(15)	0.018(2)	1.0863(9)	6.7(4)	1/2
C(12)	0.8902(10)	0.1199(16)	1.1302(10)	6.8(4)	1/2
C(13)	0.5422(6)	0.2123(7)	0.8092(3)	5.36(14)	
C(14)	0.5647(10)	0.1182(10)	0.7658(4)	10.0(3)	
C(15)	0.4698(9)	0.2476(13)	0.7527(5)	13.0(4)	
C(16)	0.6670(8)	0.3204(9)	0.8266(6)	10.6(3)	

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table S8. Anisotropic displacement parameters for **5b**

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Br(1)	0.0909(5)	0.0561(4)	0.0556(3)	0.0512(4)	0.0044(3)	-0.0030(3)
Mg(2)	0.0296(7)	0.0377(11)	0.0291(9)	0.0188(5)	0.0010(4)	0.0020(8)
N(1)	0.0268(17)	0.040(3)	0.030(2)	0.0198(15)	-0.0002(12)	-0.000(2)
N(2)	0.033(2)	0.046(2)	0.0290(16)	0.0218(17)	-0.0013(16)	0.0047(17)
C(1)	0.032(2)	0.034(2)	0.029(2)	0.016(2)	-0.0007(17)	0.0029(20)
C(2)	0.034(3)	0.044(3)	0.036(2)	0.023(2)	0.006(2)	0.006(2)

C(3)	0.037(2)	0.054(4)	0.036(3)	0.027(2)	0.0062(16)	0.012(3)
C(4)	0.024(2)	0.034(2)	0.034(2)	0.0114(19)	0.0030(19)	-0.0001(19)
C(5)	0.031(2)	0.055(3)	0.035(2)	0.025(2)	-0.001(2)	0.003(2)
C(6)	0.035(3)	0.068(4)	0.034(2)	0.026(3)	0.008(2)	0.013(2)
C(7)	0.040(3)	0.069(3)	0.035(2)	0.030(3)	-0.003(2)	0.012(2)
C(8)	0.035(3)	0.073(3)	0.042(2)	0.033(2)	0.004(2)	0.008(3)
C(9)	0.042(3)	0.091(6)	0.043(4)	0.046(3)	0.0134(19)	0.027(4)
C(10)	0.102(12)	0.113(13)	0.109(11)	0.089(11)	0.017(10)	0.013(11)
C(11)	0.067(11)	0.145(17)	0.080(9)	0.080(12)	0.016(8)	0.025(11)
C(12)	0.033(6)	0.115(12)	0.103(11)	0.033(8)	0.012(7)	0.061(10)
C(13)	0.063(4)	0.122(5)	0.040(3)	0.062(4)	0.016(3)	0.034(3)
C(14)	0.162(9)	0.202(10)	0.053(4)	0.118(8)	0.048(5)	0.026(5)
C(15)	0.151(8)	0.354(17)	0.070(4)	0.187(10)	0.066(5)	0.121(7)
C(16)	0.078(6)	0.151(8)	0.119(7)	0.016(6)	0.046(5)	0.066(6)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S9. Bond lengths (Å) for **5b**

atom	atom	distance	atom	atom	distance
Br(1)	Mg(2)	2.4571(14)	Mg(2)	N(1)	2.110(4)
Mg(2)	N(2)	2.156(3)	Mg(2)	N(2)[1]	2.155(3)
N(1)	C(1)	1.342(4)	N(1)	C(1)[1]	1.341(4)
N(2)	C(4)	1.347(7)	N(2)	C(8)	1.326(7)
C(1)	C(2)	1.384(8)	C(1)	C(4)	1.489(7)
C(2)	C(3)	1.385(6)	C(3)	C(9)	1.540(10)
C(4)	C(5)	1.362(6)	C(5)	C(6)	1.385(8)
C(6)	C(7)	1.375(9)	C(6)	C(13)	1.522(7)
C(7)	C(8)	1.370(6)	C(9)	C(10)	1.59(2)
C(9)	C(11)	1.434(16)	C(9)	C(12)	1.498(14)
C(13)	C(14)	1.508(16)	C(13)	C(15)	1.493(16)
C(13)	C(16)	1.493(9)			

Symmetry Operators:
(1) X-Y,-Y,-Z+1/3+2

Table S10. Bond angles (°) for **5b**

atom	atom	atom	angle	atom	atom	atom	angle
Br(1)	Mg(2)	Br(1)[1]	114.24(8)	Br(1)	Mg(2)	N(1)	122.88(4)
Br(1)	Mg(2)	N(2)	97.97(13)	Br(1)	Mg(2)	N(2)[1]	99.48(9)
Br(1)[1]	Mg(2)	N(1)	122.88(4)	Br(1)[1]	Mg(2)	N(2)	99.44(9)
Br(1)[1]	Mg(2)	N(2)[1]	97.99(13)	N(1)	Mg(2)	N(2)	73.79(14)
N(1)	Mg(2)	N(2)[1]	73.78(14)	N(2)	Mg(2)	N(2)[1]	147.57(11)
Mg(2)	N(1)	C(1)	120.4(3)	Mg(2)	N(1)	C(1)[1]	120.4(3)
C(1)	N(1)	C(1)[1]	119.2(3)	Mg(2)	N(2)	C(4)	118.5(3)
Mg(2)	N(2)	C(8)	123.9(4)	C(4)	N(2)	C(8)	117.6(4)
N(1)	C(1)	C(2)	121.7(4)	N(1)	C(1)	C(4)	113.6(4)
C(2)	C(1)	C(4)	124.7(4)	C(1)	C(2)	C(3)	119.3(4)
C(2)	C(3)	C(2)[1]	118.5(4)	C(2)	C(3)	C(9)	120.7(3)
C(2)[1]	C(3)	C(9)	120.7(3)	N(2)	C(4)	C(1)	113.4(4)
N(2)	C(4)	C(5)	121.4(5)	C(1)	C(4)	C(5)	124.9(5)
C(4)	C(5)	C(6)	121.6(5)	C(5)	C(6)	C(7)	116.0(4)
C(5)	C(6)	C(13)	122.5(6)	C(7)	C(6)	C(13)	121.5(6)
C(6)	C(7)	C(8)	120.1(6)	N(2)	C(8)	C(7)	123.3(6)
C(3)	C(9)	C(10)	105.3(8)	C(3)	C(9)	C(10)[1]	105.3(8)
C(3)	C(9)	C(11)	114.9(9)	C(3)	C(9)	C(11)[1]	114.9(9)

C(3)	C(9)	C(12)	108.3(8)	C(3)	C(9)	C(12)[1]	108.3(8)
C(10)	C(9)	C(10)[1]	149.3(5)	C(10)	C(9)	C(11)	52.1(11)
C(10)	C(9)	C(11)[1]	113.0(11)	C(10)	C(9)	C(12)	105.0(9)
C(10)	C(9)	C(12)[1]	64.9(9)	C(10)[1]	C(9)	C(11)	113.0(11)
C(10)[1]	C(9)	C(11)[1]	52.1(11)	C(10)[1]	C(9)	C(12)	64.9(9)
C(10)[1]	C(9)	C(12)[1]	105.0(9)	C(11)	C(9)	C(11)[1]	130.1(5)
C(11)	C(9)	C(12)	53.1(11)	C(11)	C(9)	C(12)[1]	109.7(13)
C(11)[1]	C(9)	C(12)	109.7(13)	C(11)[1]	C(9)	C(12)[1]	53.1(11)
C(12)	C(9)	C(12)[1]	143.5(5)	C(9)	C(10)	C(11)	58.0(11)
C(9)	C(10)	C(12)[1]	55.0(7)	C(11)	C(10)	C(12)[1]	106.1(14)
C(9)	C(11)	C(10)	69.9(11)	C(9)	C(11)	C(12)	66.0(11)
C(10)	C(11)	C(12)	135.6(15)	C(9)	C(12)	C(10)[1]	60.1(10)
C(9)	C(12)	C(11)	61.0(9)	C(10)[1]	C(12)	C(11)	115.8(15)
C(6)	C(13)	C(14)	110.0(6)	C(6)	C(13)	C(15)	112.9(6)
C(6)	C(13)	C(16)	107.6(5)	C(14)	C(13)	C(15)	109.2(7)
C(14)	C(13)	C(16)	105.9(8)	C(15)	C(13)	C(16)	111.0(8)

Symmetry Operators:
(1) X-Y,-Y,-Z+1/3+2

Density Functional Theory

Figure S1: Energy profile for rotation of a single aromatic ring in bipy in different solvents (lowest energy structure assigned as being at 0 kcal/mol).

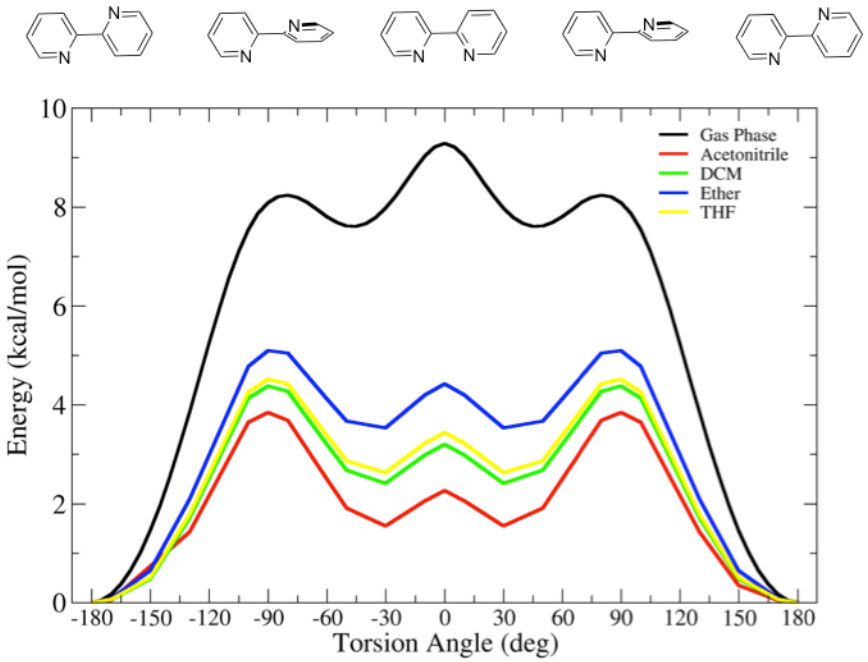


Figure S2: Energy profile for rotation of a single aromatic ring in terpy in different solvents (lowest energy structure assigned as being at 0 kcal/mol).

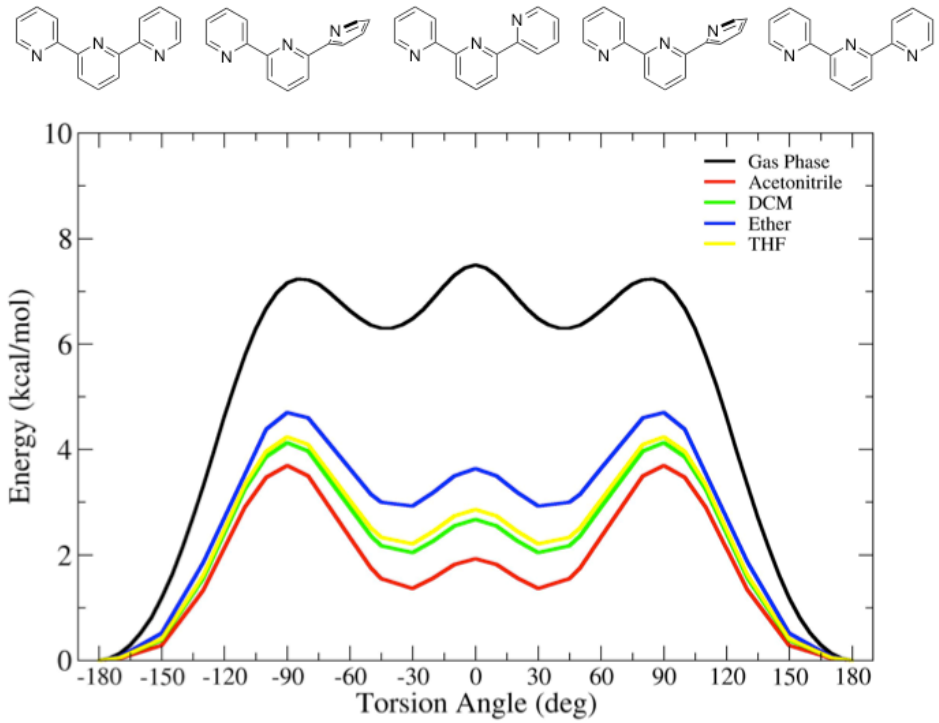


Figure S3: Energy profile for rotation of a single aromatic ring in terpy (solid lines) and mesitylterpy (pointed lines) when the other ring is fixed at a torsion angle of 0° (syn conformation) blue line, 180° (anti conformation) red line and 90° black line, in gas phase. These results show that the use of terpy as a model is sufficient to describe mesitylterpy. Lowest energy structure for each individual scan assigned as being at 0 kcal/mol.

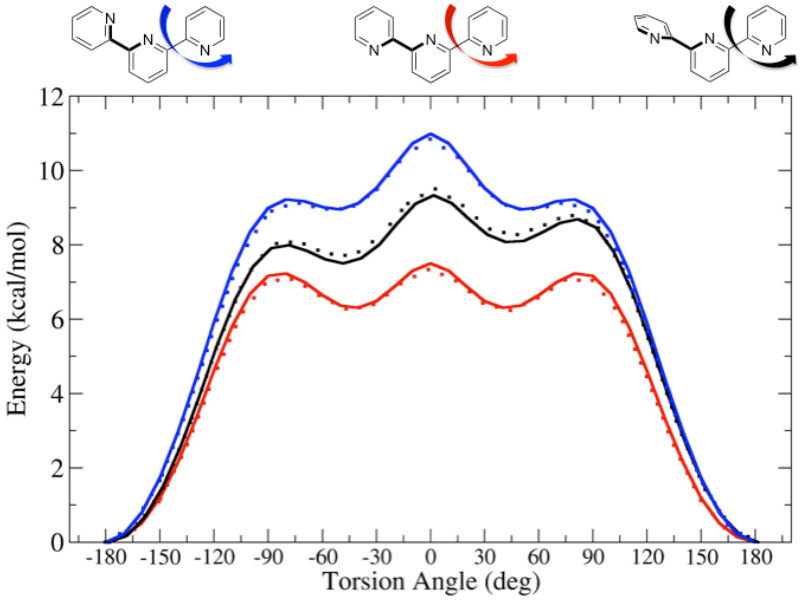


Figure S4: Energy profile for rotation of a single aromatic ring in terpy when the other ring is fixed at a torsion angle of 0° (syn conformation) blue line, 180° (anti conformation) red line and 90° black line, in gas phase (solid lines) and in diethyl ether (dashed lines). These results show how the choice of solvent can lower the energy barriers but the rotation of a second ring is still more difficult. Lowest energy structure for each individual scan assigned as being at 0 kcal/mol.

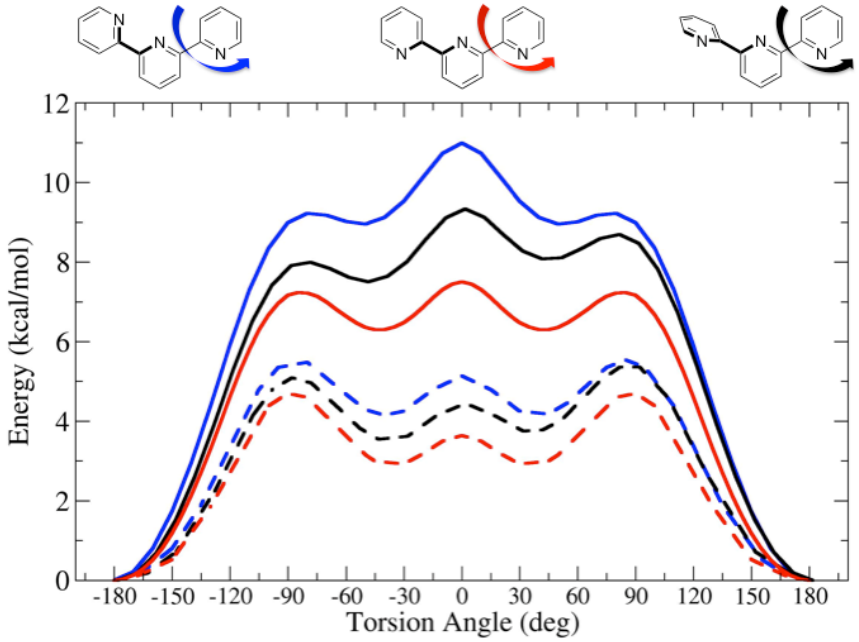
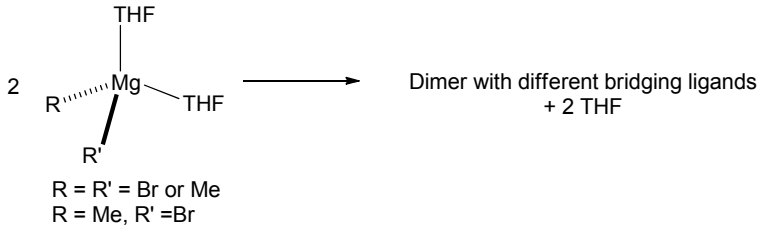
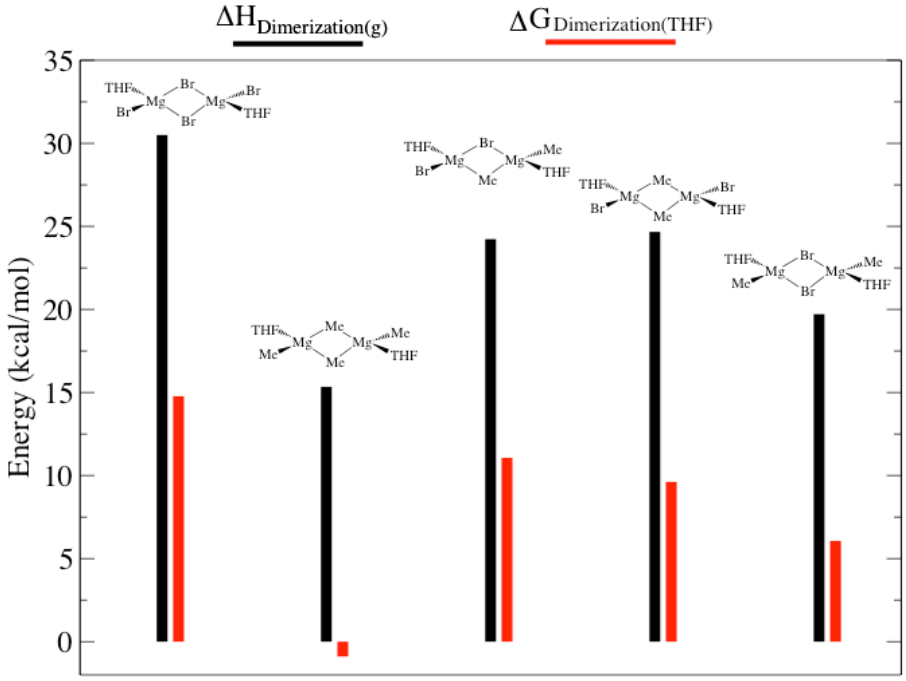


Figure S5: Enthalpies of dimerization in gas phase (black bars) and Free energies of dimerization (red bars) for different Grignard reagents. It can be seen that dimerization is highly unfavorable in all cases except for Me_2Mg where it is slightly favorable but not enough to influence our results in relation to mesitylterpy binding to Grignard reagents.



R = R' = Br or Me
R = Me, R' =Br



Optimized Structures and SCF Energies (B3LYP/TZV)
Bipy
SCF energy = -495.386947

H	-1.062443	3.062150	-1.147253
H	1.038127	1.776331	-1.558153
C	-0.941992	2.057768	-0.765395
C	0.228835	1.337240	-0.992754
N	-1.984708	1.565219	-0.068799
H	1.214549	-0.544964	-0.628472
C	0.322119	0.045778	-0.473274
C	-1.890202	0.308883	0.434812
C	-0.745908	-0.477282	0.248309
H	-0.720766	-1.469724	0.669018
C	-3.057610	-0.201083	1.196631
N	-2.963096	-1.457410	1.700259
H	-4.227062	1.577510	0.962387
C	-4.201911	0.585077	1.383117

C	-4.005813	-1.949961	2.396852
H	-3.885358	-2.954338	2.778722
C	-5.269937	0.062019	2.104701
C	-5.176647	-1.229439	2.624195
H	-6.162372	0.652755	2.259898
H	-5.985940	-1.668530	3.189592

Terpy

SCF energy = -742.485642

H	-1.666352	5.889146	-3.690035
H	-3.612829	4.954667	-2.416691
C	-1.564428	4.999045	-3.086150
C	-2.644437	4.474945	-2.375632
H	0.529382	4.710165	-3.531767
C	-0.337851	4.343643	-3.000019
C	-2.464509	3.326575	-1.611602
H	-3.270677	2.887365	-1.046966
N	-0.148766	3.231077	-2.264411
C	-1.200954	2.723301	-1.574212
H	1.117654	1.347532	-1.313639
C	-0.950592	1.495648	-0.775502
C	0.317082	0.901699	-0.746032
N	-1.994242	0.982592	-0.084216
C	0.498341	-0.246971	0.017790
C	-1.813362	-0.134514	0.657185
C	-0.572029	-0.778228	0.730391
H	-0.477152	-1.665775	1.334642
C	-2.990518	-0.657986	1.397473
N	-2.800207	-1.778674	2.138520
H	-4.340974	0.865089	0.730260
C	-4.237264	-0.022955	1.332131
C	-3.844858	-2.282652	2.823638
H	-3.644356	-3.175877	3.399081
C	-5.306602	-0.555075	2.045035
C	-5.113692	-1.707094	2.807646
H	-6.276692	-0.078564	2.006764
H	-5.920541	-2.148907	3.374339
H	1.467539	-0.725068	0.057455

Mesitylterpy (MT)

SCF energy = -1091.495943

C	5.678051	4.891519	1.512704
C	5.616346	4.255784	2.759409
N	4.874637	3.135768	2.951409
C	4.185185	2.633456	1.908745
C	4.197405	3.209816	0.640248
C	4.960849	4.361026	0.445439
C	6.362698	4.778742	3.933845
N	7.107825	5.891625	3.747369
C	7.801661	6.397005	4.792195
C	7.771034	5.801640	6.057332
C	7.002948	4.651811	6.260585
C	6.288803	4.137813	5.174709
C	6.946697	3.990291	7.603483
C	6.005792	4.420513	8.561411

C	5.968474	3.787960	9.807348
C	6.839513	2.745090	10.132072
C	7.760000	2.332579	9.167112
C	7.831019	2.936478	7.907267
C	5.037443	5.545563	8.261659
C	8.849597	2.448692	6.898370
C	6.799971	2.099167	11.499289
C	8.607005	7.621771	4.544727
N	9.296819	8.127203	5.598359
C	10.037084	9.236969	5.410643
C	10.128310	9.891991	4.184254
C	9.418060	9.370494	3.102740
C	8.649437	8.224961	3.281159
H	10.568342	9.601571	6.279042
H	10.735740	10.779847	4.083541
H	9.462954	9.850018	2.134378
H	8.084642	7.787620	2.474045
H	8.344421	6.243515	6.856944
H	5.677921	3.254086	5.270927
H	6.280843	5.778835	1.407789
H	4.996345	4.838181	-0.524481
H	3.627329	2.769271	-0.164945
H	3.609367	1.740743	2.110685
H	8.440223	1.521134	9.396819
H	5.240959	4.117925	10.539565
H	8.371350	2.053109	5.999651
H	9.463431	1.656511	7.326203
H	9.515110	3.252137	6.575770
H	5.777619	2.019326	11.872560
H	7.367724	2.684081	12.228812
H	7.230614	1.097440	11.477329
H	4.421779	5.326450	7.386726
H	5.558439	6.483138	8.055867
H	4.370866	5.712630	9.107325

Diethyl Ether

SCF energy = -233.669833

H	1.728854	1.379948	-1.625720
C	2.106378	1.233773	-0.614625
H	3.404699	-2.188049	-0.566347
H	3.199885	1.288289	-0.654495
H	4.398811	-0.759985	-0.255705
O	1.676917	-0.113432	-0.244619
H	1.831867	3.296275	-0.021649
C	3.707293	-1.472048	0.197678
H	0.455951	2.242854	0.346917
C	1.544126	2.299902	0.322926
C	2.480236	-0.775402	0.781435
H	4.246378	-2.008820	0.982246
H	1.809677	-1.504090	1.234834
H	1.915444	2.178575	1.341841
H	2.771812	-0.060048	1.558331

$(Et_2O)_2MgBr_2$

SCF energy = -5815.958204

H	4.268040	-1.701842	1.237009
C	3.676547	-1.203930	0.465595
H	3.339536	-1.960770	-0.240657
H	4.326820	-0.498150	-0.052381
H	1.834448	-1.250251	1.586396
H	2.785686	0.226015	1.851914
C	2.484935	-0.519349	1.114086
Br	0.191237	-3.077123	-0.040896
H	-2.129294	-0.218951	3.418262
H	-0.646277	0.247391	2.581080
H	-1.794672	-1.613847	1.351759
O	1.630876	0.169092	0.110024
H	3.183977	1.527746	-0.234472
C	-1.733189	0.228107	2.504110
H	1.773366	2.462177	1.660038
Mg	0.064058	-0.739978	-0.817802
C	-2.175620	-0.596546	1.305919
C	2.095222	1.525306	-0.279483
H	-2.095202	1.255620	2.448756
H	-3.261108	-0.636731	1.219193
C	1.488849	2.594469	0.615314
O	-1.642488	-0.034937	0.038238
H	1.791920	1.645644	-1.316620
H	0.401141	2.584390	0.548517
H	1.838540	3.577690	0.293712
Br	0.052582	0.260592	-3.071850
C	-2.523523	0.965125	-0.621430
H	-2.943489	1.596905	0.162719
H	-1.861181	1.559090	-1.245078
H	-4.254533	-0.336881	-0.870472
H	-3.144113	-0.296699	-2.254231
C	-3.598275	0.299774	-1.464843
H	-4.213338	1.069953	-1.935355

$(Et_2O)_2MeMgBr$

SCF energy = -3281.635889

H	-0.732084	-0.330844	-3.532263
H	0.988739	-0.018922	-3.413706
H	-0.164237	1.227478	-2.948253
C	0.030573	0.146355	-2.903486
H	-3.222179	-0.277695	-2.213845
H	-4.240672	1.127285	-1.878197
H	1.754709	1.617864	-1.374553
C	-3.642736	0.336662	-1.419460
H	-1.872281	1.557509	-1.209135
Mg	0.058194	-0.700612	-0.969374
H	-4.310239	-0.280363	-0.817516
C	-2.532193	0.959664	-0.586069
H	3.206229	1.471685	-0.379526
C	2.116563	1.506655	-0.355362
Br	0.230790	-3.066569	-0.121491
H	3.343585	-1.953476	-0.133118
H	1.967240	3.587500	0.166675
O	-1.656501	-0.063349	0.027150
O	1.619047	0.184791	0.081832

H	4.325411	-0.487150	0.069958
H	-2.926992	1.589011	0.213595
C	1.609536	2.626603	0.542737
H	0.519959	2.647891	0.552764
C	3.646252	-1.179274	0.569740
H	-3.251505	-0.756714	1.195318
C	2.421749	-0.478943	1.138257
C	-2.168092	-0.665460	1.281086
H	-1.737627	-1.663540	1.305492
H	4.196139	-1.657893	1.383156
H	1.961815	2.518135	1.569137
H	1.745713	-1.202144	1.585411
H	2.686391	0.276519	1.880345
C	-1.765553	0.153341	2.498647
H	-2.186002	1.159995	2.475342
H	-0.680929	0.232786	2.566836
H	-2.127642	-0.339512	3.403462

$(Et_2O)_2PhMgBr$

SCF energy = -3473.378488

H	-1.419844	1.950463	-4.814876
H	-2.314871	2.558866	-2.540715
H	-0.559712	2.722621	-2.615050
C	-1.381374	2.013695	-2.674693
C	-1.357101	1.242352	-3.986068
H	-4.049848	1.419386	-1.676183
Br	1.664335	3.280711	-1.067334
H	-2.193212	0.548526	-4.083069
H	-0.425603	0.685739	-4.089816
O	-1.184796	1.138477	-1.493782
C	-3.591776	0.934978	-0.814200
H	-3.423777	1.682428	-0.039622
H	2.811557	1.022203	-2.472174
H	-2.430274	-0.472285	-1.995882
H	-4.305976	0.204981	-0.428221
H	-0.658016	-0.862703	5.249573
C	-2.294574	0.217548	-1.161438
Mg	0.548600	1.146915	-0.348943
C	-0.455087	-0.518359	4.243382
H	-2.248285	0.661299	4.103370
H	5.079312	0.353181	-1.635274
H	4.028334	0.894553	-0.326575
C	2.990476	0.052101	-2.017728
H	1.415340	-1.567661	4.079415
H	-1.925521	-0.337617	-0.302144
C	-1.348400	0.335112	3.595118
H	3.127270	-0.693763	-2.801836
C	4.176996	0.112035	-1.069160
C	0.707298	-0.915059	3.581977
O	1.730458	-0.272701	-1.299418
C	-1.076184	0.777581	2.296990
H	4.345330	-0.836844	-0.557956
H	-0.088015	-1.863605	-2.597593
C	0.961999	-0.462302	2.283653
H	-1.791613	1.453919	1.837497

H	1.511303	-2.314395	-3.201647
C	1.471973	-1.715297	-1.105193
H	1.887436	-0.784641	1.813638
C	0.082248	0.394417	1.580449
C	0.848184	-2.356403	-2.337124
H	0.808333	-1.770290	-0.245171
H	2.412919	-2.197012	-0.835312
H	0.636000	-3.407754	-2.131497

$(Et_2O)_2MgCl_2$

SCF energy = -1588.112873

H	4.204104	-1.701205	1.304363
C	3.629542	-1.222783	0.508107
H	3.241900	-2.004257	-0.142953
H	4.309286	-0.586568	-0.059984
H	1.806282	-1.099889	1.652096
H	2.834035	0.340466	1.806111
C	2.484747	-0.435761	1.123764
Cl	0.271375	-2.868313	0.019221
H	-2.301953	-0.447250	3.430105
H	-0.800111	0.116524	2.693389
H	-1.811439	-1.714938	1.312846
O	1.650036	0.227020	0.086559
H	3.250431	1.487684	-0.387205
C	-1.880578	0.062327	2.561054
H	1.961525	2.587021	1.508257
Mg	0.060297	-0.696530	-0.769785
C	-2.232977	-0.712856	1.301120
C	2.161639	1.536946	-0.390362
H	-2.278764	1.077666	2.541842
H	-3.310892	-0.789240	1.159102
C	1.643236	2.679412	0.469032
O	-1.664005	-0.065644	0.091787
H	1.819767	1.618739	-1.419164
H	0.554464	2.721153	0.442723
H	2.026755	3.626290	0.083273
Cl	-0.048397	0.292540	-2.865888
C	-2.530660	0.966153	-0.537594
H	-2.996471	1.535974	0.267671
H	-1.850525	1.610990	-1.087245
H	-4.229596	-0.333979	-0.957379
H	-3.052142	-0.187758	-2.279598
C	-3.553772	0.347519	-1.475425
H	-4.155663	1.141648	-1.922771

$(Et_2O)_2MeMgCl$

SCF energy = -1167.713201

H	-0.753824	-0.214773	-3.525872
H	0.972819	0.071627	-3.426506
H	-0.156093	1.328304	-2.929593
C	0.023899	0.244192	-2.901878
H	-3.208385	-0.443420	-2.204045
H	-4.340038	0.881468	-1.907844
H	1.841769	1.662929	-1.338921
C	-3.676964	0.158749	-1.427177

H	-2.013786	1.530262	-1.261611
Mg	0.059881	-0.621343	-0.977856
H	-4.288955	-0.493127	-0.803366
C	-2.620797	0.898695	-0.618294
H	3.272522	1.445217	-0.326938
C	2.184671	1.521656	-0.316552
Cl	0.222448	-2.839562	-0.158454
H	3.217515	-2.004465	-0.184553
H	2.107481	3.599319	0.233630
O	-1.663128	-0.028556	0.023290
O	1.632521	0.214263	0.095049
H	4.300812	-0.613539	0.046753
H	-3.066027	1.517618	0.162844
C	1.708733	2.647504	0.591196
H	0.620741	2.710621	0.587719
C	3.580472	-1.272112	0.534280
H	-3.191348	-0.801830	1.229657
C	2.409780	-0.508364	1.132383
C	-2.117240	-0.626541	1.300778
H	-1.614019	-1.589033	1.351887
H	4.102716	-1.809173	1.329264
H	2.043401	2.510650	1.620151
H	1.700258	-1.197192	1.581335
H	2.729392	0.221609	1.878561
C	-1.768444	0.263361	2.484846
H	-2.264180	1.233811	2.429081
H	-0.692449	0.427891	2.537498
H	-2.084986	-0.221447	3.410839

$(Et_2O)_2PhMgCl$

SCF energy = -1359.457194

C	0.399177	0.325053	1.694127
C	-0.878111	0.355524	2.305423
C	-1.109414	-0.118111	3.600560
C	-0.059393	-0.649423	4.350566
C	1.217491	-0.701236	3.791402
C	1.430258	-0.222422	2.494297
Mg	0.625182	1.095085	-0.269083
O	1.996791	2.640058	-0.257107
C	2.959875	2.787611	0.856896
C	4.336830	2.261156	0.478456
Cl	-0.984692	2.003800	-1.739008
O	1.437047	-0.371098	-1.481529
C	1.732275	-1.723182	-0.950521
C	0.508306	-2.625988	-0.979773
C	1.493939	-0.247574	-2.957200
C	2.895240	0.111021	-3.428692
C	1.956268	3.777770	-1.210369
C	1.096440	4.921114	-0.696221
H	2.895803	0.228653	-4.514466
H	1.151716	-1.188913	-3.388518
H	0.766555	0.522324	-3.203883
H	0.131918	-2.773267	-1.992450
H	3.621904	-0.662406	-3.175452
H	3.223229	1.050400	-2.984025

H	-0.288753	-2.207186	-0.367409
H	1.531550	3.366286	-2.121571
H	2.559351	-2.134949	-1.531571
H	0.770951	-3.604828	-0.572505
H	-0.233498	-1.016933	5.354010
H	-2.105708	-0.072446	4.024151
H	1.083618	5.722409	-1.438541
H	0.073450	4.579784	-0.549850
H	2.041834	-1.111489	4.363360
H	2.066612	-1.561418	0.070425
H	2.986143	4.086373	-1.399744
H	1.475749	5.337141	0.238060
H	4.284918	1.208565	0.199989
H	-1.722249	0.761802	1.757014
H	4.770202	2.817214	-0.353876
H	2.444659	-0.283380	2.103603
H	2.528443	2.227357	1.682797
H	2.994366	3.840364	1.138085
H	5.011800	2.355019	1.331740

$(Et_2O)_2Me_2Mg$

SCF energy = -747.304402

H	3.675172	2.449789	-0.293712
H	-0.114678	-1.691829	0.247117
H	4.273443	0.899747	-0.867856
H	1.254969	-2.161189	-0.753999
C	3.648562	1.367554	-0.093169
Mg	1.716092	0.437037	-0.028308
C	0.973211	-1.569867	0.129724
H	4.186141	1.217534	0.854733
H	1.430579	-2.081330	0.989190
H	-0.496081	-0.429984	-1.822417
H	-1.866869	1.451237	-0.891899
C	-0.489015	0.550106	-2.291633
H	-2.627696	0.786348	-2.343545
C	2.175207	1.735785	-3.696539
H	-0.362188	0.417842	-3.367813
C	-1.757370	1.330021	-1.969316
O	0.715310	1.208517	-1.751267
C	1.288944	2.282219	-2.585362
H	0.470095	2.887434	-2.980432
H	-1.759480	2.319134	-2.429525
H	1.870156	2.888257	-1.895909
H	1.619579	1.107155	-4.393559
H	2.991912	1.153118	-3.273735
H	2.603493	2.565288	-4.263829
H	-0.672885	-0.332528	4.089594
H	-1.086913	1.650329	2.606651
C	0.157312	0.133310	3.553786
H	0.667548	0.803013	4.247249
H	0.849805	-0.649604	3.249201
C	-0.374233	0.869762	2.331549
H	1.248995	2.759390	3.111817
H	-0.860255	0.177595	1.649550
O	0.707085	1.484095	1.537224

C	1.198046	2.787984	2.021712
H	-0.690021	3.876913	1.912199
H	2.209579	2.859195	1.631175
C	0.330568	3.940650	1.532096
H	0.754062	4.888632	1.871325
H	0.292345	3.953098	0.443109

$(Et_2O)_2Ph_2Mg$

SCF energy = -1130.792524

H	1.159582	3.681368	-2.762830
H	2.816517	3.284991	-2.320318
C	1.791996	2.907578	-2.327581
H	-0.893993	2.823663	-2.374914
H	1.765101	2.026750	-2.967830
H	1.351036	3.434240	-0.265473
C	1.392329	2.548697	-0.902875
C	-1.088550	2.551819	-1.337545
H	-0.716766	4.549890	-0.531651
H	-2.401597	4.188581	-0.894117
H	-1.870333	1.797741	-1.326234
C	-1.474098	3.765459	-0.502936
H	2.100841	1.839640	-0.481715
O	0.096275	1.843003	-0.809158
H	-5.495846	-2.323699	-1.689791
H	-5.393792	-0.298924	-0.254350
H	2.294490	-1.654092	1.596873
C	-4.539145	-1.917733	-1.385666
C	-4.478325	-0.780259	-0.579866
C	2.685203	-1.593004	0.584276
C	1.921601	-0.948198	-0.418609
H	4.475167	-2.661754	1.142640
C	3.932423	-2.177512	0.338589
C	2.514517	-0.949879	-1.705445
H	-3.385549	-3.409810	-2.420392
C	-3.351171	-2.525299	-1.794771
H	1.986075	-0.492382	-2.538168
C	-3.235989	-0.264984	-0.193910
H	-3.239808	0.623652	0.435658
C	4.476782	-2.145245	-0.945632
C	3.759278	-1.529319	-1.972161
H	5.440498	-2.597133	-1.144662
H	4.166109	-1.507666	-2.976824
H	-1.644822	3.482497	0.535971
C	-2.118849	-1.995566	-1.398096
C	-2.002423	-0.842969	-0.582244
H	-1.219151	-2.501135	-1.736752
Mg	-0.038365	-0.135447	-0.064745
H	0.342631	2.859519	2.284797
O	-0.105271	0.172898	2.028522
H	-2.001873	-0.568055	2.228481
H	1.829639	0.839922	2.078771
C	0.599223	2.267689	3.162730
C	0.981444	0.849738	2.759898
H	1.441745	2.746210	3.666812
H	-0.249701	2.281487	3.847153

C	-1.130355	-0.486214	2.871120
H	-1.365565	0.179916	3.703445
H	-0.469785	-2.511227	2.506127
H	1.245581	0.244846	3.628714
C	-0.680028	-1.858343	3.352333
H	-1.478850	-2.313819	3.941659
H	0.209606	-1.805787	3.981297

MTMgBr$_2$

SCF energy = -6440.11748240

Br	2.586835	-0.038359	2.547731
Br	4.412113	0.017626	-1.512431
Mg	2.437020	-0.001846	0.038203
N	1.868580	2.110452	-0.204554
N	0.314392	0.004343	-0.237103
N	1.863808	-2.105533	-0.265428
C	2.753114	3.125275	-0.231954
C	2.346446	4.457135	-0.253013
C	0.983245	4.740213	-0.251838
C	0.064993	3.691792	-0.236018
C	0.535266	2.378103	-0.212247
C	-0.344295	1.180712	-0.211244
C	-1.739268	1.209335	-0.179401
C	-2.456319	0.006568	-0.179641
C	-1.741924	-1.197151	-0.218866
C	-0.346887	-1.170762	-0.248377
C	0.529935	-2.369579	-0.285336
C	0.056599	-3.680728	-0.351367
C	0.972375	-4.730454	-0.396250
C	2.336238	-4.450856	-0.383769
C	2.745998	-3.121269	-0.320641
C	-3.952456	0.006352	-0.129610
C	-4.609419	-0.082283	1.115382
C	-6.007031	-0.078608	1.139767
C	-6.767272	0.005189	-0.029425
C	-6.092873	0.096195	-1.248953
C	-4.696597	0.097821	-1.323080
C	-3.835193	-0.174635	2.413847
C	-8.277949	-0.026608	0.024051
C	-4.017147	0.198007	-2.673247
H	3.794663	2.840335	-0.245405
H	3.083938	5.244854	-0.270411
H	0.635374	5.763386	-0.266153
H	-0.993707	3.900302	-0.242705
H	-2.277661	2.143931	-0.145680
H	-2.282679	-2.130987	-0.218638
H	-1.002567	-3.886264	-0.368446
H	0.622129	-5.751823	-0.443520
H	3.071918	-5.239504	-0.422657
H	3.788258	-2.838679	-0.321827
H	-6.511839	-0.141869	2.095995
H	-6.664435	0.167955	-2.166162
H	-3.222309	-1.077469	2.461200
H	-4.515611	-0.193289	3.263943
H	-3.158121	0.671360	2.548381

H	-8.648913	-1.055458	0.035545
H	-8.717208	0.468836	-0.842269
H	-8.654785	0.464368	0.922197
H	-3.349554	-0.646516	-2.857401
H	-3.413026	1.104110	-2.759926
H	-4.756236	0.216813	-3.472997

MTMeMgBr

SCF energy = -3905.788179

H	-0.869616	5.761749	-0.028324
H	-3.320607	5.262414	0.082191
C	-1.223232	4.742101	0.031931
C	-2.588448	4.469368	0.096673
H	0.745507	3.887650	-0.023394
C	-0.313277	3.687557	0.037351
C	-3.001937	3.142234	0.176641
H	2.011759	2.132816	0.004344
H	8.380916	1.056805	-0.218002
C	-0.791979	2.376733	0.114613
H	-4.044732	2.862770	0.212769
N	-2.124697	2.119637	0.194558
H	3.105591	0.720537	2.642031
C	1.471544	1.198654	0.024315
C	8.008561	0.028976	-0.254150
C	0.076813	1.173328	0.088547
H	6.406588	-0.116007	1.947224
H	4.506144	-0.147683	3.265074
C	5.830043	-0.066208	1.031605
H	2.925675	1.006509	-2.680145
C	6.498086	-0.003816	-0.193465
C	3.762459	-0.134603	2.469441
H	8.452463	-0.507449	0.585251
C	4.434369	-0.066675	1.113733
H	8.379434	-0.419229	-1.176626
C	5.731445	0.051110	-1.359779
H	6.230918	0.092112	-2.320080
C	3.682467	-0.004771	-0.077487
C	4.333720	0.053912	-1.326576
H	-3.396839	0.863386	3.109057
C	2.186391	-0.004406	-0.015029
H	4.229344	0.129920	-3.476526
C	3.552806	0.113997	-2.623079
N	-0.588730	-0.001684	0.123381
H	3.147479	-1.030993	2.575582
C	-2.850834	-0.017306	2.747773
H	-1.865772	-0.018716	3.234092
Mg	-2.711330	-0.002724	0.608513
Br	-4.764743	0.012139	-0.929505
H	2.889690	-0.745889	-2.739836
C	1.468155	-1.205947	0.001913
C	0.073517	-1.177744	0.067884
H	-3.393945	-0.904224	3.097985
H	2.005410	-2.141199	-0.037395
N	-2.130563	-2.119683	0.160925
C	-0.798656	-2.378992	0.074426

H	-4.052545	-2.858025	0.170994
C	-3.010559	-3.139555	0.128300
C	-0.323668	-3.689656	-0.025083
H	0.734438	-3.891626	-0.091164
C	-2.600780	-4.466327	0.026233
C	-1.236448	-4.741562	-0.045725
H	-3.335091	-5.257096	0.000552
H	-0.885664	-5.761022	-0.123203

MTPhMgBr

SCF energy = -4097.534696

H	8.923618	-0.424302	-1.241958
H	8.942659	-0.498250	0.522026
C	8.524929	0.031430	-0.334791
H	8.896442	1.059462	-0.295807
H	6.811742	0.120356	-2.452718
C	7.013293	-0.000501	-0.319854
C	6.282956	0.068872	-1.508677
H	-0.359446	-5.759895	-0.404235
H	6.856676	-0.137629	1.815347
H	4.845205	0.171170	-3.669057
C	6.308223	-0.076593	0.883362
H	1.251559	-3.882994	-0.446483
H	3.480921	-0.706626	-2.981591
C	4.885108	0.073002	-1.517686
C	4.143453	0.149477	-2.836319
H	2.518579	-2.135650	-0.294451
C	-0.712275	-4.741843	-0.318452
C	4.910447	-0.077068	0.923865
C	0.196089	-3.685151	-0.340070
C	4.196533	0.000010	-0.289717
H	4.915347	-0.172991	3.075432
H	3.588139	-1.064892	2.338601
H	3.522171	1.045548	-2.902925
C	1.981050	-1.200108	-0.274913
C	4.196896	-0.161774	2.257046
H	-2.803115	-5.268750	-0.173902
C	-2.073045	-4.473918	-0.190828
C	2.699621	0.000608	-0.271263
C	-0.280806	-2.377878	-0.221904
C	0.585856	-1.171659	-0.237882
H	3.524526	0.683560	2.416197
C	-2.484422	-3.147493	-0.082252
N	-1.608736	-2.125614	-0.091602
C	1.983706	1.202483	-0.236645
H	2.523501	2.136850	-0.224176
N	-0.078752	0.002562	-0.197926
H	-3.524516	-2.871859	0.010500
C	0.588475	1.176033	-0.201504
Mg	-2.224102	-0.001446	0.251822
C	-0.275549	2.383114	-0.148772
Br	-2.012420	-0.042573	2.804833
H	1.260300	3.890932	-0.325737
C	0.204268	3.692356	-0.226574
N	-1.604159	2.129912	-0.027403

C	-2.477690	3.152931	0.011998
C	-0.701868	4.749869	-0.173733
H	-3.518477	2.876848	0.095258
H	-0.346775	5.769307	-0.227933
C	-2.063381	4.481125	-0.055888
H	-2.791764	5.276665	-0.015602
C	-4.120114	0.014948	-0.749486
C	-5.346268	-0.002272	-0.039601
C	-6.593412	0.007793	-0.675463
C	-6.668404	0.035908	-2.068825
C	-5.487183	0.053771	-2.812979
C	-4.249939	0.043421	-2.159947
H	-5.329481	-0.024055	1.046088
H	-7.503622	-0.006155	-0.086395
H	-7.630330	0.043828	-2.566814
H	-5.532185	0.075479	-3.896396
H	-3.355490	0.058078	-2.779256

MTMgCl$_2$

SCF energy = -2212.269937

Cl	2.899191	-0.028637	2.542389
Cl	4.962585	0.005458	-1.095289
Mg	2.978707	-0.004588	0.179189
N	2.429641	2.098595	-0.140573
N	0.869260	0.002250	-0.194371
N	2.423650	-2.099514	-0.183284
C	3.322260	3.105301	-0.180474
C	2.924508	4.438931	-0.248319
C	1.563410	4.729825	-0.280195
C	0.637293	3.687976	-0.253440
C	1.098310	2.373072	-0.183438
C	0.213148	1.178850	-0.174065
C	-1.181672	1.208784	-0.137163
C	-1.898392	0.005457	-0.127255
C	-1.185031	-1.199332	-0.164780
C	0.209875	-1.172641	-0.199743
C	1.091568	-2.368966	-0.233803
C	0.626629	-3.680706	-0.331733
C	1.549555	-4.724677	-0.378157
C	2.911472	-4.438727	-0.337801
C	3.313215	-3.107993	-0.242144
C	-3.393954	0.005679	-0.061742
C	-4.036450	-0.066123	1.191847
C	-5.433823	-0.062475	1.232134
C	-6.207428	0.005442	0.070831
C	-5.547103	0.080173	-1.157624
C	-4.151860	0.080757	-1.247636
C	-3.247111	-0.141043	2.482284
C	-7.717429	-0.026187	0.141532
C	-3.487725	0.162591	-2.606634
H	4.361312	2.810387	-0.165899
H	3.667017	5.221708	-0.274703
H	1.222708	5.754320	-0.330425
H	-0.419726	3.902501	-0.289068
H	-1.719831	2.143656	-0.103298

H	-1.726133	-2.133056	-0.154727
H	-0.430977	-3.891146	-0.373760
H	1.205798	-5.746857	-0.450038
H	3.651617	-5.223120	-0.378739
H	4.353140	-2.816696	-0.219795
H	-5.927506	-0.113048	2.194878
H	-6.129161	0.139776	-2.069124
H	-2.629571	-1.040488	2.532435
H	-3.917716	-0.153042	3.340270
H	-2.571746	0.708801	2.599797
H	-8.088851	-1.054946	0.147243
H	-8.166583	0.477721	-0.714875
H	-8.083413	0.456287	1.048648
H	-2.828199	-0.688531	-2.789763
H	-2.878295	1.063414	-2.709396
H	-4.236006	0.178351	-3.397908

MTMeMgCl

SCF energy = -1791.864073

H	-1.281461	5.752825	-0.321725
H	-3.731125	5.239374	-0.277553
C	-1.630175	4.732871	-0.241094
C	-2.995146	4.452318	-0.213430
H	0.345561	3.891718	-0.208184
C	-0.713427	3.685956	-0.173965
C	-3.402802	3.125185	-0.103675
H	1.624731	2.134681	-0.061944
H	7.999911	1.049029	0.031254
C	-1.186039	2.374965	-0.071323
H	-4.443862	2.836549	-0.092029
N	-2.519128	2.111521	-0.024295
H	2.638712	0.989283	2.602616
C	1.084059	1.200548	-0.047312
C	7.626720	0.022009	-0.016536
C	-0.312066	1.175003	-0.039270
H	5.928023	0.073839	2.113310
H	3.970481	0.107479	3.344682
C	5.392632	0.040405	1.172188
H	2.621349	0.741367	-2.724825
C	6.114942	-0.007143	-0.022798
C	3.262926	0.097165	2.516713
H	8.031652	-0.510753	0.844975
C	3.995008	0.044956	1.191857
H	8.036789	-0.432539	-0.918843
C	5.401439	-0.059888	-1.221951
H	5.943384	-0.103986	-2.158762
C	3.296922	-0.004346	-0.032725
C	4.003235	-0.058473	-1.251240
H	-3.770008	0.907728	2.933553
C	1.799420	-0.003224	-0.035887
H	3.994854	-0.128151	-3.404111
C	3.281110	-0.117030	-2.581433
N	-0.977187	0.000221	-0.009972
H	2.603720	-0.762733	2.652832
C	-3.231735	0.018332	2.582117

H	-2.245507	0.014402	3.065672
Mg	-3.107950	0.005788	0.439016
Cl	-5.039021	-0.000681	-0.993426
H	2.659784	-1.011143	-2.669037
C	1.081280	-1.205362	-0.028933
C	-0.314804	-1.176440	-0.022232
H	-3.781448	-0.860442	2.942461
H	1.619736	-2.140895	-0.027681
N	-2.524166	-2.107158	0.003329
C	-1.191676	-2.374603	-0.038053
H	-4.450650	-2.828137	-0.057448
C	-3.410315	-3.119557	-0.063600
C	-0.722264	-3.688087	-0.121771
H	0.336252	-3.896991	-0.151310
C	-3.005901	-4.449092	-0.154574
C	-1.641605	-4.733480	-0.176075
H	-3.743792	-5.235074	-0.209183
H	-1.295386	-5.755334	-0.242075

MTPhMgCl

SCF energy = -1983.611032

H	-8.279936	-0.571747	1.719034
H	-8.594406	-0.371232	-0.006585
C	-8.027165	0.020253	0.838257
H	-8.374965	1.040865	1.021769
H	-5.978477	-0.024390	2.634255
C	-6.540706	-0.006409	0.563198
C	-5.618268	-0.014471	1.612737
H	0.719670	-5.754391	-0.958279
H	-6.749956	-0.003222	-1.571662
H	-3.832149	-0.020559	3.500549
C	-6.050767	-0.002621	-0.744399
H	-0.872132	-3.898807	-0.575057
H	-2.635953	-0.899736	2.552757
C	-4.239245	-0.011115	1.385300
C	-3.283212	-0.020071	2.559991
H	-2.122394	-2.139631	-0.250186
C	1.070107	-4.731888	-0.959129
C	-4.679641	0.000818	-1.020558
C	0.173257	-3.687648	-0.740560
C	-3.769511	-0.002686	0.055322
H	-5.051239	0.006648	-3.142205
H	-3.594017	-0.872958	-2.687743
H	-2.627330	0.853155	2.558603
C	-1.590087	-1.204703	-0.336513
C	-4.203510	0.004004	-2.458445
H	3.132658	-5.231020	-1.366479
C	2.414829	-4.445840	-1.183971
C	-2.295830	-0.001825	-0.210067
C	0.647971	-2.374359	-0.745144
C	-0.213165	-1.176088	-0.568060
H	-3.592469	0.881054	-2.683101
C	2.827085	-3.115156	-1.169999
N	1.965169	-2.105240	-0.946461
C	-1.591578	1.202190	-0.333993

H	-2.125040	2.136255	-0.245528
N	0.440937	0.000346	-0.662320
H	3.851544	-2.821386	-1.347148
C	-0.214638	1.175759	-0.565743
Mg	2.608353	0.001717	-0.609372
C	0.644940	2.375464	-0.740669
Cl	4.356164	0.004328	-2.243284
H	-0.877110	3.897611	-0.567474
C	0.168523	3.688124	-0.733562
N	1.962444	2.108425	-0.942744
C	2.823000	3.119876	-1.164578
C	1.063967	4.733934	-0.950368
H	3.847810	2.827770	-1.342455
H	0.712206	5.755979	-0.947563
C	2.409012	4.450049	-1.176010
H	3.125784	5.236496	-1.357212
C	3.096036	0.000604	1.488345
C	4.442658	0.001619	1.924087
C	4.799413	0.001102	3.276945
C	3.811190	-0.000479	4.263125
C	2.469319	-0.001552	3.879986
C	2.131319	-0.001022	2.521869
H	5.238848	0.002856	1.185855
H	5.845570	0.001930	3.562042
H	4.082529	-0.000873	5.311855
H	1.692017	-0.002799	4.636688
H	1.072238	-0.001933	2.269872

MTMe$_2$Mg

SCF energy = -1371.450994

H	7.828330	-0.490007	0.905395
H	7.841993	-0.453976	-0.859809
C	7.427444	0.021912	0.029496
H	5.718801	0.071555	2.152002
H	7.800378	1.049906	0.054169
H	3.755611	0.105433	3.373935
C	5.187757	0.038749	1.208309
C	5.915586	-0.007979	0.016811
H	2.392868	-0.766332	2.674651
C	3.051792	0.094430	2.542636
C	3.789865	0.043295	1.221038
C	5.207478	-0.060039	-1.185627
H	5.753669	-0.103662	-2.120085
H	-1.363113	-5.783985	-0.023109
H	0.207379	-3.876614	-0.036325
H	2.425857	0.985663	2.624981
H	1.415133	-2.137682	0.000145
C	3.096588	-0.005035	-0.006164
C	3.809415	-0.058437	-1.221128
C	-1.740437	-4.771064	-0.014990
C	-0.856652	-3.696895	-0.022036
C	0.877892	-1.201769	-0.011924
C	1.599139	-0.003590	-0.017333
H	2.471412	-1.009635	-2.644293
H	3.810268	-0.127086	-3.374228

C	3.093104	-0.116103	-2.554396
C	-3.114676	-4.526560	0.001089
H	-3.828665	-5.336470	0.005948
C	-1.365524	-2.391795	-0.011391
C	-0.518754	-1.175395	-0.018500
H	-3.359520	0.019881	2.823891
H	2.433854	0.742328	-2.699354
C	0.881451	1.196681	-0.029668
H	1.421567	2.131005	-0.033034
C	-3.554430	-3.207402	0.010212
N	-2.704381	-2.161601	0.004787
H	-4.796982	-0.865971	2.283686
N	-1.193527	0.000522	-0.027641
C	-4.174667	0.017453	2.087525
C	-0.515257	1.174421	-0.034916
H	-4.604880	-2.956911	0.020383
H	-4.793251	0.905639	2.273713
Mg	-3.410987	0.004374	0.045256
H	0.219167	3.872833	-0.091029
C	-1.358290	2.393399	-0.043500
C	-0.845387	3.696645	-0.072290
N	-2.697817	2.167630	-0.021994
C	-4.492029	-0.004336	-1.843079
C	-1.725791	4.773590	-0.077529
C	-3.544594	3.216083	-0.028587
H	-1.345330	5.785128	-0.099610
H	-4.595803	2.969068	-0.013334
C	-3.100745	4.533632	-0.055594
H	-3.812201	5.345772	-0.059827
H	-3.802982	-0.005474	-2.699007
H	-5.138595	0.878336	-1.942611
H	-5.134719	-0.890420	-1.937145

MTPh$_2$Mg

SCF energy = -1754.944381

H	-0.342212	-5.640766	-1.347049
H	-2.790976	-5.169135	-1.121692
C	-0.695315	-4.639725	-1.142999
C	-2.059085	-4.382350	-1.018034
H	1.271481	-3.780433	-1.119489
C	0.214153	-3.592701	-1.011919
C	-2.469725	-3.077303	-0.757287
H	-3.511713	-2.808275	-0.664331
H	-3.343646	-2.093373	4.780497
H	-1.702899	-0.776355	6.102265
C	-0.263075	-2.306029	-0.746658
C	-2.707630	-1.366976	4.286472
C	-1.787427	-0.628288	5.032564
N	-1.593614	-2.064130	-0.617839
H	-3.543444	-1.762427	2.364463
C	-2.810952	-1.168348	2.905060
C	-0.981290	0.306709	4.381579
H	-0.265676	0.891443	4.949938
C	-2.014611	-0.234531	2.200410
C	-1.101672	0.490813	2.999191

H	-0.456618	1.235251	2.536050
H	2.533745	-2.088992	-0.667632
C	0.607703	-1.112016	-0.606640
C	2.003115	-1.152796	-0.585360
H	-7.477395	0.487457	-0.364773
H	-7.601385	0.428823	-2.845624
C	-6.570669	0.384341	-0.950887
C	-6.644354	0.350626	-2.344151
H	-5.316002	0.310862	0.774661
C	-5.328784	0.283480	-0.311657
C	-5.467427	0.214164	-3.083268
H	3.630461	-0.373692	-3.154327
H	-5.511071	0.187109	-4.166849
C	-4.105574	0.144953	-1.015125
C	-4.236116	0.114393	-2.426079
H	3.490468	-1.332529	2.090267
H	-3.345980	0.009418	-3.042472
Mg	-2.209846	0.023749	0.036097
N	-0.052051	0.060604	-0.480895
C	2.731044	0.033582	-0.438714
C	4.313693	0.437904	-2.895301
C	4.227145	0.014268	-0.381257
H	5.058403	0.511924	-3.686776
C	4.982003	0.207992	-1.555543
C	4.090801	-0.420955	2.130033
H	8.919367	-0.723793	0.556654
C	4.875126	-0.203452	0.852782
H	4.763609	-0.505785	2.982276
H	8.996398	-0.288656	-1.152705
C	6.377868	0.180644	-1.473965
H	6.956854	0.323596	-2.378251
C	6.272507	-0.220521	0.886200
C	7.042407	-0.027436	-0.263509
H	6.769355	-0.389435	1.833844
C	8.552815	-0.021304	-0.193118
H	3.727588	1.359816	-2.904539
C	0.626839	1.222170	-0.357184
H	3.399452	0.399626	2.330834
C	2.023376	1.235371	-0.328873
N	-1.558278	2.187486	-0.144950
H	8.930160	0.969110	0.077292
C	-0.225391	2.432502	-0.240052
H	-3.464553	2.951895	-0.005100
H	2.568650	2.158895	-0.207266
C	-2.419507	3.219486	-0.060554
C	0.269934	3.740170	-0.247069
H	1.328898	3.930718	-0.331206
C	-1.990643	4.544167	-0.057476
C	-0.624106	4.803520	-0.149481
H	-2.710746	5.345305	0.012922
H	-0.257879	5.820546	-0.152063

$THF_2MeMgBr$

SCF energy = -3279.216116

H	4.328116	2.775481	1.189704

C	3.279820	2.542739	1.369490
H	3.211191	1.728121	-0.685427
H	3.834469	0.541404	2.041167
H	2.813361	3.418219	1.824074
H	3.190857	1.555153	3.339057
C	3.098941	1.309772	2.281886
C	2.557491	2.153079	0.070946
H	1.981384	2.965092	-0.366657
Br	2.043049	0.060641	-2.885554
O	1.598638	1.073988	0.460528
C	1.697011	0.827353	1.921681
H	1.518906	-0.232184	2.076977
H	0.921124	1.410515	2.420760
H	-0.307289	1.655181	-3.104262
Mg	0.636694	-0.236623	-0.808911
H	-1.230158	2.756712	-2.038563
H	0.918812	-2.466589	0.716296
C	-1.194410	1.762255	-2.487279
O	-1.071934	0.764670	-1.390278
C	0.053993	-1.930394	0.303705
H	-0.606957	-1.696053	1.150442
H	-2.929499	2.228542	-3.727198
H	-2.349112	0.563823	-3.859400
C	-2.507092	1.393649	-3.169790
H	-0.480622	-2.659215	-0.319274
C	-2.428727	0.260447	-1.024124
H	-2.604298	0.499464	0.022136
H	-2.408143	-0.819385	-1.148445
C	-3.400476	0.962246	-1.985836
H	-3.845546	1.838108	-1.511299
H	-4.208233	0.300226	-2.293983

$THF_2PhMgBr$

SCF energy = -3470.960937

C	-4.080953	-2.903866	3.203444
C	-3.245723	-2.968447	2.062241
C	-2.844052	-4.272827	1.686889
C	-3.240009	-5.416881	2.387057
C	-4.064718	-5.302790	3.507065
C	-4.486689	-4.037176	3.915882
Mg	-2.621828	-1.266708	0.963966
Br	-1.134738	-1.144968	-1.064087
O	-1.667895	0.024474	2.243200
C	-0.782015	1.153688	1.821259
C	0.077429	1.482288	3.051407
C	0.013773	0.197165	3.906028
C	-1.411026	-0.293745	3.673529
O	-4.284037	-0.248530	0.315079
C	-5.668405	-0.704858	0.652898
C	-6.580060	-0.077142	-0.414034
C	-5.619098	0.276086	-1.570323
C	-4.346039	0.687004	-0.840483
H	-2.906385	-6.394844	2.060628
H	-4.374021	-6.185811	4.052125
H	-2.202428	-4.404263	0.821336

H	-5.127448	-3.935398	4.784417
H	-4.434261	-1.937532	3.558635
H	-1.421648	1.976683	1.509211
H	-5.892131	-0.371301	1.663666
H	-5.653560	-1.791046	0.627776
H	-0.207386	0.793493	0.972108
H	-7.365650	-0.764612	-0.723221
H	-0.343228	2.323349	3.604638
H	1.096370	1.741215	2.768497
H	-3.429245	0.547563	-1.405328
H	-7.055388	0.826637	-0.030097
H	-1.559486	-1.362437	3.792241
H	-2.137968	0.250605	4.278524
H	-5.424399	-0.596703	-2.194150
H	-4.405334	1.704472	-0.449713
H	0.729107	-0.542231	3.544468
H	0.216186	0.386362	4.959310
H	-6.005514	1.073213	-2.203898

$THF_2MeMgCl$

SCF energy = -1165.292918

H	4.421725	2.617423	1.147887
C	3.358863	2.488161	1.345283
H	3.189111	1.699928	-0.719276
H	3.748494	0.462064	2.061905
H	2.985243	3.411187	1.791219
H	3.188583	1.553405	3.335424
C	3.078004	1.293030	2.283581
C	2.583047	2.151520	0.060279
H	2.043315	3.001387	-0.351497
Cl	1.923836	0.170401	-2.751073
O	1.575804	1.121101	0.461876
C	1.642812	0.916570	1.929176
H	1.377386	-0.119449	2.115974
H	0.915928	1.578532	2.403851
H	-0.312912	1.686072	-3.052986
Mg	0.630755	-0.211560	-0.796475
H	-1.257950	2.752554	-1.970779
H	0.985167	-2.421770	0.743309
C	-1.210509	1.772058	-2.447754
O	-1.099874	0.745167	-1.375485
C	0.105736	-1.931504	0.305205
H	-0.590634	-1.731616	1.132071
H	-2.933139	2.269024	-3.693154
H	-2.336557	0.615573	-3.879872
C	-2.510814	1.417390	-3.161542
H	-0.372982	-2.686236	-0.332066
C	-2.451787	0.193696	-1.069099
H	-2.651947	0.364025	-0.013970
H	-2.410028	-0.876282	-1.259799
C	-3.416324	0.933640	-2.007628
H	-3.867854	1.787274	-1.499750
H	-4.219137	0.283669	-2.352265

$THF_2PhMgCl$

SCF energy = -1357.037933

C	-4.078096	-2.923287	3.215793
C	-3.246071	-2.968752	2.071469
C	-2.840510	-4.266541	1.677160
C	-3.229880	-5.421798	2.362291
C	-4.051826	-5.326296	3.486130
C	-4.477242	-4.068074	3.913618
Mg	-2.630622	-1.255615	0.990651
Cl	-1.212951	-1.077637	-0.893280
O	-1.696241	0.040341	2.277628
C	-0.819828	1.172331	1.842049
C	0.070956	1.487744	3.053375
C	0.029376	0.193666	3.895604
C	-1.402075	-0.292626	3.696523
O	-4.281245	-0.249317	0.300294
C	-5.673851	-0.648596	0.667211
C	-6.576372	-0.027360	-0.409942
C	-5.620688	0.232295	-1.595358
C	-4.319769	0.625050	-0.904446
H	-2.893202	-6.393827	2.021476
H	-4.356132	-6.217980	4.019811
H	-2.200255	-4.383632	0.808463
H	-5.115650	-3.980870	4.785452
H	-4.433449	-1.963257	3.585575
H	-1.466754	1.998717	1.555078
H	-5.875442	-0.274323	1.668442
H	-5.696279	-1.735312	0.676581
H	-0.270308	0.816978	0.974339
H	-7.397546	-0.691138	-0.675602
H	-0.336808	2.321862	3.626481
H	1.082265	1.750799	2.747813
H	-3.415510	0.417589	-1.468496
H	-7.003693	0.912965	-0.058392
H	-1.549248	-1.362417	3.807950
H	-2.110834	0.246757	4.327053
H	-5.473068	-0.675612	-2.181036
H	-4.329947	1.663312	-0.568014
H	0.733909	-0.542392	3.507141
H	0.260353	0.371902	4.944929
H	-5.985365	1.014533	-2.259628

THF_2Me_2Mg

SCF energy = -744.883694

H	-1.153529	-3.545162	-0.921365
C	-1.518456	-2.509529	-0.983665
H	-2.615630	-2.576693	-0.938444
H	3.492677	-2.487583	0.954720
H	1.504185	-2.578302	-1.325647
H	-0.062923	-2.231406	3.108146
H	-1.269376	-2.155634	-1.996363
H	3.907838	-2.364735	-1.449706
C	3.564418	-1.481074	0.540320
C	3.405728	-1.511417	-0.996083
C	1.884205	-1.566503	-1.207269
H	4.513110	-1.047414	0.854221

Mg	-0.732996	-1.304737	0.608593
C	-0.648549	-1.371045	2.751541
H	-1.650332	-1.490143	3.189531
H	2.001728	-0.854334	1.983885
O	1.288740	-1.022568	0.044083
C	2.368233	-0.642095	0.984577
H	-2.460228	0.071738	-1.558160
H	1.538781	-0.955669	-2.038164
H	-0.209997	-0.478178	3.224087
H	3.822816	-0.603336	-1.434744
H	-4.221136	1.215378	-0.316825
O	-1.540944	0.614012	0.219573
C	-2.200318	0.995434	-1.050993
H	2.559030	0.427801	0.877795
H	-2.379875	1.038947	2.079278
C	-3.386791	1.852005	-0.614330
H	-1.488159	1.562997	-1.653642
H	-3.728675	2.518783	-1.404986
C	-1.894907	1.595806	1.281231
C	-2.823089	2.616759	0.603877
H	-0.972557	2.031156	1.658806
H	-3.606045	2.960740	1.278189
H	-2.258311	3.489271	0.271090

THF_2Ph_2Mg

SCF energy = -1128.372650

H	-3.058265	-6.694142	3.283436
H	-2.758340	-6.692373	0.818521
C	-2.971238	-5.758619	2.744864
C	-2.803678	-5.753788	1.359092
H	-3.151305	-4.532921	4.504609
C	-3.023929	-4.542578	3.427627
H	-2.552912	-4.583541	-0.406656
C	-2.690056	-4.541575	0.670015
C	-2.909167	-3.340741	2.720218
C	-2.739564	-3.281822	1.315057
H	-2.954426	-2.415584	3.292612
H	-3.215226	-2.458243	-2.728337
Mg	-2.549612	-1.425694	0.252252
H	-2.541786	-1.941519	-5.021732
C	-2.494580	-1.659206	-2.883309
C	-2.117050	-1.375880	-4.200128
C	-1.975210	-0.962141	-1.764134
C	-1.186380	-0.368192	-4.458623
C	-1.033228	0.046776	-2.079738
H	-0.888398	-0.144568	-5.475447
H	-0.579970	0.624104	-1.276900
C	-0.642221	0.345044	-3.389699
H	-4.916992	1.511983	-0.134178
H	0.085444	1.126780	-3.577628
H	-7.045580	0.748631	-1.088787
H	1.249648	0.909647	1.942078
C	-4.954491	0.488649	-0.513444
C	-6.387098	-0.010923	-0.669471
H	-4.331233	0.394327	-1.397312

H	-6.409131	-0.883586	-1.323182
H	0.442805	-1.250269	1.269676
H	-7.115872	0.484581	1.320258
C	0.600804	0.439506	2.682297
O	-4.373064	-0.413188	0.514955
H	1.208733	0.171199	3.544848
C	-0.105415	-0.780570	2.082693
C	-6.775120	-0.397192	0.775384
H	-0.249047	2.423321	3.132419
O	-1.380144	-0.248860	1.518789
H	-7.571055	-1.139487	0.806576
C	-0.563544	1.383853	3.050399
C	-5.470157	-0.939740	1.382407
H	-0.370632	-1.530605	2.824584
H	-1.314601	1.789412	1.035211
C	-1.551560	1.171252	1.902112
H	-5.290820	-0.592715	2.398077
H	-5.392613	-2.023250	1.355862
H	-1.011990	1.085539	3.999186
H	-2.594001	1.310003	2.176513

^{1}H NMR spectra

Figure S6: ^{1}H NMR spectrum of (mesitylterpy)$MgBr_2$ (**5a**)

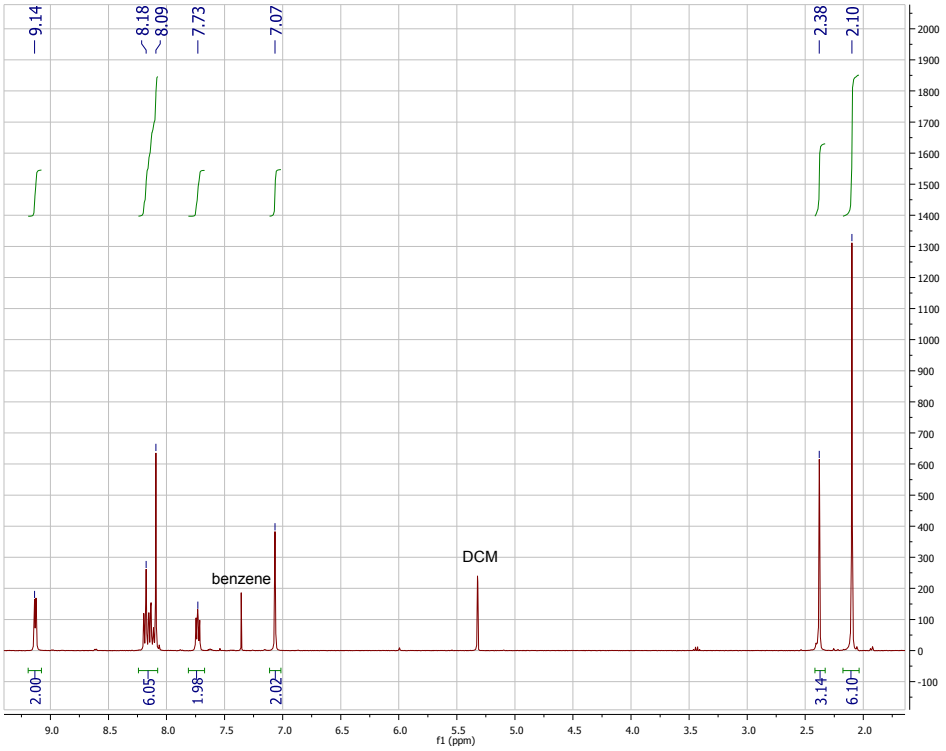


Figure S7: ^{1}H NMR spectrum of (tri-^{t}Buterpy)$MgBr_2$ (**5b**)

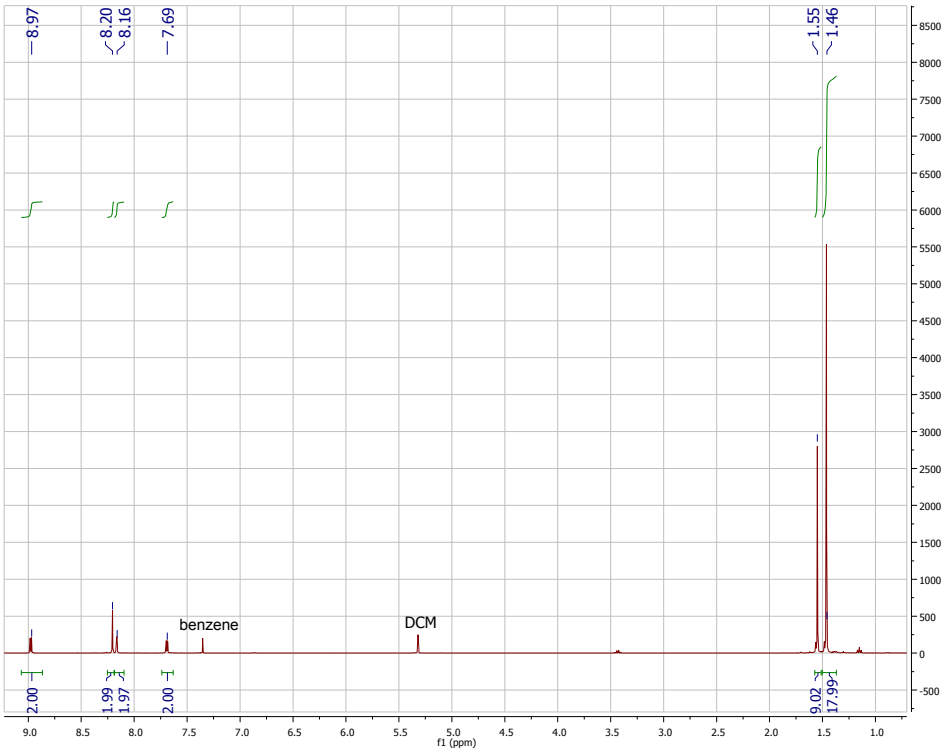


Figure S8: ^{1}H NMR spectrum of (phenylterpy)$MgBr_2$ (**5c**) (peaks which are not picked, represent impurities)

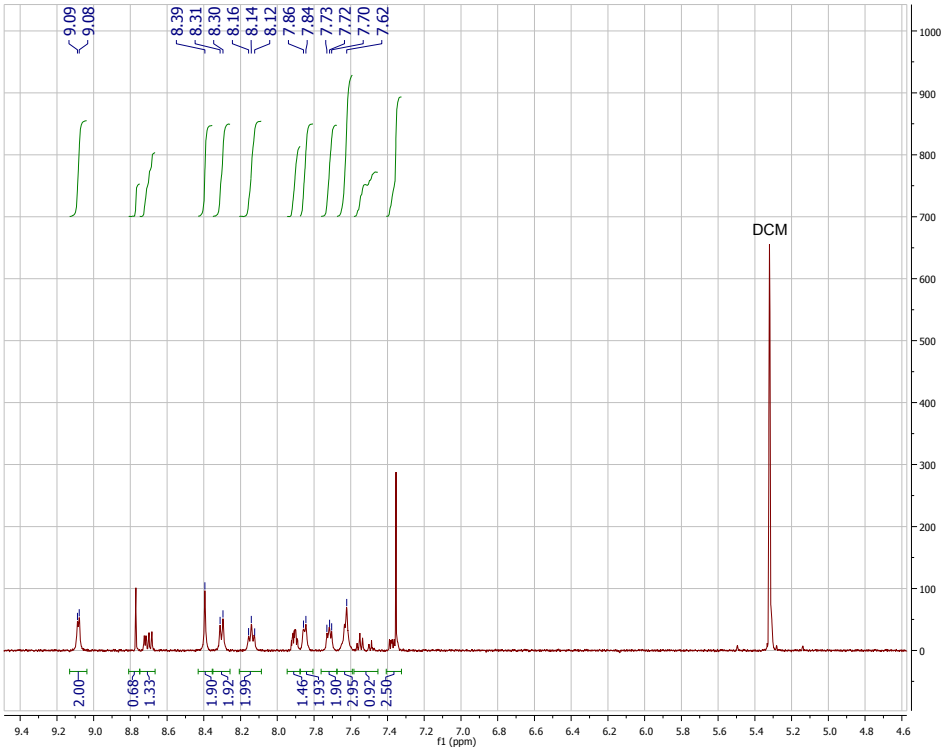


Figure S9: ^{1}H NMR spectrum of (mesitylterpy)$MgCl_2$ (**6a**)

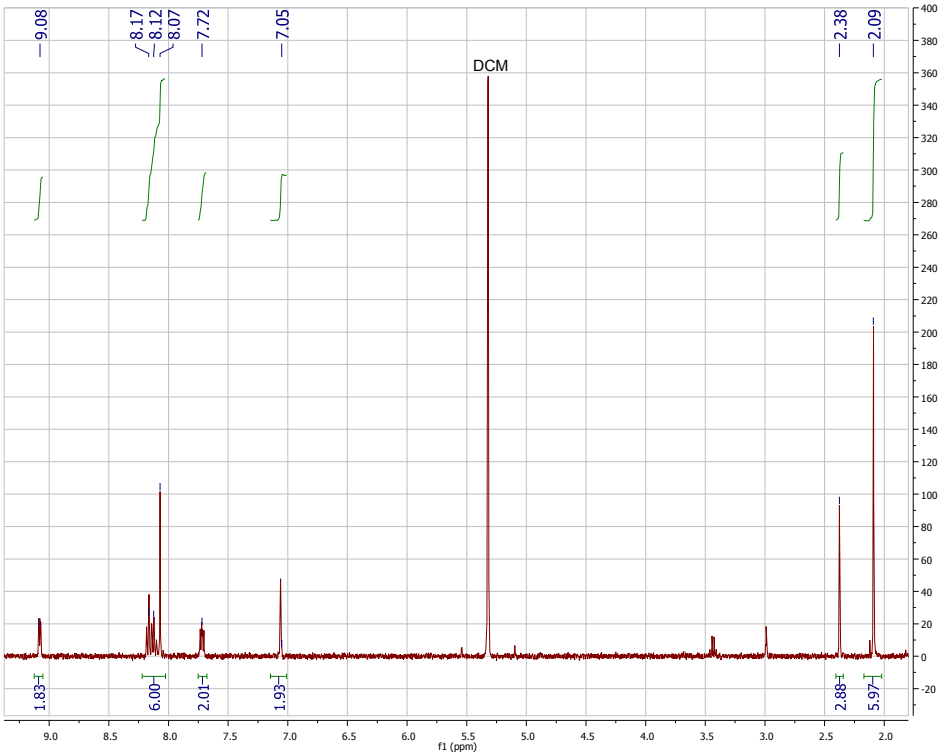


Figure S10: ^{1}H NMR spectrum of (tri-^{t}Buterpy)$MgCl_2$ (**6b**)

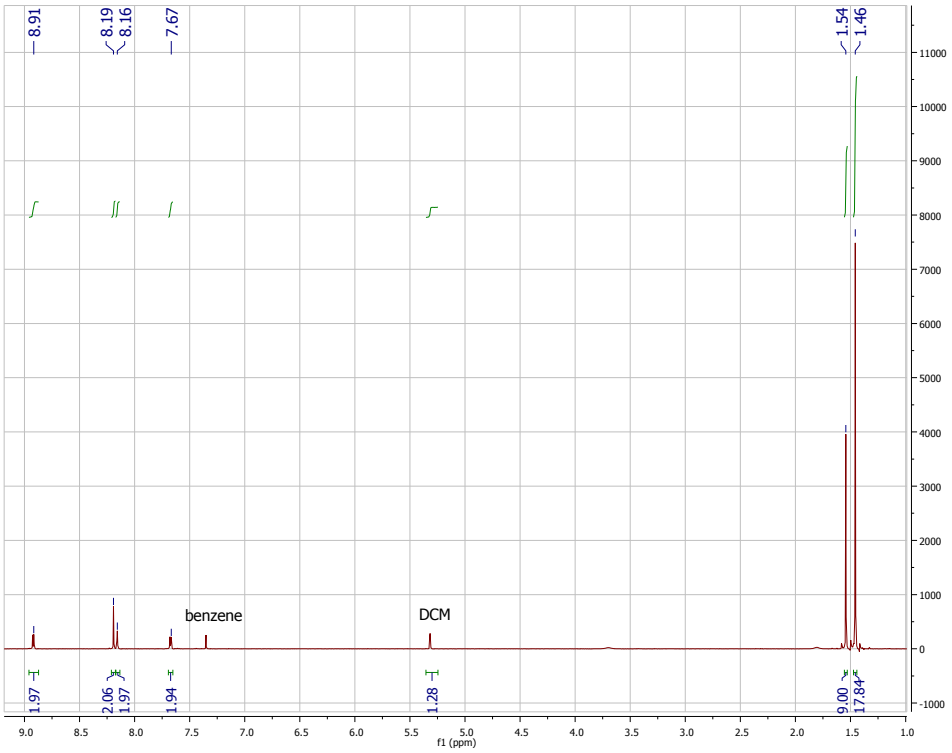


Figure S11: ^{1}H NMR spectrum of (phenylterpy)$MgCl_2$ (**5c**) (peaks which are not picked, represent impurities)