Supporting Information

Synthesis and Reactivity of a Heteroleptic Magnesium Hydride on a Dearomatized Picolyl-Based NNN-Chelator.

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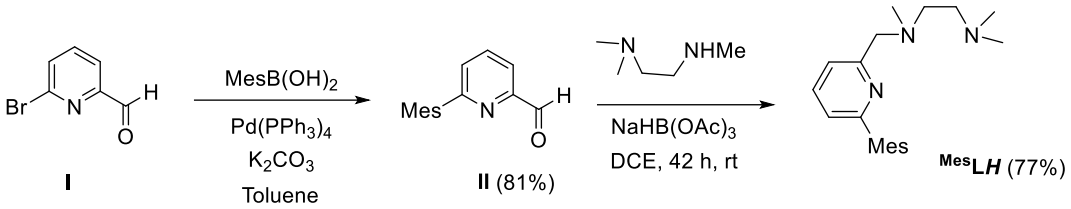
Table of Contents

1. Synthesis and characterization of ^{Mes}L*H*.



Scheme S1. Synthesis of ^{Mes}L*H*.

Step-1

A 250 mL Schlenk flask equipped with a magnetic stir bar was charged with **I** (5.0 g, 26.88 mmol), $MesB(OH)_2$ (6.61g, 40.32 mmol), K_2CO_3 (11.14 g, 80.64 mmol), 70 mL toluene, 30 mL ethanol, and 30 mL H_2O. The mixture was degassed following three freeze-pump-thaw cycle, followed by the addition of 0.912 g of $Pd(PPh_3)_4$ (0.79 mmol) and the reaction mixture was degassed again. The reaction mixture was then heated to 120 ^{0}C for 48 h under N_2 with constant stirring. Upon cooling back to ambient temperature, the volatiles were removed under reduced pressure. The residue was extracted with ethyl acetate, dried by $MgSO_4$, and purified by column chromatography (silica mesh 100-200, EtOAc/hexane = 2/98 (v/v)) to give 4.90 g of **II** (21.76 mmol, 81%).

^{1}H NMR ($CDCl_3$, 500 MHz): δ 10.13 (s, Ar-*CHO*), 7.96 (m, 1H, Ar*H*), 7.95 (m, 1H, Ar*H*), 7.49-7.47 (m, 1H, Ar*H*), 6.99 (m, 2H, Ar*H*), 2.35 (s, 3H, ^{Me}Mes), 2.05 (s, 6H, ^{Me}Mes). ^{13}C{^{1}H} NMR ($CDCl_3$, 126 MHz): δ 194.1, 161.0, 153.0, 138.2, 137.4, 136.7, 135.7, 129.2, 128.7, 119.6, 21.2, 20.3.

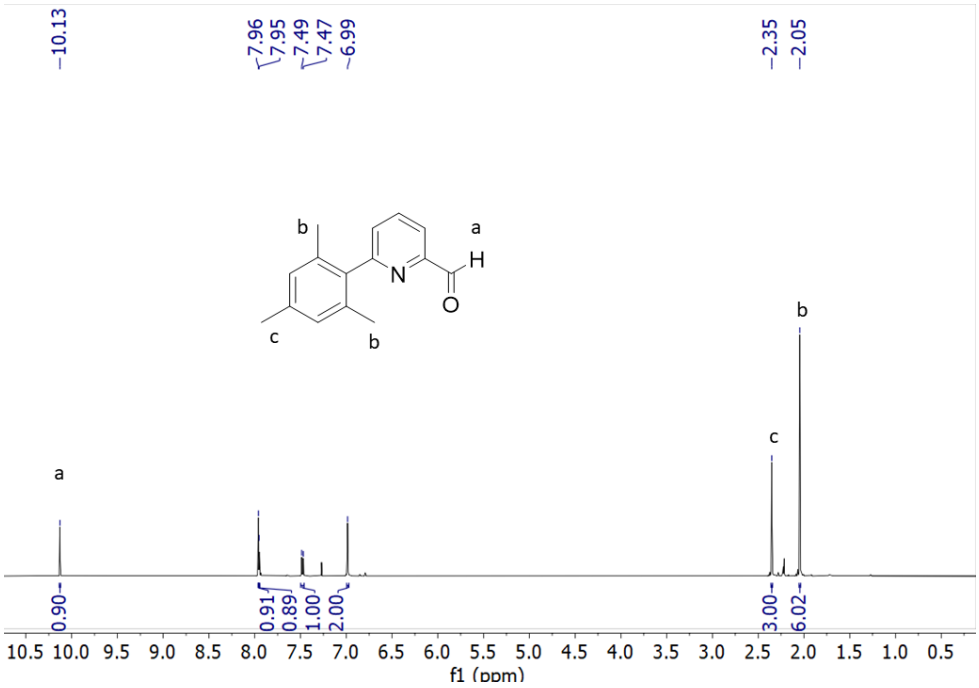


Figure S1. ^{1}H NMR spectrum of **II** in $CDCl_3$.

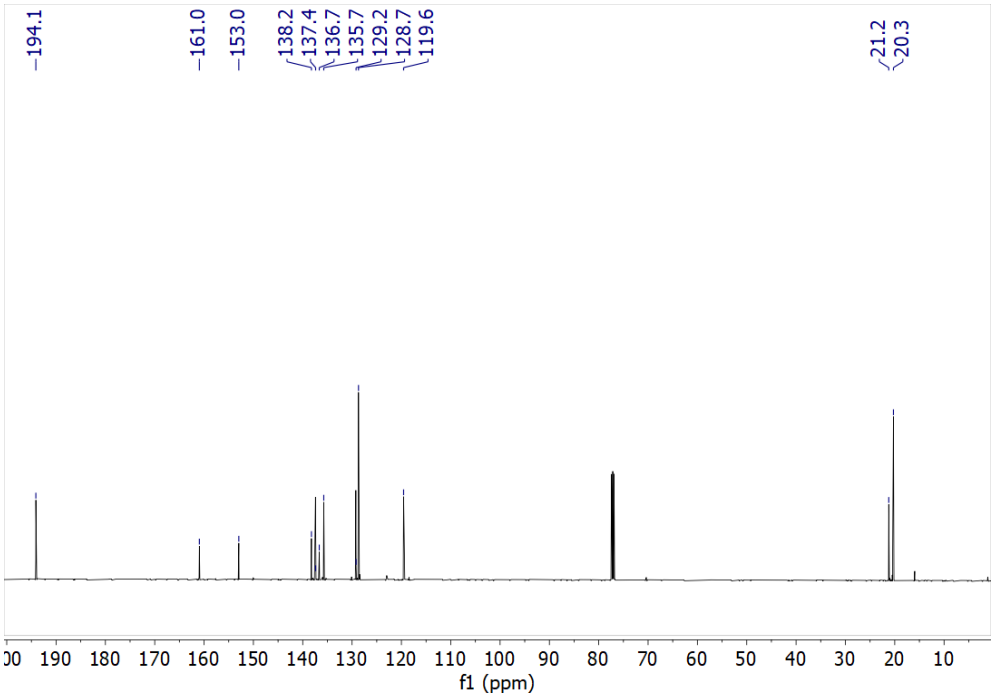


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of **II** in $CDCl_3$.

Step 2.

A 250 mL Schlenk flask equipped with a magnetic stir bar was charged under N_2 atmosphere with **II** (1.81 g, 8.04 mmol) and N,N,N'-trimethylethylenediamine (1.0 mL,7.7 mmol) in 50 mL of Dry DCE. To this, $NaHB(OAc)_3$ (5.11 g, 24.12 mmol) was added slowly under ice cold

condition. The reaction mixture was set for stirring under N_2 atmosphere for 60 hours at room temperature. The reaction mixture was then quenched by a saturated solution of $NaHCO_3$ the mixture was filtered and the volatiles were removed under reduced pressure. The residue was then extracted with EtOAc, dried by $MgSO_4$, and subsequently purified by column chromatography (silica mesh 60-120, MeOH/DCM = 5/95 (v/v)) to give 1.92 g of pure ^{Mes}**L*H*** (6.164 mmol, 77%).

^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.7 (t, $^3J_{HH}$ = 7.5 Hz, 1H, Ar*H*), 7.41 (d, $^3J_{HH}$ = 7.5 Hz, 1H, Ar*H*), 7.07 (d, $^3J_{HH}$ = 7.5 Hz, 1H, Ar*H*), 6.91 (m, 2H, Ar*H*), 3.74 (s, 2H, picolyl-CH_2), 2.59 (t, $^3J_{HH}$ = 7.5 Hz, 2H, CH_2), 2.48 (t, $^3J_{HH}$ = 6.0 Hz, 2H, CH_2), 2.31 (d, $^3J_{HH}$ = 7.5 Hz, 6H, *Me*), 2.23 (s, 6H, *Me*), 2.0 (s, 6H, *Me*). ^{13}C{^{1}H} NMR ($CDCl_3$, 126 MHz): δ 159.3, 159.2, 137.9, 137.4, 136.7, 135.7, 129.0, 128.4, 123.0, 121.2, 64.5, 57.4, 55.4, 45.7, 42.8, 21.1, 20.2. HRMS-(m/z): [M+nH] calc. for [$C_{20}H_{29}N_3$], 311.2361, Found 312.2417.

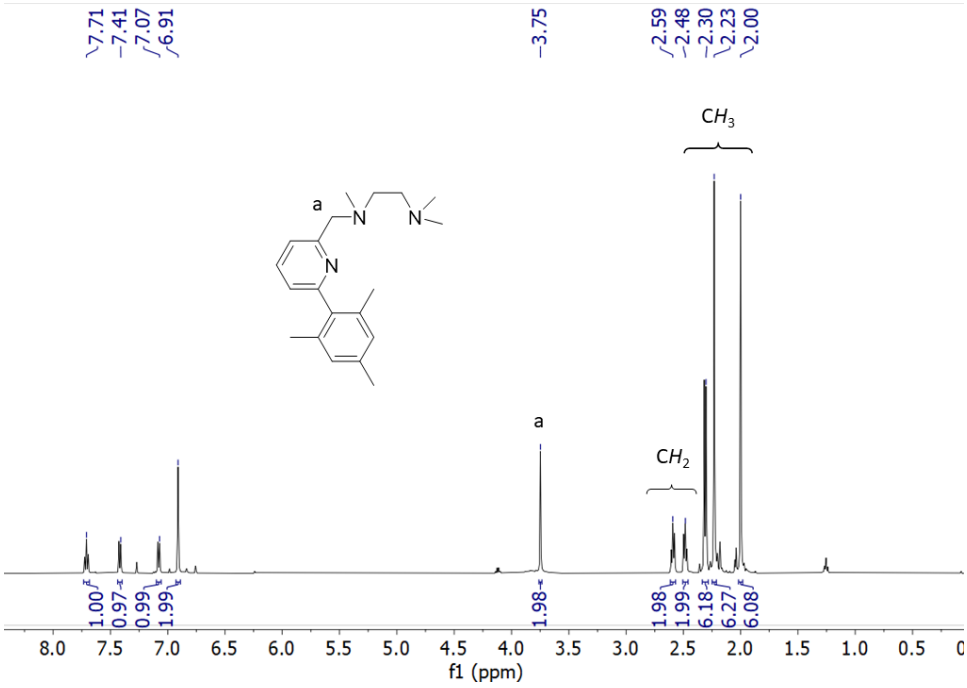


Figure S3. ^{1}H NMR spectrum of ^{Mes}**L*H*** in $CDCl_3$.

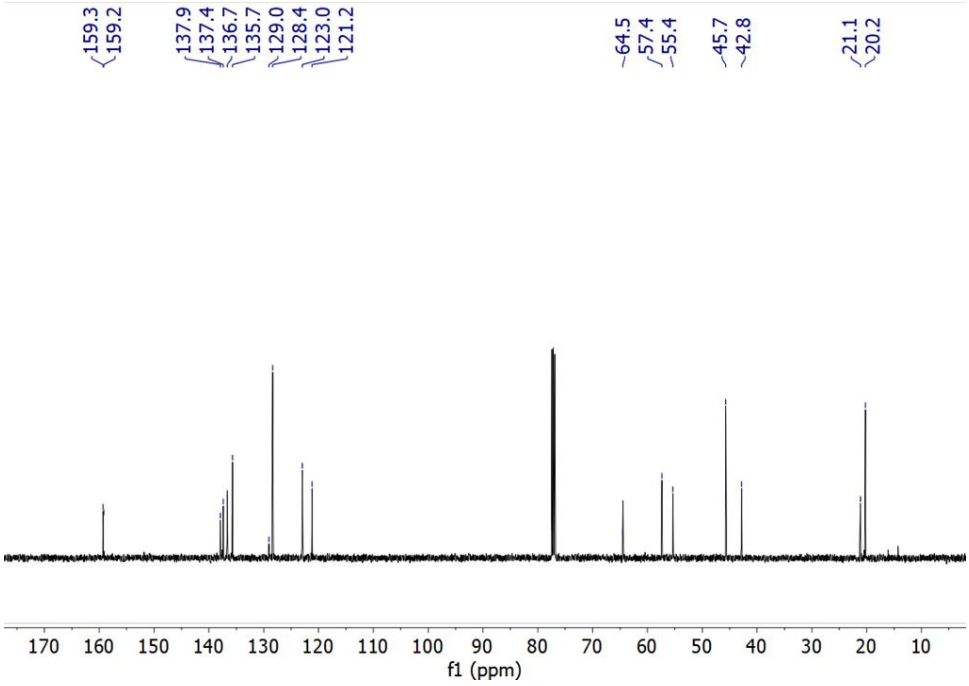


Figure S4. $^{13}C\{^{1}H\}$ NMR of ^{Mes}**L*H*** in $CDCl_3$.

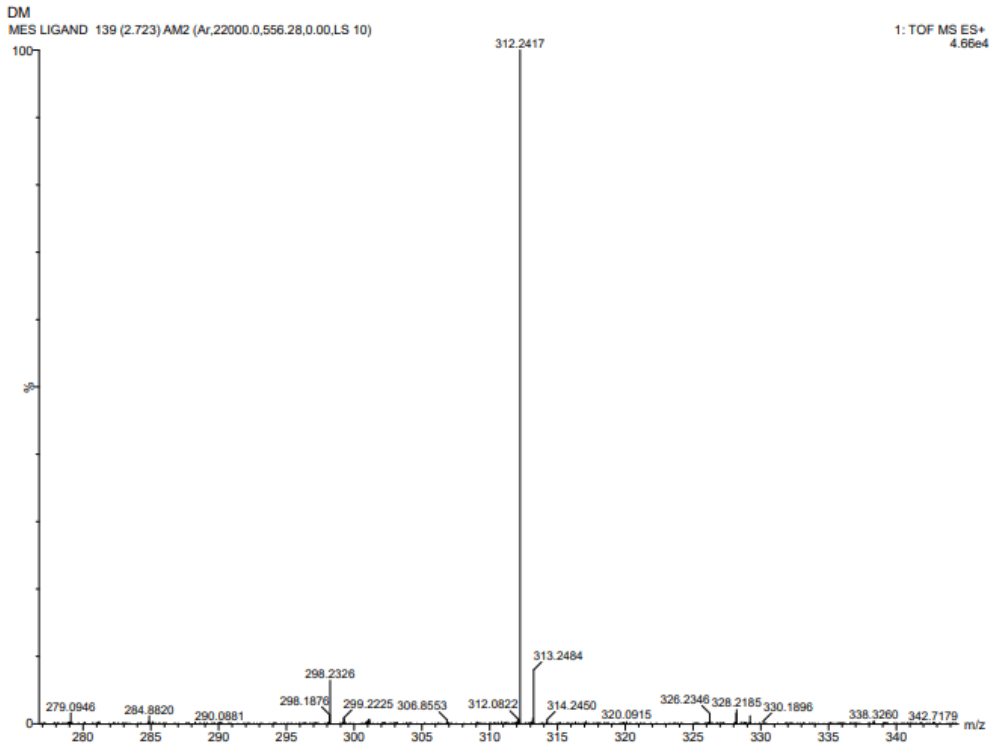


Figure S5. HRMS data of ^{Mes}**L*H***.

2. Spectroscopic characterization data.

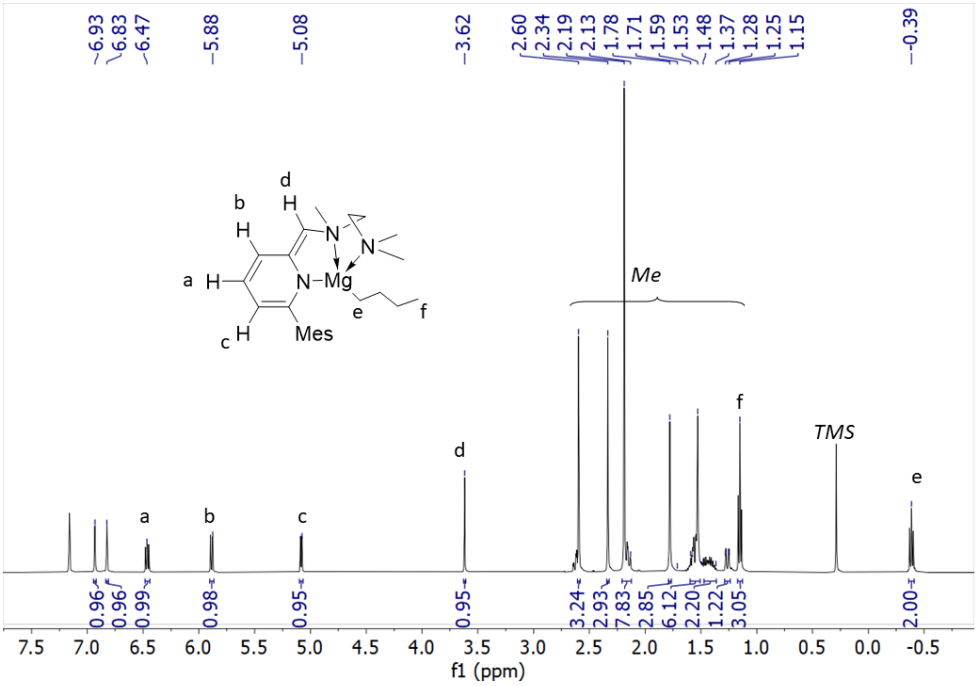


Figure S6. ^{1}H NMR spectrum of **1** in C_6D_6.

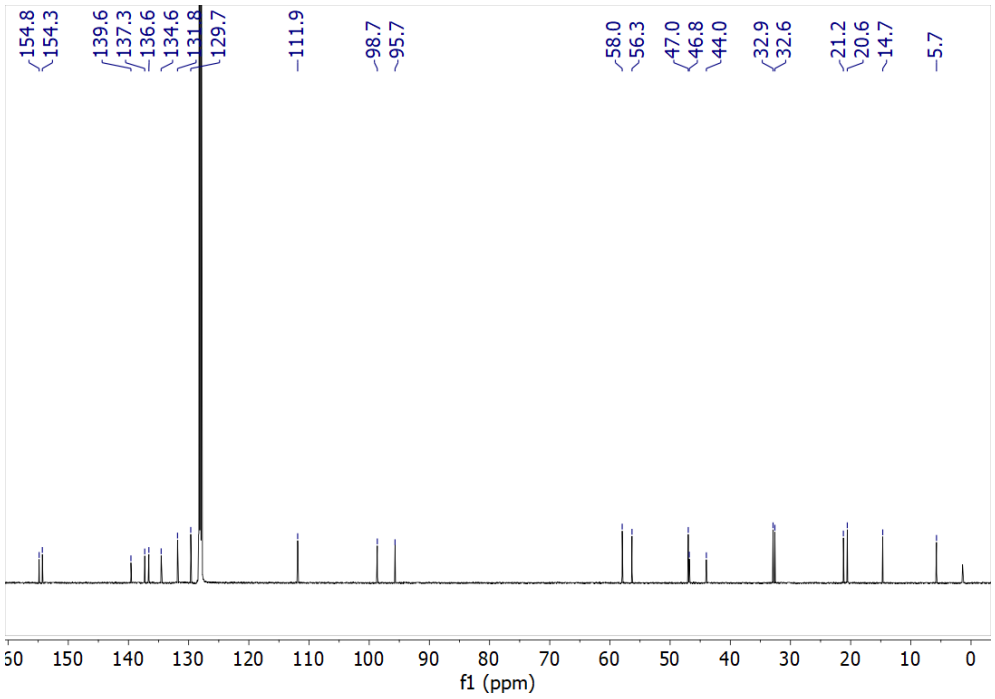


Figure S7. ^{13}C{^{1}H} NMR spectrum of **1** in C_6D_6.

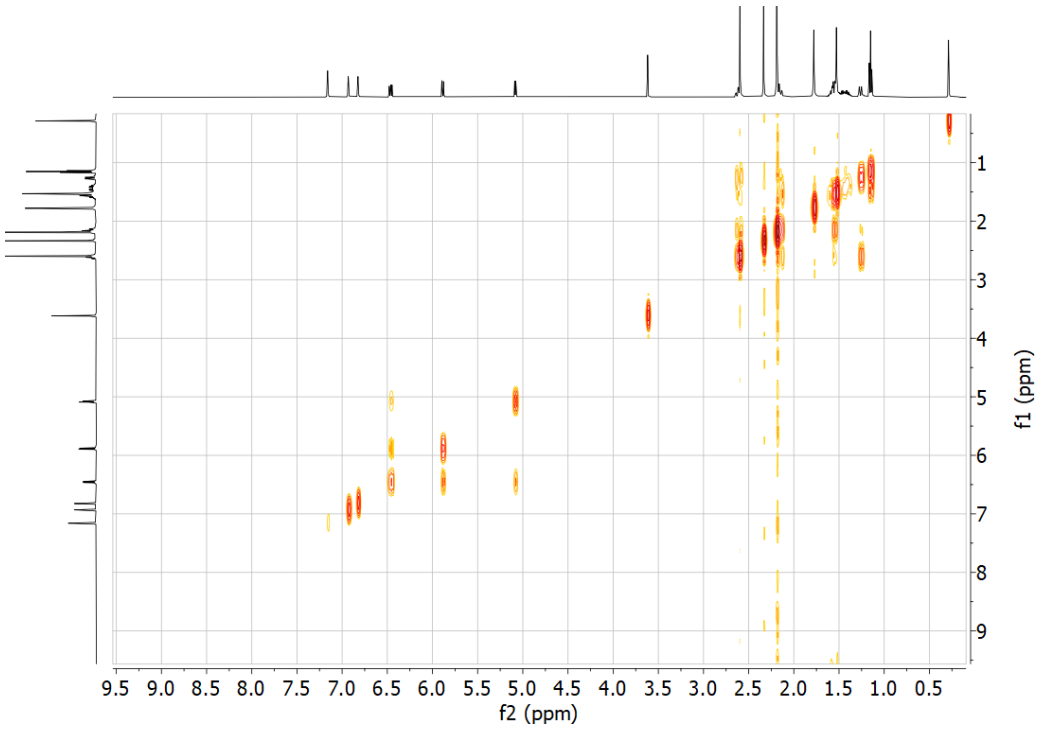


Figure S8. ^{1}H-^{1}H COSY NMR spectrum of **1** in C_6D_6.

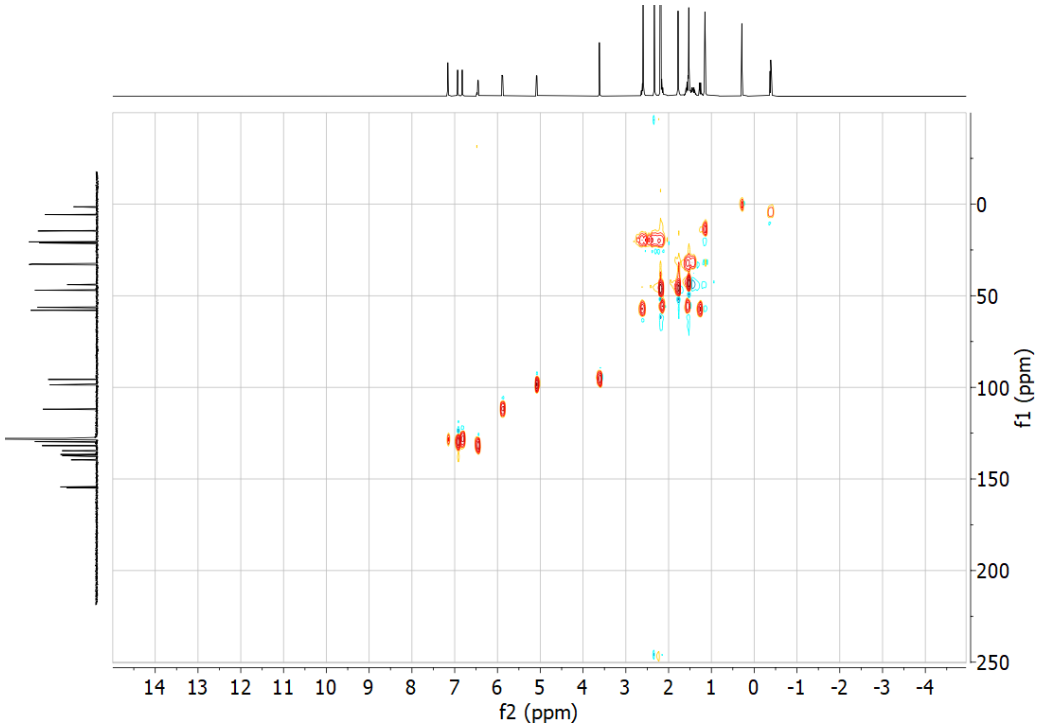


Figure S9. ^{1}H-^{13}C HSQC NMR spectrum of **1** in C_6D_6.

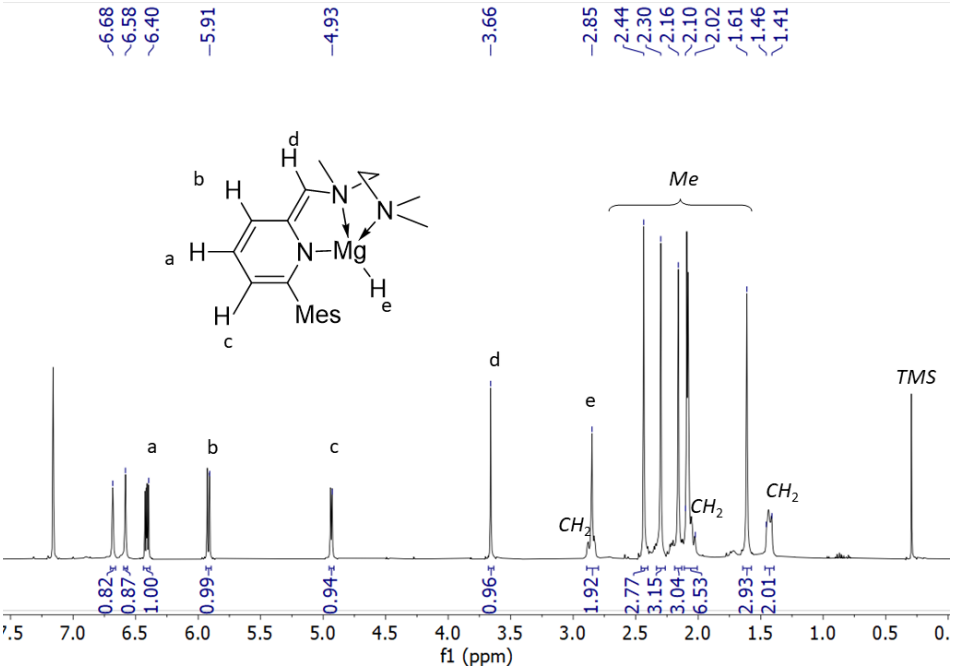


Figure S10. ^{1}H NMR spectrum of **2₂** in C_6D_6. The monomeric form is shown in the picture for peak assignment.

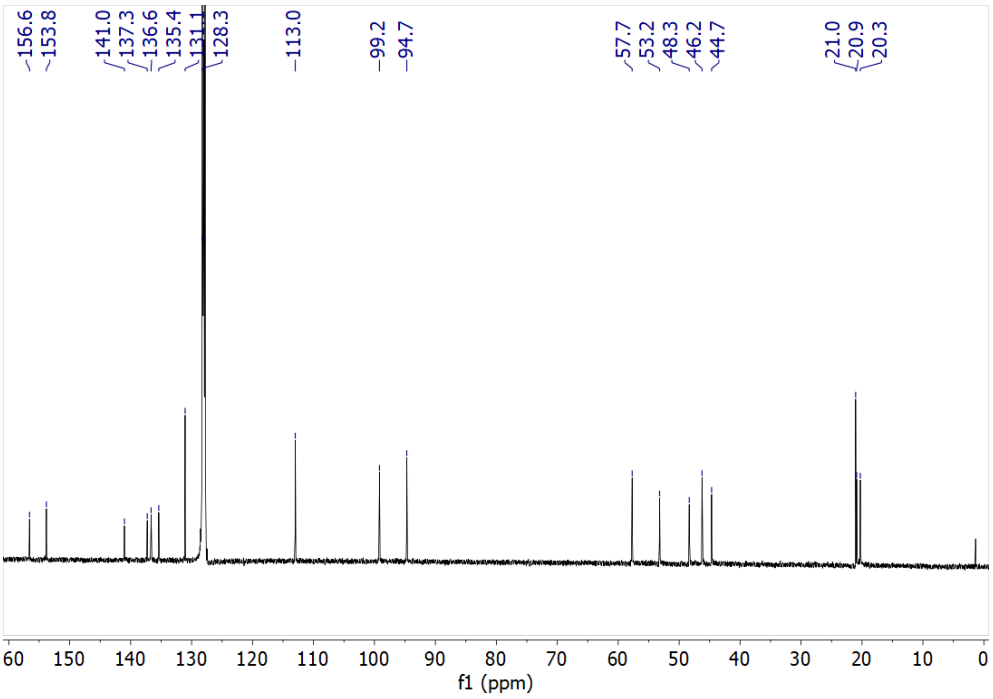


Figure S11. ^{13}C{^{1}H} NMR spectrum of **2₂** in C_6D_6.

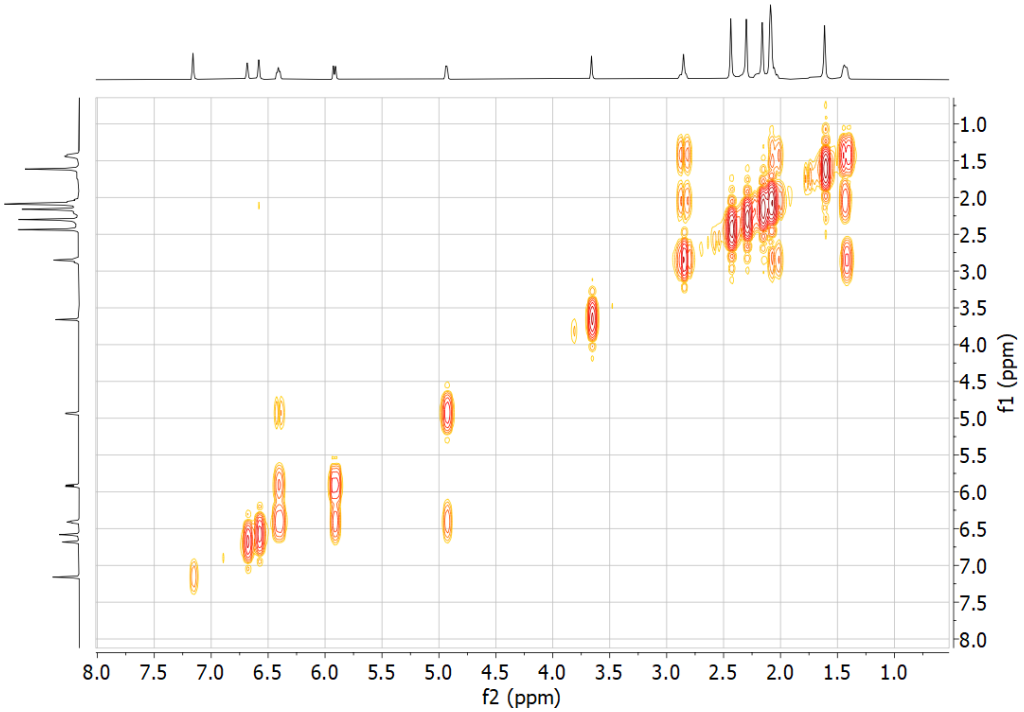


Figure S12. ^{1}H-^{1}H COSY NMR spectrum of **2₂** in C_6D_6.

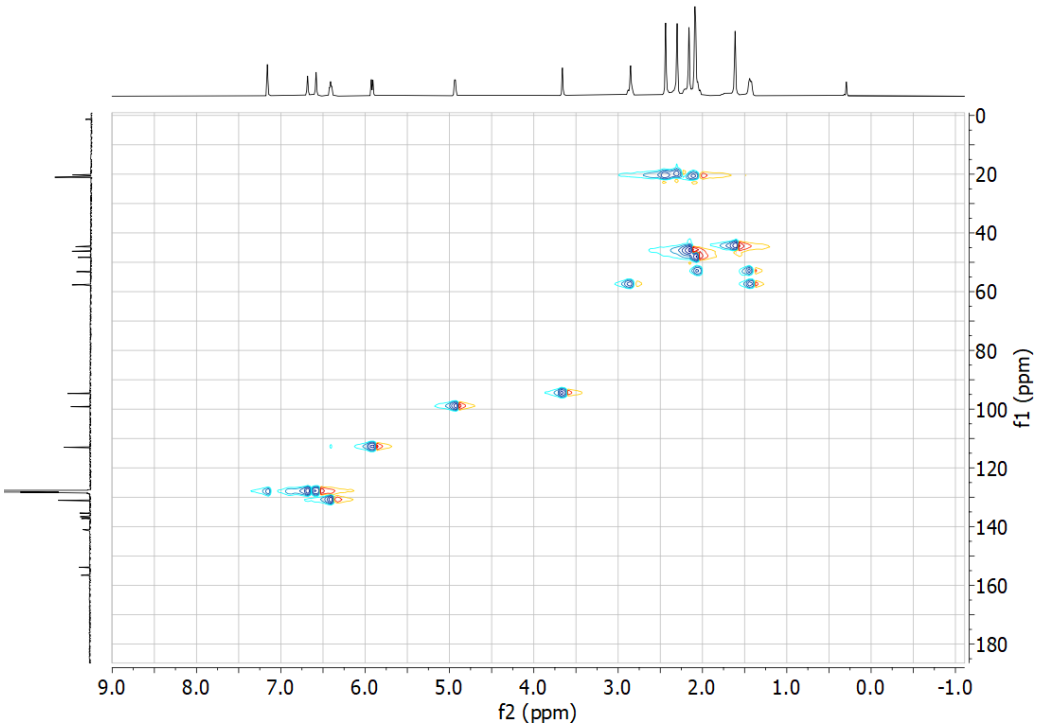
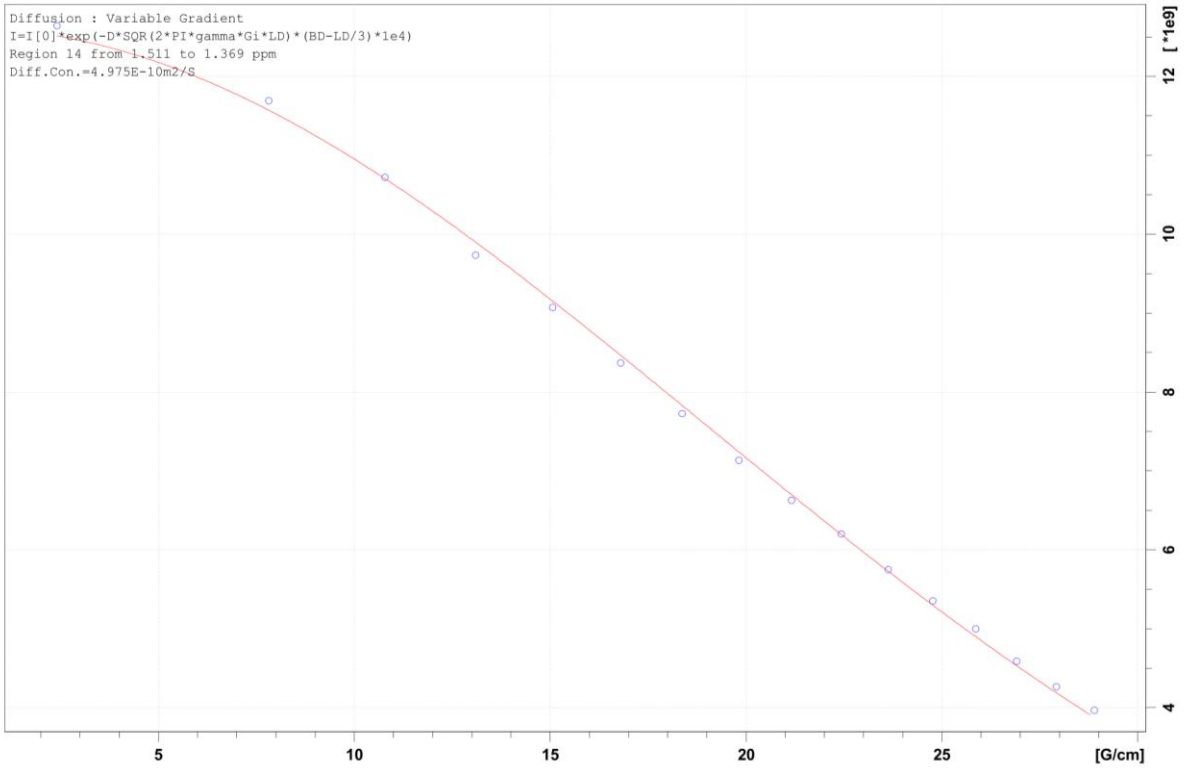


Figure S13. ^{1}H-^{13}C HSQC NMR spectrum of **2₂** in C_6D_6.



$$r = \frac{kT}{6\pi\eta D}$$

$$= \frac{1.3806488 * 10^{-23} * 300}{6 * \frac{22}{7} * 596.2 * 10^{-6} * 4.975 * 10^{-10}} \text{ m}$$

$$= 7.40 * 10^{-10} \text{ m} \quad = 7.40 \text{ Å}$$

For the dimeric **2**$_2$, the crystallographic diameter is estimated as 14.14 Å. That makes the approximated radius value as ~ 7.07 Å, which is close to what is found through the DOSY analysis.

Figure S14. DOSY analysis of **2**$_2$ in C_6D_6.

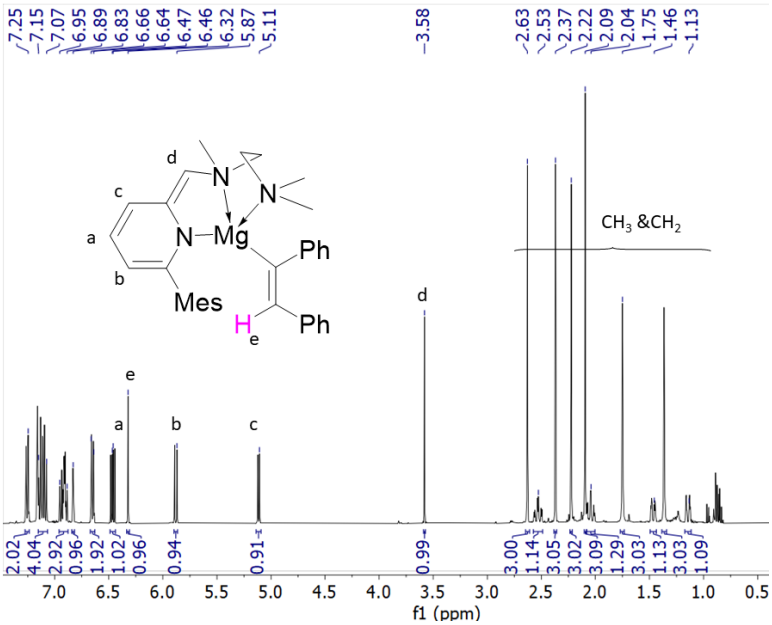


Figure S15. ^{1}H NMR spectrum of **3** in C_6D_6.

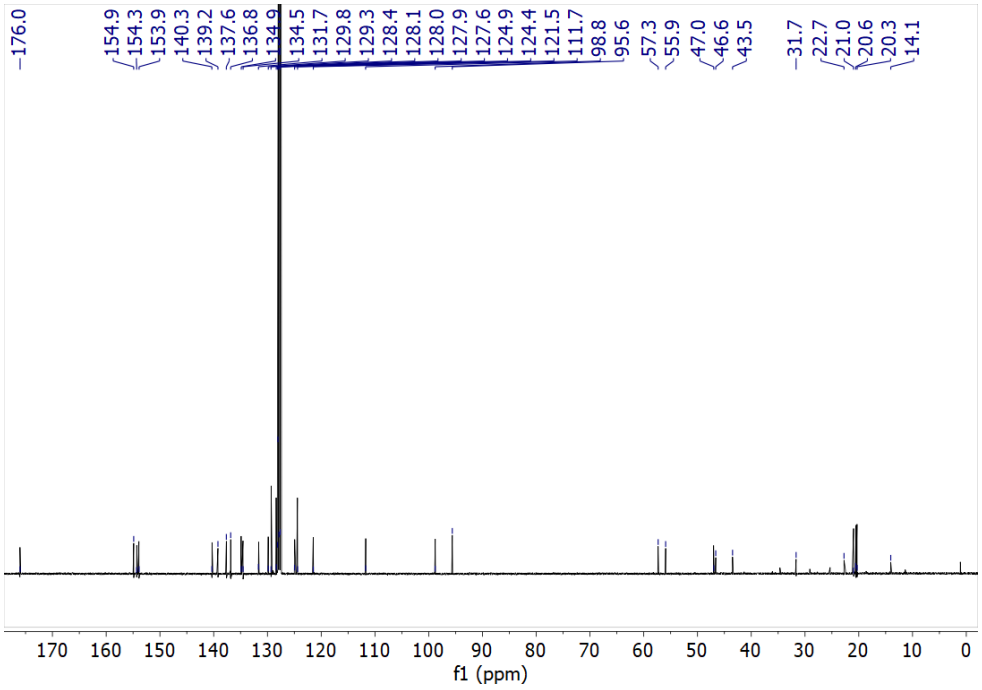


Figure S16. ^{13}C{^{1}H} NMR spectrum of **3** in C_6D_6.

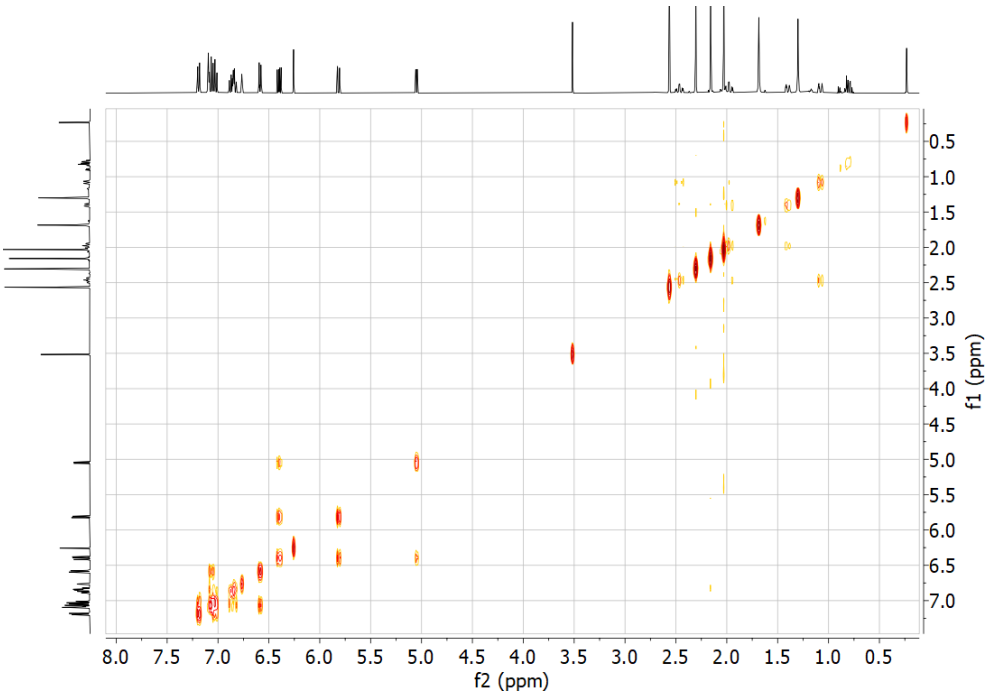


Figure S17. ^{1}H-^{1}H COSY NMR spectrum of **3** in C_6D_6.

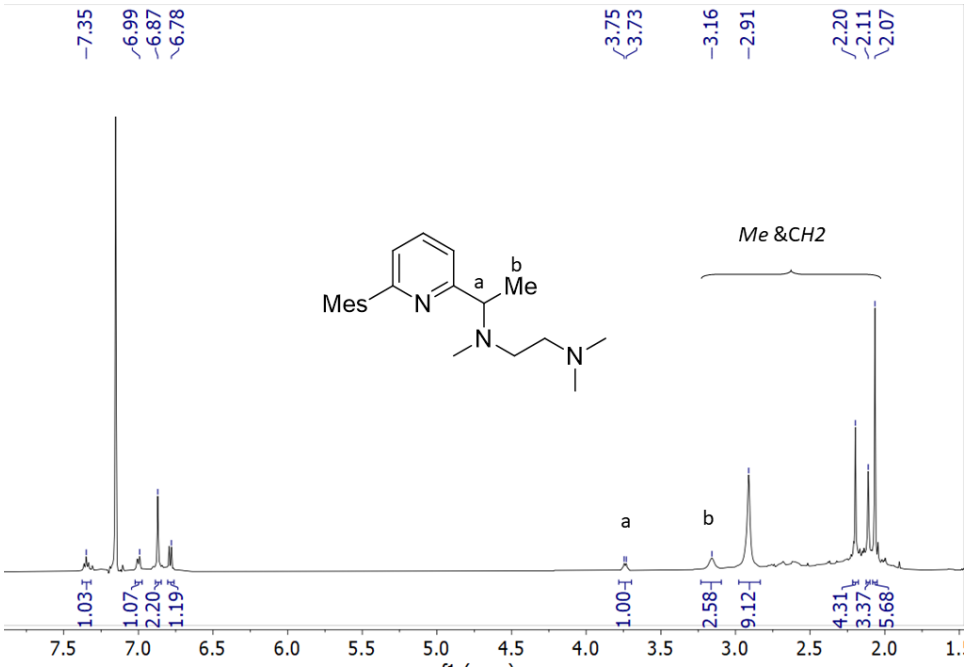


Figure S18. ^{1}H NMR spectrum of (**^{Mes}L^{Me}**)***H*** in C_6D_6.

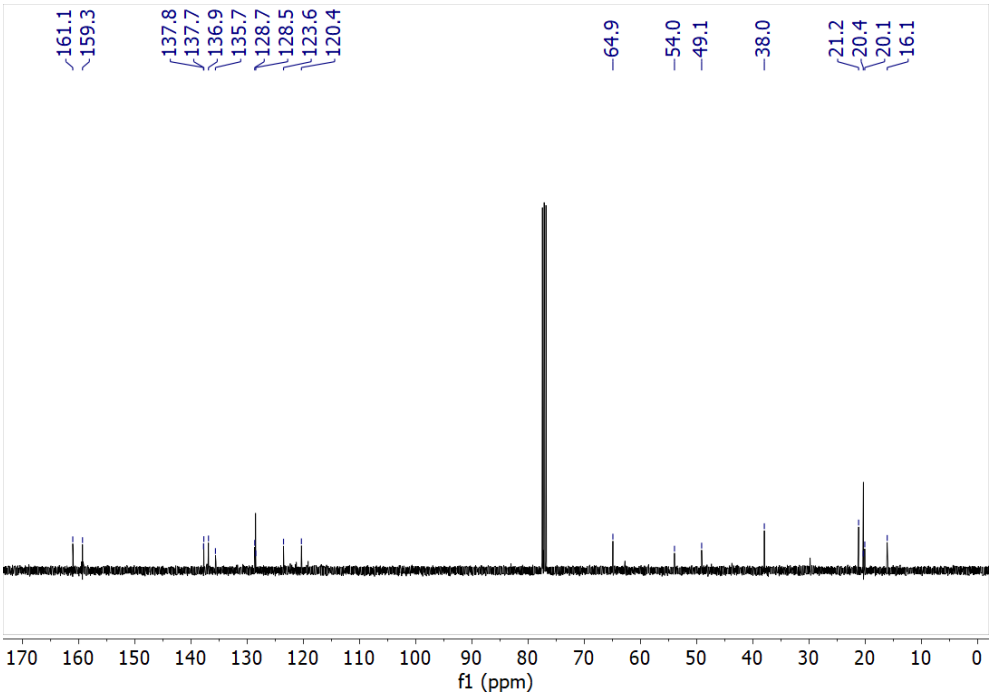
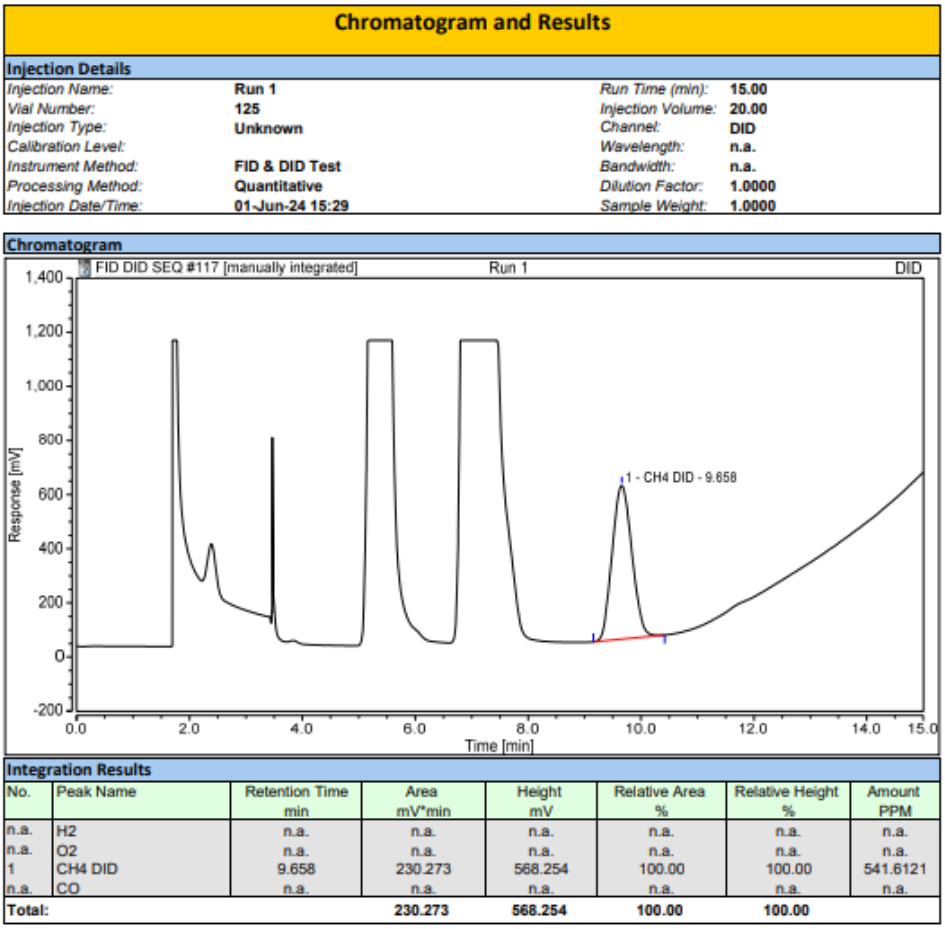


Figure S19. $^{13}C\{^{1}H\}$ NMR spectrum of **($^{Mes}L^{Me}$)*H*** in $CDCl_3$.



Chromatogram and Results

Injection Details

Injection Name:	**Run 1**	*Run Time (min):*	**15.00**
Vial Number:	**125**	*Injection Volume:*	**20.00**
Injection Type:	**Unknown**	*Channel:*	**DID**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**FID & DID Test**	*Bandwidth:*	**n.a.**
Processing Method:	**Quantitative**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**01-Jun-24 15:29**	*Sample Weight:*	**1.0000**

Chromatogram

Integration Results

No.	Peak Name	Retention Time min	Area mV*min	Height mV	Relative Area %	Relative Height %	Amount PPM
n.a.	H2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	O2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1	CH4 DID	9.658	230.273	568.254	100.00	100.00	541.6121
n.a.	CO	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Total:			**230.273**	**568.254**	**100.00**	**100.00**	

Figure S20. GC-TCD data of CH_4 gas detection.

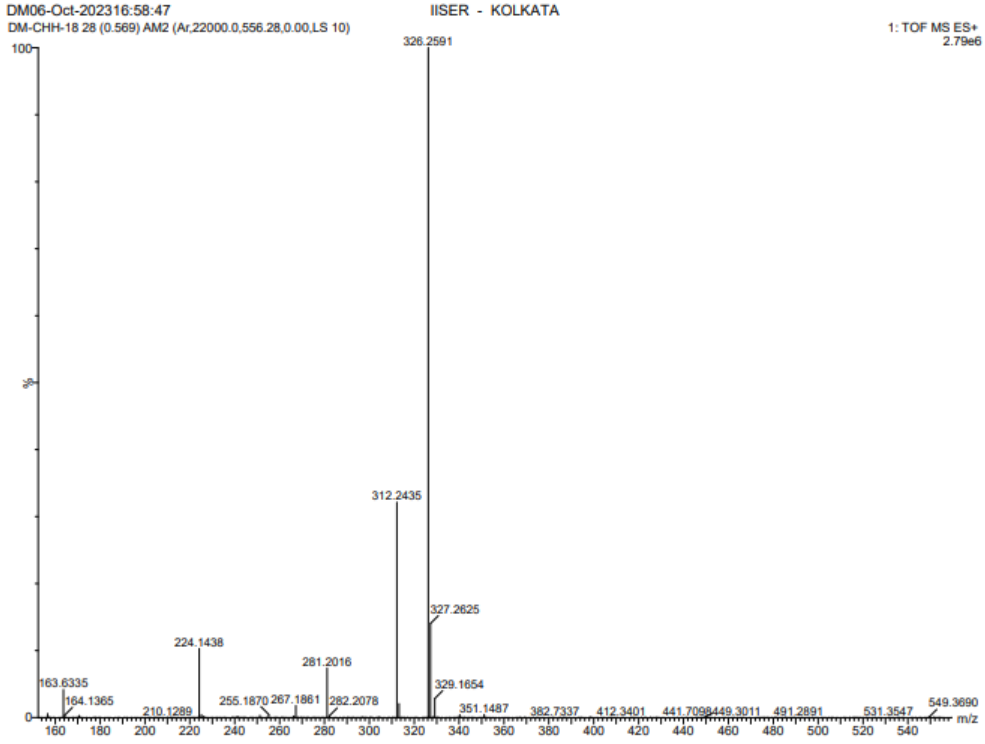


Figure S21. HRMS data of **($^{Mes}L^{Me}$)*H***.

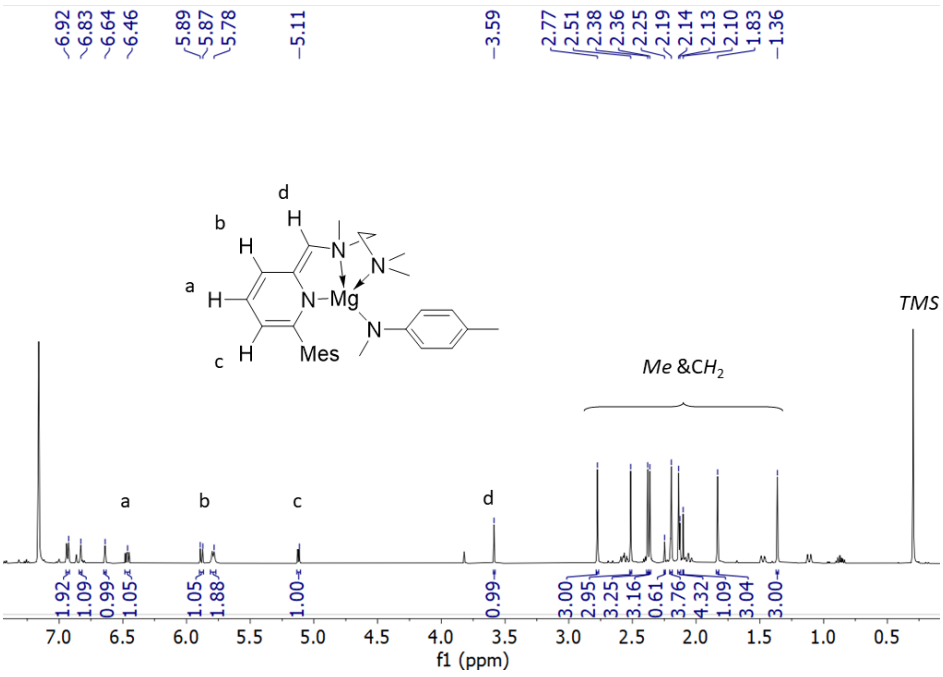


Figure S22. ^{1}H NMR spectrum of **4** in C_6D_6.

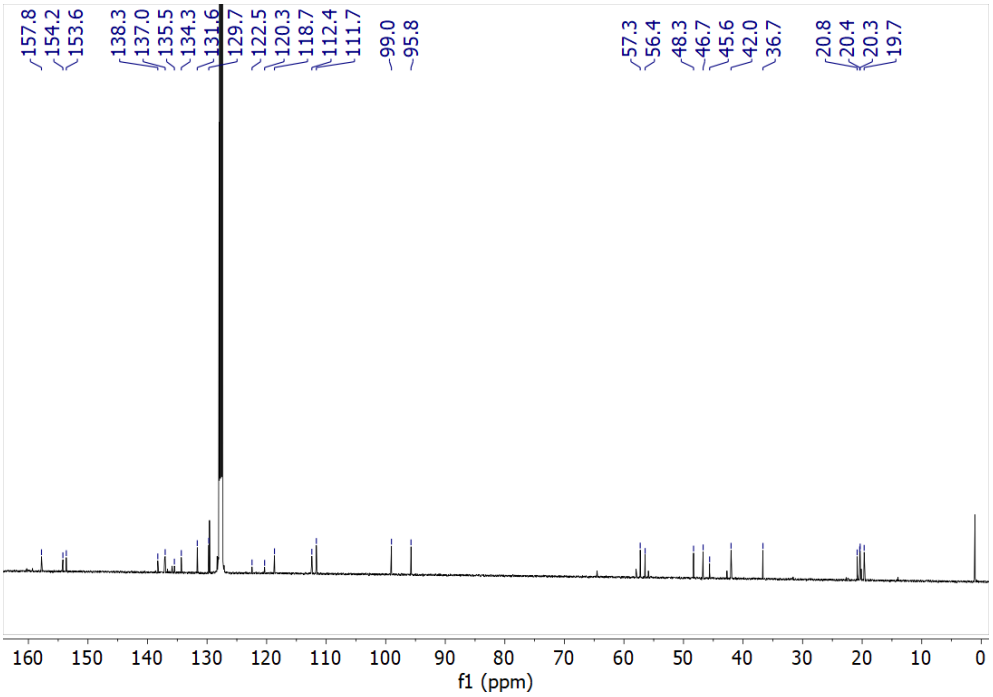


Figure S23. $^{13}C\{^{1}H\}$ NMR spectrum of **4** in C_6D_6.

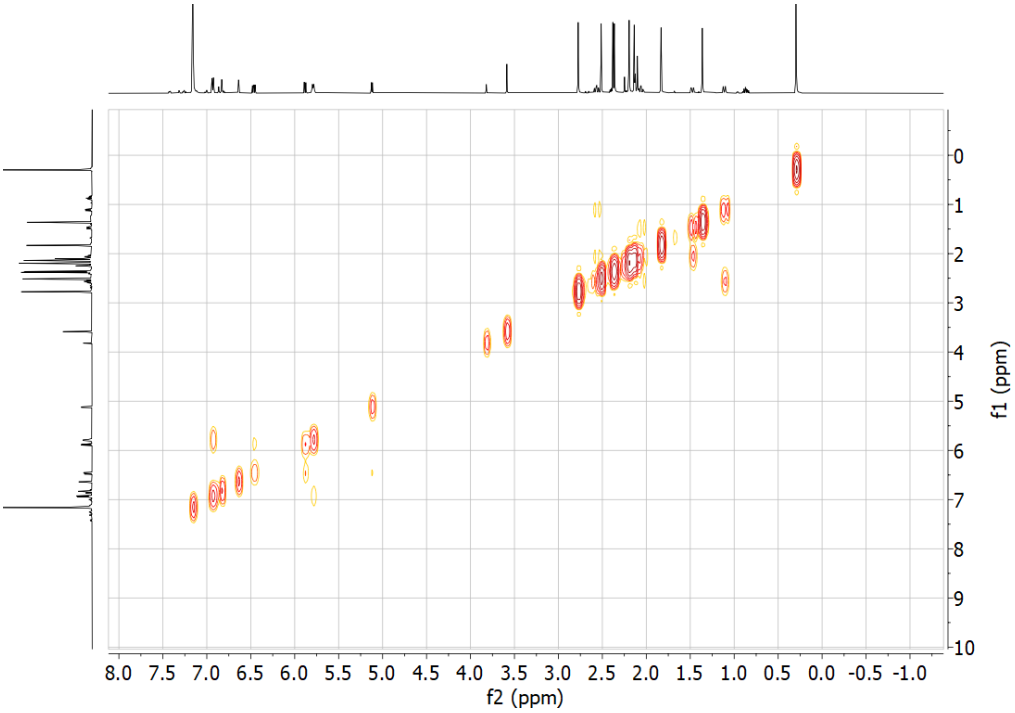


Figure S24. ^{1}H-^{1}H COSY NMR spectrum of **4** in C_6D_6.

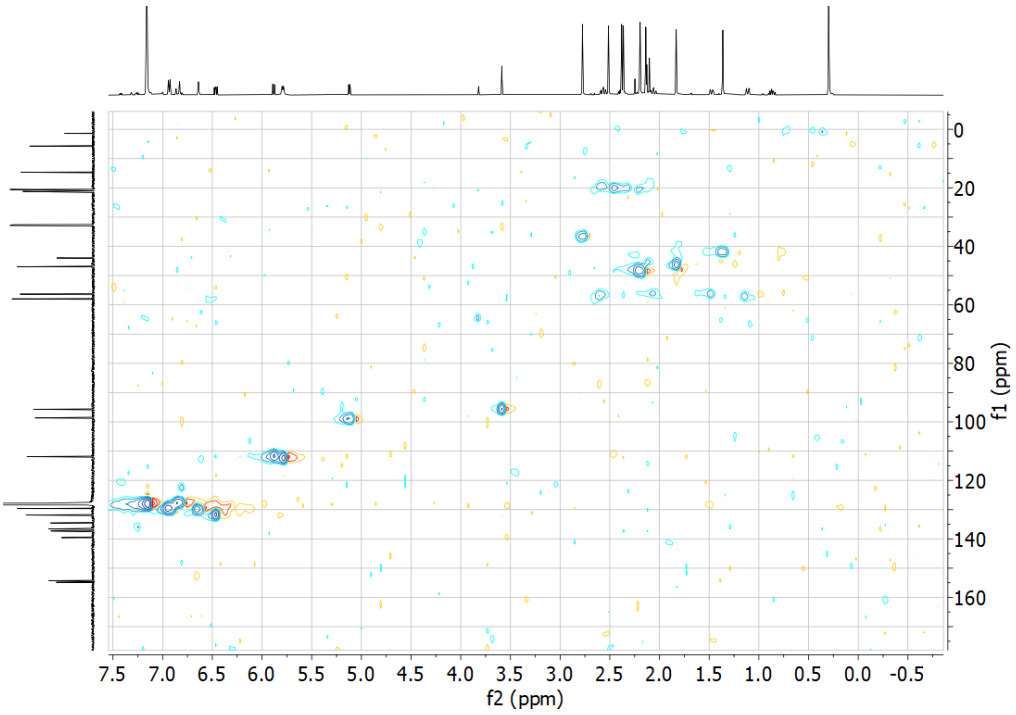


Figure S25. ^{1}H-^{13}C HSQC NMR spectrum of **4** in C_6D_6.

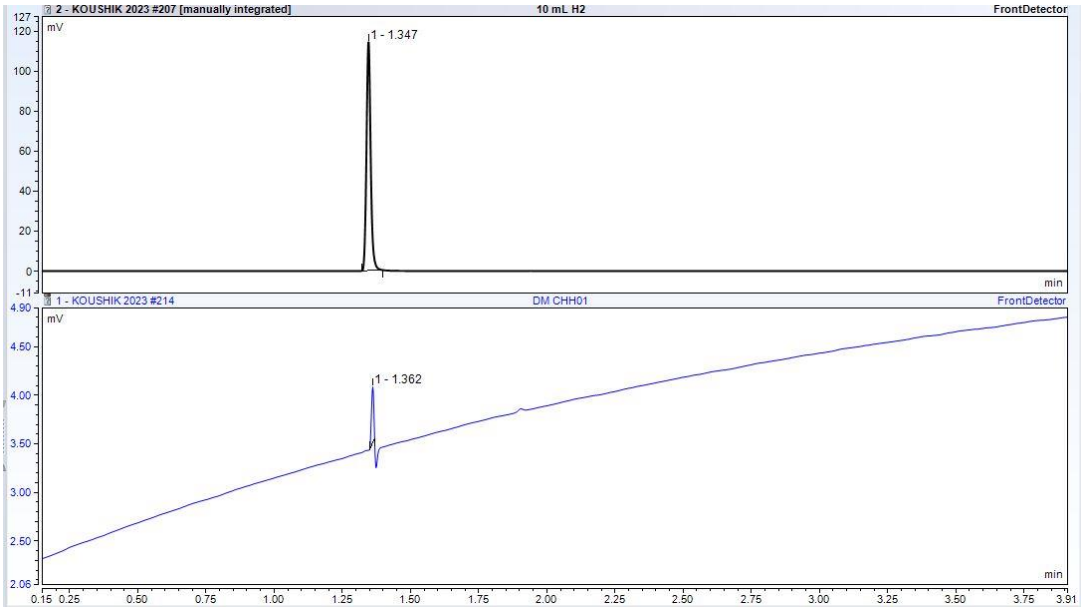


Figure S26. GC-TCD data of H_2 gas detection.

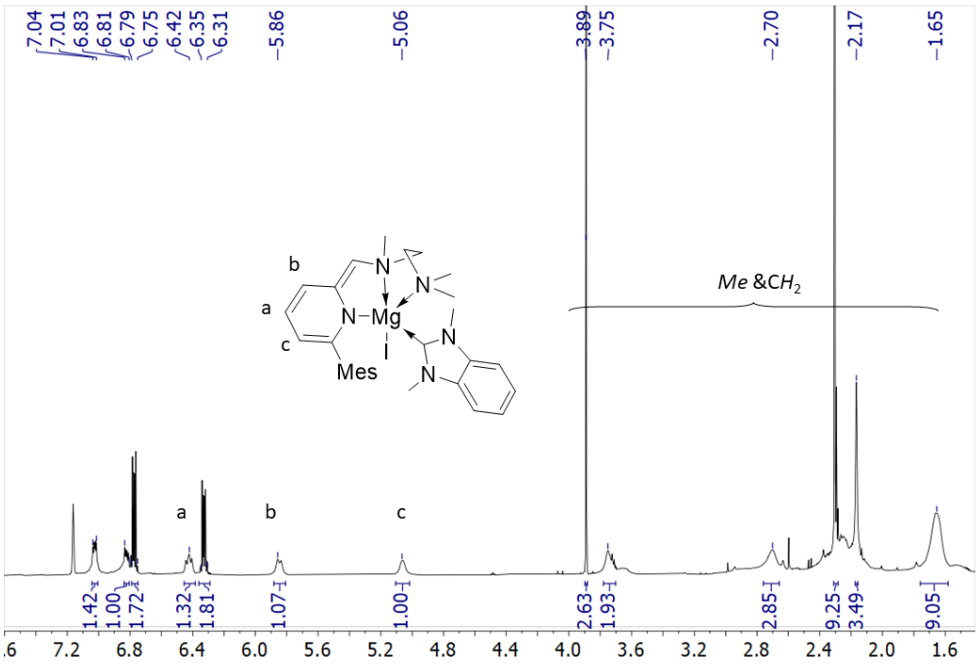


Figure S27. ^{1}H NMR spectrum of **5** in C_6D_6.

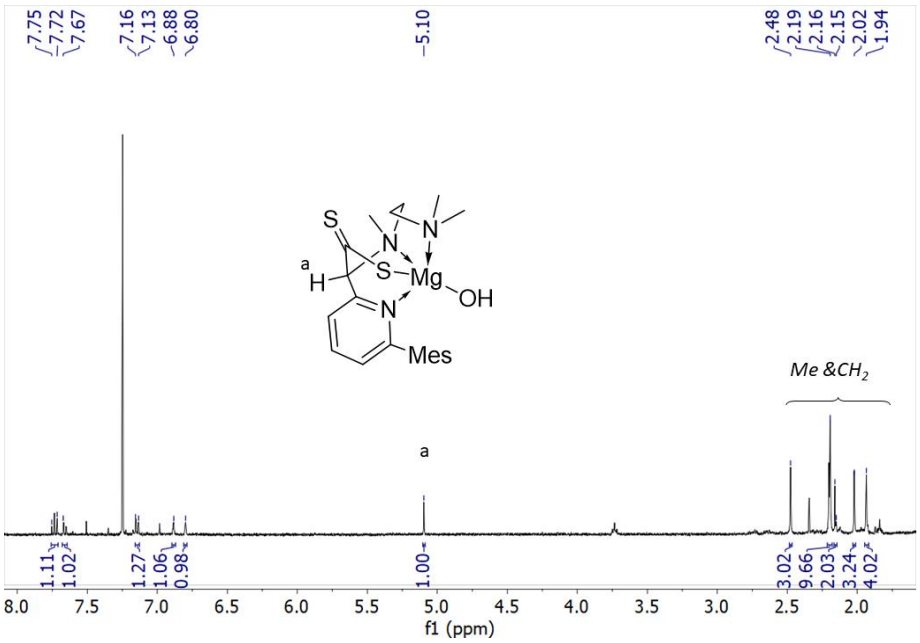


Figure S28. ^{1}H NMR spectrum of **6$_2$** in $CDCl_3$. The monomeric form is shown in the picture for peak assignment.

3. Crystallographic Data.

X-ray diffraction data were collected on a Rigaku XtaLAB Synergy, Dualflex four-circle diffractometer with HyPix3000 detector and Cu-K$_\alpha$ radiation for all. Measurements were

carried out at 100 K for all the compounds. The structures were solved by intrinsic phasing using SHELXT.[1] all refinements were carried out against F^2 with ShelXL[2] as implemented in the program system Olex2.[3] The non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were included in calculated positions and treated as riding throughout the refinement. Potential solvent accessible area or void space was calculated using PLATON[4] executable in Olex2. Graphical representations were performed with the program DIAMOND.[5] The crystallographic data can be obtained free of charge from the Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif using the CCDC numbers (given in the tables S1 and S2) as reference.

Table S1: Crystallographic data of 1, 2, and 3.

	1	**2_2**	**4**
formula	$C_{24}H_{37}MgN_3$	$C_{40}H_{58}Mg_2N_6$	$C_{31.5}H_{42}MgN_4$
Fw /g·mol^{-1}	391.87	671.557	501.017
cryst. color, habit	Red	Red	Red
crystal size / mm^3	0.164 × 0.142× 0.124	0.24 × 0.22 × 0.14	0.4 × 0.32 × 0.18
crystal system	monoclinic	orthorhombic	monoclinic
space group	$P2_1/n$	Pbca	$P2_1/c$
a / Å	12.2110(3)	14.1364(2)	14.6445(2)
b / Å	11.1972(3)	15.1179(2)	11.4598(1)
c / Å	17.5444(5)	18.5001(2)	18.6091(2)
α / °	90	90	90
β / °	103.866(3)	90	111.524((1)
γ / °	90	90	90
V / Å^3	2328.92(11)	3953.71(9)	2905.25(6)
Z	4	4	4
d_{calc}/Mg·m^{-3}	1.118	1.128	1.145
μ/mm^{-1}	0.740 (CuKα)	0.798 (CuKα)	0.711(CuKα)
F (000)	856.0	1461.3	1087.7
2θ range / °	8.0 to 136.742	9.56 to 136.48	6.48 to 136.3

index ranges	$-14 \le h \le 14, -13 \le k \le 13, -17 \le l \le 21$	$-16 \le h \le 17, -17 \le k \le 18, -22 \le l \le 22$	$-17 \le h \le 17, -13 \le k \le 13, -20 \le l \le 22$
Reflections collected	23984	47379	32463
independ.reflns (R_{int})	4230 [R_{int} = 0.0735, R_{sigma} = 0.0351]	3601 [R_{int} = 0.0340, R_{sigma} = 0.0167]	5281 [R_{int} = 0.0494, R_{sigma} = 0.0253]
observed reflns	12024	21729	20415
data/ restr./ param.	4230/0/260	3601/0/331	5281/303/456
$R1$, $wR2$ [$I > 2\sigma(I)$]	R_1 = 0.0675, wR_2 = 0.1857	R_1 = 0.0341, wR_2 = 0.0832	R_1 = 0.0442, wR_2 = 0.1187
$R1$, $wR2$ (all data)	R_1 = 0.0739, wR_2 = 0.1952	R_1 = 0.0383, wR_2 = 0.0834	R_1 = 0.0492, wR_2 = 0.1224
GooF-of-fit on F^2	1.037	1.080	1.044
largest diff. peak, hole/ e·Å^3	0.74/-0.43	0.28/-0.17	0.41/-0.30
CCDC number	2313143	2313144	2313152

Table S2: Crystallographic data of 5 and 6.

	5	**6$_2$**
formula	$C_{33}H_{46}IMgN_5O$	$C_{58.06}H_{77.94}Mg_2N_6O_{2.97}S_4$
Fw /g·mol^{-1}	679.976	1084.359
cryst. color, habit	Red	Clear Colourless
crystal size / mm^3	0.168 × 0.148× 0.128	0.146 × 0.126 × 0.118
crystal system	monoclinic	triclinic
space group	$P2_1/n$	*P-1*
a / Å	11.2666(2)	8.9855(2)
b / Å	21.1640(3)	13.0705(2)
c / Å	15.6557(2)	13.5358(2)
α / °	90	111.931(2)
β / °	106.939(2)	91.736(1)
γ / °	90	100.183(2)
V / Å^3	3571.09(10)	1443.34(5)
Z	4	1
d_{calc}/Mg·m^{-3}	1.265	1.248
μ/mm^{-1}	7.447 (CuKα)	2.100 (CuKα)

$F(000)$	1413.2	583.3
2θ range / °	7.24 to 136.66	11.24 to 136.432
index ranges	$-10 \leq h \leq 13, -25 \leq k \leq 25, -18 \leq l \leq 18$	$-10 \leq h \leq 9, -15 \leq k \leq 15, -16 \leq l \leq 16$
Reflections collected	42246	28990
independ.reflns (R_{int})	6464 [R_{int} = 0.0465, R_{sigma} = 0.0219]	5241 [R_{int} = 0.0439, R_{sigma} = 0.0273]
observed reflns	22983	17100
data/ restr./ param.	6464/0/333	5241/153/417
$R1$, $wR2$ [$I > 2\sigma(I)$]	R_1 = 0.0522, wR_2 = 0.1437	R_1 = 0.0448, wR_2 = 0.1216
$R1$, $wR2$ (all data)	R_1 = 0.0582, wR_2 = 0.1545	R_1 = 0.0487, wR_2 = 0.1250
GooF-of-fit on F^2	1.037	1.070
largest diff. peak, hole/ e·Å^3	2.04/-0.47	0.56/-0.38
CCDC number	2313153	2313150

Table S3: Crystallographic data of 3.

	3
formula	$C_{136}H_{156}Mg_4N_{12}$
Fw /g·mol^{-1}	2062.23
cryst. color, habit	reddish
crystal size / mm^3	0.0148 × 0.0136 × 0.0125
crystal system	orthorhombic
space group	$Pca2_1$
a / Å	30.5242(3)
b / Å	9.16760(10)
c / Å	21.0090(2)
α / °	90
β / °	90
γ / °	90
V / Å^3	5879.03(10)
Z	2

d_{calc}/Mg·m^{-3}	1.165
μ/mm^{-1}	0.711(CuKα)
F(000)	2214..0
2θ range / °	5.79 to 136.692
index ranges	*-36 ≤ h ≤ 36, -11 ≤ k ≤ 9, -25 ≤ l ≤ 25*
Reflections collected	69482
independ.reflns (R_{int})	10290 [R_{int} = 0.0618, R_{sigma} = 0.0395]
observed reflns	10774
data/ restr./ param.	10290/19/699
*R*1, *wR*2 [*I*> 2σ(*I*)]	R_1 = 0.2354, wR_2 = 0.4646
*R*1, *wR*2 (all data)	R_1 = 0.2390, wR_2 = 0.4708
GooF-of-fit on F^2	1.060
largest diff. peak, hole/ e·Å^3	6.75/-0.76
Flack parameter	0.53(3)

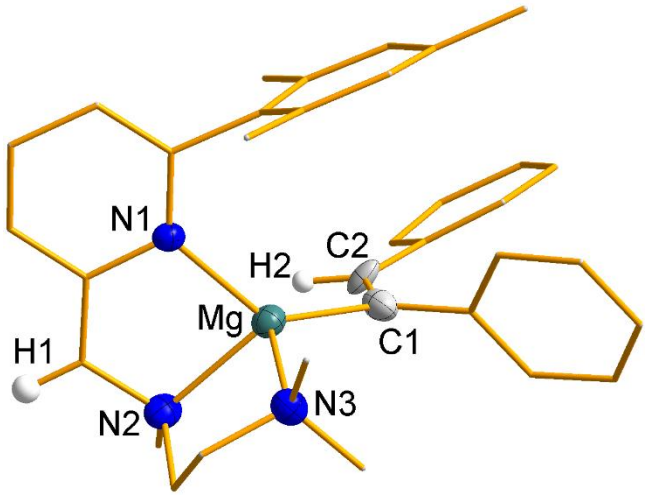


Figure S29. DIAMOND-rendered molecular structures of **3**. Relevant ellipsoids are set at 50% probability level while the rest of the skeleton is shown in sticks for clarity. H atoms except the dearomatized picolyl C-*H* and the alkenyl C-*H* are omitted for clarity. Unfortunately, the data collection could not be completed due to an icing issue at the time of data acquisition. But the structure and bond connectivity are confirmed from the existing data set as depicted above. We, however, refrain from reporting this to CCDC.

4. DFT analyses.

Density Functional Theory (DFT) calculations were performed using M06-2X functional[6] as implemented in the Gaussian 16 package[7] The structures were optimized in the gas phase using the 6-31+G**[8] basis set (B1) for all the atoms. This method is referred to as the M06-2X/B1 level of theory. Frequency calculations were done to characterize the stationary points as minima. Energy values were refined by single-point calculations using the def2-TZVPP[9] basis set (B2). The Fukui functions were calculated at M06-2X/B2//M06-2X/B1 level using the Multiwfn program.[10]

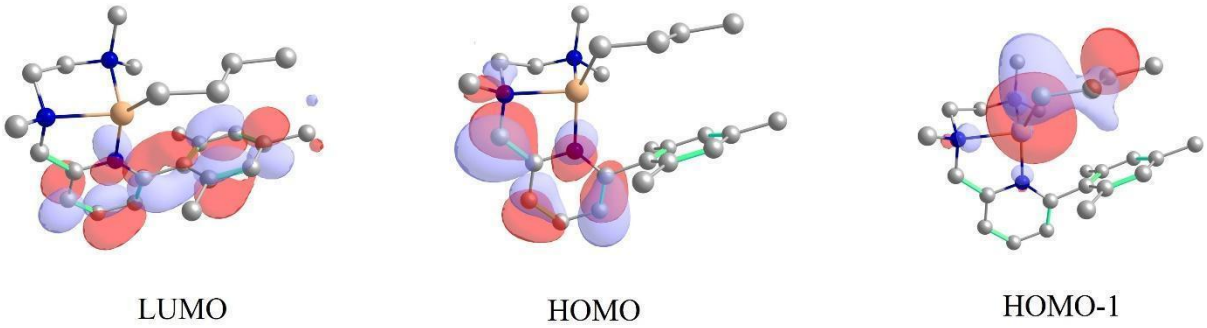


Figure S30. MOs of **1**.

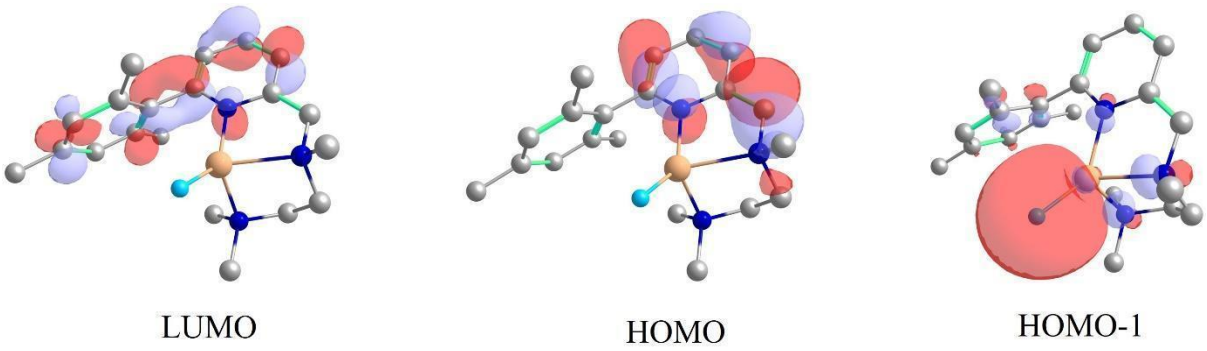


Figure S31. MOs of **2**.

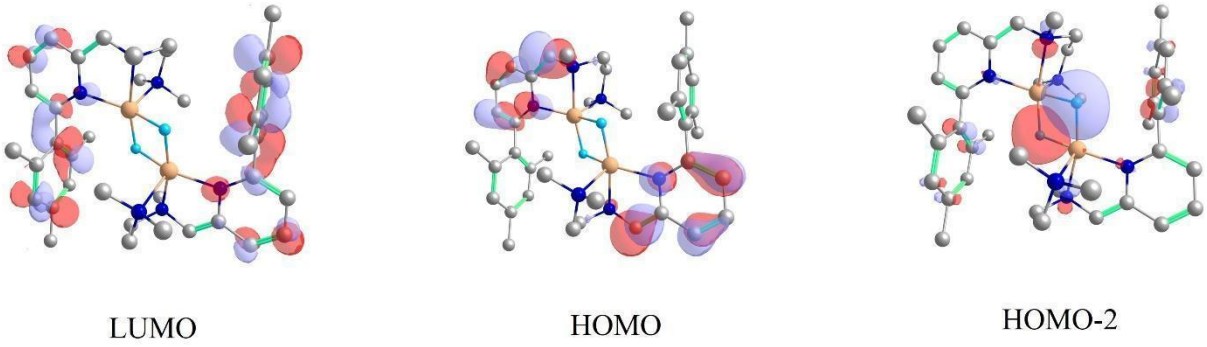


Figure S32. MOs of **2**$_2$.

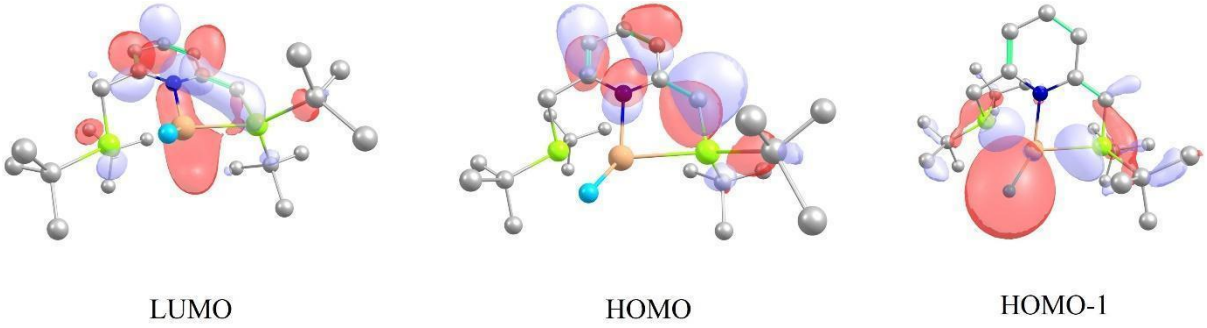


Figure S33. MOs of (PNP)MgH.

Table S4. Relative energies of the frontier Molecular Orbitals (FMOs) in eV

FMO	**1**	**2**	**2**$_2$	**(PNP)MgH**
LUMO	0.2061	0.2066	0.2058	0.2066
HOMO	0	0	0	0
HOMO-1	-0.0548	-0.0798	-0.0003	-0.0570
HOMO-2	-0.0924	-0.0903	-0.0768	-0.0863

The Fukui function analysis

Theoretical Background:

The Fukui functions are descriptors that help us to assign reactive sites in a molecule as either electrophilic or nucleophilic. It is expressed mathematically as follows

$f(r) = [\partial\rho(r)/\partial N]_v$

which simply means the change of electron density ρ(*r*) induced by the change of absolute electron number (N) with a fixed geometry and potential *v*.

For Nucleophilic attack it is defined as: $f^{+}(r) = \rho_{N+1}(r) - \rho_{N}(r)$

For Electrophilic attack it is defined as: $f^{-}(r) = \rho_{N}(r) - \rho_{N-1}(r)$

The dual descriptor is a much more accurate descriptor than the Fukui function in predicting the reactive sites of a molecule. It is also less affected by orbital contraction or dilatation than the Fukui function and seems more reasonable. With a finite difference approximation, $f^{(2)}(r)$ can be described as

$f^{(2)}(r) = \mathrm{D}\, f(r) = f^{+}(r) - f^{-}(r)$

$f^{(2)}(\mathrm{r}) > 0$, the reactive site for the nucleophilic attack.

$f^{(2)}(\mathrm{r}) < 0$, the reactive site for the electrophilic attack.

Analysis

A positive value of f^{+} and f^{-} indicates that a site is reactive towards nucleophiles and electrophiles respectively (Whereas negative values have no meaning as such). Condensed Dual Descriptor (CDD) is defined as ($f^{+} - f^{-}$). CDD is positive if the site is electrophilic and is negative if the site is nucleophilic.

Table S5. The condensed Fukui functions and dual descriptor (both in 10^{-3} a.u.) based on Hirshfeld charges

Atom	$f^{+}(r)$	$f^{-}(r)$	$f^{(2)}(\mathrm{r})$
1			
Mg	14.9	3.2	11.8
N2	-0.1	5.5	-5.6
N3 (pyridyl)	27.2	67.5	-40.4
N4	-4.1	-4.3	0.2
C6 (picolyl)	32.8	162.8	-130.0

C33 (butyl)	4.8	4.0	0.8
2			
Mg	28.4	12.2	16.2
N2(pyridyl)	29.4	66.8	-37.4
N3	0.3	5.3	-4.9
N4	-4.3	-4.7	0.3
C15 (picolyl)	35.2	163.7	-128.5
H53 (hydride)	17.6	21.6	-4.0
(PNP)MgH			
Mg	98.1	12.9	85.2
P1 (coordinated)	34.2	26.3	8.0
P2 (non-coordinated)	17.8	4.5	13.3
N4 (pyridyl)	31.6	55.0	-23.4
C5 (picolyl)	20.3	158.5	-138.1
H70 (hydride)	22.6	19.8	2.8
2_2			
Mg1/Mg54	28.6	7.6	21.0
N2/N55 (pyridyl)	3.0	32.3	-29.3
N3/N56	-1.3	2.0	-3.4
N4/N57	-2.1	-3.4	1.2
C15/C68 (picolyl)	8.7	74.3	-65.6
H53/H106 (hydride)	6.4	0.9	5.5

Cartesian coordinates of the optimized structures

1 (optimized geometry in gas phase)

E@B2 = -1301.126074 a.u.

12 -0.956865000 -0.901919000 -0.418439000

7 -3.133284000 -0.834482000 -0.610557000

7 -1.156221000 1.151498000 -0.341645000

7 -1.407723000 -1.405327000 1.681882000

6	-2.488924000	1.530206000	-0.499060000
6	-3.466467000	0.574704000	-0.620719000
1	-4.514923000	0.837788000	-0.745891000
6	1.901312000	1.665960000	1.122877000
6	1.843581000	1.027374000	-1.230508000
6	-3.637592000	-1.514232000	0.601991000
1	-3.547387000	-2.597671000	0.456697000
1	-4.703194000	-1.287513000	0.756138000
6	-0.188523000	2.096830000	-0.226908000
6	1.207977000	1.575229000	-0.098635000
6	3.165362000	0.588954000	-1.120360000
1	3.661448000	0.190256000	-2.003725000
6	-1.796829000	3.864569000	-0.394681000
1	-2.033363000	4.925059000	-0.415721000
6	3.866844000	0.659264000	0.082955000
6	-0.439508000	3.446834000	-0.244594000
1	0.373326000	4.157043000	-0.153423000
6	-2.792482000	2.948315000	-0.517912000
1	-3.827802000	3.251223000	-0.638761000

6	-2.839954000	-1.062206000	1.817414000
1	-2.918172000	0.027991000	1.884319000
1	-3.252923000	-1.498296000	2.740518000
6	-3.616547000	-1.515106000	-1.822749000
1	-3.201100000	-1.011242000	-2.697238000
1	-4.714257000	-1.480282000	-1.885184000
1	-3.287625000	-2.559747000	-1.823484000
6	3.211953000	1.188044000	1.195378000
1	3.745717000	1.259527000	2.142467000
6	-0.046101000	-2.477558000	-1.520429000
1	-0.476851000	-3.410851000	-1.112748000
1	-0.414767000	-2.436117000	-2.557889000
6	-0.597206000	-0.586423000	2.592974000
1	0.464125000	-0.805352000	2.435676000
1	-0.853037000	-0.786863000	3.644805000
1	-0.770687000	0.467897000	2.370718000
6	1.300623000	2.312239000	2.350648000
1	1.731207000	3.307992000	2.502977000
1	1.520423000	1.720513000	3.245471000

1	0.221154000	2.442568000	2.264802000
6	1.141022000	0.948364000	-2.565492000
1	0.528511000	0.041414000	-2.641496000
1	1.872597000	0.915692000	-3.376856000
1	0.481992000	1.807013000	-2.719187000
6	1.480803000	-2.619807000	-1.533048000
1	1.804020000	-3.548148000	-2.033336000
1	1.932556000	-1.800749000	-2.112314000
6	5.304223000	0.213580000	0.183553000
1	5.664310000	-0.180705000	-0.769851000
1	5.422588000	-0.570013000	0.938427000
1	5.950255000	1.049633000	0.469639000
6	-1.171019000	-2.829201000	1.955170000
1	-1.718710000	-3.452743000	1.245890000
1	-1.481796000	-3.086939000	2.979271000
1	-0.107531000	-3.044842000	1.836115000
6	2.103559000	-2.601788000	-0.137248000
1	1.905679000	-1.623168000	0.331831000
1	1.606497000	-3.361053000	0.483605000

6	3.606764000	-2.868667000	-0.146798000
1	3.820263000	-3.875904000	-0.520216000
1	4.045362000	-2.778389000	0.852395000
1	4.117845000	-2.156692000	-0.803846000

2 (optimized geometry in gas phase)

E@B2 = -1143.883100 a.u.

12	0.884552000	-0.838368000	0.932186000
7	0.639262000	1.029201000	0.103540000
7	3.004604000	-0.313053000	0.813312000
7	1.323160000	-2.032347000	-0.851383000
6	-2.466654000	0.311413000	-1.072777000
6	1.862326000	1.672948000	-0.067356000
6	-1.747216000	0.836957000	0.014269000
6	-0.520639000	1.661434000	-0.213678000
6	-3.555472000	-0.530109000	-0.821543000
1	-4.105779000	-0.943610000	-1.665188000
6	-3.956858000	-0.846229000	0.474797000
6	-2.153393000	0.552205000	1.334273000
6	-3.250019000	-0.284275000	1.539512000

1	-3.559939000	-0.502589000	2.560027000
6	3.028615000	1.023128000	0.251401000
1	4.001468000	1.497084000	0.138760000
6	1.844414000	3.024395000	-0.593707000
1	2.791323000	3.537410000	-0.729376000
6	-1.443024000	1.145203000	2.528366000
1	-0.706093000	0.441232000	2.933636000
1	-0.927241000	2.073066000	2.271378000
1	-2.161639000	1.354142000	3.325413000
6	3.580657000	-1.316936000	-0.108683000
1	4.562420000	-0.982609000	-0.475817000
1	3.735633000	-2.249655000	0.446948000
6	2.646495000	-1.539703000	-1.290401000
1	3.095342000	-2.237013000	-2.015075000
1	2.495120000	-0.575042000	-1.786203000
6	-0.575046000	2.940653000	-0.707119000
1	-1.527647000	3.400171000	-0.940831000
6	-5.124544000	-1.765145000	0.732477000
1	-5.622254000	-2.044291000	-0.199354000

1	-4.795684000	-2.683215000	1.229747000
1	-5.863477000	-1.287110000	1.382619000
6	0.663966000	3.626941000	-0.895085000
1	0.661024000	4.642812000	-1.281172000
6	-2.123904000	0.647368000	-2.506002000
1	-1.086843000	0.967919000	-2.619655000
1	-2.306804000	-0.212767000	-3.157866000
1	-2.750254000	1.471537000	-2.865162000
6	3.693080000	-0.359279000	2.114272000
1	3.229562000	0.368110000	2.782765000
1	3.600616000	-1.357735000	2.553650000
1	4.758162000	-0.107300000	2.005222000
6	0.318111000	-1.805004000	-1.898253000
1	-0.666521000	-2.116142000	-1.535428000
1	0.279962000	-0.738531000	-2.128885000
1	0.559732000	-2.369418000	-2.811929000
6	1.361776000	-3.458405000	-0.498723000
1	2.070317000	-3.632536000	0.313250000
1	0.375927000	-3.767454000	-0.144997000

1	1.648449000	-4.068454000	-1.368800000
1	0.335273000	-1.829563000	2.241558000

2_2 (optimized geometry in gas phase)

E@B2 = -2287.820692 a.u.

12	-1.312926000	0.534426000	-0.152258000
7	-2.992777000	1.090613000	0.952149000
7	-1.859801000	2.296560000	-1.320653000
7	-2.119250000	-0.490590000	-1.947029000
6	-2.526422000	-1.553795000	2.996514000
6	-3.777131000	1.920972000	0.141911000
6	-2.622530000	-0.156485000	3.030679000
6	-3.528138000	0.595477000	2.101266000
6	-1.743969000	-2.207825000	3.955764000
1	-1.671124000	-3.294106000	3.922596000
6	-1.048300000	-1.507695000	4.937567000
6	-1.927952000	0.571259000	4.017248000
6	-1.148781000	-0.113257000	4.949394000
1	-0.608114000	0.454309000	5.705935000
6	-3.244075000	2.504715000	-0.979249000

1	-3.831068000	3.178604000	-1.602021000
6	-5.164691000	2.135187000	0.509345000
1	-5.776291000	2.751442000	-0.142592000
6	-2.017519000	2.076999000	4.060203000
1	-1.787836000	2.512084000	3.081279000
1	-1.325423000	2.487168000	4.800048000
1	-3.031740000	2.400416000	4.314857000
6	-1.656544000	1.822158000	-2.701049000
1	-0.583390000	1.639527000	-2.836561000
1	-1.962820000	2.591354000	-3.431024000
6	-2.453308000	0.551361000	-2.946367000
1	-3.517349000	0.779992000	-2.849742000
1	-2.267486000	0.177733000	-3.964641000
6	-4.830468000	0.798080000	2.489542000
1	-5.189406000	0.381507000	3.422969000
6	-0.190748000	-2.222022000	5.951900000
1	-0.167698000	-3.298018000	5.762220000
1	-0.566604000	-2.064463000	6.967824000
1	0.840086000	-1.851648000	5.924230000

6	-5.669261000	1.581521000	1.640601000
1	-6.709188000	1.745432000	1.910395000
6	-3.203922000	-2.368220000	1.926021000
1	-4.036394000	-1.826148000	1.471300000
1	-3.578285000	-3.313330000	2.329205000
1	-2.475388000	-2.600644000	1.139402000
6	-1.034907000	3.487832000	-1.078057000
1	-1.127523000	3.774501000	-0.027348000
1	-1.368974000	4.329908000	-1.702357000
1	0.012591000	3.257623000	-1.303398000
6	-3.305143000	-1.296131000	-1.627784000
1	-3.025027000	-2.081990000	-0.923459000
1	-3.723639000	-1.762693000	-2.532657000
1	-4.061951000	-0.658107000	-1.161467000
6	-1.035602000	-1.351525000	-2.439326000
1	-0.154280000	-0.740783000	-2.653272000
1	-1.331458000	-1.876529000	-3.361433000
1	-0.781068000	-2.088150000	-1.671551000
1	-0.520161000	-0.994686000	0.587957000

12	1.312926000	-0.534426000	0.152258000
7	2.992777000	-1.090613000	-0.952149000
7	1.859801000	-2.296560000	1.320653000
7	2.119250000	0.490590000	1.947029000
6	2.526422000	1.553795000	-2.996514000
6	3.777131000	-1.920972000	-0.141911000
6	2.622530000	0.156485000	-3.030679000
6	3.528138000	-0.595477000	-2.101266000
6	1.743969000	2.207825000	-3.955764000
1	1.671124000	3.294106000	-3.922596000
6	1.048300000	1.507695000	-4.937567000
6	1.927952000	-0.571259000	-4.017248000
6	1.148781000	0.113257000	-4.949394000
1	0.608114000	-0.454309000	-5.705935000
6	3.244075000	-2.504715000	0.979249000
1	3.831068000	-3.178604000	1.602021000
6	5.164691000	-2.135187000	-0.509345000
1	5.776291000	-2.751442000	0.142592000
6	2.017519000	-2.076999000	-4.060203000

1	1.787836000	-2.512084000	-3.081279000
1	1.325423000	-2.487168000	-4.800048000
1	3.031740000	-2.400416000	-4.314857000
6	1.656544000	-1.822158000	2.701049000
1	0.583390000	-1.639527000	2.836561000
1	1.962820000	-2.591354000	3.431024000
6	2.453308000	-0.551361000	2.946367000
1	3.517349000	-0.779992000	2.849742000
1	2.267486000	-0.177733000	3.964641000
6	4.830468000	-0.798080000	-2.489542000
1	5.189406000	-0.381507000	-3.422969000
6	0.190748000	2.222022000	-5.951900000
1	0.167698000	3.298018000	-5.762220000
1	0.566604000	2.064463000	-6.967824000
1	-0.840086000	1.851648000	-5.924230000
6	5.669261000	-1.581521000	-1.640601000
1	6.709188000	-1.745432000	-1.910395000
6	3.203922000	2.368220000	-1.926021000
1	4.036394000	1.826148000	-1.471300000

1	3.578285000	3.313330000	-2.329205000
1	2.475388000	2.600644000	-1.139402000
6	1.034907000	-3.487832000	1.078057000
1	1.127523000	-3.774501000	0.027348000
1	1.368974000	-4.329908000	1.702357000
1	-0.012591000	-3.257623000	1.303398000
6	3.305143000	1.296131000	1.627784000
1	3.025027000	2.081990000	0.923459000
1	3.723639000	1.762693000	2.532657000
1	4.061951000	0.658107000	1.161467000
6	1.035602000	1.351525000	2.439326000
1	0.154280000	0.740783000	2.653272000
1	1.331458000	1.876529000	3.361433000
1	0.781068000	2.088150000	1.671551000
1	0.520161000	0.994686000	-0.587957000

(PNP)MgH (optimized geometry in gas phase)

E@B2 = -1839.807201 a.u.

15	-2.487094000	-0.309013000	-0.001291000
15	2.373433000	-0.498915000	-0.162347000

12	-0.169546000	-0.732528000	-1.044980000
7	0.045972000	1.328999000	-0.661742000
6	-2.208616000	1.422107000	0.238656000
1	-2.988256000	2.057799000	0.650347000
6	-1.004154000	2.035557000	-0.103523000
6	-0.799694000	3.448077000	0.125963000
1	-1.623224000	4.023081000	0.536561000
6	0.398090000	4.035850000	-0.153257000
1	0.533825000	5.098686000	0.027426000
6	1.479871000	3.260981000	-0.651960000
1	2.454721000	3.694184000	-0.841804000
6	1.246153000	1.924103000	-0.872593000
6	2.346578000	0.984780000	-1.306516000
1	3.311237000	1.499134000	-1.358433000
1	2.119804000	0.591493000	-2.305143000
6	-3.866996000	-0.431719000	-1.295605000
6	-4.989946000	0.586642000	-1.067604000
1	-5.530241000	0.418121000	-0.133008000
1	-5.713965000	0.510481000	-1.888826000

1	-4.595090000	1.606530000	-1.061394000
6	-4.447384000	-1.845714000	-1.389726000
1	-3.660337000	-2.604431000	-1.467709000
1	-5.071050000	-1.919097000	-2.289221000
1	-5.083100000	-2.084896000	-0.531926000
6	-3.171910000	-0.091881000	-2.625314000
1	-2.669544000	0.881193000	-2.570913000
1	-3.921792000	-0.037929000	-3.424200000
1	-2.434605000	-0.852090000	-2.905896000
6	-3.027661000	-1.056605000	1.649417000
6	-4.387409000	-0.543524000	2.132501000
1	-4.424494000	0.551131000	2.142621000
1	-4.569234000	-0.895093000	3.156047000
1	-5.205237000	-0.914374000	1.508143000
6	-3.040068000	-2.590369000	1.568275000
1	-3.832580000	-2.974361000	0.924292000
1	-3.201165000	-3.002322000	2.572400000
1	-2.083616000	-2.976249000	1.197973000
6	-1.947742000	-0.653517000	2.663005000

1	-0.972204000	-1.065430000	2.377769000
1	-2.205175000	-1.063272000	3.647260000
1	-1.849299000	0.432536000	2.744049000
6	2.894255000	0.210708000	1.514200000
6	1.653073000	0.868756000	2.149174000
1	1.353231000	1.784152000	1.633892000
1	1.894196000	1.132365000	3.186445000
1	0.794912000	0.191071000	2.164265000
6	4.008146000	1.262302000	1.441475000
1	4.937863000	0.869293000	1.026158000
1	4.221673000	1.620229000	2.456469000
1	3.695859000	2.129307000	0.851735000
6	3.320410000	-0.949542000	2.426210000
1	2.546752000	-1.724129000	2.480448000
1	3.475726000	-0.563109000	3.440328000
1	4.255523000	-1.415609000	2.105940000
6	3.721556000	-1.603649000	-0.895033000
6	5.161343000	-1.130689000	-0.668887000
1	5.315467000	-0.110186000	-1.034989000

1	5.839557000	-1.787373000	-1.227968000
1	5.459458000	-1.171050000	0.381832000
6	3.471088000	-1.680268000	-2.412756000
1	2.423291000	-1.893016000	-2.649806000
1	4.085387000	-2.489952000	-2.824281000
1	3.766919000	-0.756390000	-2.918797000
6	3.529660000	-3.017467000	-0.320468000
1	3.666402000	-3.055974000	0.762870000
1	4.265435000	-3.692741000	-0.773530000
1	2.531057000	-3.399332000	-0.556061000
1	0.071723000	-1.705624000	-2.458648000

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