Supporting Information

Reactivity of $Mg(AlMe_4)_2$ towards neutral Tris(pyrazolyl)alkanes

Felix Kracht, Christoph Stuhl, Cäcilia Maichle-Mössmer and Reiner Anwander*

Institut für Anorganische Chemie, Eberhard Karls Universität Tübingen, Auf der Morgenstelle 18, 72076 Tübingen (Germany)

* to whom correspondence should be addressed: E-Mail reiner.anwander@uni-tuebingen.de

Table of Contents

Table S1. Crystallographic Data for Compounds **3a**, **3b**, **3c** and **3e**

	3a	**3b**	**3c***	**3e**
formula	$C_{17}H_{24}N_6$	$C_{20}H_{24}N_6$	$C_{29}H_{42}N_6$	$C_{30}H_{26}N_6$
CCDC	2386227	2386220	2386219	2386222
M [g mol^{-1}]	312.42	348.39	474.68	470.57
color/shape	colorless/needle	colorless/rod	colorless/block	colorless/block
Crystal dimensions [mm]	0.232 x 0.176 x 0.088	0.389 x 0.235 x 0.186	0.360 x 0.340 x 0.280	0.549 x 0.256 x 0.216
cryst. system	orthorhombic	hexagonal	trigonal	triclinic
space group	*P*ca2$_1$	*P*6$_3$	*R*3*c*	$P\bar{1}$
a [Å]	10.2106(6)	12.7968(10)	13.0173(14)	11.6713(8)
b [Å]	30.7802(17)	12.7968(10)	13.0173(14)	13.0857(9)
c [Å]	11.0809(6)	6.5617(5)	27.493(5)	17.0523(12)
α [°]	90	90	90	92.633(2)
β [°]	90	90	90	97.331(2)
γ [°]	90	120	120	100.998(2)
V [Å^3]	3482.6(3)	930.57(16)	4034.5(11)	2529.0(3)
Z	8	2	6	4
T [K]	100(2)	100(2)	100(2)	100(2)
wavelength [Å]	0.71073	0.71073	0.71073	0.71073
ρ_{calcd} [g cm^{-3}]	1.192	1.243	1.172	1.236
μ [mm^{-1}]	0.075	0.078	0.071	0.076
F (000)	1344	372	1548	992
θ range [°]	1.323/26.361	3.184/30.049	2.336/28.774	1.795/28.282
unique reflns	7074	1824	2338	12609
observed reflns	76630	25103	10181	12609
[a]R_1/[b]wR_2 (I>2σ)[a]	0.0406/0.0923	0.0404/0.0914	0.0832/0.2389	0.0517/0.01166
[a]R_1/[b]wR_2 (all data)	0.0513/0.0989	0.0486/0.0989	0.0989/0.2587	0.0689/0.1279
GOF[c]	1.034	1.054	1.077	1.042

[a]$R_1 = \Sigma(||F_o| - |F_c||) / \Sigma|F_o|$, $F_o > 4\sigma(F_o)$, [b]$wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2 / \Sigma[w(F_o^2)^2]\}^{1/2}$. [c]$GOF = [\Sigma w(F_o^2 - F_c^2)^2 / (n_o - n_p)]^{1/2}$ *connectivity only.

Table S2. Crystallographic data for compounds **3f**, **3g**, **4** and **5a**

	3f	**3g**	**4**	**5a**
formula	$C_{31}H_{28}N_6$	$C_{32}H_{30}N_6$	$C_{86}H_{108}Al_2MgN_{12}$ ·0.5(C_7H_8)	$C_{42}H_{72}Al_2MgN_6$ ·2(C_4H_8O)
CCDC	2386225	2386224	2386228	2386223
M [g mol^{-1}]	484.59	498.62	1434.17	967.59
color/shape	colorless/block	colorless/block	colorless/block	colorless/plate
Crystal dimensions [mm]	0.390 x 0.263 x 0.209	0.232 x 0.174 x 0.169	0.263 x 0.259 x 0.196	0.348 x 0.153 x 0.110
cryst. system	triclinic	triclinic	tetragonal	triclinic
space group	$P\bar{1}$	$P\bar{1}$	$I\bar{4}2d$	$P\bar{1}$
a [Å]	10.0945(6)	9.9371(2)	34.119(3)	9.7777(12)
b [Å]	10.6005(6)	10.2888(2)	34.119(3)	12.1692(14)
c [Å]	14.4819(8)	14.6512(4)	15.6274(12)	13.3741(16)
α [°]	68.975(2)	71.1880(10)	90	111.897(2)
β [°]	84.913(2)	87.3140(10)	90	103.651(2)
γ [°]	66.2510(10)	68.6040(10)	90	97.092(2)
V [Å^3]	1321.17(13)	1315.95(5)	18192(3)	1394.8(3)
Z	2	2	8	1
T [K]	101(2)	101(2)	100(2)	100(2)
wavelength [Å]	0.71073	0.71073	0.71073	0.71073
ρ_{calcd} [g cm^{-3}]	1.218	1.258	1.047	1.152
μ [mm^{-1}]	0.074	0.077	0.086	0.111
F (000)	512	528	6168	526
θ range [°]	1.510/27.102	1.473/28.700	3.470/28.350	2.205/29.026
unique reflns	5840	6810	11311	7374
observed reflns	47758	47259	77626	34685
[a]R_1/[b]wR_2 ($I>2\sigma$)[a]	0.0520/0.1240	0.0414/0.1039	0.0570/0.1290	0.0406/0.0961
[a]R_1/[b]wR_2 (all data)	0.0600/0.1317	0.0518/0.1113	0.0774/0.1392	0.0540/0.1045
GOF[c]	1.040	1.022	1.044	1.060

[a]$R_1 = \Sigma(||F_0| - |F_c||) / \Sigma|F_0|$, $F_0 > 4\sigma(F_0)$, [b]$wR_2 = \{\Sigma[w(F_0^2 - F_c^2)^2 / \Sigma[w(F_0^2)^2]\}^{1/2}$. [c]$GOF = [\Sigma w(F_0^2 - F_c^2)^2 / (n_0 - n_p)]^{1/2}$

Table S3. Crystallographic Data for Compounds **5b**, **6**, **7** and **8**

	5b*	**6**	**7***	**8**
formula	$C_{48}H_{72}Al_2MgN_{12}$ ·1.5(C_7D_8)	$C_{33}H_{55}AlMgN_6O_2$ ·2(C_4H_8O)	$C_{77}H_{99}Al_3Mg_2N_{12}$	$C_{37}H_{66}Al_2MgN_6$
CCDC		2386221		2386230
M [g mol^{-1}]	1045.72	763.32	1322.24	673.22
color	colorless/plate	colorless/plate	colorless/block	colorless/plate
crystal dimensions [mm]	0.098 x 0.118 x 0.140	0.329 x 0.189 x 0.155	0.212 x 0.273 x 0.291	0.186 x 0.056 x 0.053
cryst. system	triclinic	triclinic	monoclinic	orthorhombic
space group	$P\bar{1}$	$P\bar{1}$	$P2_1/n$	$P2_12_12_1$
a [Å]	13.275(3)	12.099(4)	18.0198(13)	11.1027(12)
b [Å]	13.327(3)	12.786(4)	23.3262(17)	17.3897(19)
c [Å]	17.445(5)	15.286(4)	24.3189(17)	20.542(2)
α [°]	85.470(6)	90.005(5)	90	90
β [°]	86.305(5)	109.607(4)	108.3360(10)	90
γ [°]	83.301(5)	103.636(4)	90	90
V [Å^3]	3050.8(14)	2156.8(11)	9703.1(12)	3966.1(7)
Z	2	2	4	4
T [K]	100(2)	100(2)	100(2)	100(2)
wavelength [Å]	0.71073	0.71073	0.71073	0.71073
ρ_{calcd} [g cm^{-3}]	1.138	1.175	0.905	1.127
μ [mm^{-1}]	0.104	0.107	0.091	0.122
F (000)	1114	832	2832	1472
θ range [°]	1.173/25.184	1.419/24.712	1.746/23.852	2.085/27.166
unique reflns	9558	7361	14946	8754
observed reflns	48977	49371	157365	95948
[a]R_1/[b]wR_2 (I>2σ)[a]	0.1806/0.3484	0.0737/0.1292	0.0981/0.2943	0.0525/0.1223
[a]R_1/[b]wR_2 (all data)	0.2128/0.3571	0.1093/0.1438	0.1276/0.3271	0.0756/0.1350
GOF[c]	2.154	1.084	1.022	1.019

[a]$R_1 = \Sigma(||F_o| - |F_c||) / \Sigma|F_o|$, $F_o > 4\sigma(F_o)$, [b]$wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2 / \Sigma[w(F_o^2)^2]\}^{1/2}$. [c]$GOF = [\Sigma w(F_o^2 - F_c^2)^2 / (n_o - n_p)]^{1/2}$ *connectivity only.

Table S4. Crystallographic Data for Compounds **9** and **10**

	9	**10**
formula	$C_{49}H_{72}Al_2MgN_6 \cdot 2.5(C_6D_6)$	$C_{45}H_{59}AlMgN_6 \cdot 2(C_7H_8)$
CCDC	2386229	2386226
M [g mol^{-1}]	1033.75	919.54
color	colorless/plate	colorless/block
crystal dimensions [mm]	0.488 x 0.102 x 0.065	0.273 x 0.103 x 0.089
cryst. system	monoclinic	triclinic
space group	$P2_1/c$	$P\bar{1}$
a [Å]	21.4977(15)	12.9915(16)
b [Å]	18.5064(13)	13.6495(17)
c [Å]	15.4454(11)	15.6799(19)
α [°]	90	88.421(3)
β [°]	97.1020(10)	83.625(3)
γ [°]	90	78.741(3)
V [Å^3]	6097.7(7)	2710.1(6)
Z	4	2
T [K]	100(2)	100(2)
wavelength [Å]	0.71073	0.71073
ρ_{calcd} [g cm^{-3}]	1.126	1.127
μ [mm^{-1}]	0.100	0.091
F (000)	2204	992
θ range [°]	1.457/27.463	1.307/25.081
unique reflns	13915	9624
observed reflns	85399	59387
[a]R_1/[b]wR_2 (I>2σ)[a]	0.0471/0.1032	0.0423/0.1017
[a]R_1/[b]wR_2 (all data)	0.0859/0.1232	0.0636/0.1148
GOF[c]	1.015	1.020

[a]$R_1 = \Sigma(||F_0| - |F_c||) / \Sigma|F_0|$, $F_0 > 4\sigma(F_0)$, [b]$wR_2 = \{\Sigma[w(F_0^2 - F_c^2)^2 / \Sigma[w(F_0^2)^2]\}^{1/2}$. [c]$GOF = [\Sigma w(F_0^2 - F_c^2)^2 / (n_0 - n_p)]^{1/2}$

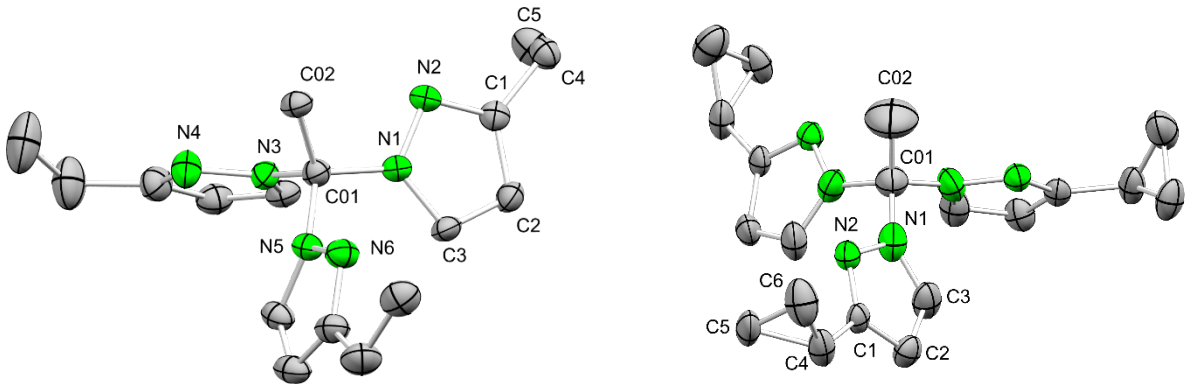


Figure S1. Crystal structures of **3a** (left) and **3b** (right), thermal ellipsoids set at 50% probability. Hydrogen atoms are omitted for clarity.

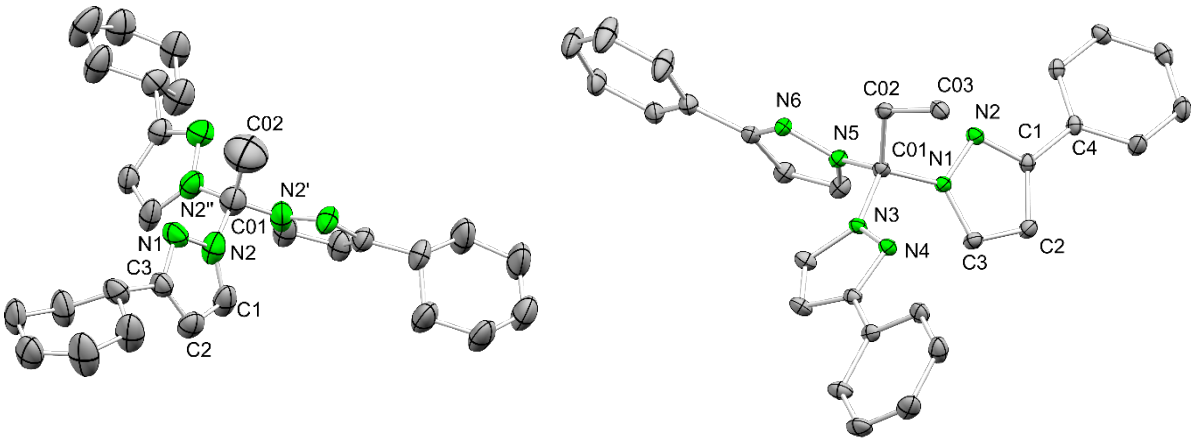


Figure S2. Connectivity structure of **3c** (left) and crystal structure **3e** (right), thermal ellipsoids set at 50% probability. Hydrogen atoms are omitted for clarity.

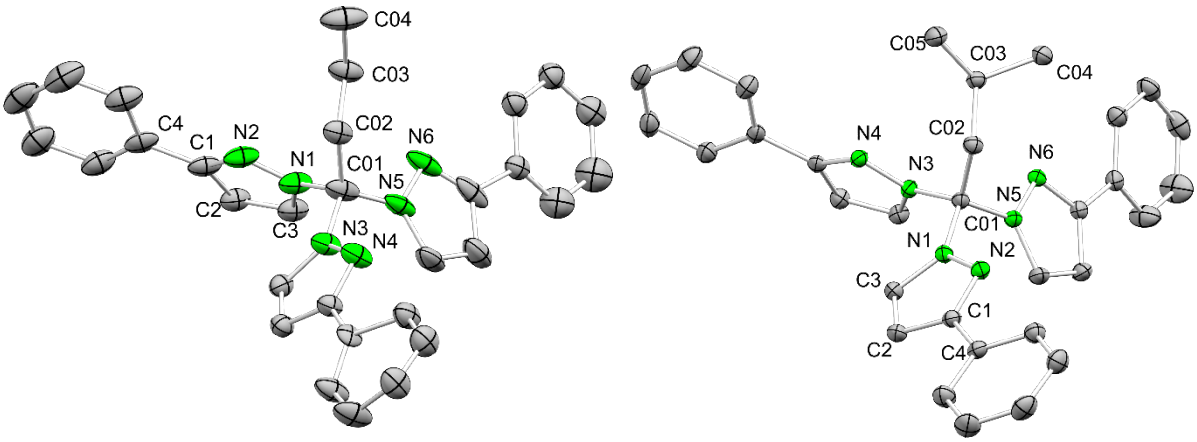


Figure S3. Crystal structures of **3f** (left) and **3g** (right), thermal ellipsoids set at 50% probability. Hydrogen atoms are omitted for clarity.

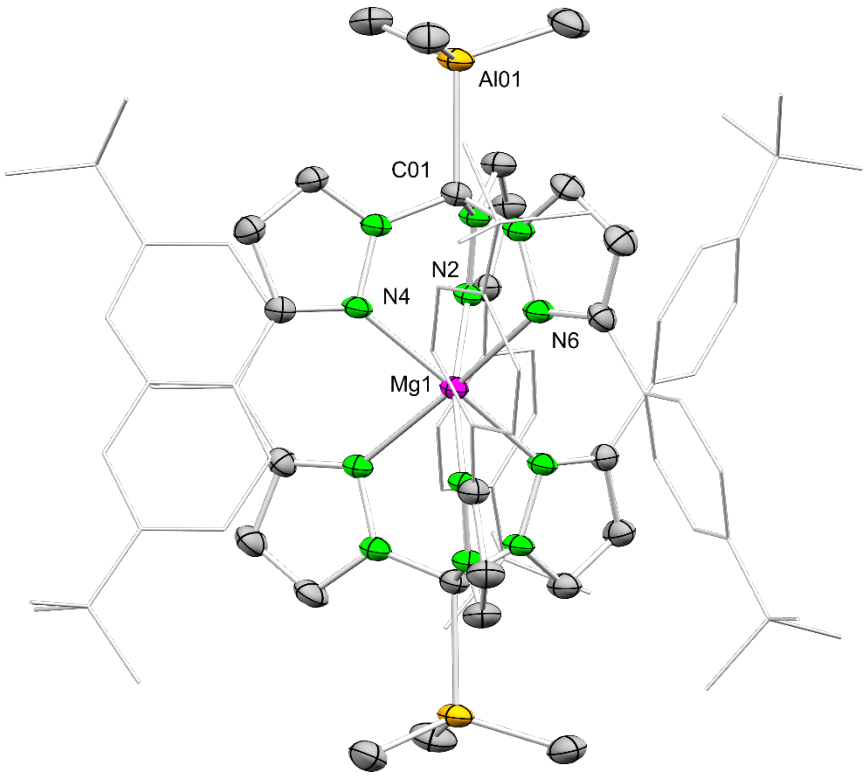


Figure S4. Crystal structures of **4**. Thermal ellipsoids set at 50% probability. Hydrogen atoms and one lattice toluene are omitted and *p*-*t*BuPh moieties are set as wireframe for clarity. Selected interatomic distances [Å]: Mg1–N2 2.221(3), Mg1–N4 2.2214(3), Mg1–N6 2.222(2), Al01–C01 2.209(4).

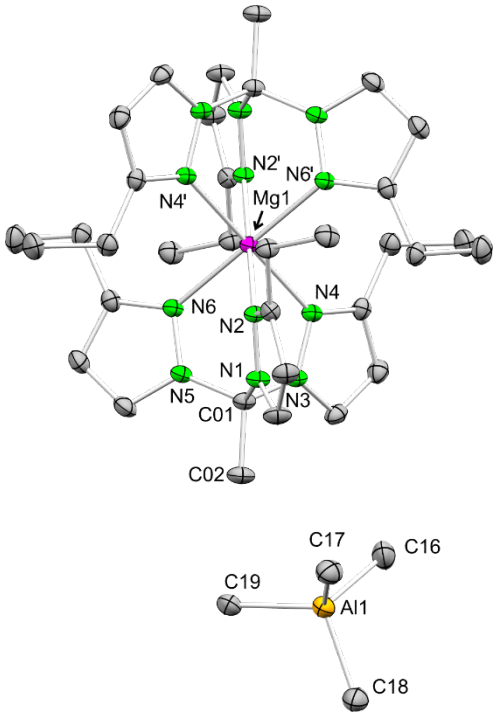


Figure S5. Crystal structure of **5a**, thermal ellipsoids set at 50% probability. Hydrogen atoms are omitted for clarity. Selected interatomic distances [Å]: Mg1–N2 2.1666(10), Mg1–N4 2.1676(10), Mg1–N6 2.1458(10).

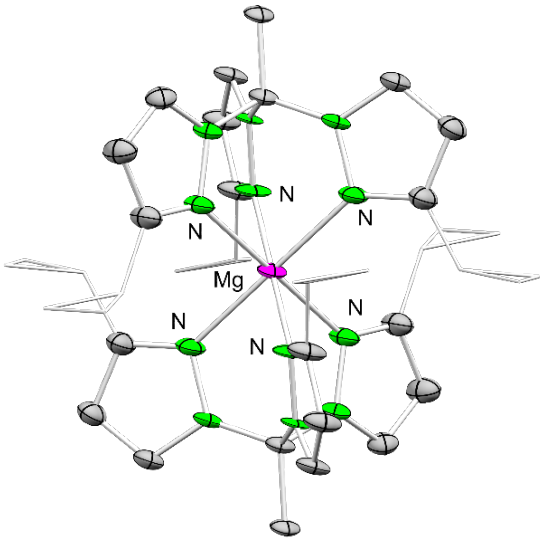


Figure S6. Connectivity of **5b**, hydrogen atoms are omitted for clarity. Thermal ellipsoids set at 50%. $[AlMe_4]^-$ and C_6D_6 are omitted for clarity.

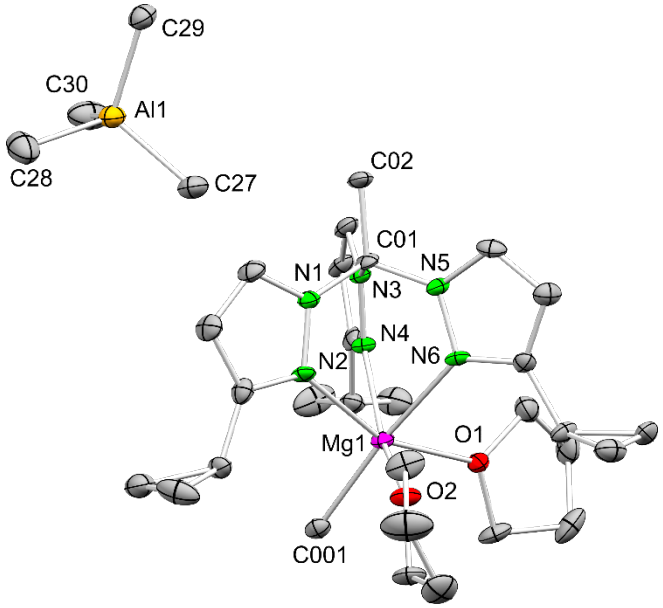


Figure S7. Crystal structure of **6**, thermal ellipsoids set at 50% probability. Hydrogen atoms are omitted for clarity. Selected interatomic distances [Å]: Mg1–N2 2234(4), Mg1–N4 2.230(4), Mg1–N6 2.233(3), Mg1–C001 2.182(4), Mg1–O1 2.184(4), Mg1–O2 2.186(4).

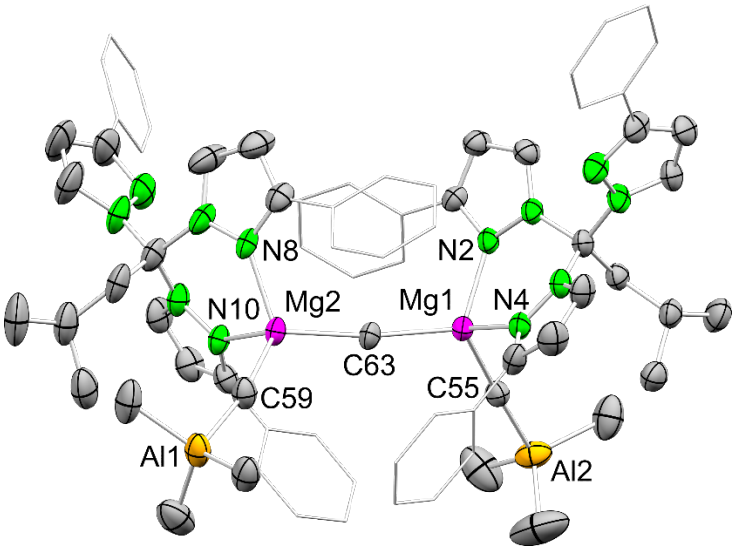


Figure S8. Connectivity of **7**, thermal ellipsoids set at 50% probability. Hydrogen atoms and the counter ion $[AlMe_4]^-$ are omitted for clarity. Phenyl moieties are set as wireframe.

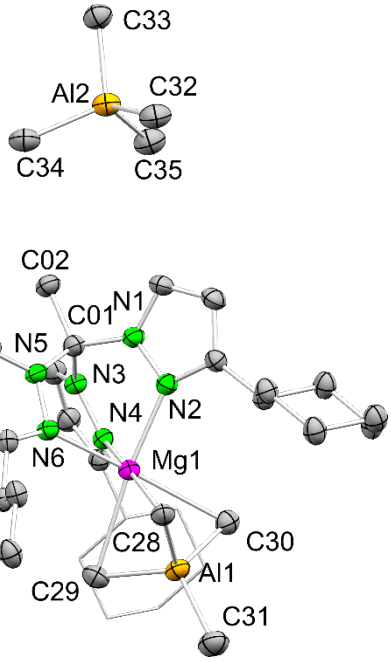


Figure S9. Crystal structures of **8**, thermal ellipsoids set at 50% probability. Hydrogen atoms are omitted for clarity. Selected interatomic distances [Å] and angles [°]: Mg1–N2 2123(3), Mg1–N4 2.128(3), Mg1–N6 2.143(3), Mg1–C28 2.545(4), Mg1–C29 2.633(4), Mg1–C30 2.442(4); Mg1–C28–Al1 66.84(13), Mg1–C29–Al1 65.13(12), Mg1–C30–Al1 68.74(13).

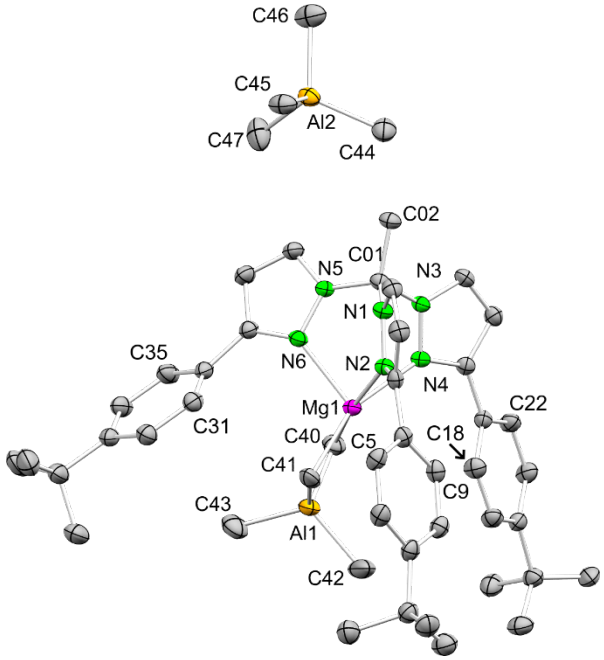


Figure S10. Crystal structures of **9**, thermal ellipsoids set at 50% probability. Hydrogen atoms and 2.5 lattice solvent C_6D_6 are omitted for clarity. Selected interatomic distances [Å] and angles [°]: Mg1–N2 2.1933(15), Mg1–N4 2.1882(15), Mg1–N6 2.1387(15), Mg1–C40 2.346(2), Mg1–C41 2.284(2); Mg1–C40–Al1 77.85(7), Mg1–C41–Al1 78.65(7).

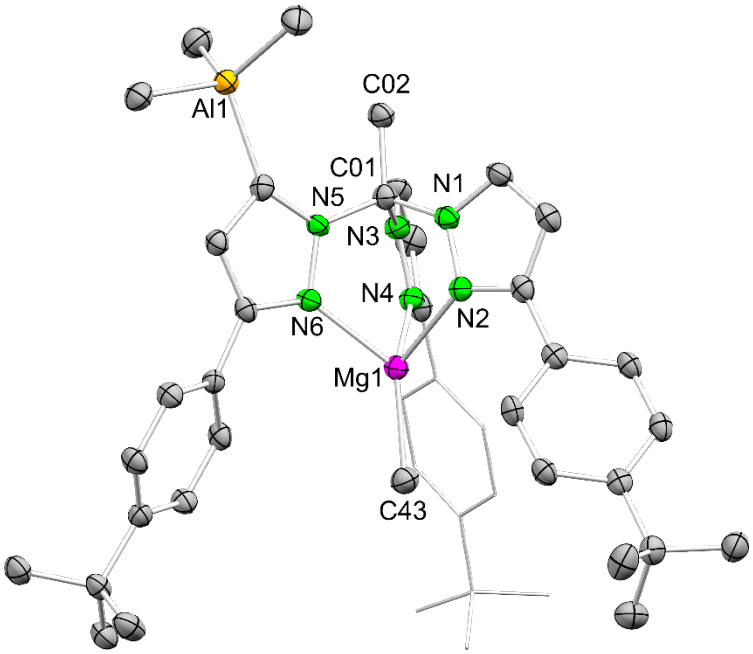


Figure S11. Crystal structures of **10**, thermal ellipsoids set at 50% probability. Hydrogen atoms are omitted for clarity. Selected interatomic distances [Å]: Mg1–N2 2.1398(16), Mg1–N4 2.1231(16), Mg1–N6 2.0965(16), Mg1–C43 2.090 (2).

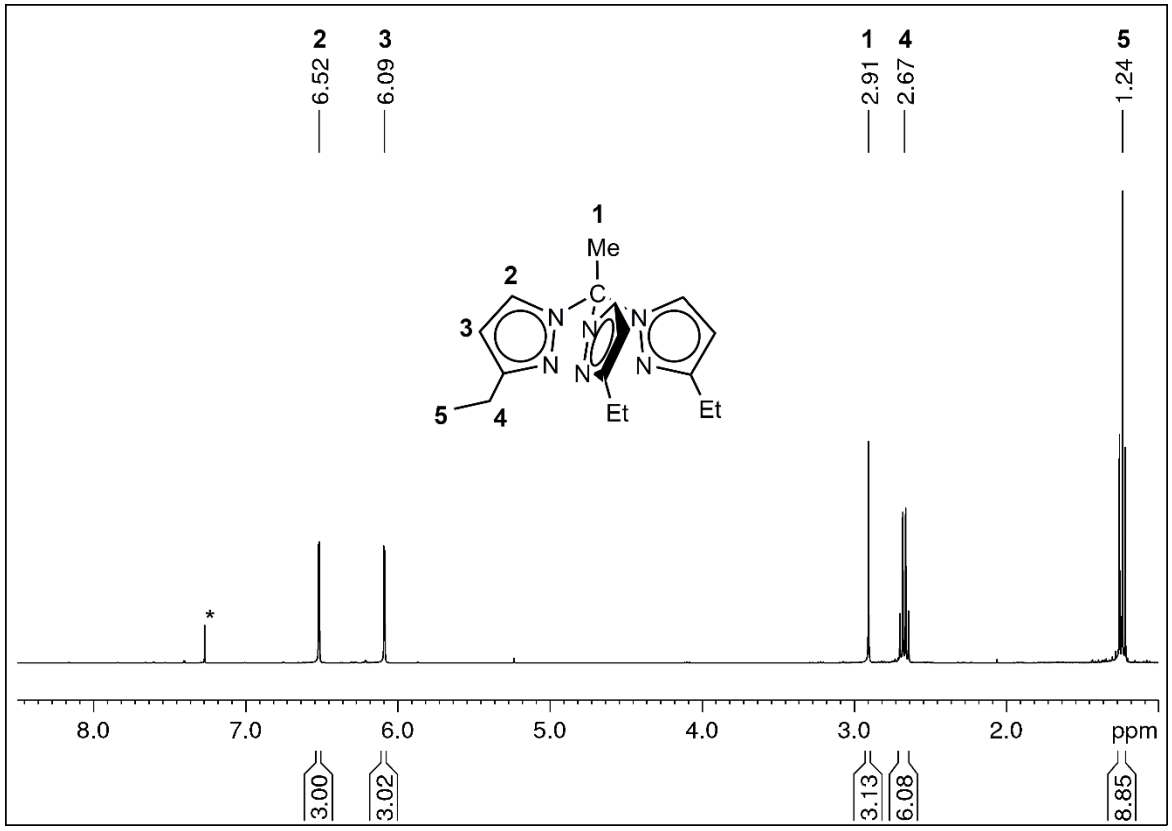


Figure S12. ^{1}H NMR spectrum (400 MHz) of **3a** in $CDCl_3$ (*) at 26 °C.

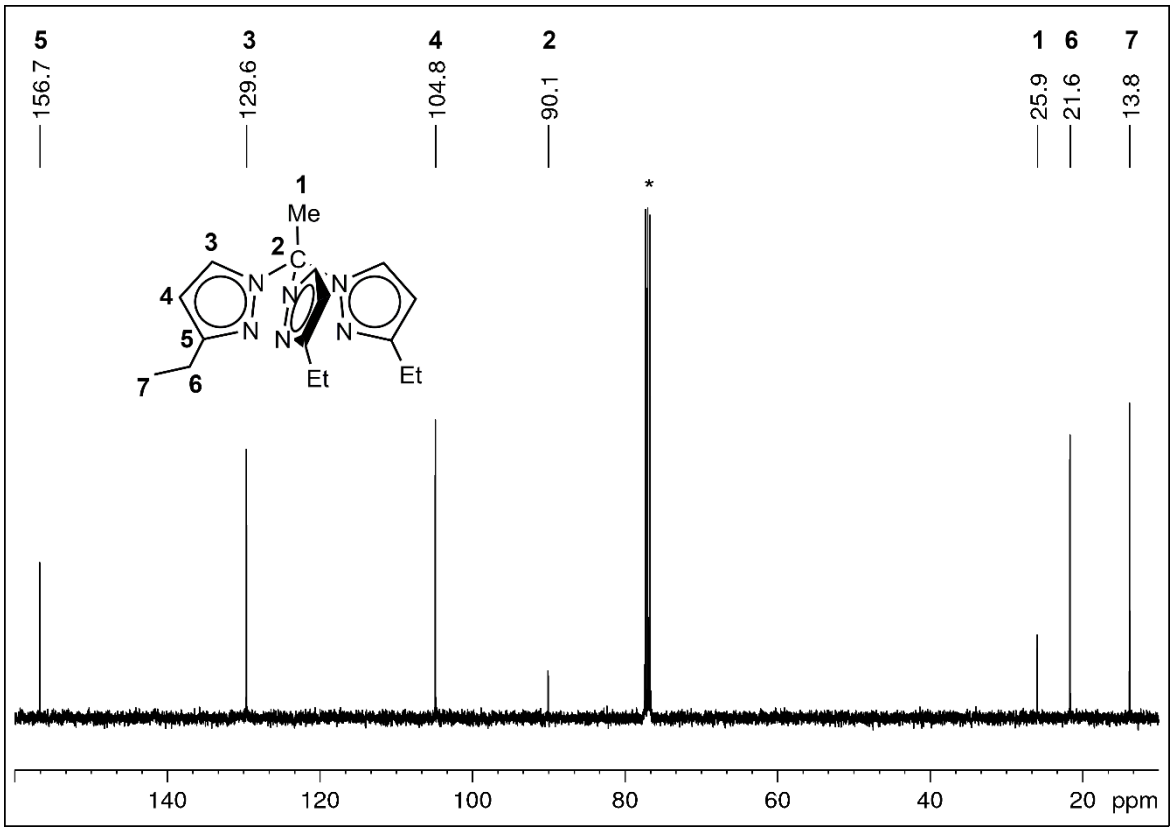


Figure S13. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz) of **3a** in $CDCl_3$ (*) at 26 °C.

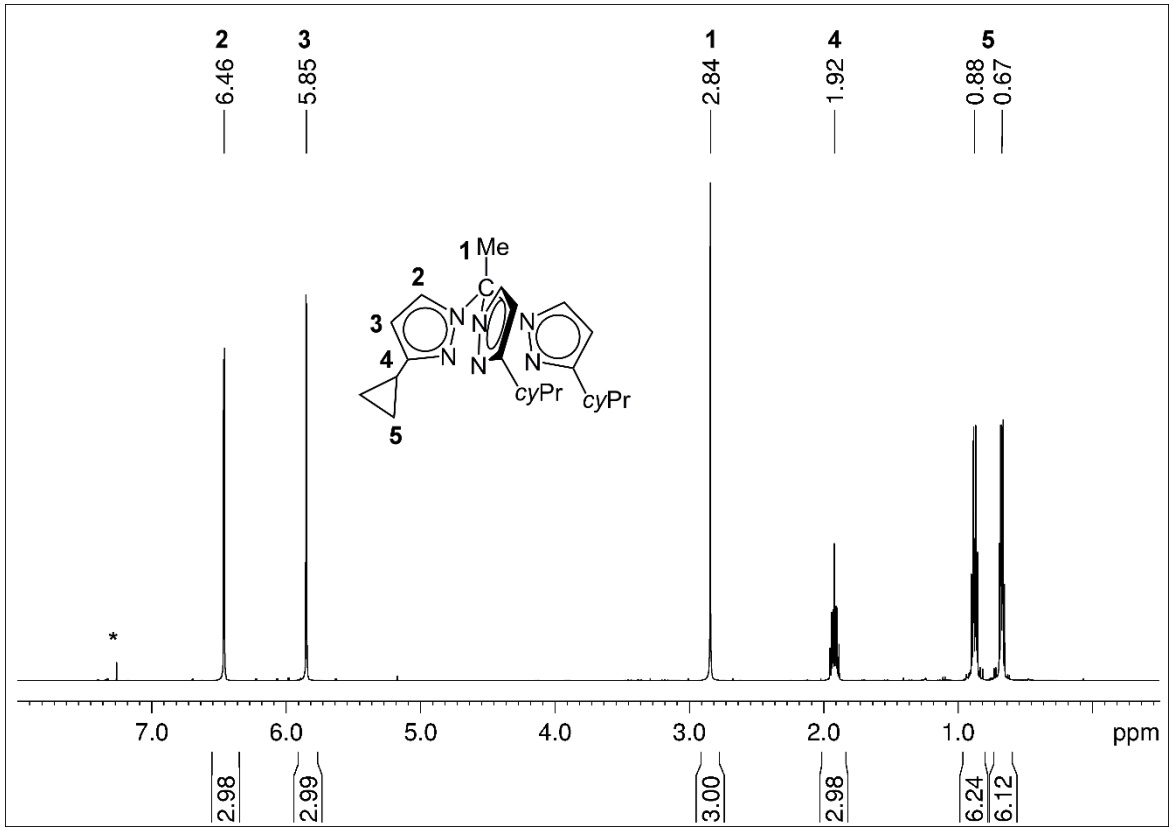


Figure S14. ^{1}H NMR spectrum (400 MHz) of **3b** in $CDCl_3$ (*) at 26 °C.

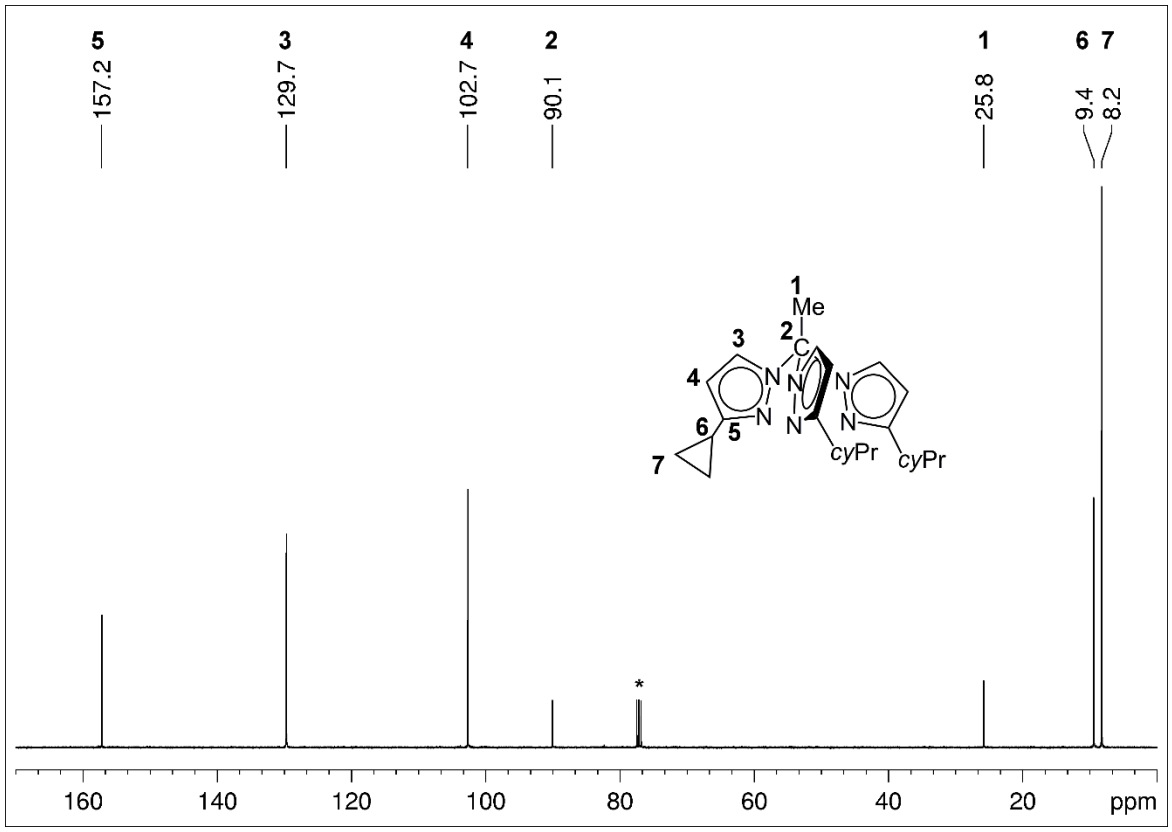


Figure S15. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz) of **3b** in $CDCl_3$ (*) at 26 °C.

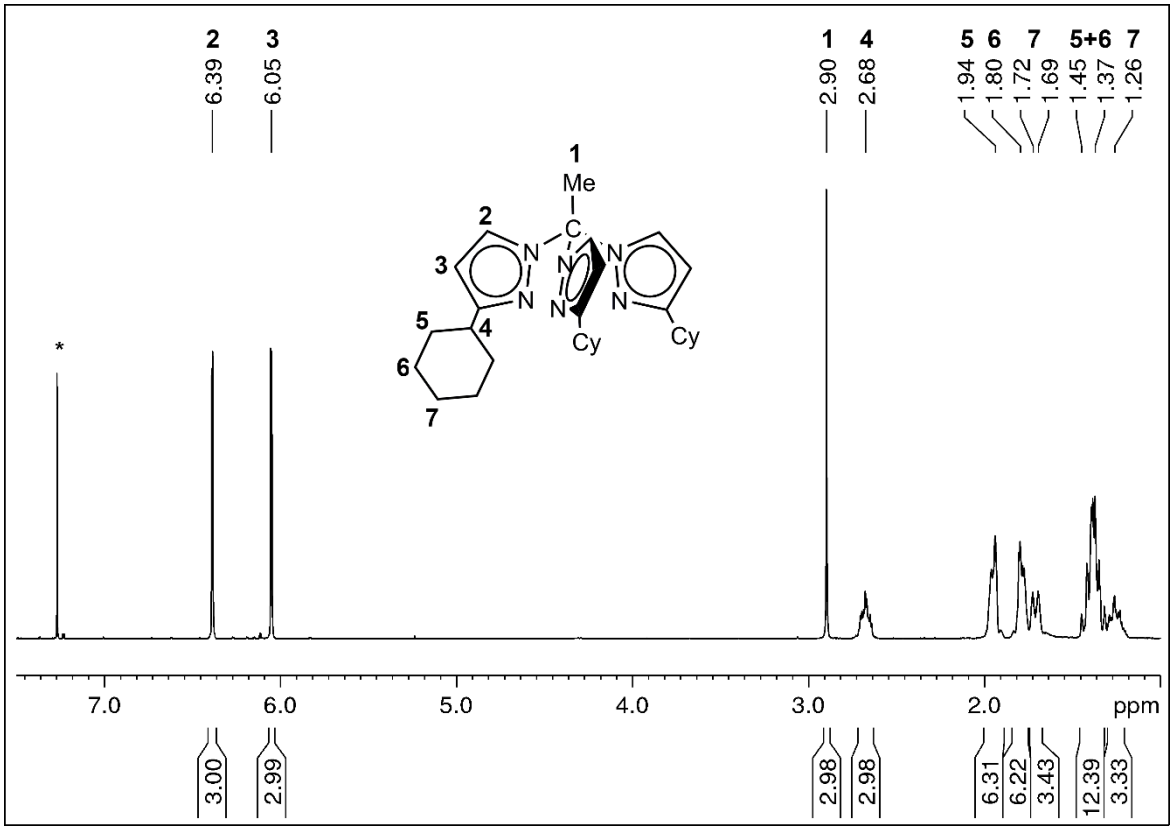


Figure S16. ^{1}H NMR spectrum (400 MHz) of **3c** in $CDCl_3$ (*) at 26 °C.

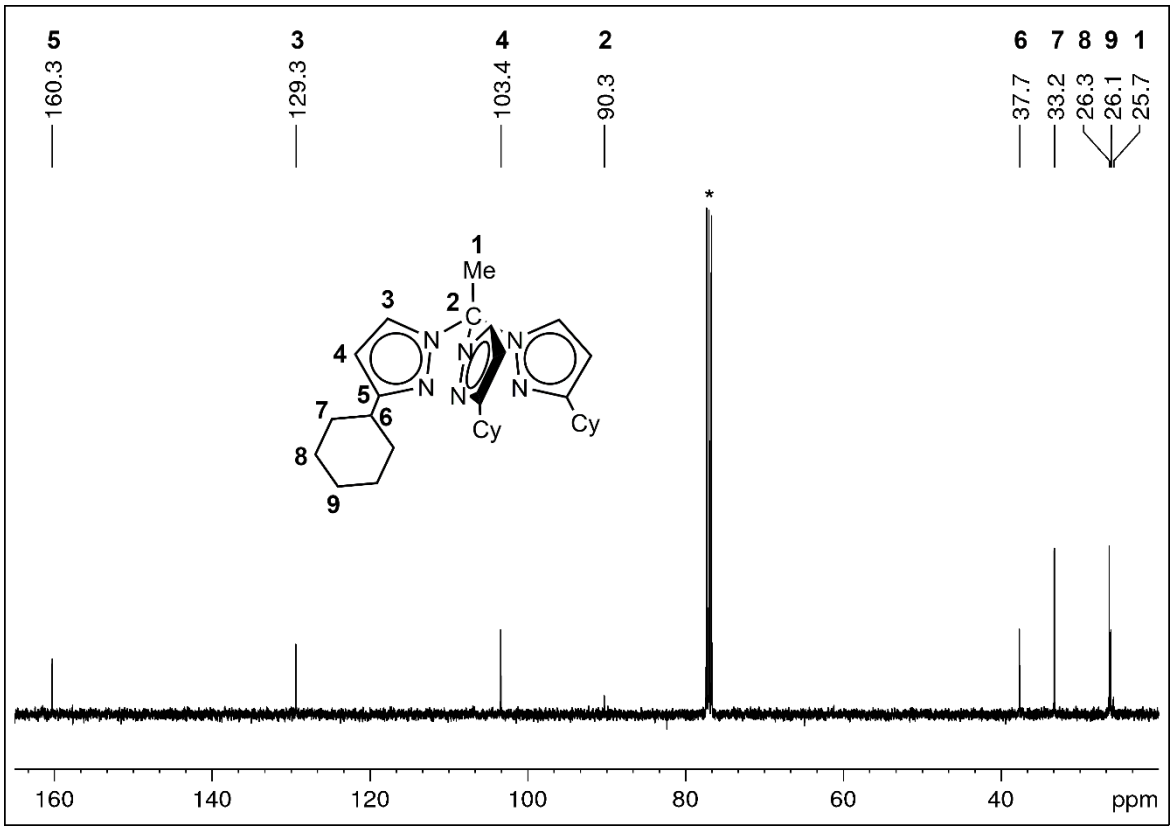


Figure S17. ^{13}C{^{1}H} NMR spectrum (101 MHz) of **3c** in $CDCl_3$ (*) at 26 °C.

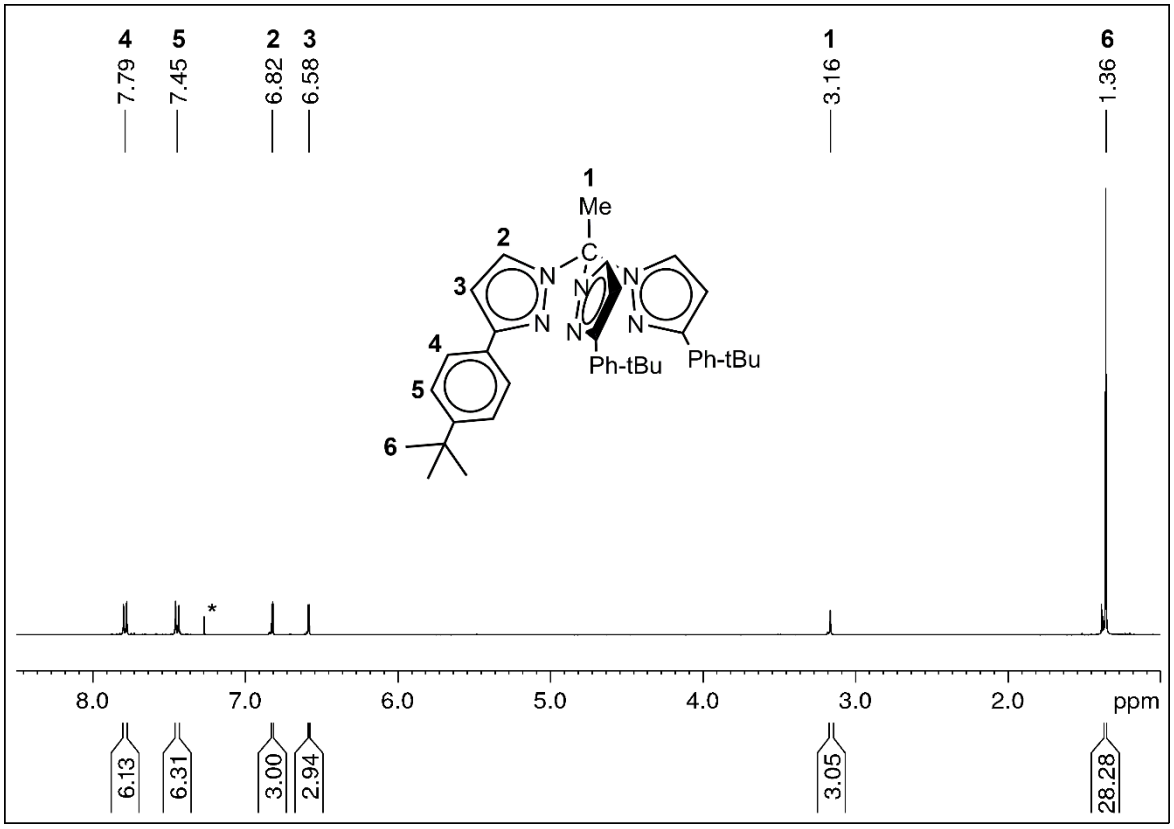


Figure S18. ^{1}H NMR spectrum (400 MHz) of **3d** in $CDCl_3$ (*) at 26 °C.

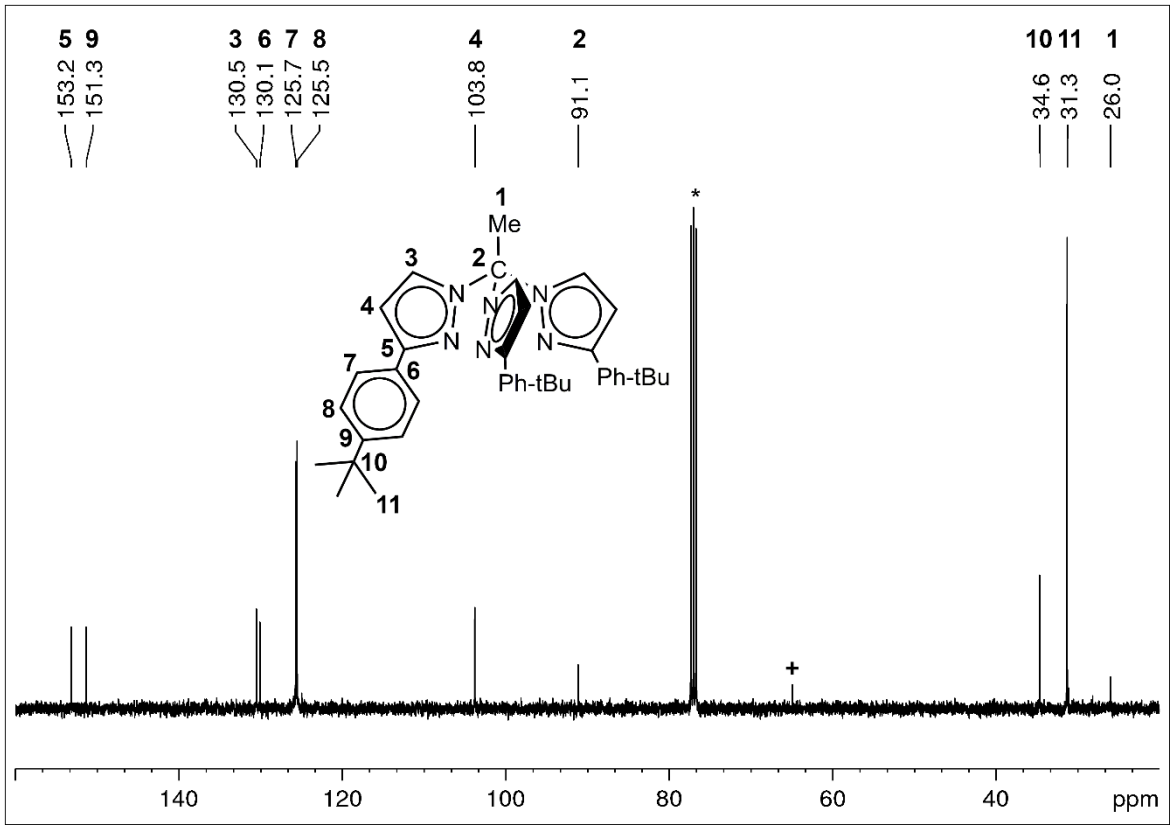


Figure S19. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz) of **3d** in $CDCl_3$ (*) at 26 °C (+ impurities).

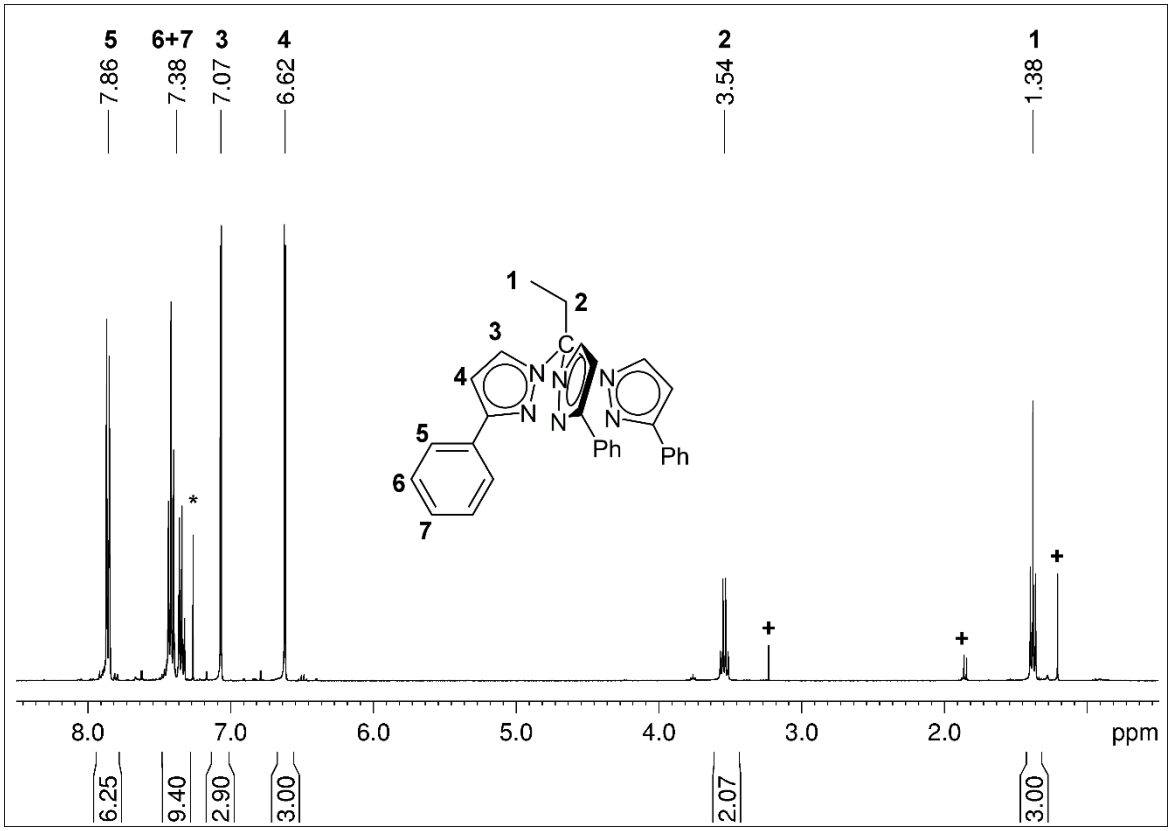


Figure S20. ^{1}H NMR spectrum (400 MHz) of **3e** in $CDCl_3$ (*) at 26 °C (+ impurities).

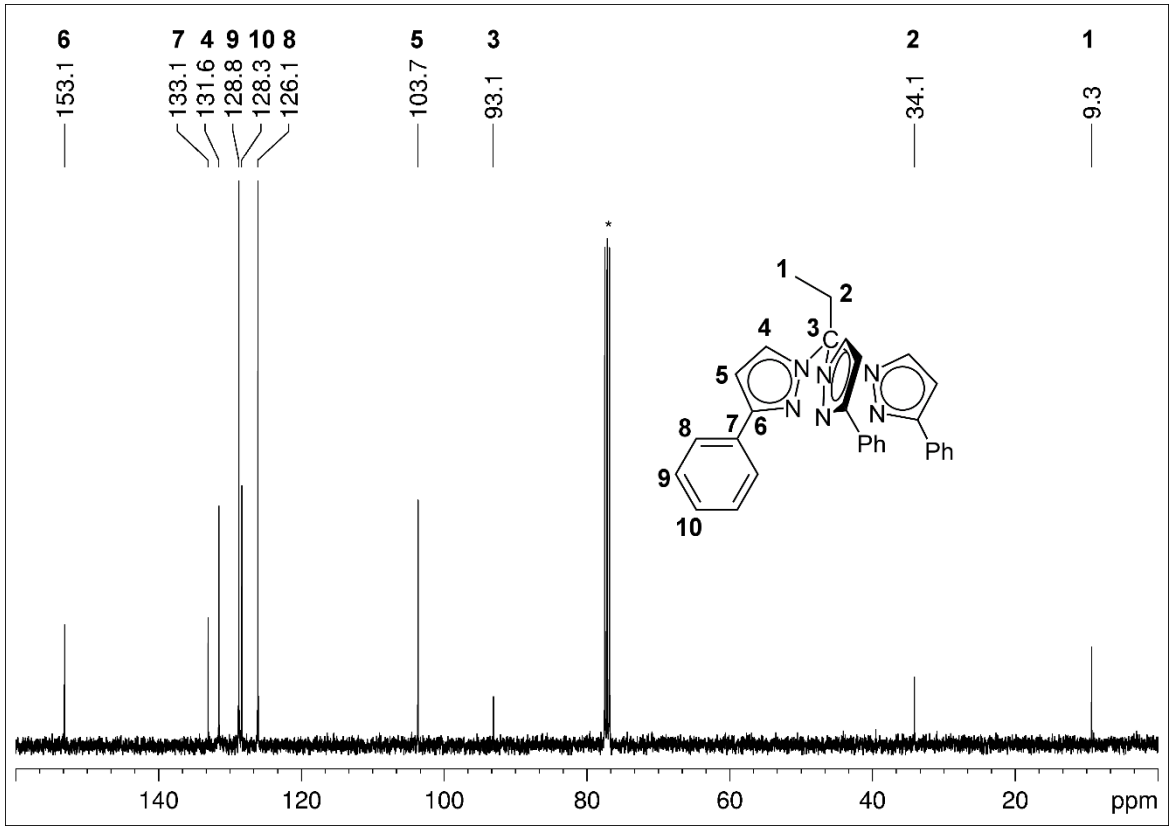


Figure S21. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz) of **3e** in $CDCl_3$ (*) at 26 °C.

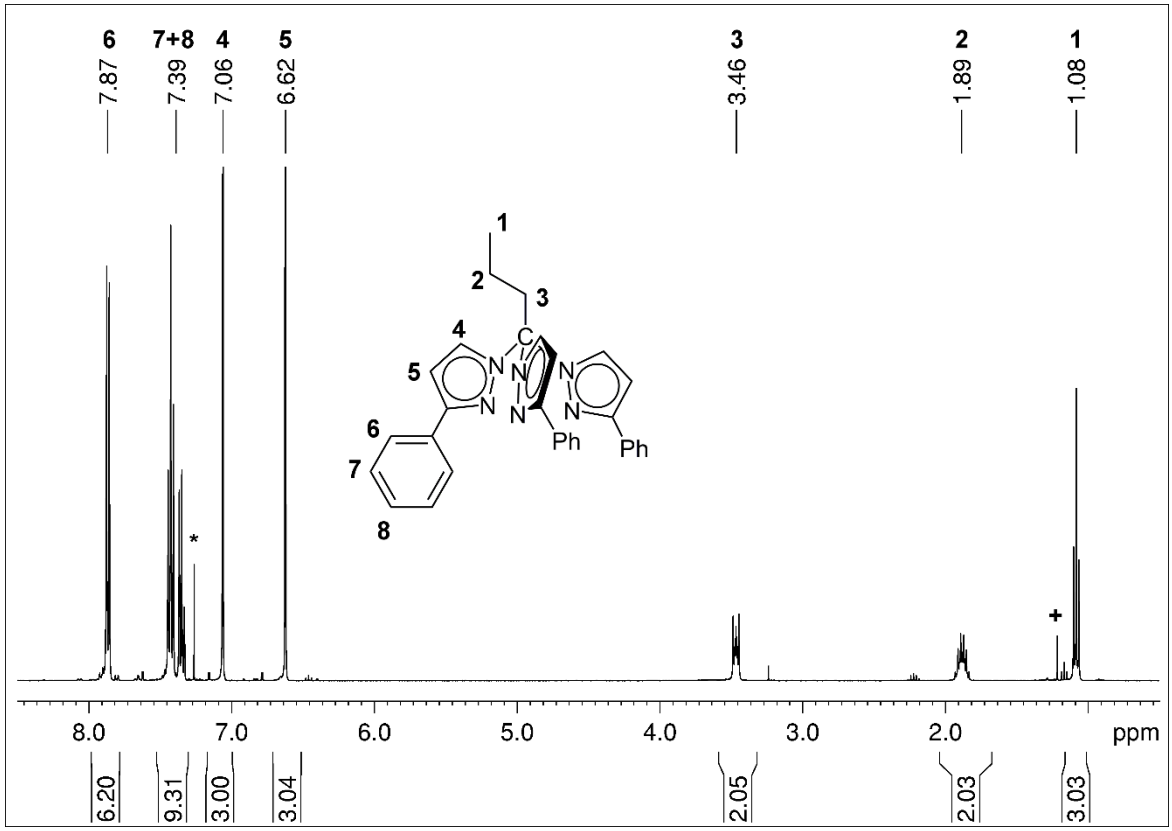


Figure S22. ^{1}H NMR spectrum (400 MHz) of **3f** in $CDCl_3$ (*) at 26 °C (+ mtbe).

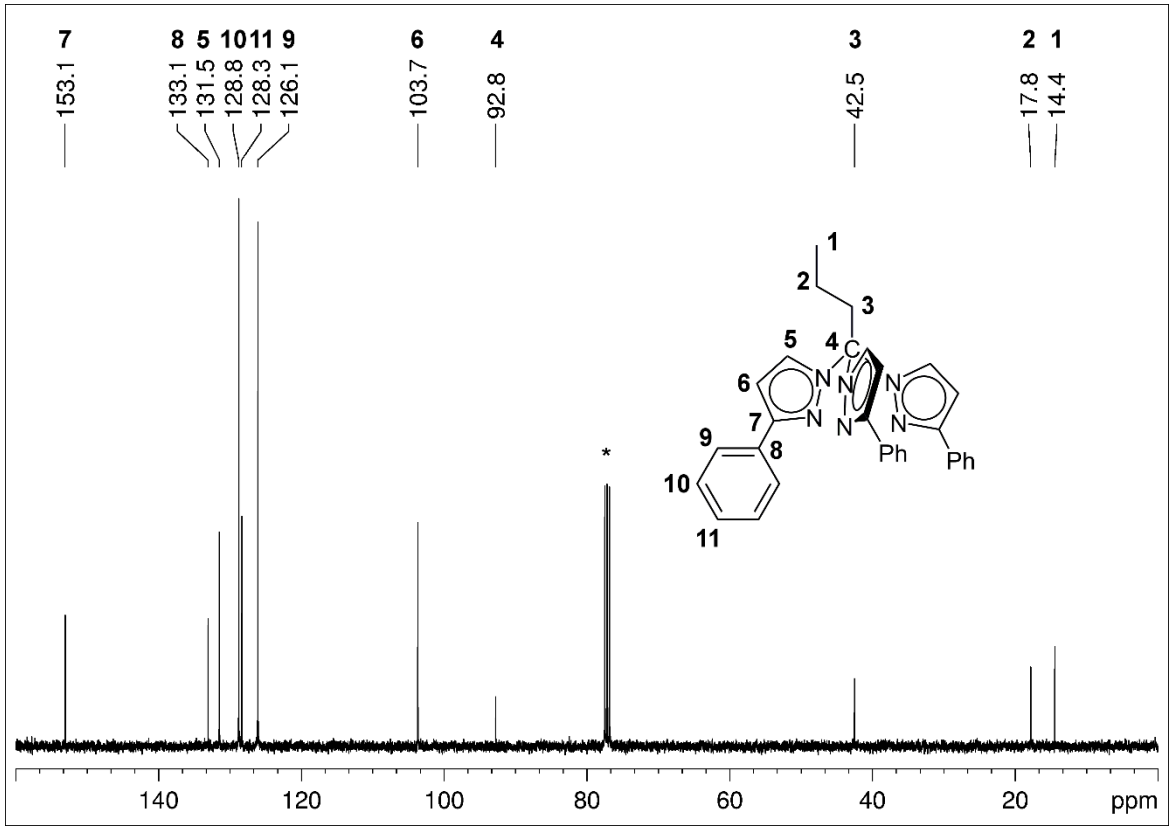


Figure S23. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz) of **3f** in $CDCl_3$ (*) at 26 °C.

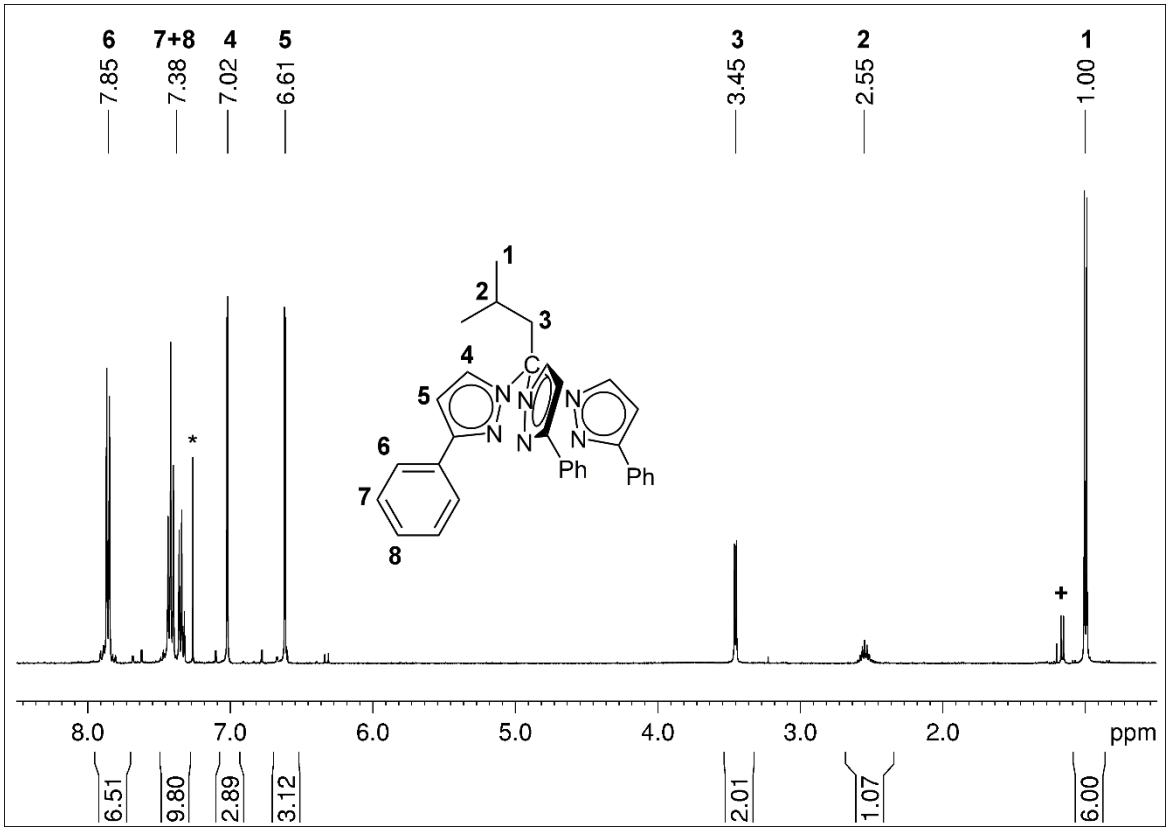


Figure S24. ^{1}H NMR spectrum (400 MHz) of **3g** in $CDCl_3$ (*) at 26 °C (+ impurities).

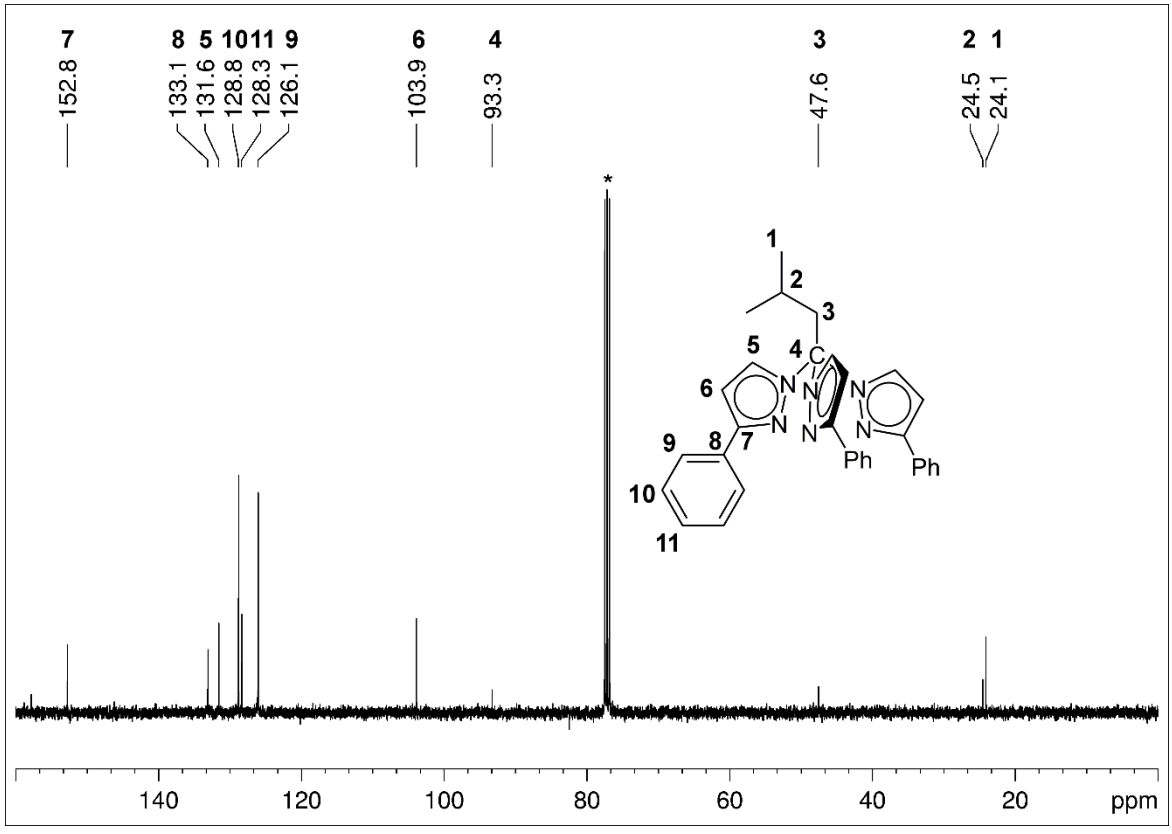


Figure S25. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz) of **3g** in $CDCl_3$ (*) at 26 °C.

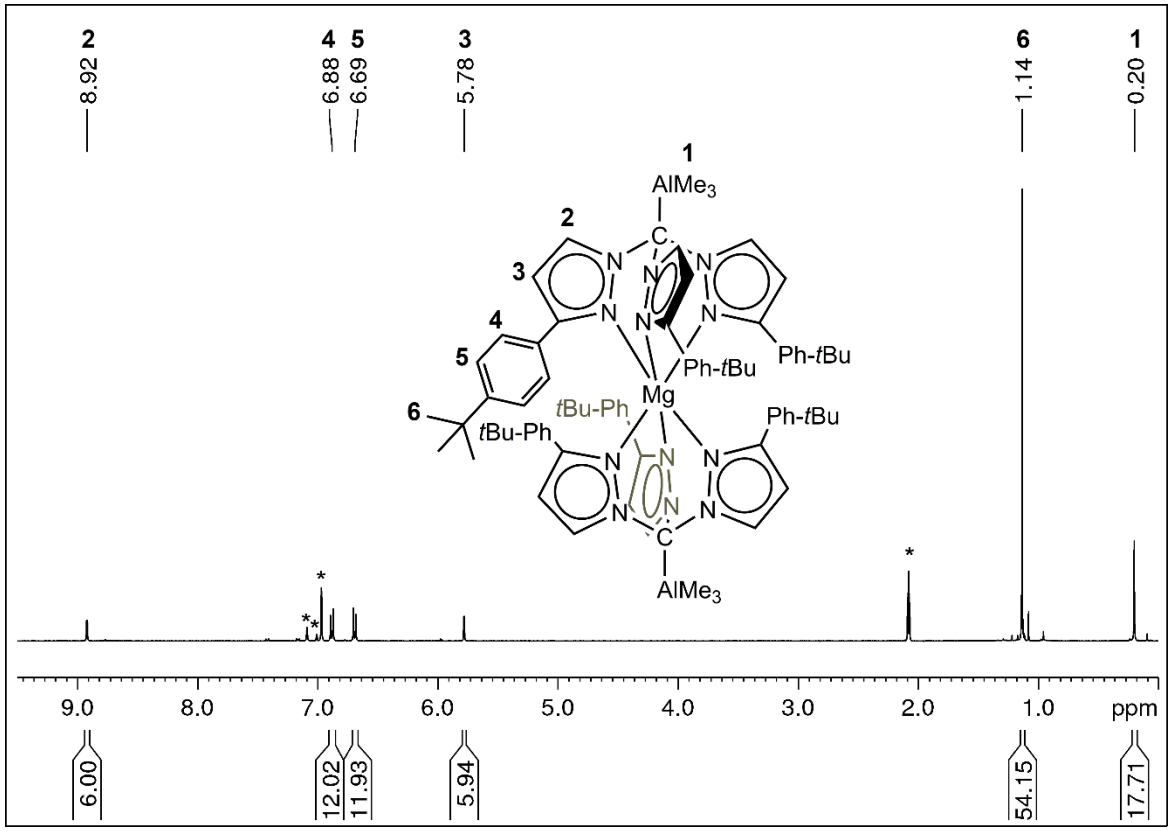


Figure S26. ^{1}H NMR spectrum (400 MHz) of **4** in [D$_8$]toluene (*) at 26 °C.

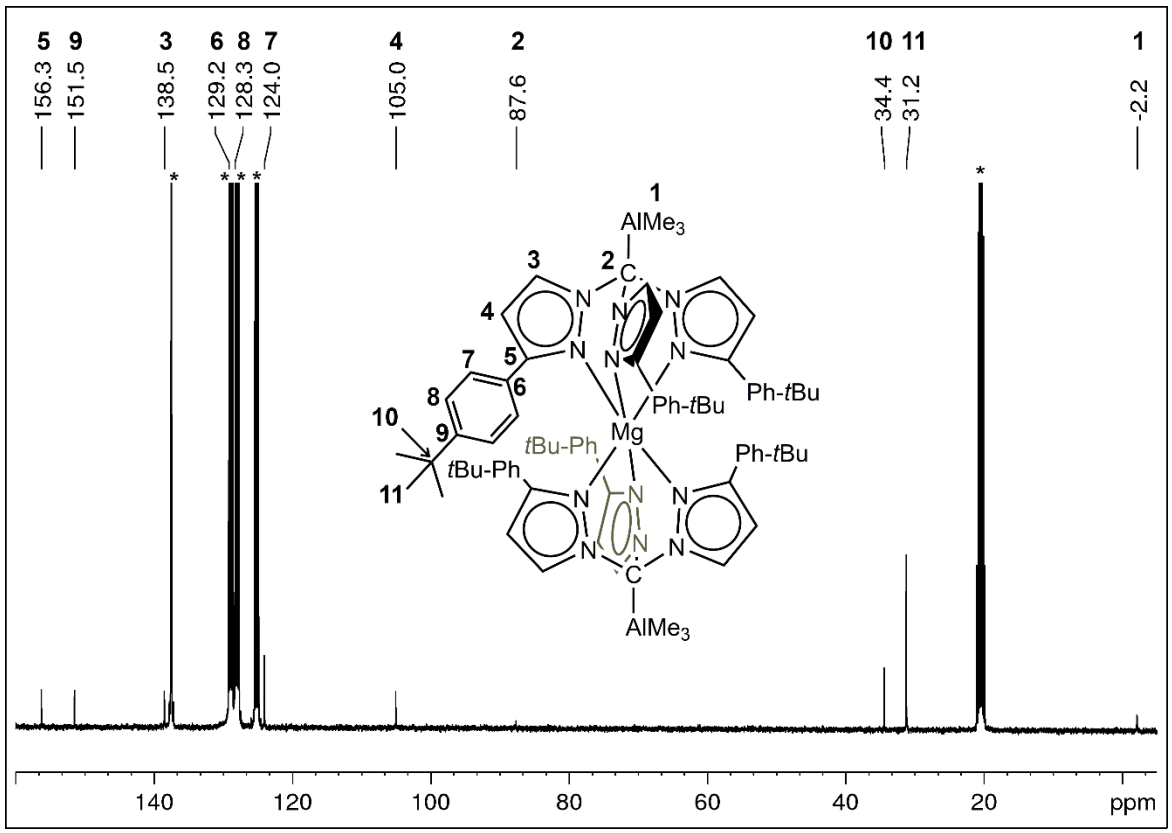


Figure S27. ^{13}C{^{1}H} NMR spectrum (101 MHz) of **4** in [D$_8$]toluene (*) at 26 °C.

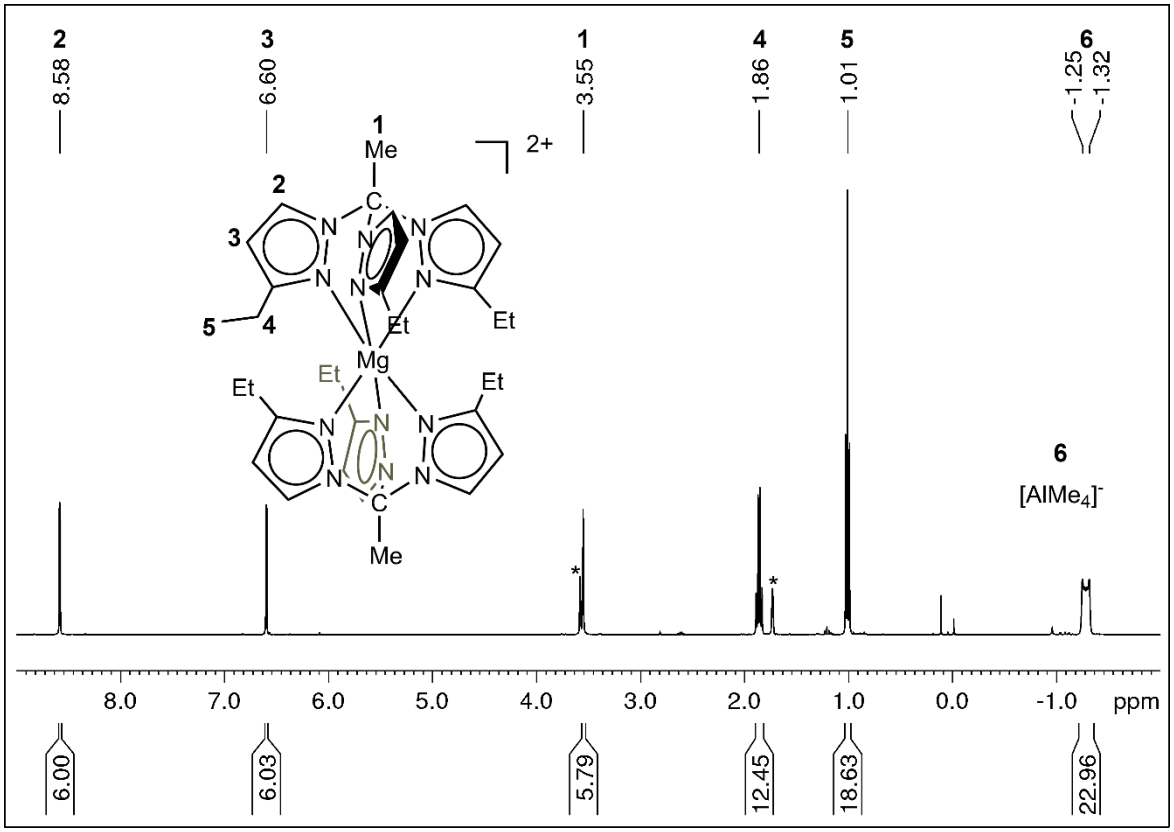


Figure S28. ^{1}H NMR spectrum (400 MHz) of **5a** in [D_8]thf (*) at 26 °C.

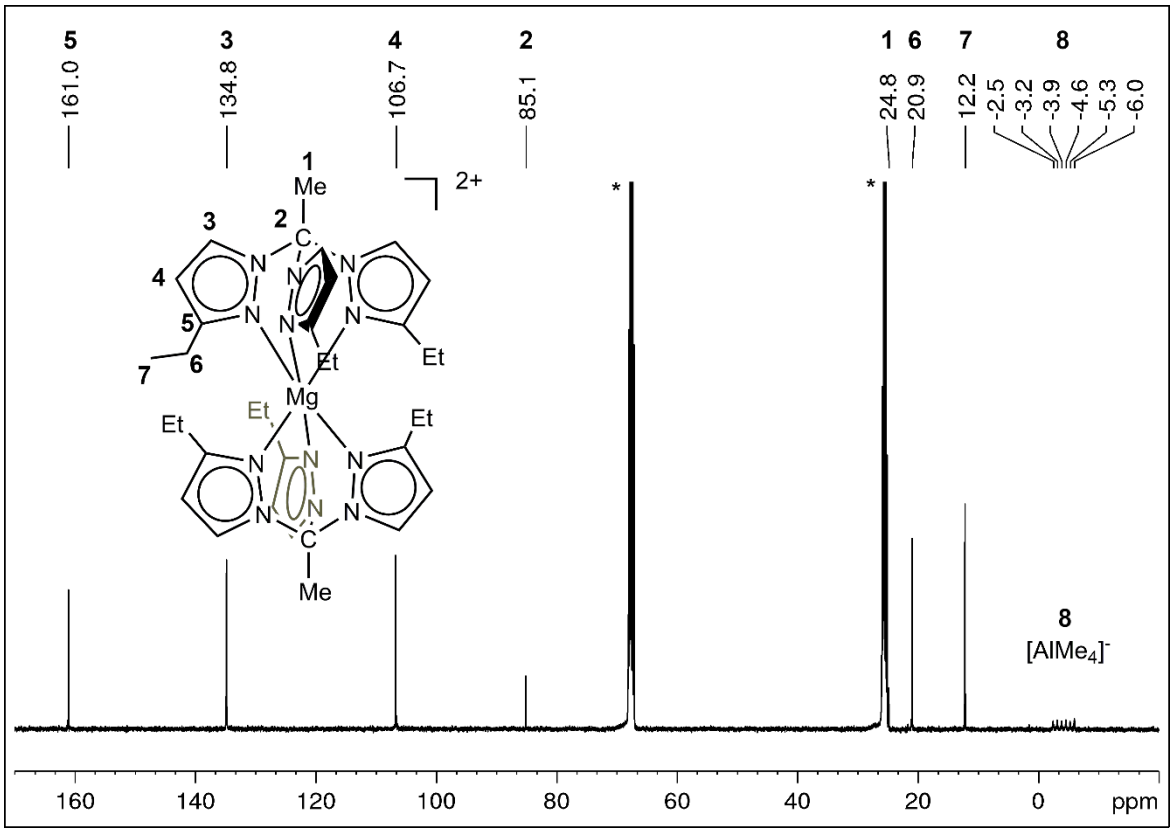


Figure S29. ^{13}C{^{1}H} NMR spectrum (101 MHz) of **5a** in [D_8]thf (*) at 26 °C.

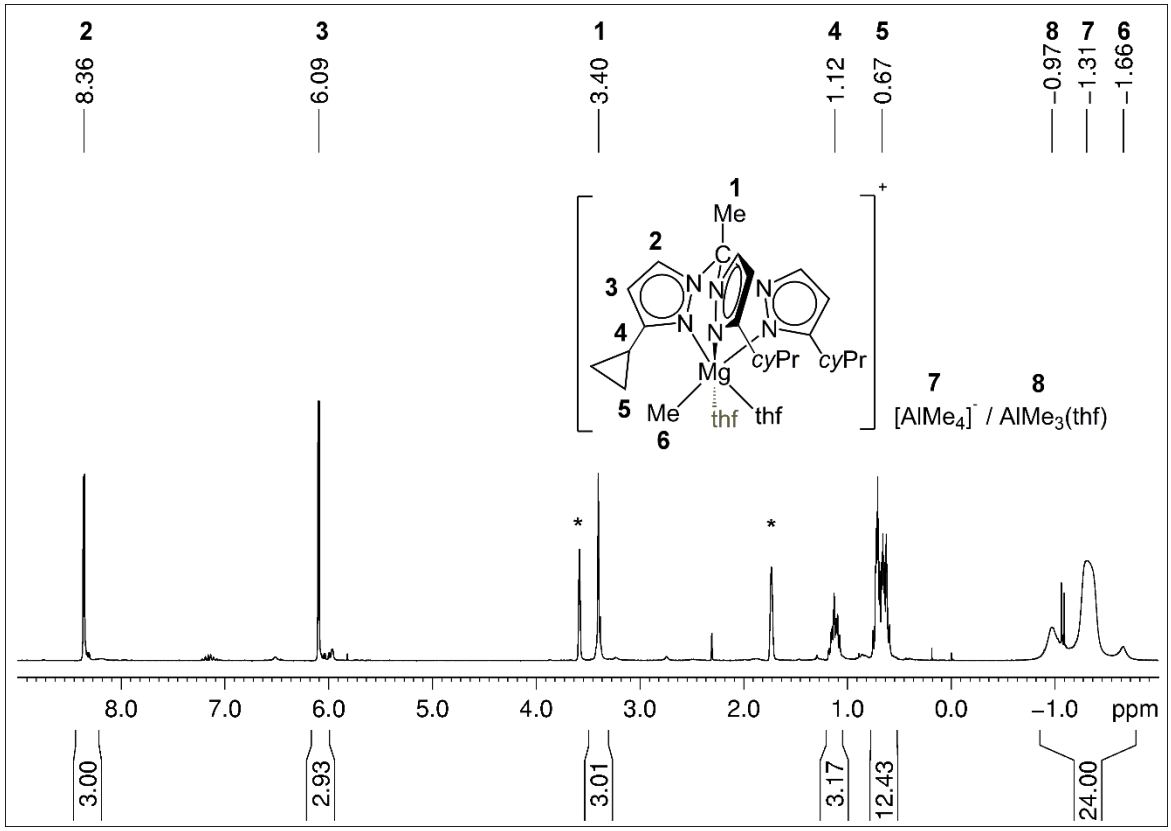


Figure S30. ^{1}H NMR spectrum (400 MHz) of **6** in [D$_8$]thf (*) at 26 °C.

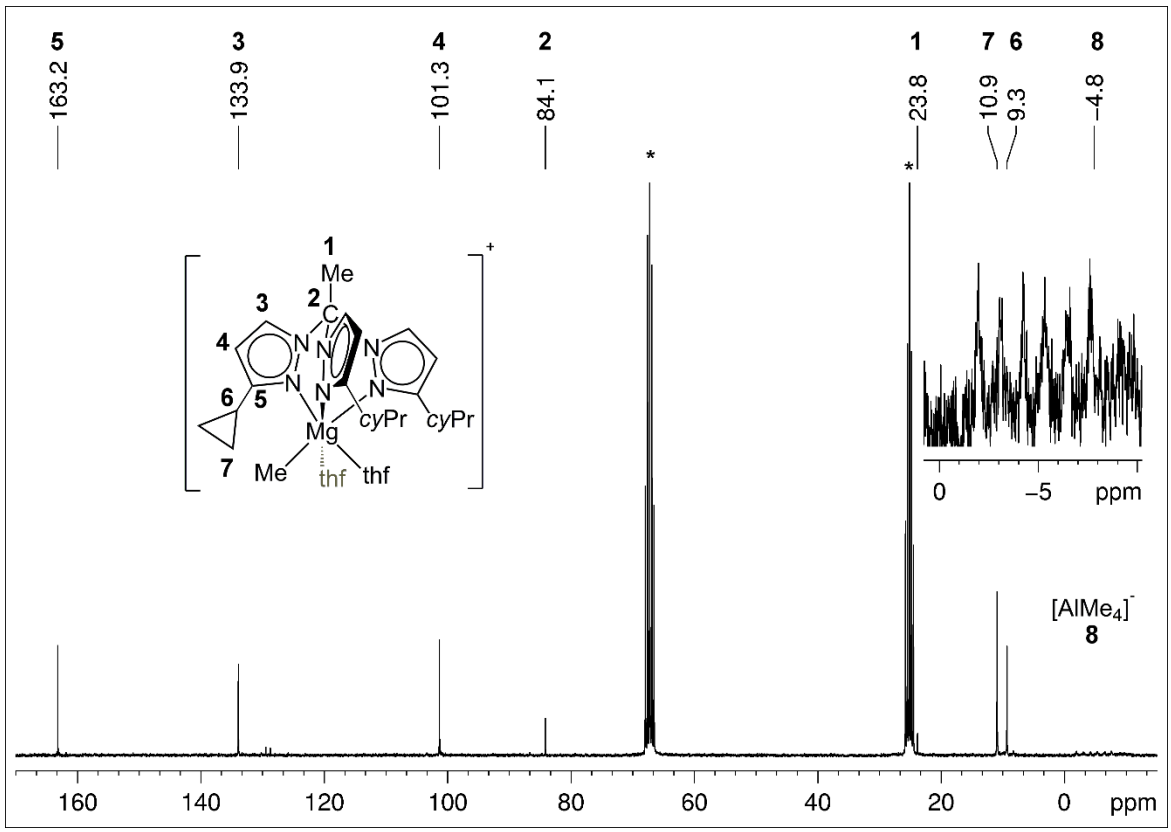


Figure S31. ^{13}C{^{1}H} NMR spectrum (101 MHz) of **6** in [D$_8$]thf (*) at 26 °C.

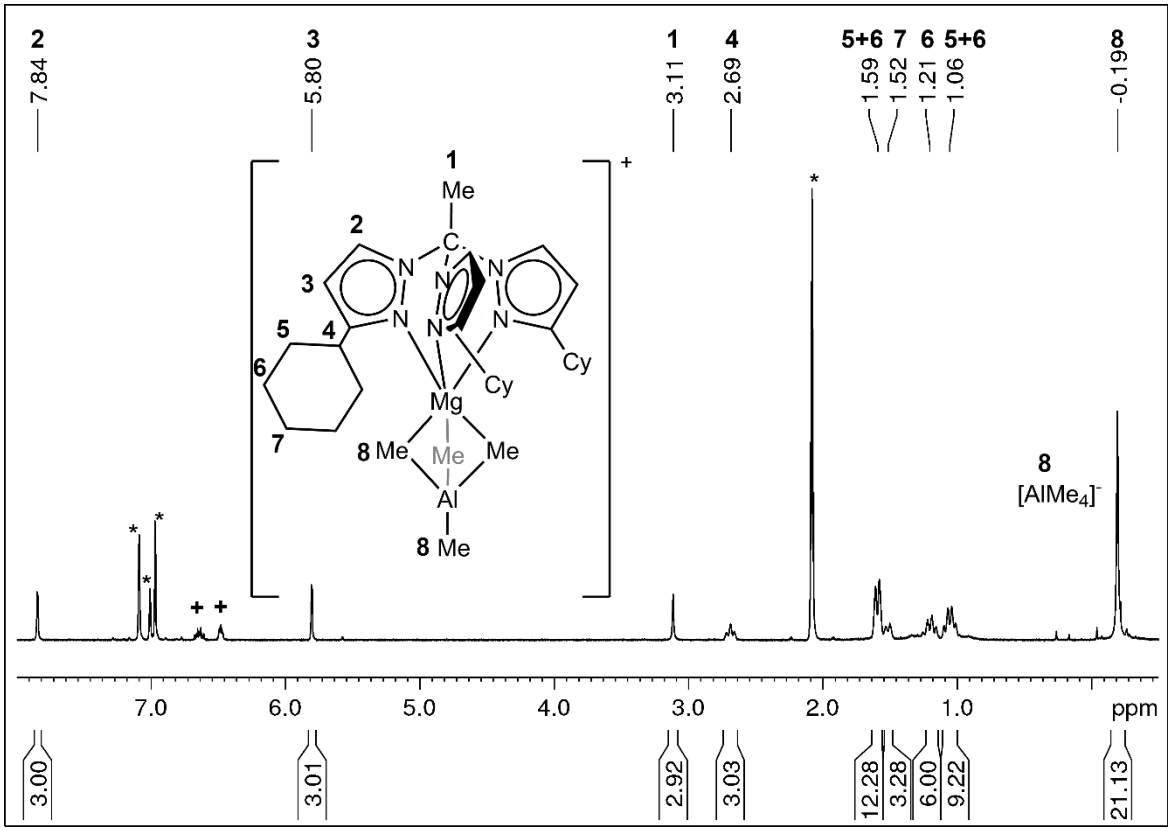


Figure S32. ^{1}H NMR spectrum (400 MHz) of **8** in [D$_8$]toluene (*) at 26 °C (+ 1,2DFB).

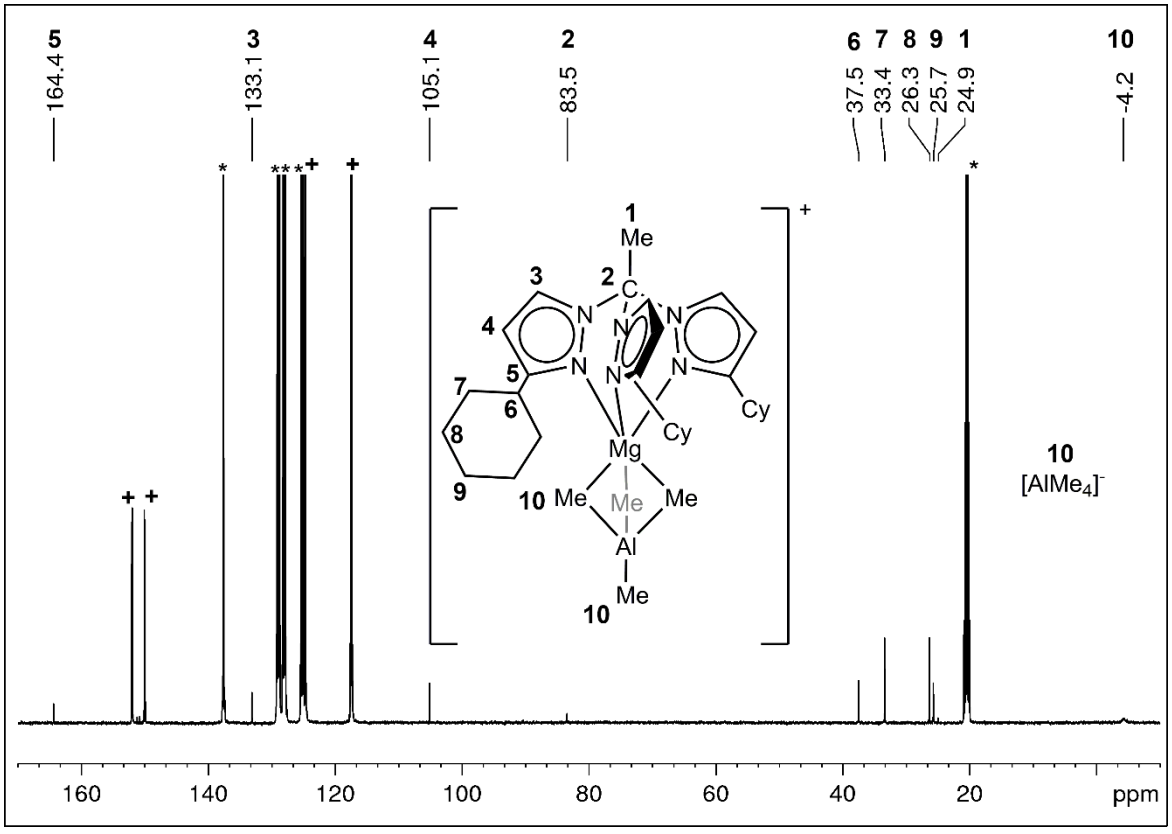


Figure S33. ^{13}C{^{1}H} NMR spectrum (101 MHz) of **8** in [D$_8$]toluene(*)/1,2DFB(+) at 26 °C.

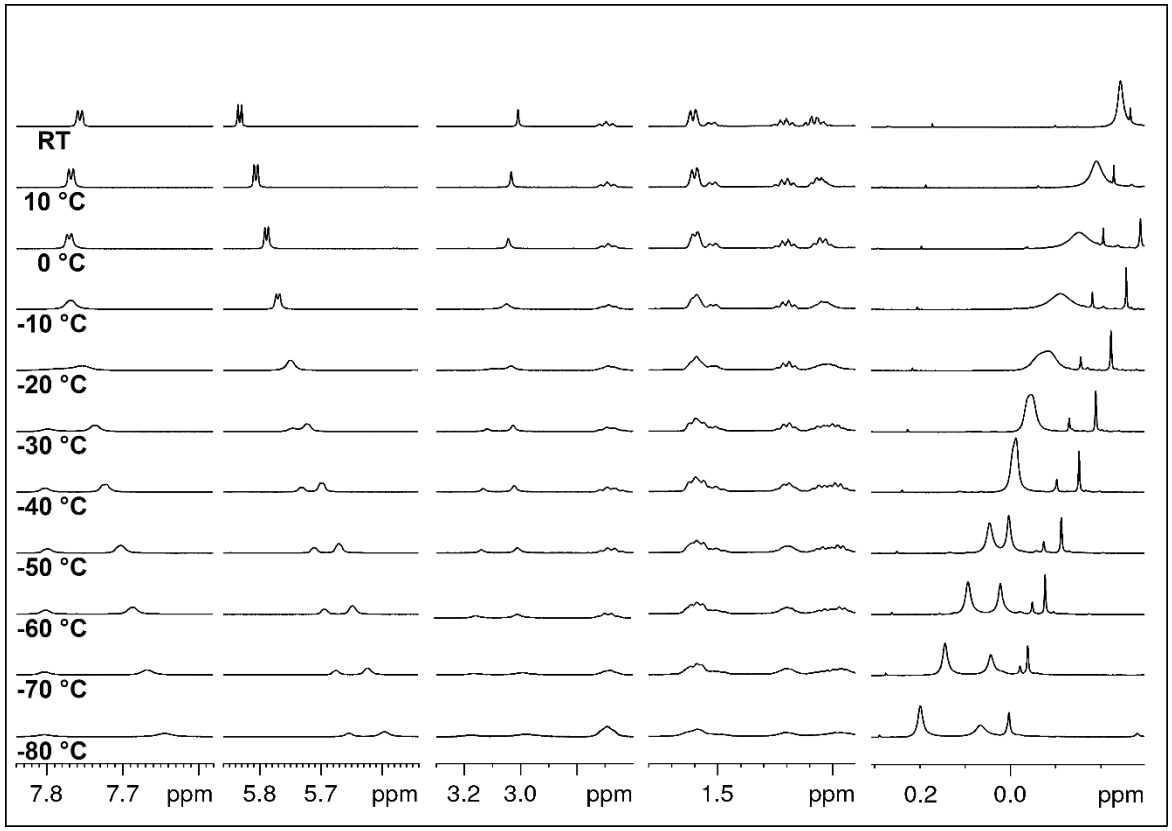


Figure S34. VT ^{1}H NMR spectrum (500 MHz) of **8** in [D_8]toluene/1,2DFB.

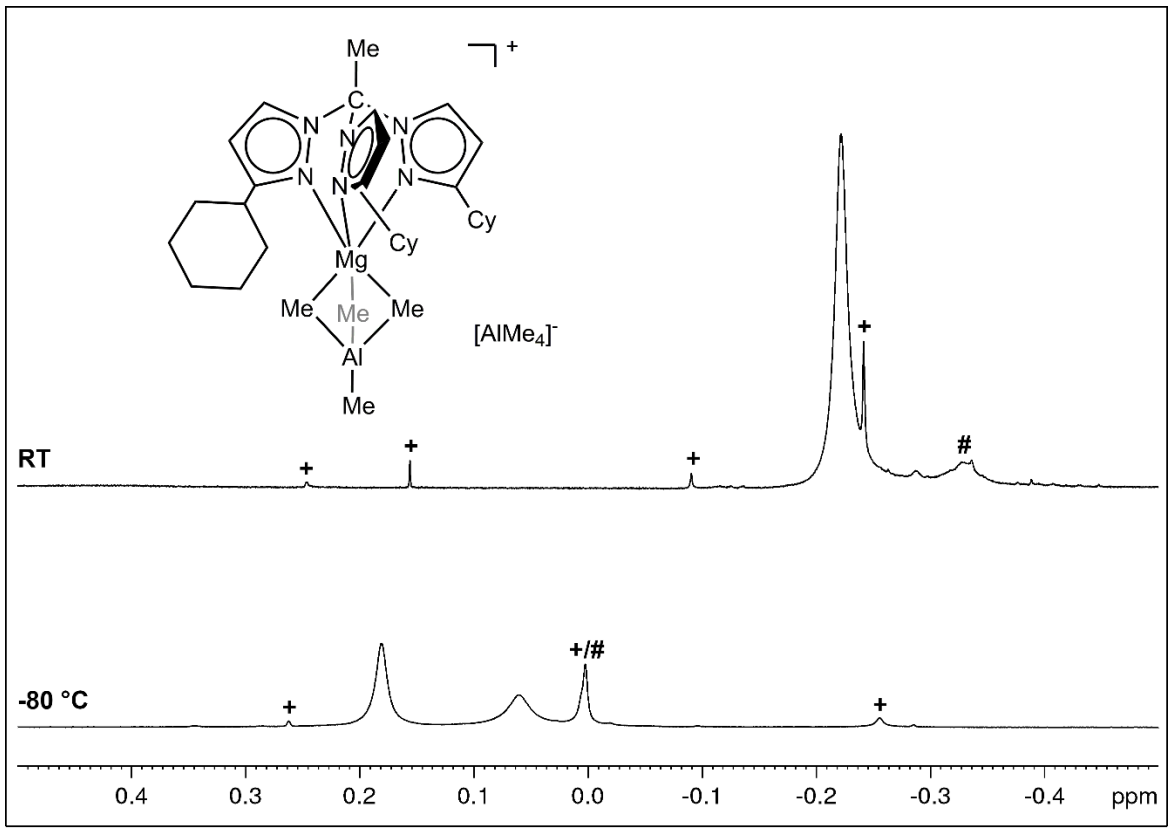


Figure S35. VT ^{1}H NMR spectrum (500 MHz) of **8** in [D_8]toluene/1,2DFB.

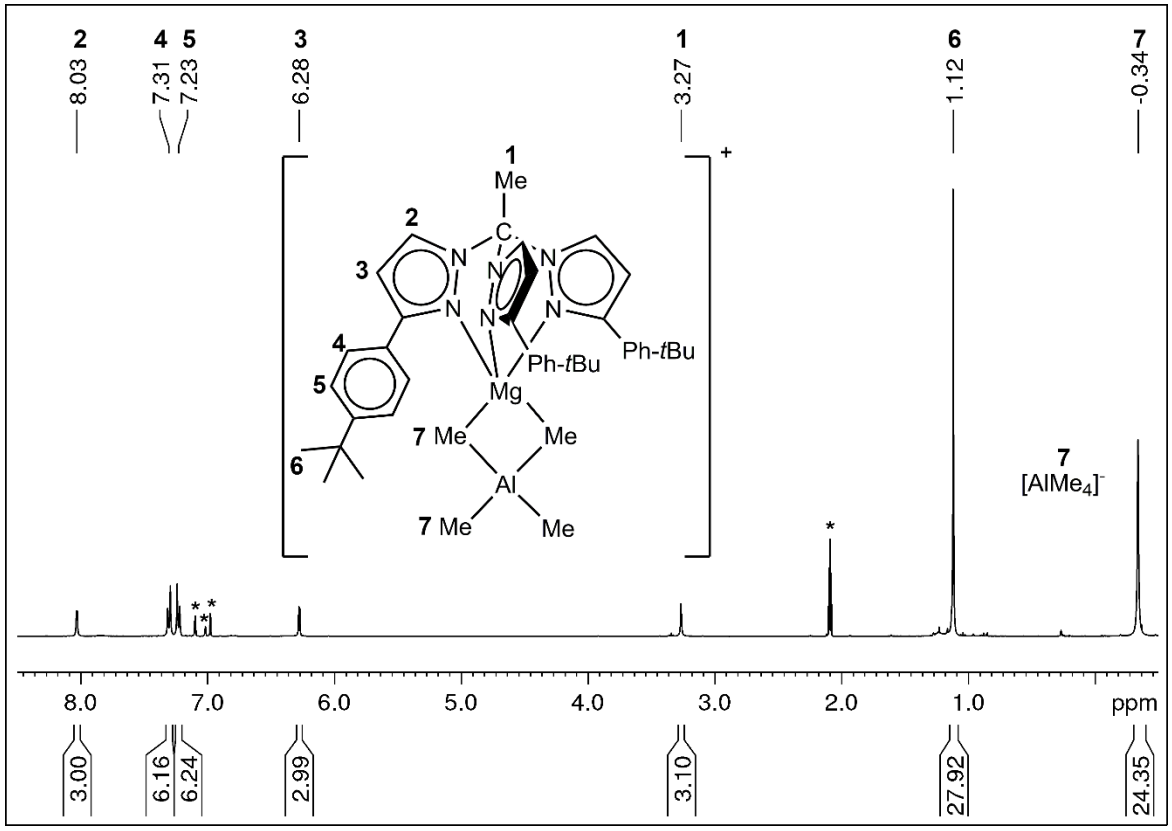


Figure S36. ^{1}H NMR spectrum (400 MHz) of **9** in [D_8]toluene (*) at 26 °C.

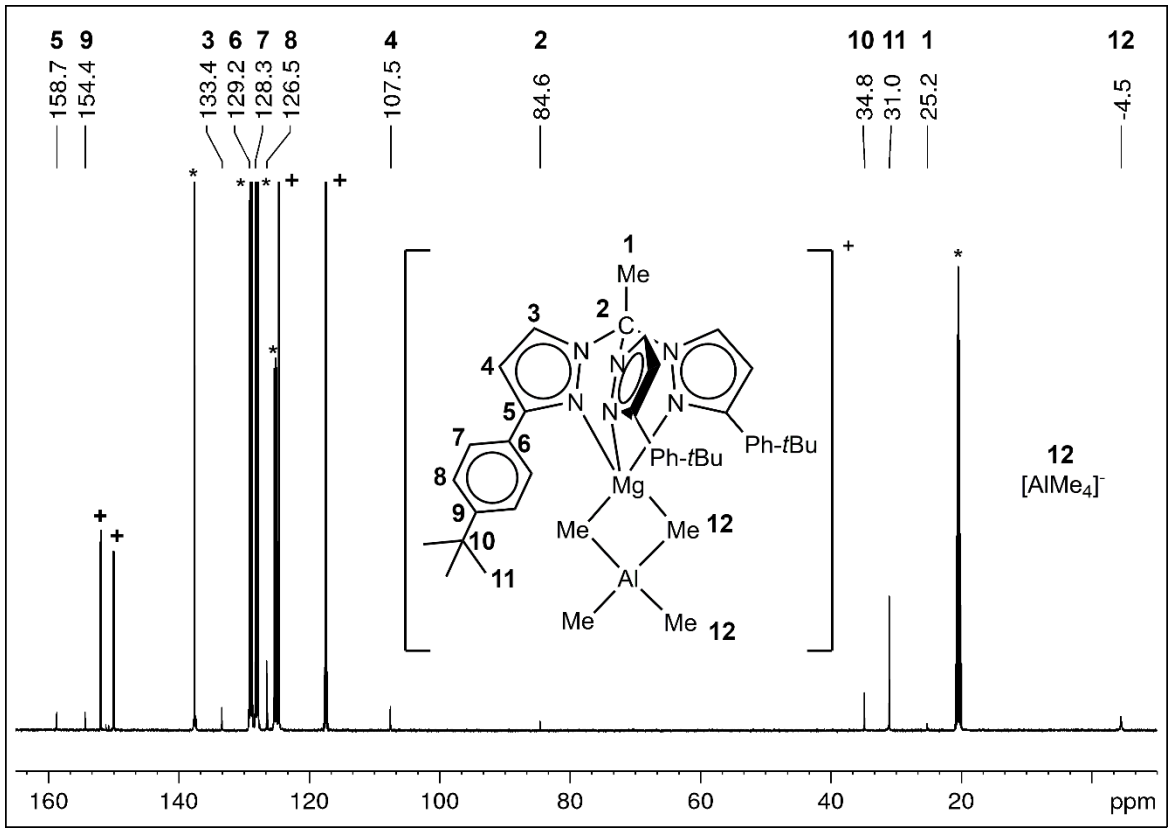


Figure S37. ^{13}C{^{1}H} NMR spectrum (101 MHz) of **9** in [D_8]toluene(*)/1,2DFB(+) at 26 °C.

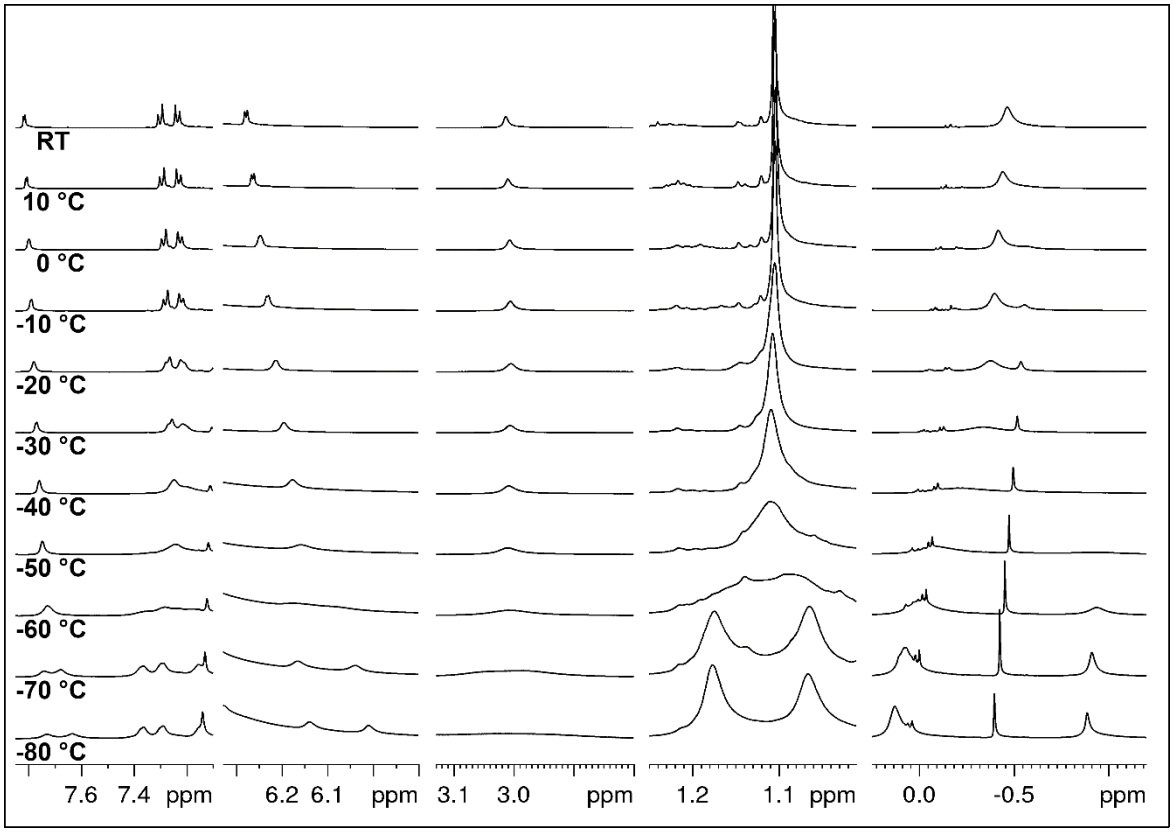


Figure S38. VT ^{1}H NMR spectrum (500 MHz) of **9** in [D_8]toluene/1,2DFB.

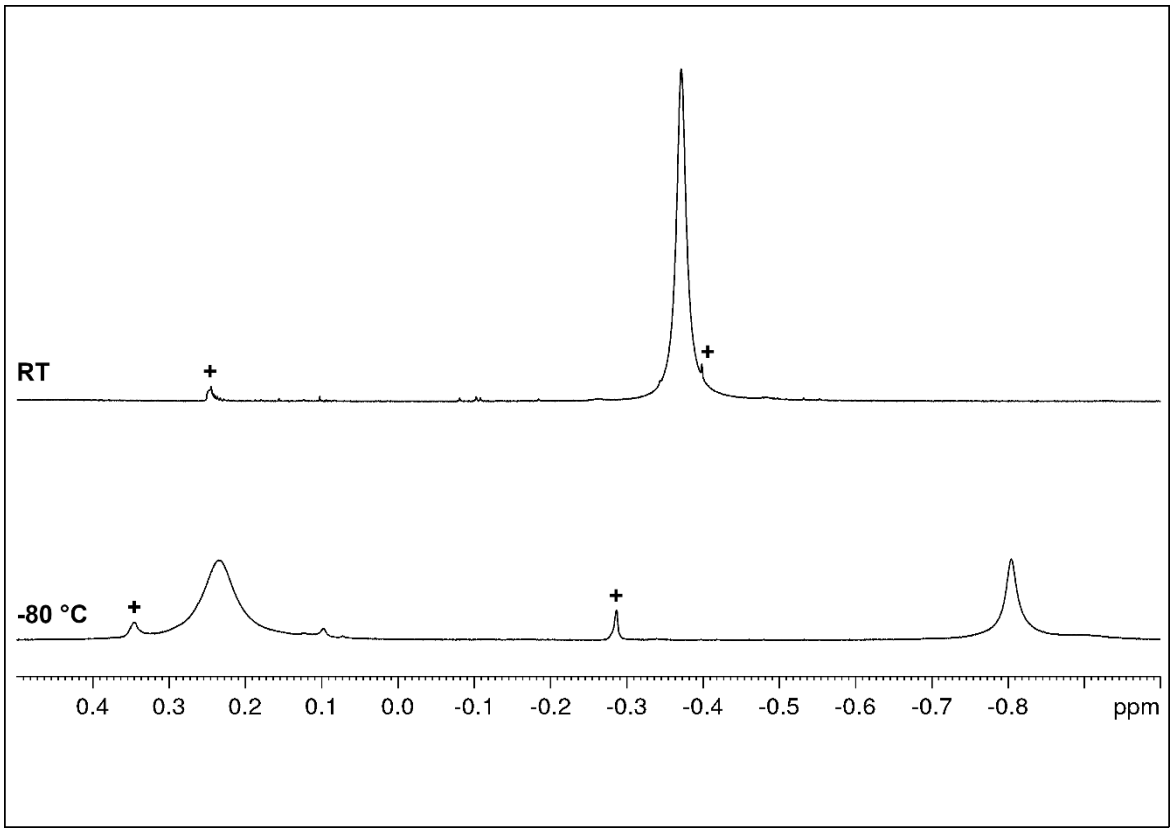


Figure S39. VT ^{1}H NMR spectrum (500 MHz) of **9** in [D_8]toluene/1,2DFB (+ impurities).

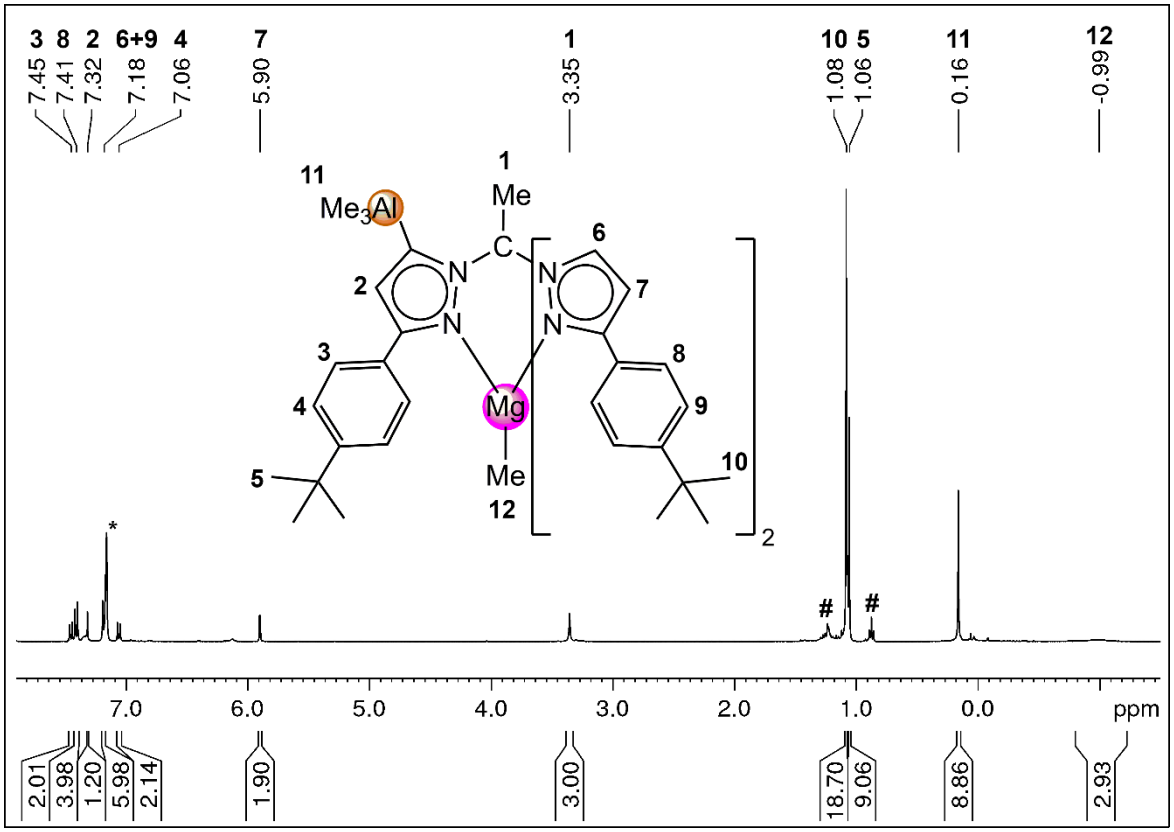


Figure S40. ^{1}H NMR spectrum (400 MHz) of **10** in [D_6]benzene (*) at 26 °C (# impurities).

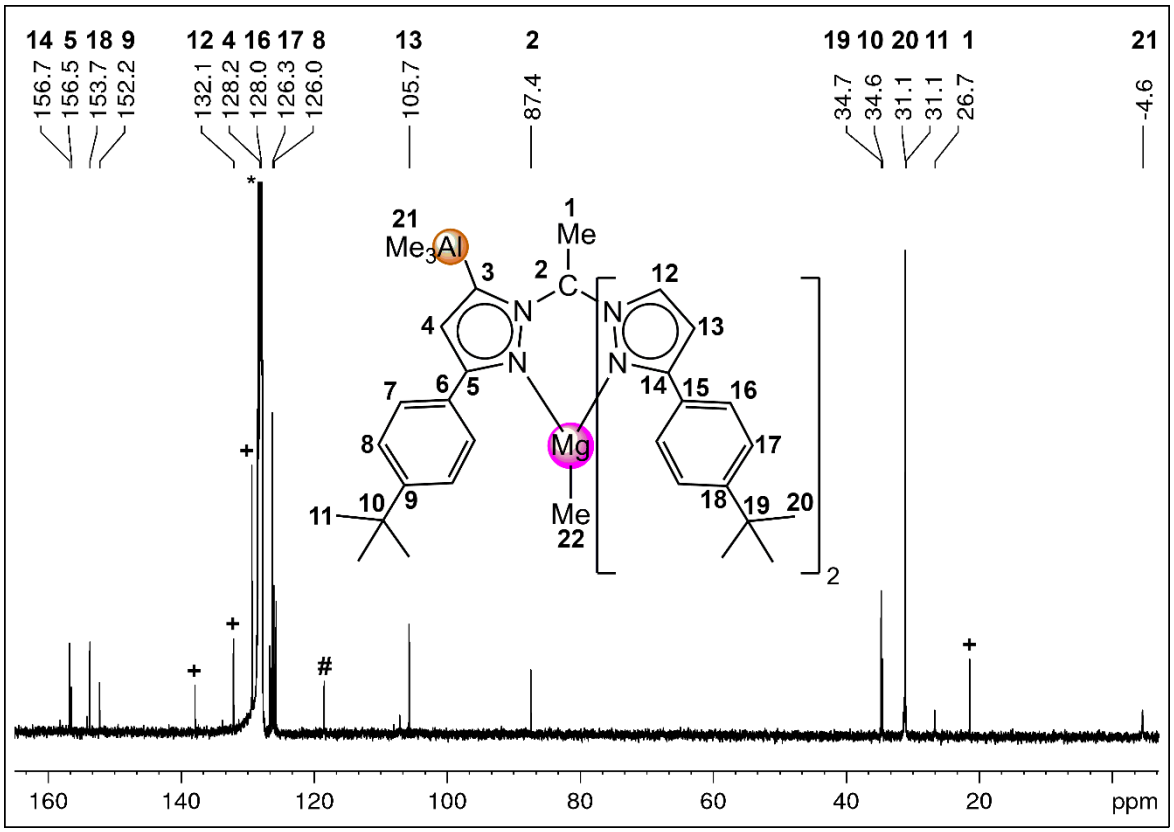


Figure S41. ^{13}C{^{1}H} NMR spectrum (101 MHz) of **10** in [D_6]benzene(*) at 26 °C (+ toluene/# impurities).

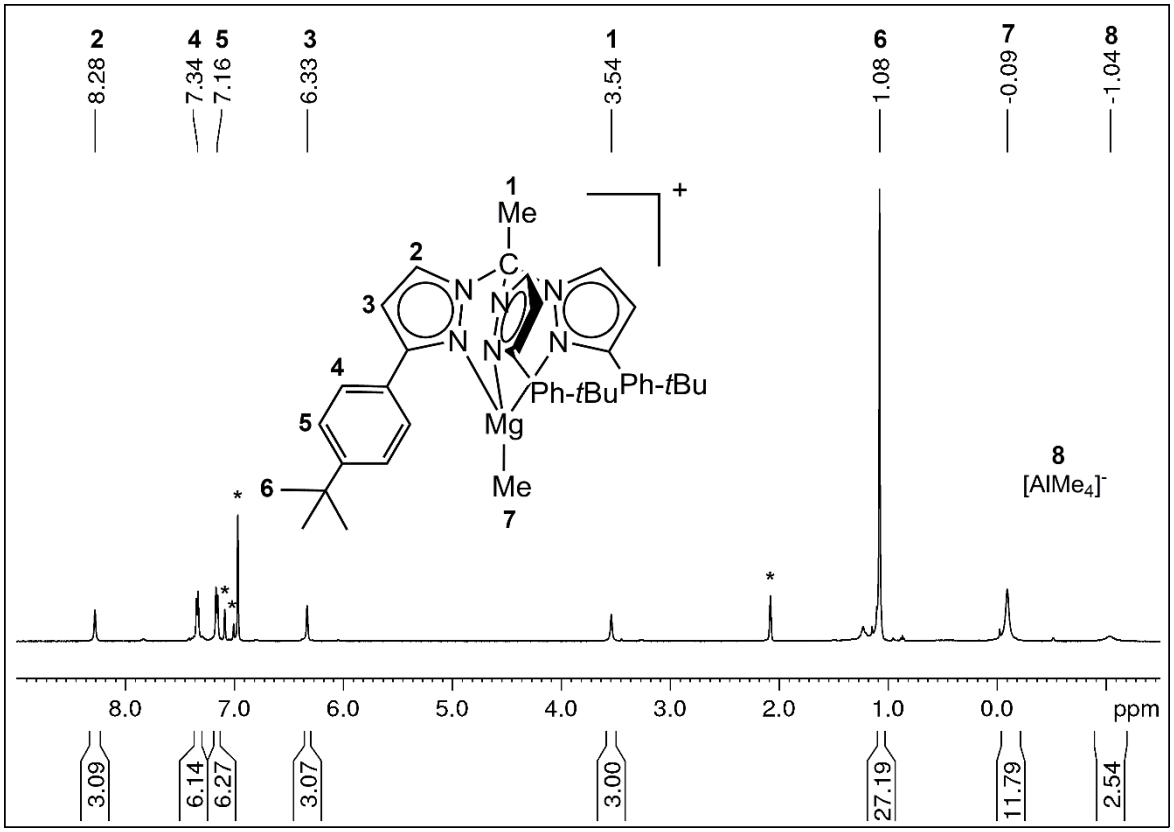


Figure S42. ^{1}H NMR spectrum (400 MHz) of **11** in [D_8]toluene (*) at 26 °C.

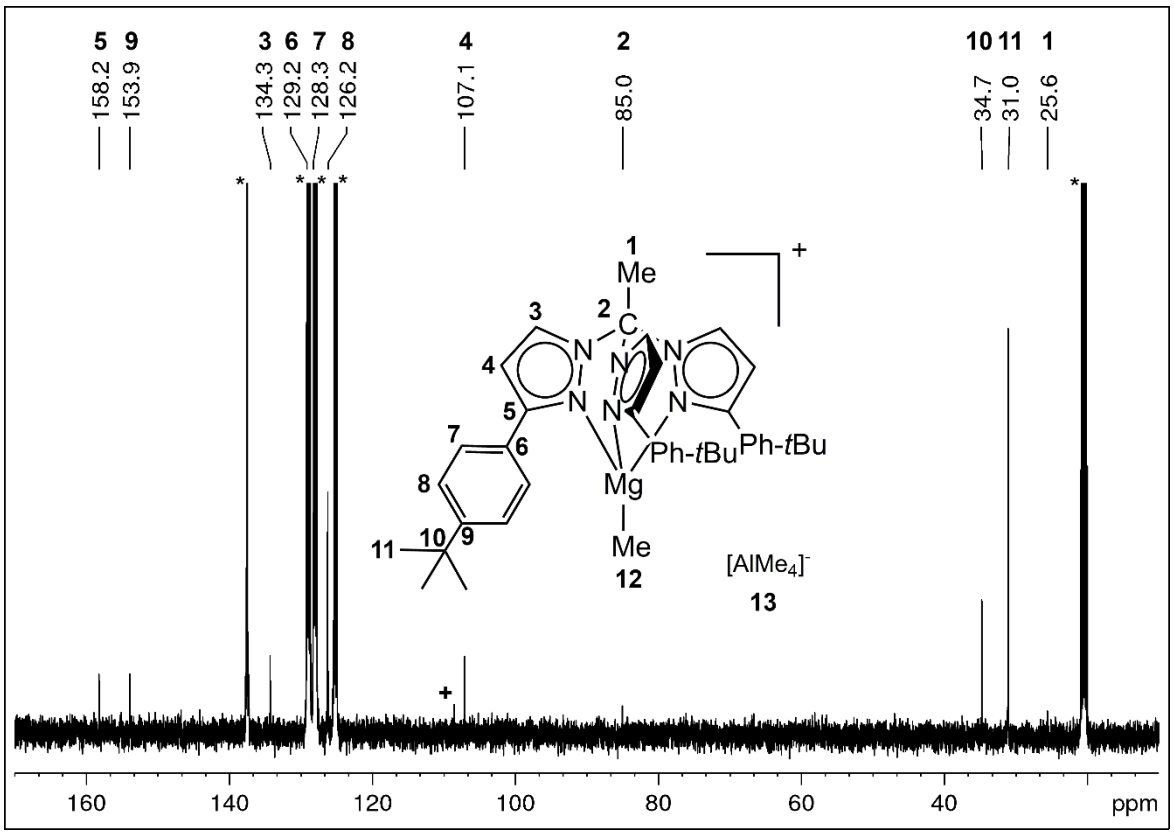


Figure S43. ^{13}C{^{1}H} NMR spectrum (101 MHz) of **11** in [D_8]toluene(*) at 26 °C (+ impurities).

Cone-Angle Calculation

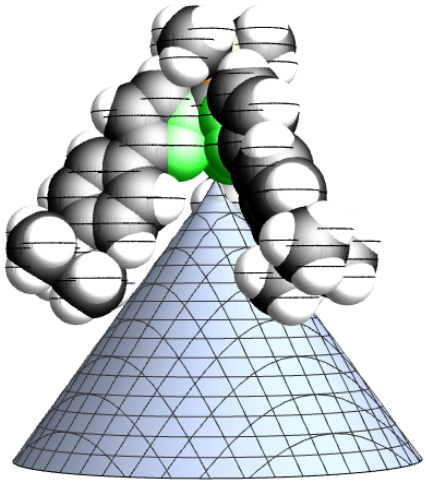
For the calculation of the mathematically exact cone angles .xyz files were generated from the final .cif files with Mercury. The Mathematica package was downloaded free of charge from http://www.ccqc.uga.edu/references/software.php. The adopted van der Waals radii were r = 1.20, 1.70, 1.55, 1.52, 1.84, 1.73 Å for H, C, N O, Al and Mg in this order.

$[(AlMe_3CTp^{3\text{-}ptBuPh})_2Mg]$_(**4**)

Ligand atoms forming cone = {31, 55, 90}

Cone angle (deg) = 288.022

Cone axis = {–0.00734705, 0.157434, –0.987502}

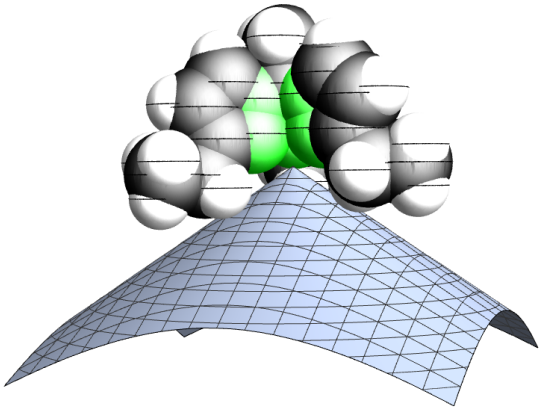


$[(MeCTp^{3\text{-}Et})_2Mg][AlMe_4]_2$ (**5a**)

Ligand atoms forming cone = {15, 26, 38}

Cone angle (deg) = 247.949

Cone axis = {0.395488, –0.110808, 0.911762}

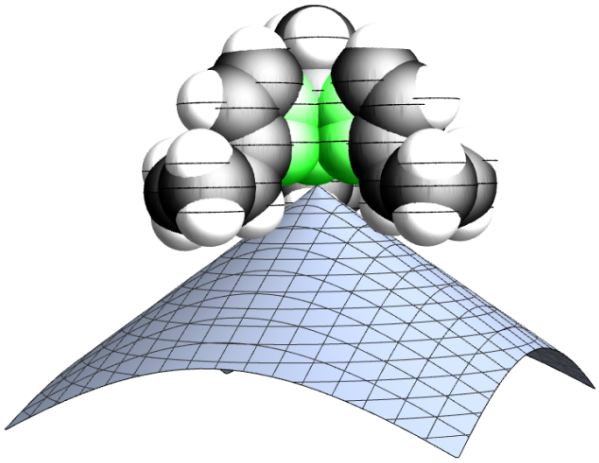


$[MeCTp^{3\text{-}cyPr}Me(thf)_2][AlMe_4]$ (**6**)

Ligand atoms forming cone = {13, 26, 39}

Cone angle (deg) = 250.799

Cone axis = {0.15295, –0.986949, –0.0503766}

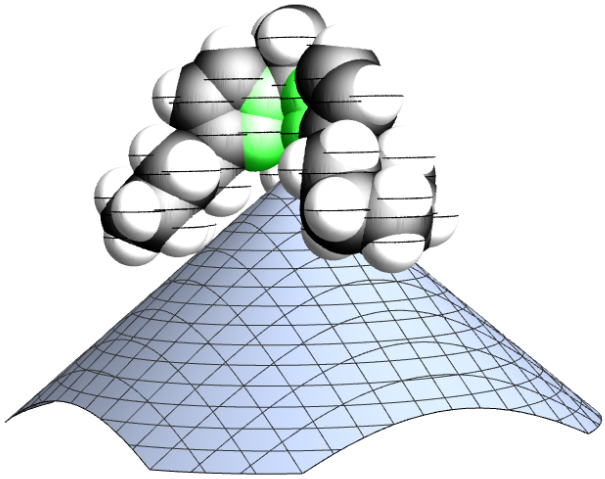


[(MeCTp$^{3\text{-}Cy}$)Mg(AlMe$_4$)] (**8**)

Ligand atoms forming cone = {20, 41, 58}

Cone angle (deg) = 260.64

Cone axis = {0.259263, –0.0918334, 0.961431}



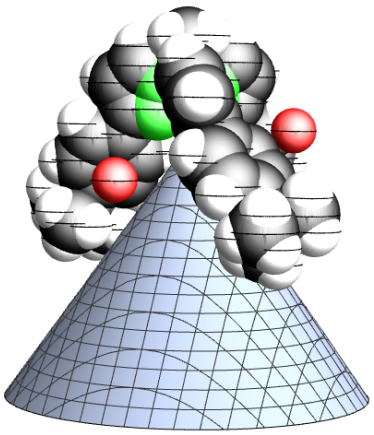
Because of the ample distance between two of the *p*-*t*BuPh substituents in complex **9** it was necessary to place two dummy germanium atoms between those substituents; otherwise the program would not find an appropriate cone.

[(MeCTp$^{3\text{-}ptBuPh}$)Mg(AlMe$_4$)][AlMe$_4$]_1 (**9**)

Ligand atoms forming cone = {34, 78, 90}

Cone angle (deg) = 289.6

Cone axis = {0.862318, 0.272602, –0.426728}

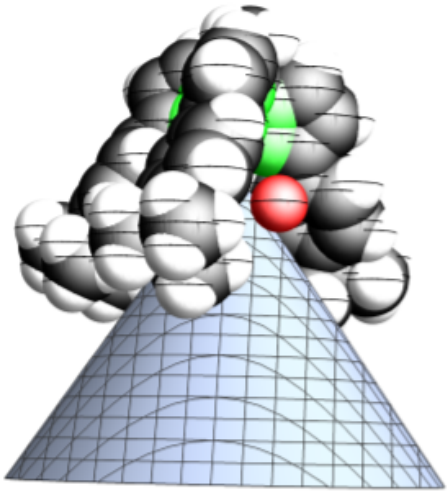


[(MeCTp$^{3\text{-}ptBuPh}$)Mg(AlMe$_4$)][AlMe$_4$]_2 (**9**)

Ligand atoms forming cone = {34, 78, 87}

Cone angle (deg) = 291.336

Cone axis = {0.870764, 0.248934, –0.42403}

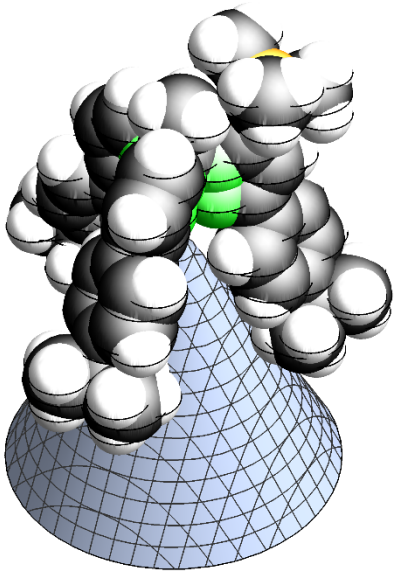


[MeC(pz3-p-tBuPh)2(pz3-p-tBuPh,5-AlMe3)]MgMe_**10**

Ligand atoms forming cone = {19, 54, 76}

Cone angle (deg) = 299.101

Cone axis = {0.282265, –0.854919, –0.435247}



Raw Data Files for Cone Angle Calculations

ComplexDataBase1.txt
(X1) [(AlMe3CTp-3-ptBuPh)2Mg]_4

1	Mg	16.549421	25.589250	9.767125
2	N	17.881427	25.590274	7.051083
3	N	18.153696	25.094866	8.318465
4	N	15.532675	25.128985	6.947942
5	N	15.163848	24.792571	8.235640
6	N	16.320824	27.362073	7.307372
7	N	16.364155	27.519362	8.679458
8	C	19.429747	24.676908	8.273146
9	C	19.987934	24.934165	7.004201
10	H	20.877416	24.756746	6.719782
11	C	18.986882	25.492352	6.271276
12	H	19.052050	25.766669	5.363324
13	C	20.152046	24.009540	9.379565
14	C	19.525963	23.338078	10.410974
15	H	18.581207	23.238451	10.389096
16	C	20.233932	22.805822	11.478325
17	H	19.765137	22.354769	12.170619
18	C	21.614045	22.918756	11.554900
19	C	22.261965	23.532898	10.482860
20	H	23.211156	23.583053	10.484423
21	C	21.555361	24.078461	9.407695
22	H	22.023815	24.497442	8.695085
23	C	22.416865	22.459514	12.773837
24	C	22.917732	23.709293	13.531766
25	H	23.456812	23.429517	14.300634
26	H	22.150055	24.231314	13.842751
27	H	23.463636	24.258609	12.931674
28	C	21.549560	21.689448	13.777116
29	H	22.081817	21.464263	14.567862
30	H	21.222018	20.863769	13.359864
31	H	20.785295	22.245588	14.044344
32	C	23.572817	21.580267	12.378464
33	H	24.060719	21.300492	13.181712
34	H	24.176723	22.081817	11.789311
35	H	23.238451	20.788707	11.906516
36	C	14.113666	23.964162	8.101244
37	C	13.821266	23.764566	6.730721
38	H	13.135815	23.221391	6.360352
39	C	14.737702	24.517231	6.057180
40	H	14.800822	24.596387	5.113285
41	C	13.359294	23.352750	9.206101
42	C	13.314940	23.904113	10.484423
43	H	13.719250	24.749923	10.643822
44	C	12.687150	23.234698	11.534584
45	H	12.685444	23.627408	12.400342
46	C	12.064478	22.007779	11.347055

47	C	12.052878	21.500088	10.045293
48	H	11.603872	20.679526	9.873391
49	C	12.680326	22.161655	8.987318
50	H	12.641090	21.795217	8.112183
51	C	11.469784	21.170498	12.489418
52	C	11.743760	21.791805	13.842751
53	H	11.358215	21.228842	14.544421
54	H	11.341156	22.682311	13.880257
55	H	12.712739	21.863455	13.977147
56	C	12.112245	19.758313	12.442536
57	H	11.753996	19.212409	13.172335
58	H	13.084637	19.840198	12.539426
59	H	11.904119	19.335237	11.583029
60	C	9.978784	21.020716	12.283136
61	H	9.590851	20.539638	13.042628
62	H	9.812624	20.519167	11.458010
63	H	9.566968	21.907810	12.215939
64	C	16.161829	28.832261	8.898242
65	C	15.974175	29.508500	7.680867
66	H	15.807333	30.437560	7.560536
67	C	16.079944	28.562038	6.711968
68	H	15.998399	28.711139	5.777450
69	C	16.135899	29.501676	10.231259
70	C	15.352526	30.625556	10.381282
71	H	14.855413	30.956169	9.640543
72	C	15.281559	31.288147	11.614284
73	H	14.753056	32.075272	11.692421
74	C	15.979634	30.807751	12.736331
75	C	16.792348	29.690695	12.537863
76	H	17.301745	29.362811	13.267663
77	C	16.881058	29.049599	11.326740
78	H	17.451868	28.294887	11.231412
79	C	15.859876	31.459424	14.117793
80	C	17.240331	31.942208	14.586615
81	H	17.144798	32.440345	15.424244
82	H	17.632699	32.522231	13.902135
83	H	17.823766	31.167706	14.733513
84	C	14.889532	32.604116	14.167801
85	H	14.838353	32.948718	15.083566
86	H	14.002438	32.293633	13.884945
87	H	15.193191	33.317203	13.566146
88	C	15.350138	30.393205	15.136700
89	H	15.309195	30.792397	16.032150
90	H	15.964280	29.628940	15.146076
91	H	14.456220	30.089546	14.872597
92	C	16.588999	26.101035	6.615078
93	C	17.021628	24.624023	3.642747
94	H	17.700937	24.726039	2.944202
95	H	16.209937	24.238138	3.253625
96	H	17.359747	24.030012	4.344417
97	C	18.024385	27.789243	4.083440

98	H	17.670230	28.489365	3.494287
99	H	18.792745	27.360026	3.652123
100	H	18.304844	28.189118	4.932007
101	C	14.775233	27.071721	3.984987
102	H	14.387982	26.507051	3.281754
103	H	14.828117	27.998051	3.669314
104	H	14.210564	27.029072	4.785110
105	Al	16.601282	26.418683	4.428961

0

(X2) [(MeCTp3-Et)2Mg][AlMe4]2_5a

1	Mg	4.137628	6.038048	0.000000
2	N	4.086232	5.393307	2.977860
3	N	3.268001	5.398417	1.878453
4	N	5.864076	6.882195	2.380492
5	N	5.296724	7.387616	1.238442
6	N	6.021866	4.548128	1.847149
7	N	5.680649	4.641693	0.523066
8	C	2.024768	5.274417	2.363836
9	C	2.046068	5.228883	3.765648
10	H	1.298454	5.162812	4.348249
11	C	3.364102	5.297939	4.122391
12	H	3.709871	5.281894	5.007397
13	C	0.834088	5.135950	1.461583
14	H	0.540432	4.190979	1.462410
15	H	1.104938	5.365203	0.537477
16	C	-0.345004	6.017990	1.862506
17	H	-0.114697	6.958786	1.715202
18	H	-0.551263	5.876803	2.810238
19	H	-1.126979	5.784173	1.319477
20	C	5.769926	8.634976	1.123623
21	C	6.630968	8.927930	2.195860
22	H	7.093378	9.743032	2.350724
23	C	6.667941	7.801400	2.972071
24	H	7.163649	7.684399	3.774153
25	C	5.409066	9.497735	-0.050558
26	H	4.657112	9.076058	-0.536296
27	H	6.181727	9.533512	-0.667417
28	C	5.014042	10.918345	0.322250
29	H	4.788814	11.418217	-0.490226
30	H	5.762741	11.356709	0.778456
31	H	4.236894	10.895462	0.917846
32	C	6.276276	3.604640	-0.080917
33	C	6.995524	2.846615	0.855475
34	H	7.505253	2.062946	0.686317
35	C	6.812616	3.465928	2.060250
36	H	7.173176	3.190041	2.894108
37	C	6.123972	3.339423	-1.548997
38	H	6.245302	4.187686	-2.044776
39	H	5.204931	3.015574	-1.724652

40	C	7.122919	2.310706	-2.071118
41	H	6.999633	2.196255	-3.037041
42	H	6.976144	1.453669	-1.618338
43	H	8.034685	2.622096	-1.893573
44	C	5.543912	5.524520	2.833981
45	C	6.209874	5.255059	4.170586
46	H	5.965057	4.358357	4.482914
47	H	5.912154	5.921387	4.824300
48	H	7.182721	5.310561	4.068289

0

(X3) [MeCTp-3-cyPrMe(thf)2][AlMe4]_6

1	Mg	4.708899	6.565086	10.130630
2	C	5.211565	3.259387	9.986026
3	C	4.239381	5.191196	7.171404
4	C	5.451727	1.752426	9.911428
5	H	5.662178	1.410151	10.805164
6	H	6.202559	1.570028	9.307475
7	H	4.645905	1.308410	9.572870
8	C	4.245122	3.922925	6.566017
9	H	4.017725	3.722824	5.665108
10	C	4.638475	3.041366	7.517135
11	H	4.737554	2.102636	7.409542
12	C	3.894021	6.502473	6.594708
13	H	3.992083	7.286766	7.207268
14	C	2.773956	6.590544	5.594814
15	H	2.315335	5.750256	5.340896
16	H	2.189548	7.389254	5.626375
17	C	4.140269	6.774541	5.150098
18	H	4.421158	7.688749	4.896180
19	H	4.547854	6.050993	4.610701
20	C	2.642720	4.728038	11.918389
21	C	2.386700	3.388364	12.235428
22	H	1.701702	3.053368	12.802082
23	C	3.323822	2.665218	11.562616
24	H	3.410958	1.719754	11.561181
25	C	1.933570	5.927128	12.390362
26	H	2.159294	6.777393	11.914085
27	C	1.607551	6.067961	13.845013
28	H	1.867119	5.327137	14.448966
29	H	1.662742	6.971338	14.245258
30	C	0.528296	5.812334	12.868073
31	H	-0.090504	6.555928	12.661495
32	H	0.113572	4.912970	12.865203
33	C	7.707010	5.537010	11.059083
34	C	8.446649	4.349842	11.179586
35	H	9.345055	4.262176	11.473673
36	C	7.616065	3.360850	10.792253
37	H	7.828534	2.436765	10.759258
38	C	8.119874	6.919418	11.351734

39	H	7.413214	7.616025	11.228362
40	C	9.124883	7.191543	12.453483
41	H	9.005428	8.011886	12.994315
42	H	9.487009	6.415331	12.949843
43	C	9.521564	7.350286	11.026088
44	H	10.132931	6.674294	10.640189
45	H	9.651349	8.270850	10.684660
46	N	4.864680	3.754221	8.651878
47	N	4.608084	5.091011	8.453908
48	N	4.104948	3.544228	10.898411
49	N	3.695526	4.834705	11.104989
50	N	6.424793	3.915478	10.457999
51	N	6.466683	5.278033	10.621540

0

(X4) [(MeCTp-3-Cy)Mg(AlMe4)]_8

1	Mg	5.119677	6.696426	4.109222
2	C	4.109109	3.923116	5.437878
3	C	4.195710	3.314477	6.695870
4	H	3.807116	2.486727	6.953467
5	C	4.944032	4.138749	7.475850
6	H	5.171638	3.997892	8.387299
7	C	3.397426	3.432727	4.219121
8	H	3.625032	4.048322	3.463381
9	C	3.844865	2.018944	3.822866
10	H	4.821903	2.013727	3.662639
11	H	3.652788	1.391176	4.564432
12	C	3.123190	1.558117	2.567750
13	H	3.407419	0.634724	2.350005
14	H	3.378552	2.142411	1.811804
15	C	1.606561	1.587680	2.738249
16	H	1.170225	1.333790	1.885756
17	H	1.334545	0.935566	3.430514
18	C	1.162453	2.982334	3.144980
19	H	0.184305	2.982334	3.296991
20	H	1.354529	3.613580	2.407522
21	C	1.865254	3.460550	4.406259
22	H	1.613222	2.877995	5.166313
23	H	1.574363	4.383943	4.617842
24	C	8.349230	6.839369	4.466036
25	C	9.235226	6.938490	5.547778
26	H	10.174514	7.074130	5.503202
27	C	8.483573	6.802851	6.674917
28	H	8.805551	6.811545	7.567673
29	C	8.682311	6.867193	3.007965
30	H	7.828514	6.844586	2.487636
31	C	9.516124	5.642958	2.626089
32	H	10.341055	5.625568	3.173739
33	H	9.000959	4.820425	2.822471
34	C	9.891395	5.663825	1.143368

35	H	10.469846	4.886506	0.940824
36	H	9.069796	5.585572	0.595718
37	C	10.621953	6.943707	0.777309
38	H	11.491295	6.973270	1.248954
39	H	10.800707	6.954141	-0.197203
40	C	9.803684	8.164464	1.150352
41	H	8.974312	8.185332	0.610097
42	H	10.321070	8.983519	0.949040
43	C	9.440626	8.145335	2.639647
44	H	10.268887	8.202721	3.179902
45	H	8.881050	8.933089	2.853284
46	C	3.839314	8.986997	6.016341
47	C	3.778249	9.242626	7.392655
48	H	3.280848	9.927780	7.822394
49	C	4.573202	8.312277	7.992071
50	H	4.723089	8.213155	8.925499
51	C	3.165380	9.750405	4.924945
52	H	3.491799	9.400872	4.046774
53	C	1.634317	9.592159	4.975272
54	H	1.396720	8.637464	4.870508
55	H	1.299016	9.898217	5.856524
56	C	0.977038	10.400780	3.876275
57	H	-0.006662	10.313831	3.948172
58	H	1.251274	10.040813	2.995024
59	C	1.360081	11.875426	3.962552
60	H	0.959273	12.365816	3.200444
61	H	1.003684	12.263216	4.800665
62	C	2.864497	12.033672	3.931739
63	H	3.207570	11.738048	3.050487
64	H	3.095433	12.990106	4.042666
65	C	3.530659	11.228529	5.022519
66	H	3.250871	11.578062	5.905825
67	H	4.513248	11.329390	4.952676
68	C	6.016553	6.416799	7.129307
69	C	6.462882	6.262031	8.577312
70	H	7.104618	5.524708	8.644074
71	H	5.684582	6.069005	9.141190
72	H	6.887005	7.091520	8.878252
73	N	5.307091	5.198825	6.711071
74	N	4.785264	5.081096	5.445068
75	N	7.188998	6.651039	6.288112
76	N	7.091294	6.679036	4.908305
77	N	5.112793	7.554433	7.005644
78	N	4.656472	7.960657	5.776000

0

(X5) [(MeCTp3-ptBuPh)Mg(AlMe4)][AlMe4]_9_1

1	Mg	15.170285	9.647016	5.566269
2	C	17.782064	10.312506	3.873413
3	C	18.987124	10.647287	3.014954

4	H	19.142422	9.923132	2.374136
5	H	19.776038	10.754069	3.586494
6	H	18.820017	11.481371	2.528938
7	C	16.903935	12.219406	6.737244
8	C	17.875075	13.082914	6.211991
9	H	18.176958	13.902008	6.585968
10	C	18.295548	12.504219	5.052665
11	H	18.967369	12.839740	4.469323
12	C	16.167986	12.287139	8.014741
13	C	15.525768	13.457854	8.415693
14	H	15.633941	14.257331	7.913277
15	C	14.726145	13.453598	9.552029
16	H	14.288059	14.255480	9.812280
17	C	14.549982	12.298798	10.322359
18	C	15.269298	11.168057	9.961717
19	H	15.218967	10.387642	10.501990
20	C	16.063006	11.163060	8.821089
21	H	16.542921	10.376538	8.589193
22	C	13.541417	12.301944	11.477547
23	C	13.906972	13.407517	12.474102
24	H	13.983120	14.262882	12.000960
25	H	14.763180	13.193213	12.900649
26	H	13.209062	13.474510	13.158141
27	C	13.511260	10.971889	12.226879
28	H	13.260239	10.254396	11.608592
29	H	12.856100	11.020561	12.954293
30	H	14.398602	10.787381	12.600242
31	C	12.136312	12.556777	10.903095
32	H	12.124488	13.420841	10.440682
33	H	11.481473	12.567696	11.633115
34	H	11.907060	11.844096	10.270554
35	C	17.609693	7.426618	5.922926
36	C	18.883271	7.218421	5.378975
37	H	19.475572	6.499448	5.566729
38	C	19.099848	8.256075	4.527565
39	H	19.882225	8.405607	4.011049
40	C	16.965164	6.598642	6.951514
41	C	16.152907	7.140694	7.944237
42	H	16.001699	8.078044	7.963856
43	C	15.564142	6.335111	8.901402
44	H	15.019056	6.730778	9.570115
45	C	15.752964	4.956754	8.906000
46	C	16.591163	4.428952	7.929370
47	H	16.755739	3.494008	7.916342
48	C	17.190357	5.231944	6.976497
49	H	17.765996	4.841274	6.330008
50	C	15.024779	4.077145	9.917575
51	C	14.498885	10.260133	2.483111
52	C	15.240279	10.070072	1.303399
53	H	14.896795	9.973099	0.423022
54	C	16.545484	10.054527	1.678908

55	H	17.293034	9.943489	1.102004
56	C	13.051433	10.497755	2.572926
57	C	12.532823	11.516348	3.360422
58	H	13.107912	11.993998	3.945143
59	C	11.188352	11.846132	3.305245
60	H	10.856665	12.539937	3.862378
61	C	10.312191	11.181197	2.450464
62	C	10.835428	10.148540	1.687951
63	H	10.258032	9.662191	1.109667
64	C	12.179106	9.806541	1.746040
65	H	12.504455	9.090344	1.213890
66	C	8.833713	11.584266	2.402798
67	C	8.695215	13.100125	2.223779
68	H	9.149205	13.374575	1.399346
69	H	9.101663	13.557789	2.988745
70	H	7.746283	13.337562	2.168756
71	C	8.098452	10.905822	1.250522
72	H	8.529509	11.144554	0.403097
73	H	7.165670	11.203775	1.238413
74	H	8.129543	9.934236	1.370225
75	C	8.175661	11.156768	3.719378
76	H	7.231329	11.420299	3.713707
77	H	8.633425	11.592409	4.469323
78	H	8.241825	10.184072	3.816397
79	N	17.580778	11.359043	4.881617
80	N	16.701954	11.176385	5.920321
81	N	17.992713	9.035565	4.553468
82	N	17.045359	8.529600	5.414073
83	N	16.591177	10.224601	3.018632
84	N	15.324792	10.321760	3.542812
85	C	13.957213	3.221964	9.016814
86	H	13.360540	3.840078	8.543212
87	H	13.426365	2.642714	9.602301
88	H	14.442338	2.674175	8.366953
89	C	14.167907	4.830170	10.897424
90	H	13.486962	5.337246	10.410028
91	H	14.726986	5.446434	11.413940
92	H	13.733275	4.195401	11.504369
93	C	15.945066	3.120179	10.523448
94	H	16.387620	2.602000	9.818410
95	H	15.446465	2.513169	11.108935
96	H	16.617129	3.601345	11.047627
97	Ge	14.045359	5.529600	5.414073
98	Ge	14.045359	14.52960	5.414073

0

(X6) [(MeCTp3-ptBuPh)Mg(AlMe4)][AlMe4]_9_2

1	Mg	15.170285	9.647016	5.566269
2	C	17.782064	10.312506	3.873413
3	C	18.987124	10.647287	3.014954

4	H	19.142422	9.923132	2.374136
5	H	19.776038	10.754069	3.586494
6	H	18.820017	11.481371	2.528938
7	C	16.903935	12.219406	6.737244
8	C	17.875075	13.082914	6.211991
9	H	18.176958	13.902008	6.585968
10	C	18.295548	12.504219	5.052665
11	H	18.967369	12.839740	4.469323
12	C	16.167986	12.287139	8.014741
13	C	15.525768	13.457854	8.415693
14	H	15.633941	14.257331	7.913277
15	C	14.726145	13.453598	9.552029
16	H	14.288059	14.255480	9.812280
17	C	14.549982	12.298798	10.322359
18	C	15.269298	11.168057	9.961717
19	H	15.218967	10.387642	10.501990
20	C	16.063006	11.163060	8.821089
21	H	16.542921	10.376538	8.589193
22	C	13.541417	12.301944	11.477547
23	C	13.906972	13.407517	12.474102
24	H	13.983120	14.262882	12.000960
25	H	14.763180	13.193213	12.900649
26	H	13.209062	13.474510	13.158141
27	C	13.511260	10.971889	12.226879
28	H	13.260239	10.254396	11.608592
29	H	12.856100	11.020561	12.954293
30	H	14.398602	10.787381	12.600242
31	C	12.136312	12.556777	10.903095
32	H	12.124488	13.420841	10.440682
33	H	11.481473	12.567696	11.633115
34	H	11.907060	11.844096	10.270554
35	C	17.609693	7.426618	5.922926
36	C	18.883271	7.218421	5.378975
37	H	19.475572	6.499448	5.566729
38	C	19.099848	8.256075	4.527565
39	H	19.882225	8.405607	4.011049
40	C	16.965164	6.598642	6.951514
41	C	16.152907	7.140694	7.944237
42	H	16.001699	8.078044	7.963856
43	C	15.564142	6.335111	8.901402
44	H	15.019056	6.730778	9.570115
45	C	15.752964	4.956754	8.906000
46	C	16.591163	4.428952	7.929370
47	H	16.755739	3.494008	7.916342
48	C	17.190357	5.231944	6.976497
49	H	17.765996	4.841274	6.330008
50	C	15.024779	4.077145	9.917575
51	C	14.498885	10.260133	2.483111
52	C	15.240279	10.070072	1.303399
53	H	14.896795	9.973099	0.423022
54	C	16.545484	10.054527	1.678908

55	H	17.293034	9.943489	1.102004
56	C	13.051433	10.497755	2.572926
57	C	12.532823	11.516348	3.360422
58	H	13.107912	11.993998	3.945143
59	C	11.188352	11.846132	3.305245
60	H	10.856665	12.539937	3.862378
61	C	10.312191	11.181197	2.450464
62	C	10.835428	10.148540	1.687951
63	H	10.258032	9.662191	1.109667
64	C	12.179106	9.806541	1.746040
65	H	12.504455	9.090344	1.213890
66	C	8.833713	11.584266	2.402798
67	C	8.695215	13.100125	2.223779
68	H	9.149205	13.374575	1.399346
69	H	9.101663	13.557789	2.988745
70	H	7.746283	13.337562	2.168756
71	C	8.098452	10.905822	1.250522
72	H	8.529509	11.144554	0.403097
73	H	7.165670	11.203775	1.238413
74	H	8.129543	9.934236	1.370225
75	C	8.175661	11.156768	3.719378
76	H	7.231329	11.420299	3.713707
77	H	8.633425	11.592409	4.469323
78	H	8.241825	10.184072	3.816397
79	N	17.580778	11.359043	4.881617
80	N	16.701954	11.176385	5.920321
81	N	17.992713	9.035565	4.553468
82	N	17.045359	8.529600	5.414073
83	N	16.591177	10.224601	3.018632
84	N	15.324792	10.321760	3.542812
85	C	13.543348	4.158573	9.674491
86	H	13.343218	3.841929	8.768518
87	H	13.246659	5.087409	9.767831
88	H	13.073769	3.599495	10.327263
89	C	15.483384	2.619766	9.870522
90	H	15.287250	2.242976	8.987692
91	H	15.007865	2.106028	10.557167
92	H	16.448453	2.576091	10.037585
93	C	15.324651	4.604762	11.356771
94	H	16.285723	4.545172	11.533490
95	H	14.837392	4.062155	12.011689
96	H	15.036793	5.538966	11.429267
97	Ge	14.045359	5.529600	5.414073
98	Ge	14.045359	14.52960	5.414073

0
(X7) [MeC(pz3-p-tBuPh)2(pz3-p-tBuPh,5-AlMe3)]MgMe_10

1	Mg	9.921594	8.286851	3.133050
2	C	8.417664	5.660597	4.305021
3	C	8.382184	4.288323	3.995550
4	H	7.791439	3.635323	4.352237

5	C	9.371052	4.090964	3.078822
6	H	9.599875	3.263743	2.670868
7	C	7.567657	6.396576	5.255252
8	C	8.088728	7.372256	6.107156
9	H	9.009313	7.600056	6.055421
10	C	7.276022	8.007094	7.023416
11	H	7.652494	8.672203	7.587197
12	C	5.914725	7.703973	7.149324
13	C	5.408377	6.742751	6.275293
14	H	4.485902	6.522657	6.317210
15	C	6.210098	6.101426	5.348904
16	H	5.830854	5.451754	4.769852
17	C	5.056161	8.428448	8.189778
18	C	4.932609	9.907281	7.788837
19	H	5.823607	10.315855	7.767956
20	H	4.373384	10.377476	8.441127
21	H	4.522626	9.971945	6.901560
22	C	5.718747	8.333469	9.577570
23	H	5.811097	7.391227	9.831100
24	H	5.161466	8.796617	10.237807
25	H	6.603970	8.752285	9.545937
26	C	3.647985	7.841400	8.294806
27	H	3.183297	7.951100	7.439162
28	H	3.151443	8.308562	8.998986
29	H	3.707591	6.887977	8.514365
30	C	9.375715	8.117982	-0.052358
31	C	9.804578	7.298279	-1.100603
32	H	9.659020	7.436189	-2.028862
33	C	10.475375	6.260948	-0.521240
34	H	10.886985	5.533590	-0.973916
35	C	8.622568	9.383676	-0.123726
36	C	7.622311	9.696517	0.785210
37	H	7.391630	9.071692	1.463212
38	C	6.954163	10.911489	0.716179
39	H	6.271081	11.103115	1.347900
40	C	7.266347	11.859664	-0.262879
41	C	8.247067	11.516575	-1.193008
42	H	8.464046	12.129121	-1.887060
43	C	8.910606	10.307064	-1.128496
44	H	9.573005	10.101677	-1.777981
45	C	6.541507	13.215055	-0.289058
46	C	7.241154	14.218992	-1.211708
47	H	7.216311	13.888002	-2.133266
48	H	8.173589	14.327658	-0.928727
49	H	6.781938	15.082604	-1.162466
50	C	5.103275	12.988941	-0.779289
51	H	4.621887	13.842600	-0.782250
52	H	4.649209	12.360291	-0.180759
53	H	5.121634	12.620281	-1.687602
54	C	6.504473	13.819286	1.123821
55	H	6.075281	14.699939	1.090786

56	H	7.418869	13.913701	1.463212
57	H	5.994936	13.229837	1.718767
58	C	13.033777	7.896159	3.677508
59	C	13.959437	6.858621	3.556430
60	H	14.835337	6.861638	3.923714
61	C	13.406559	5.822987	2.818591
62	C	13.229096	9.217318	4.301593
63	C	14.083085	9.345482	5.398301
64	H	14.479687	8.568918	5.776492
65	C	14.360884	10.590262	5.943538
66	H	14.934502	10.648096	6.698985
67	C	13.818501	11.757590	5.410299
68	C	12.961925	11.618629	4.321383
69	H	12.567397	12.394511	3.940855
70	C	12.671090	10.375199	3.778016
71	H	12.080719	10.315435	3.035502
72	C	14.181398	13.126704	6.017244
73	C	13.619855	14.288651	5.191051
74	H	13.959977	14.231853	4.274324
75	H	13.900333	15.139385	5.591058
76	H	12.641426	14.238650	5.179676
77	C	15.710660	13.280231	6.058382
78	H	16.064349	13.270577	5.145394
79	H	16.099315	12.538863	6.568091
80	H	15.942207	14.130076	6.488619
81	C	13.618418	13.196600	7.441187
82	H	12.646584	13.068737	7.415788
83	H	13.822427	14.072569	7.830286
84	H	14.025449	12.492536	7.987671
85	C	15.108049	4.341268	0.387229
86	H	14.529338	3.731529	-0.118428
87	H	16.045593	4.085857	0.255556
88	H	14.972436	5.258762	0.070122
89	C	13.913540	2.467293	2.903829
90	H	13.456317	2.042396	2.148849
91	H	13.276472	2.604234	3.635434
92	H	14.643813	1.890829	3.210028
93	C	16.275303	4.637599	3.420550
94	H	16.964830	3.964643	3.242751
95	H	16.039471	4.622044	4.370936
96	H	16.616778	5.525188	3.183537
97	C	11.036966	5.601911	1.876152
98	C	11.538290	4.320346	1.246924
99	H	10.810803	3.894717	0.747968
100	H	11.851675	3.711867	1.949391
101	H	12.278709	4.523230	0.637331
102	N	9.970508	5.285718	2.853652
103	N	9.380580	6.270687	3.603334
104	N	10.445146	6.460343	0.821985
105	N	9.769407	7.609831	1.126626
106	N	12.137397	6.296436	2.545116

107	N	11.885647	7.556082	3.069316
108	Al	14.655052	4.233154	2.327582
0				