Electronic Supplementary Material (ESI) for Dalton Transactions.

SUPPORTING INFORMATION

Bulky cationic ß-diketiminate magnesium complexes

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Contents

1. Supporting Experimental data

1.1. NMR spectra of synthesized compounds

1.1.1. Spectra of [(^{tBu}BDI)Mg·benzene]$^{+}$[B(C_6F_5)$_4$]$^{-}$

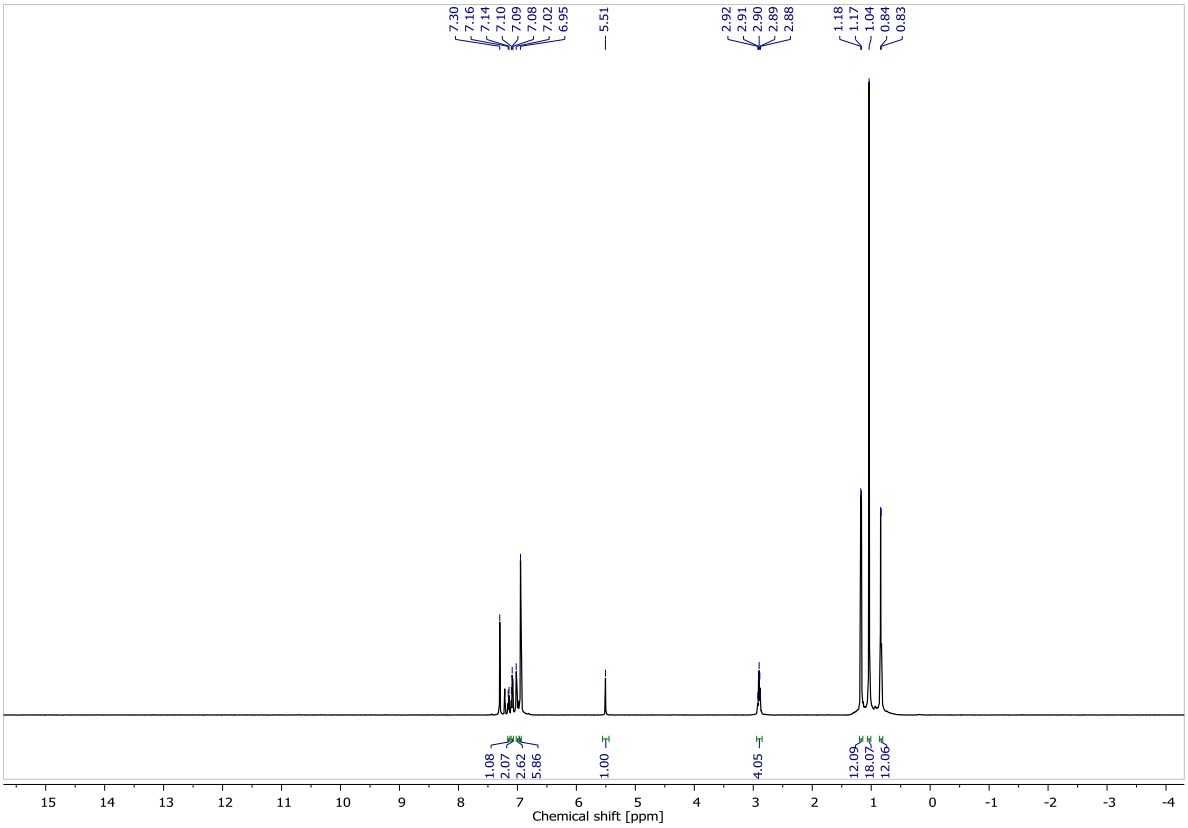

Figure S1: ^{1}H NMR spectrum of [(^{tBu}BDI)Mg·benzene]$^{+}$[B(C_6F_5)$_4$]$^{-}$ in C_6D_5Br.

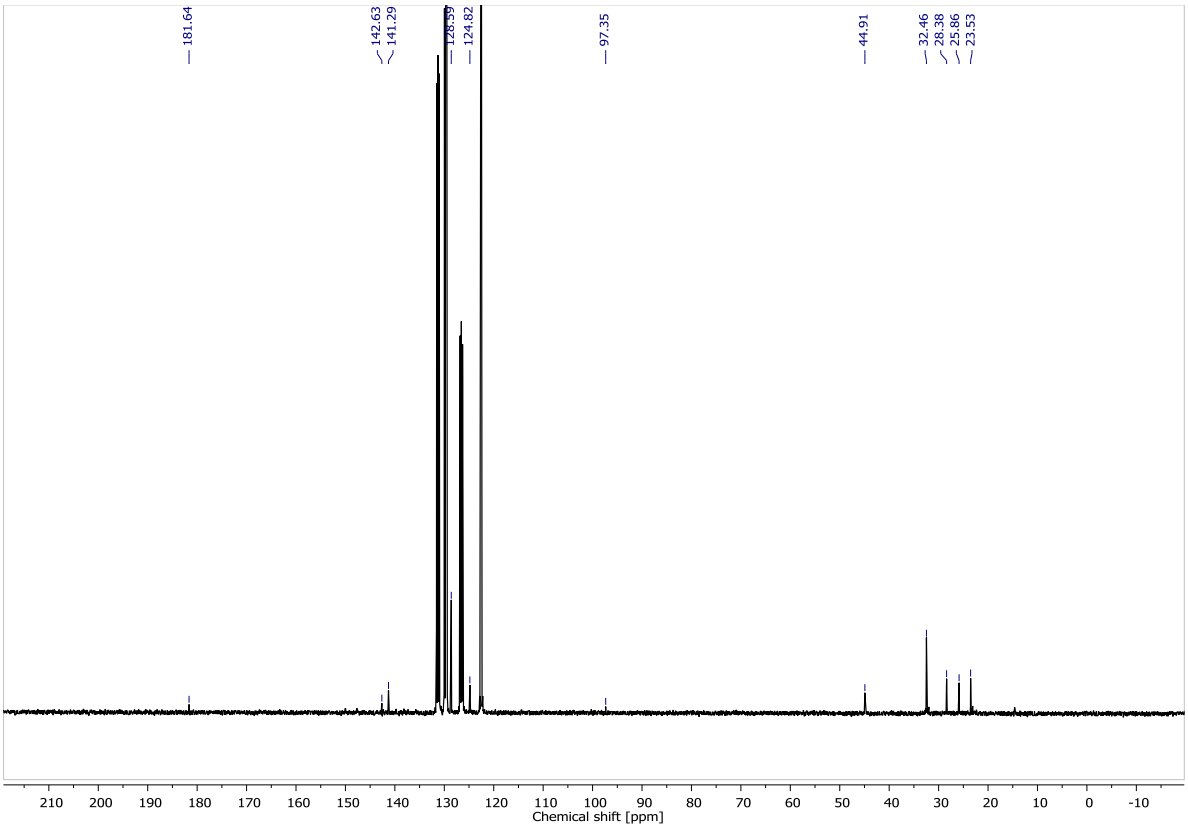

Figure S2: $^{13}C\{^{1}H\}$ NMR spectrum of $[(^{tBu}BDI)Mg{\cdot}benzene]^{+}[B(C_6F_5)_4]^{-}$ in C_6D_5Br

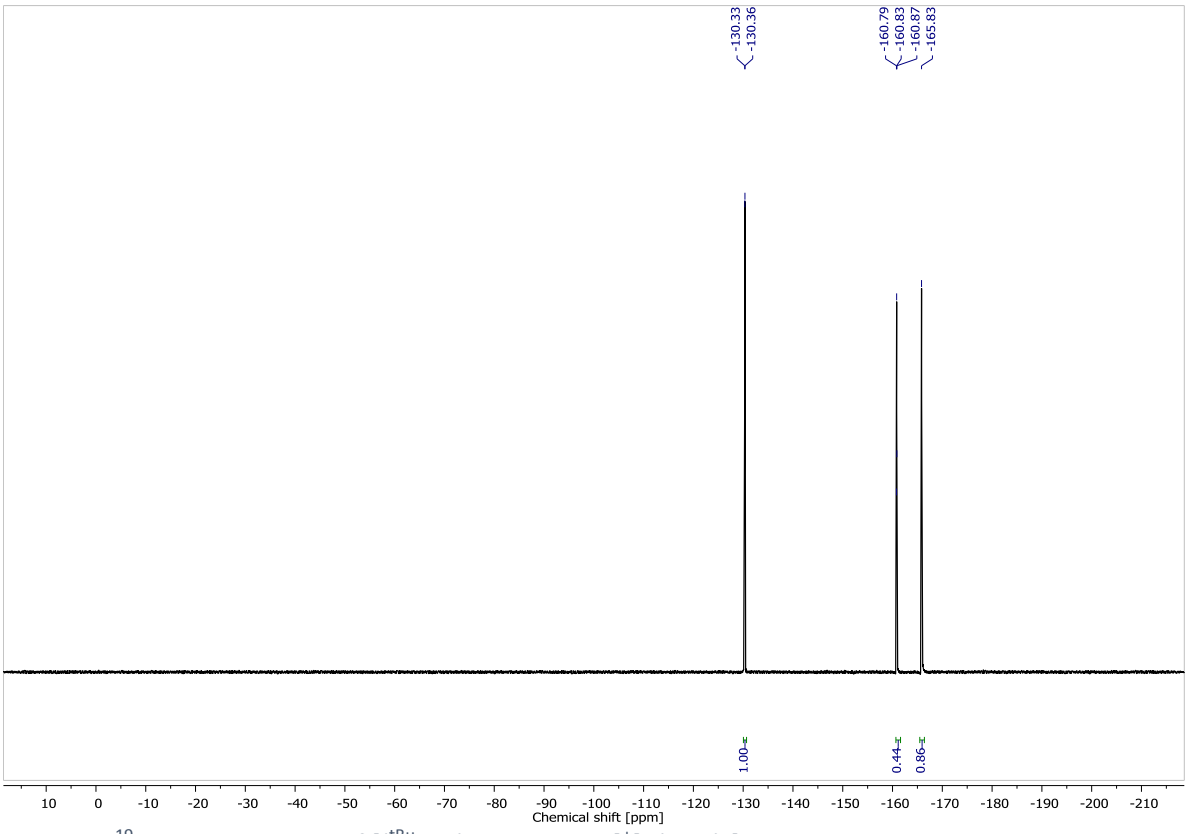

Figure S3: ^{19}F NMR spectrum of $[(^{tBu}BDI)Mg{\cdot}benzene]^{+}[B(C_6F_5)_4]^{-}$ in C_6D_5Br

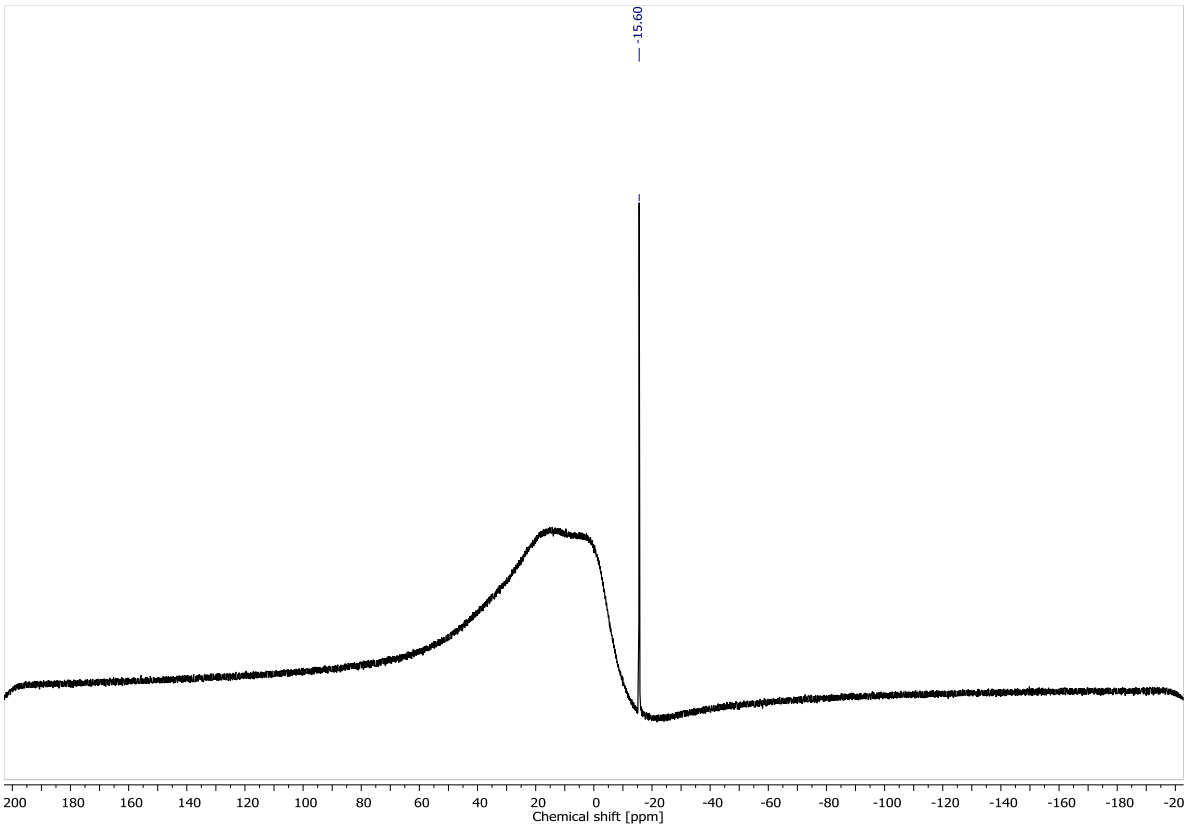

Figure S4: ^{11}B NMR spectrum of [(^{tBu}BDI)Mg·benzene]$^{+}$[B(C_6F_5)$_4$]$^{-}$ in C_6D_5Br

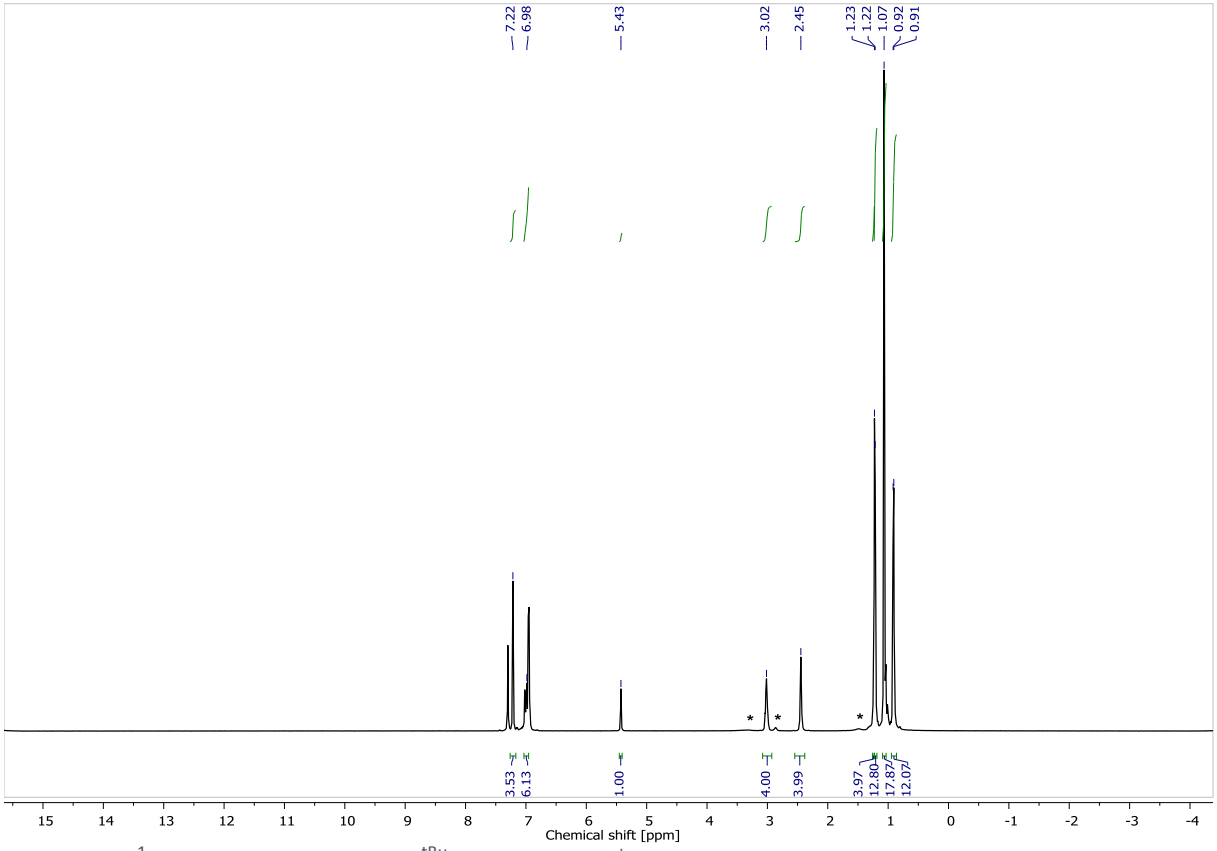

Figure S5: ^{1}H NMR spectrum of [(^{tBu}BDI)Mg·(THF)]$^{+}$[B(C_6F_5)$_4$]$^{-}$ in C_6D_5Br. Resonances marked with a star can be assigned to a species with two coordinated THF ligands (as has been proven by subsequent addition of a second eq of THF)

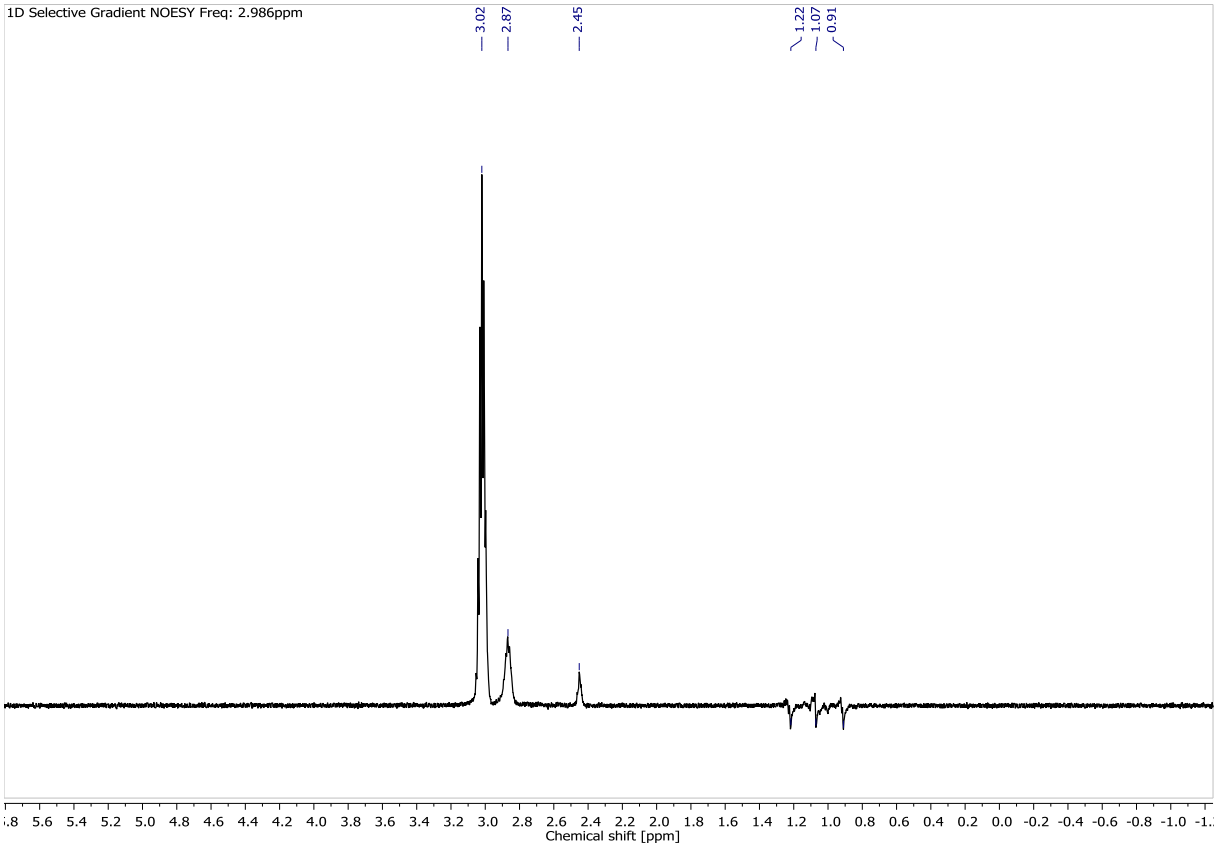

Figure S6: ^{1}D Selective Gradient NOESY NMR spectrum of $[(^{tBu}BDI)Mg\cdot(THF)]^{+}[B(C_6F_5)_4]^{-}$ in C_6D_5Br. Irradiation at the THF OCH_2 signal (2.87 ppm) gave strong enlargement of the *i*Pr CH signal at 3.02 ppm.

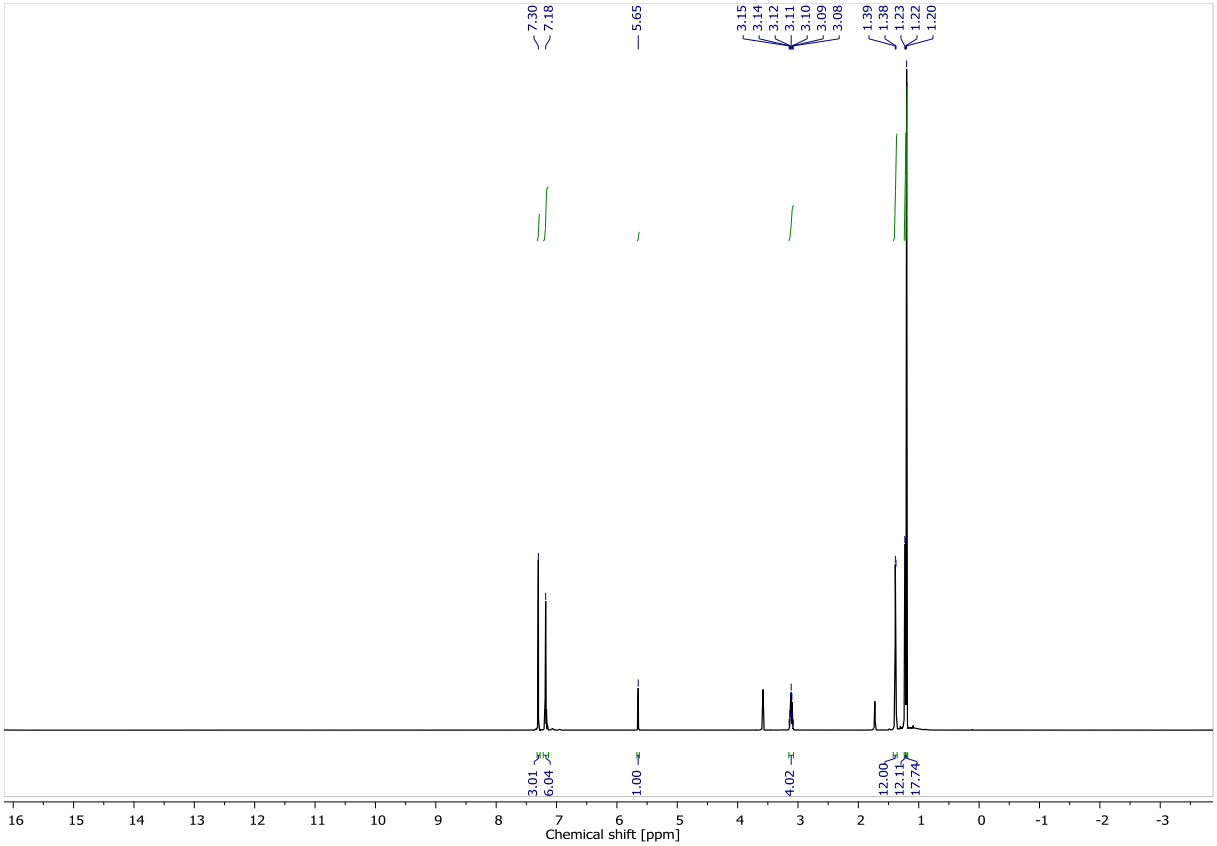

Figure S5: ^{1}H NMR spectrum of $[(^{tBu}BDI)Mg]^{+}[B(C_6F_5)_4]^{-}$ in THF-d_8

1.1.2. Spectra of [(^{tBu}BDI)Mg·toluene]$^{+}$[B(C_6F_5)$_4$]$^{-}$

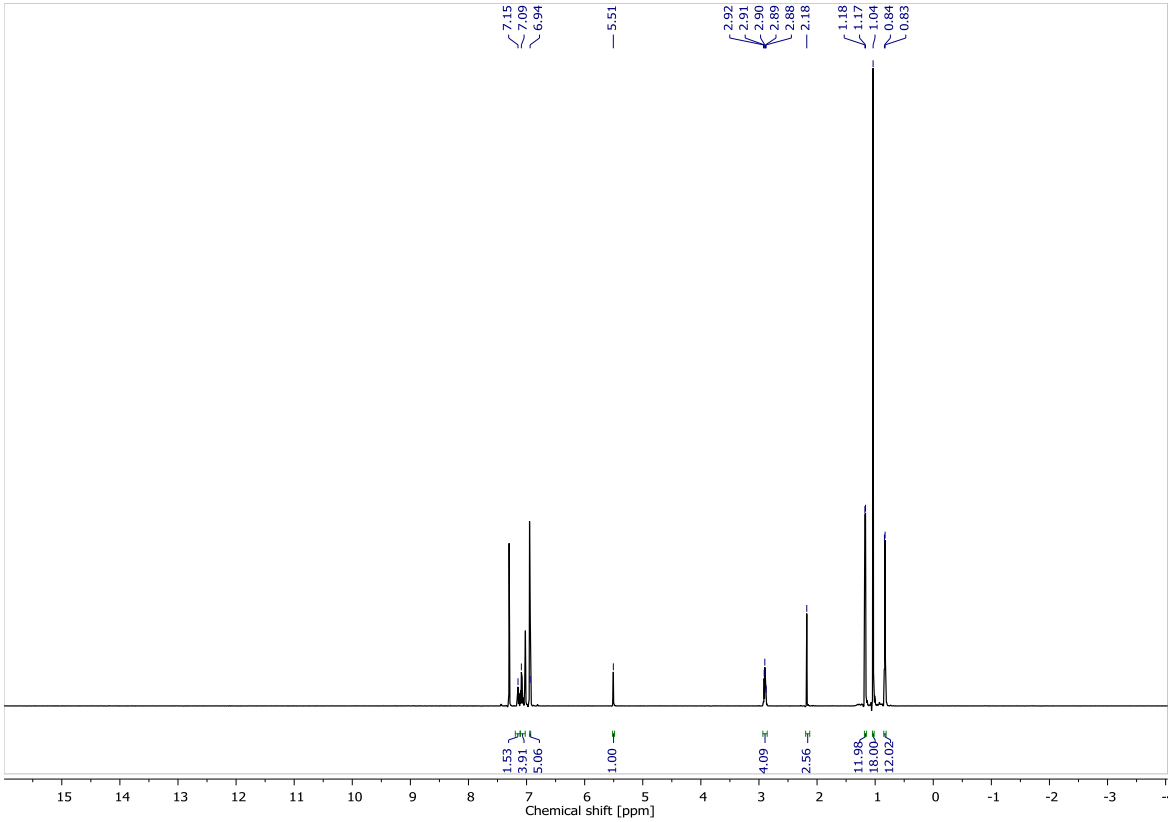

Figure S8: ^{1}H NMR spectrum of [(^{tBu}BDI)Mg·toluene]$^{+}$[B(C_6F_5)$_4$]$^{-}$ in C_6D_5Br

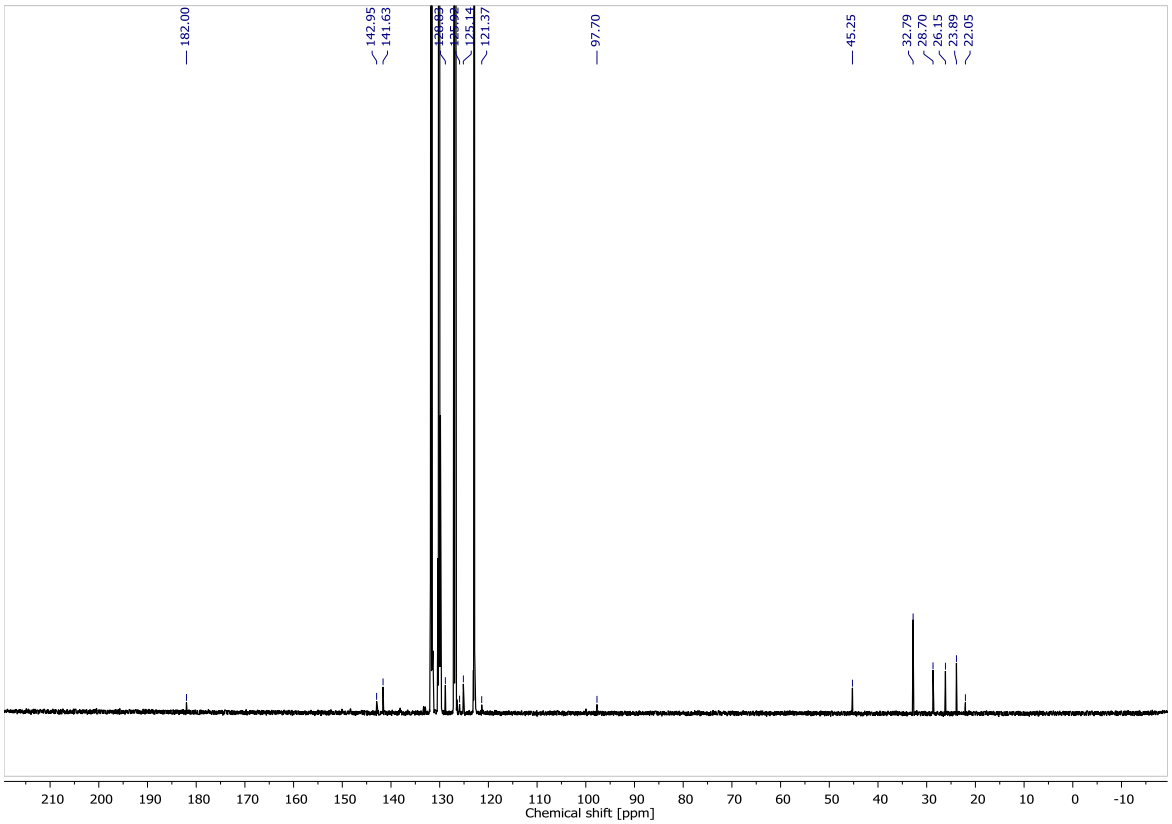

Figure S9: ^{13}C{^{1}H} NMR spectrum of [(^{tBu}BDI)Mg·toluene]$^{+}$[B(C_6F_5)$_4$]$^{-}$ in C_6D_5Br

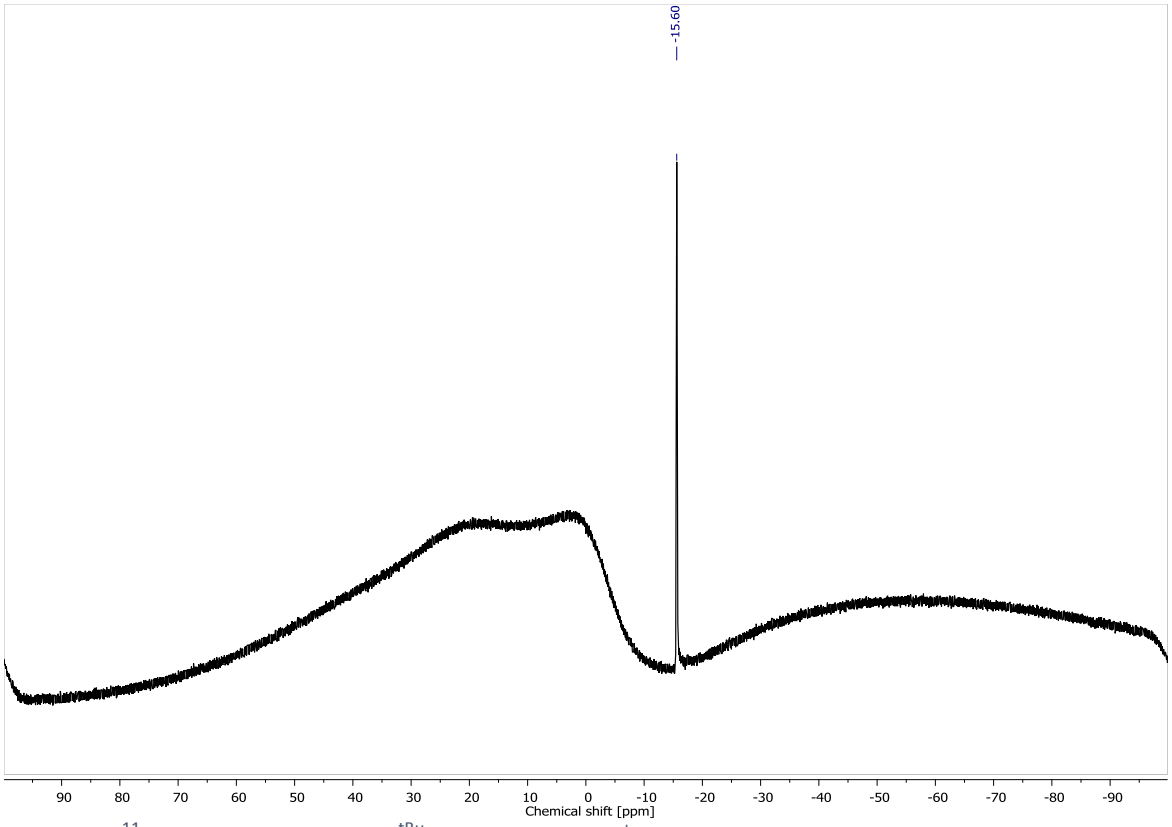

Figure S10: ^{11}B NMR spectrum of [(^{tBu}BDI)Mg·toluene]$^{+}$[B(C_6F_5)$_4$]$^{-}$ in C_6D_5Br

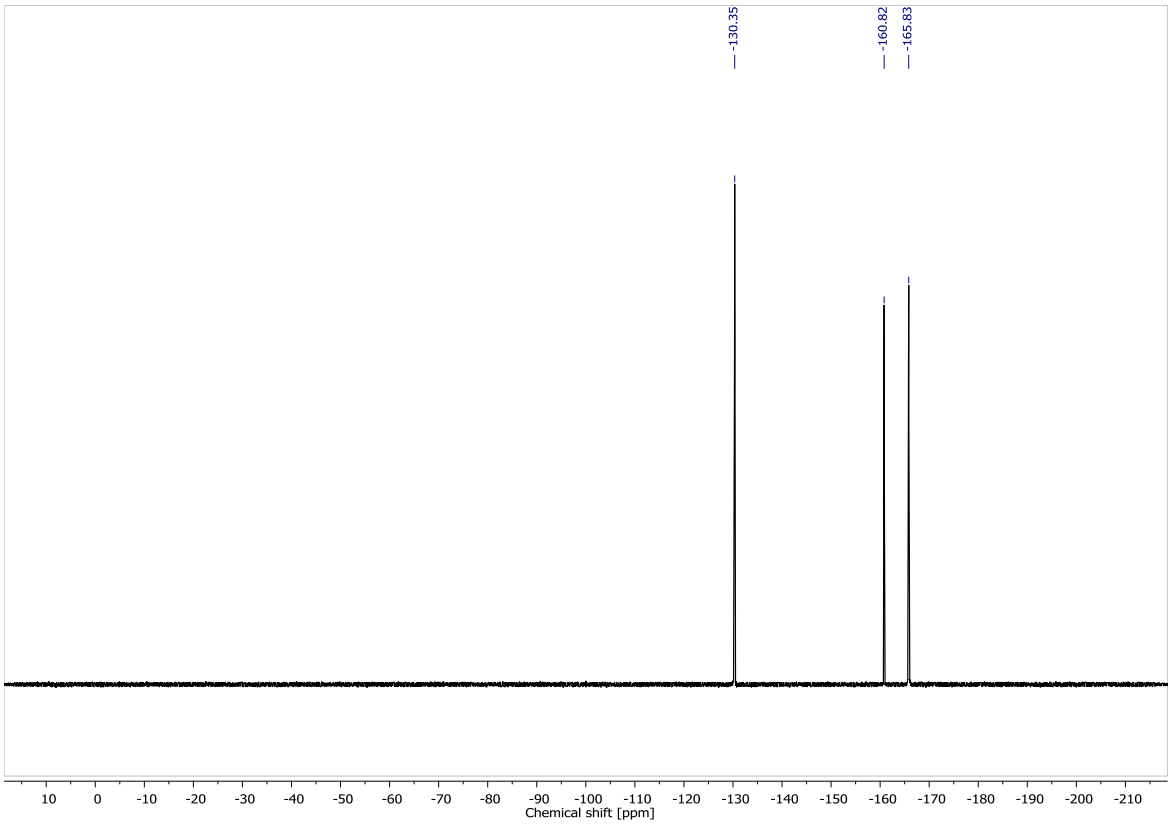

Figure S11: ^{19}F NMR spectrum of [(^{tBu}BDI)Mg·toluene]$^{+}$[B(C_6F_5)$_4$]$^{-}$ in C_6D_5Br

1.1.3. Spectra of [(^{tBu}BDI)Mg·*m*-xylene]$^{+}$[B(C_6F_5)$_4$]$^{-}$

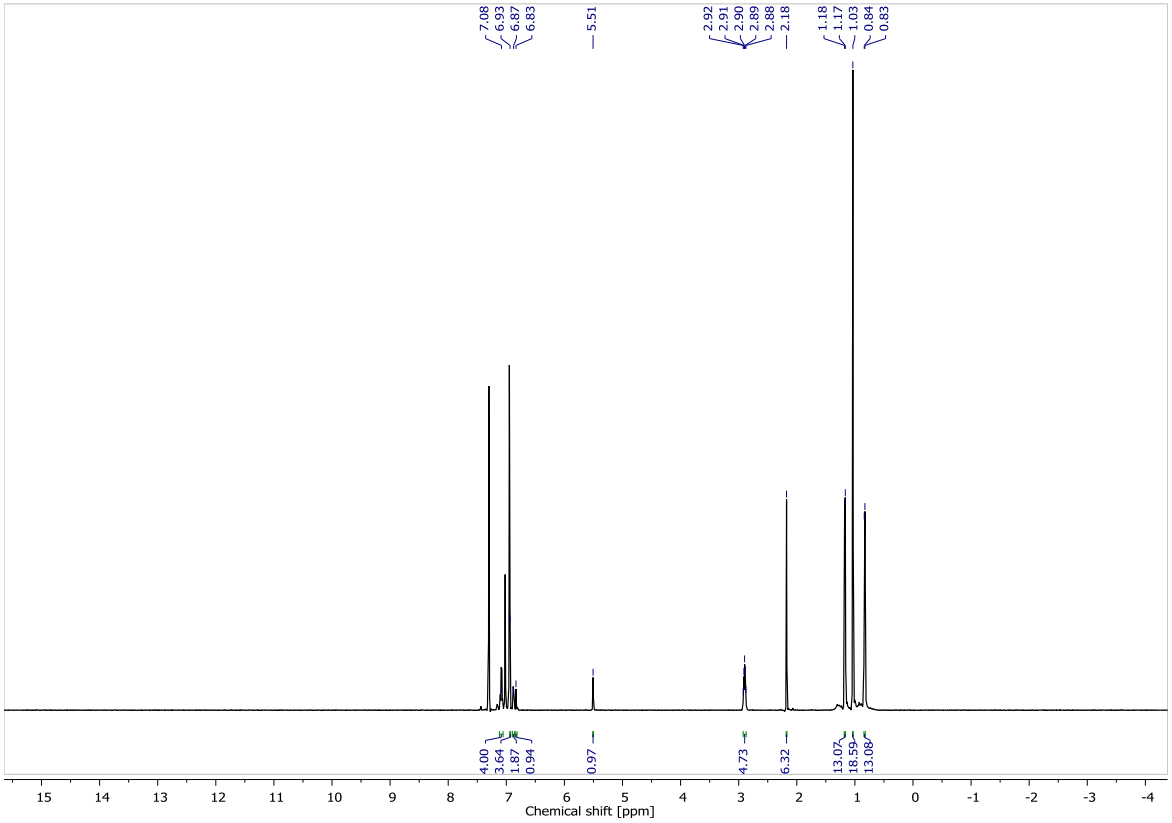

Figure S12: ^{1}H NMR spectrum of [(^{tBu}BDI)Mg·*m*-xylene]$^{+}$[B(C_6F_5)$_4$]$^{-}$ in C_6D_5Br.

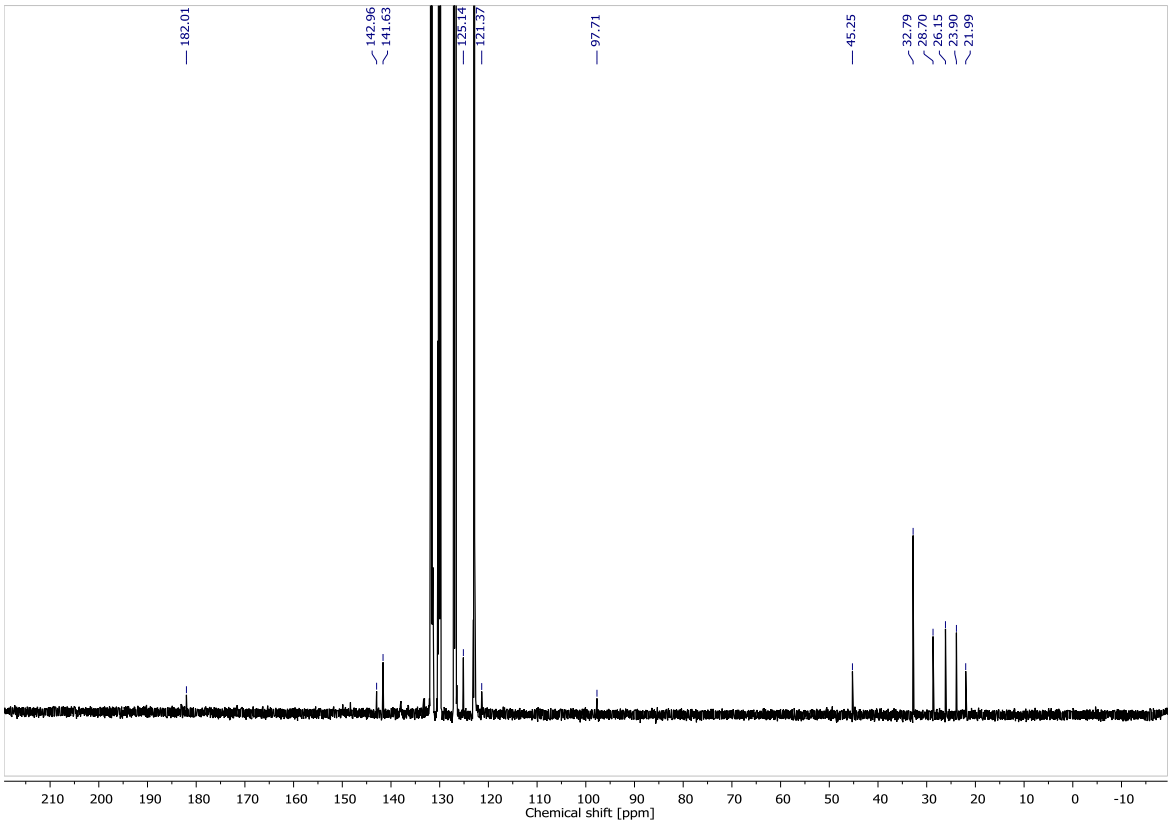

Figure S13: ^{13}C{^{1}H} NMR spectrum of [(^{tBu}BDI)Mg·*m*-xylene]$^{+}$[B(C_6F_5)$_4$]$^{-}$ in C_6D_5Br.

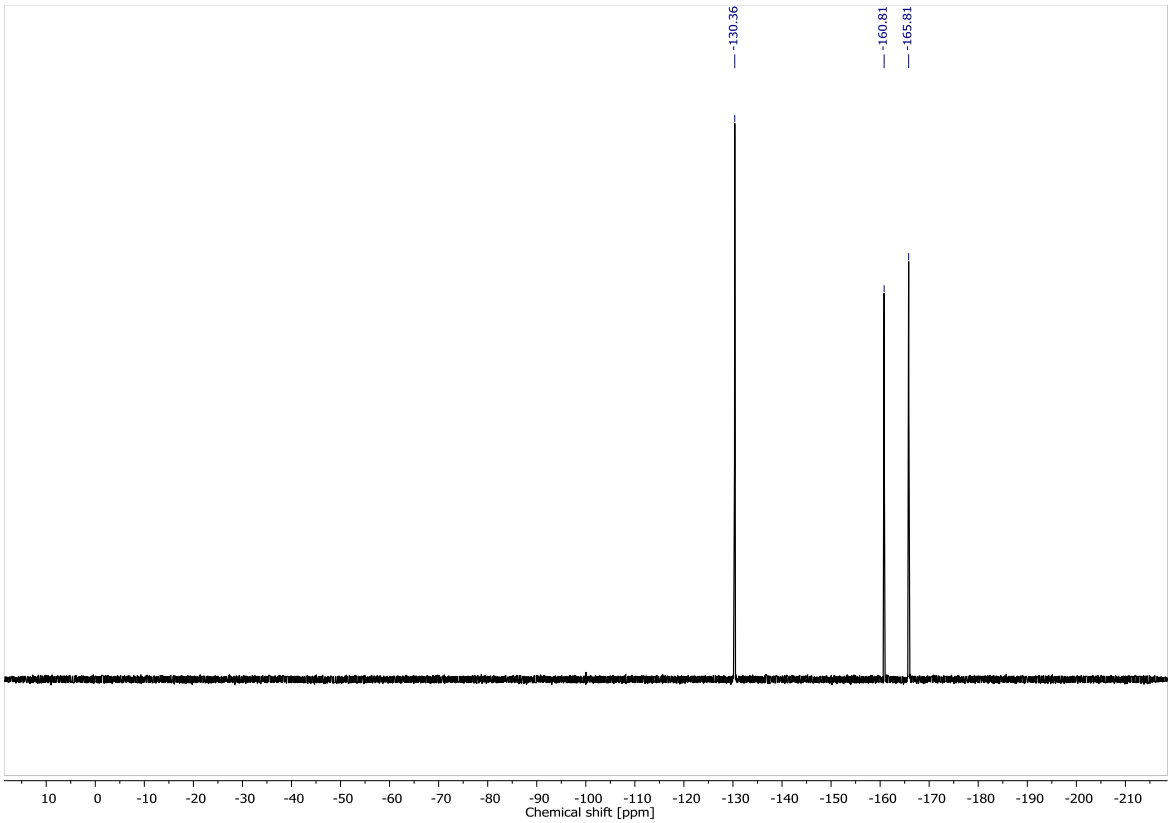

Figure S14: ^{19}F NMR spectrum of [(^{tBu}BDI)Mg·*m*-xylene]$^{+}$[B(C_6F_5)$_4$]$^{-}$ in C_6D_5Br.

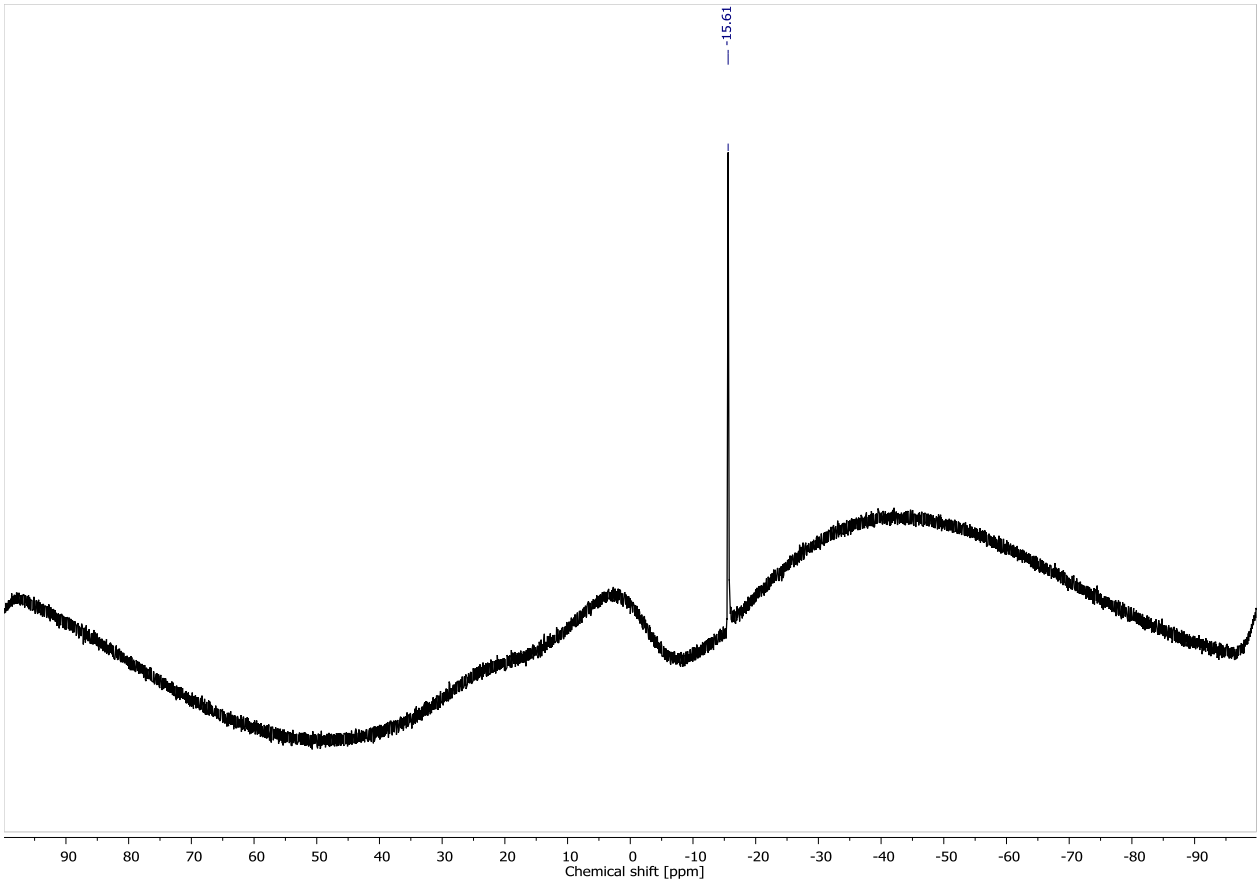

Figure S15: ^{11}B NMR spectrum of [(^{tBu}BDI)Mg·*m*-xylene]$^{+}$[B(C_6F_5)$_4$]$^{-}$ in C_6D_5Br.

1.1.4. Spectra of $[(^{tBu}BDI)Mg\cdot(PhCl)]^+[B(C_6F_5)_4]^-$

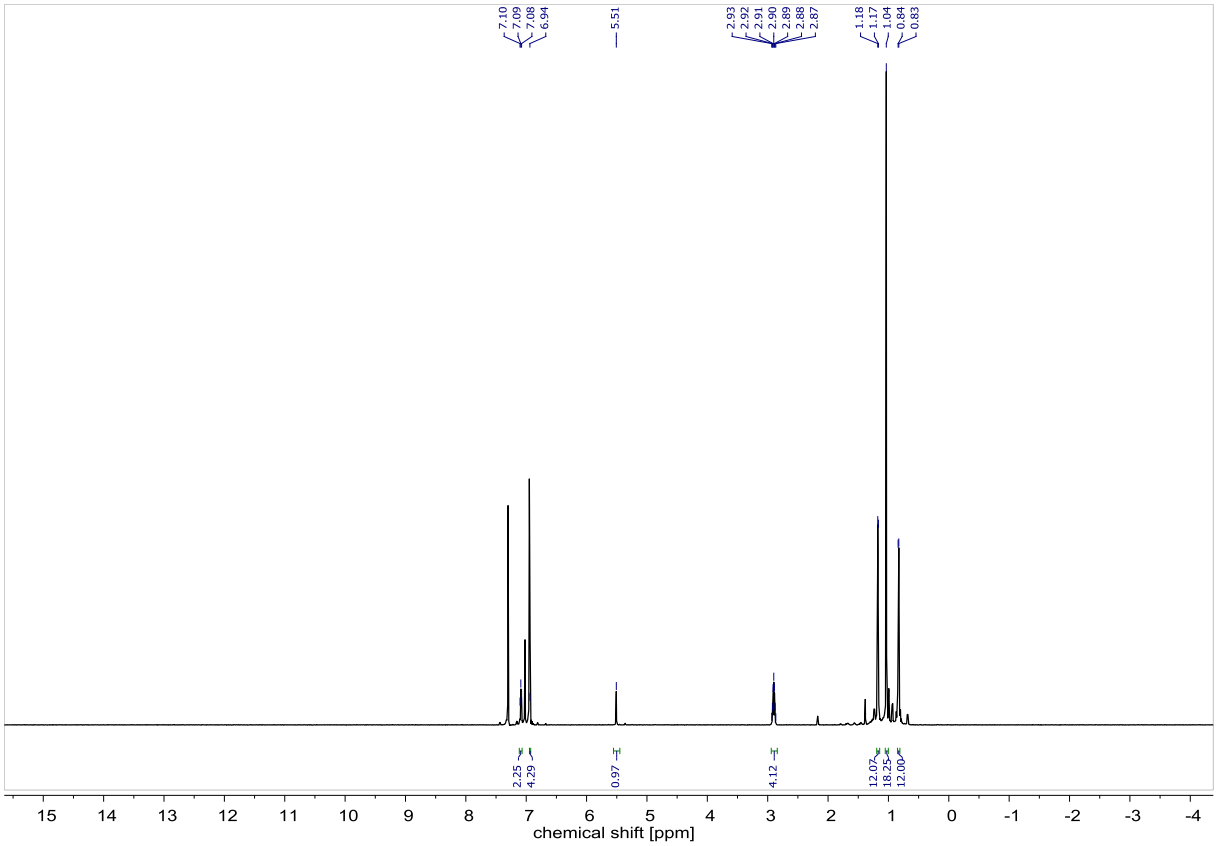

Figure S16: ^{1}H NMR spectrum of $[(^{tBu}BDI)Mg\cdot(PhCl)]^+[B(C_6F_5)_4]^-$ in C_6D_5Br.

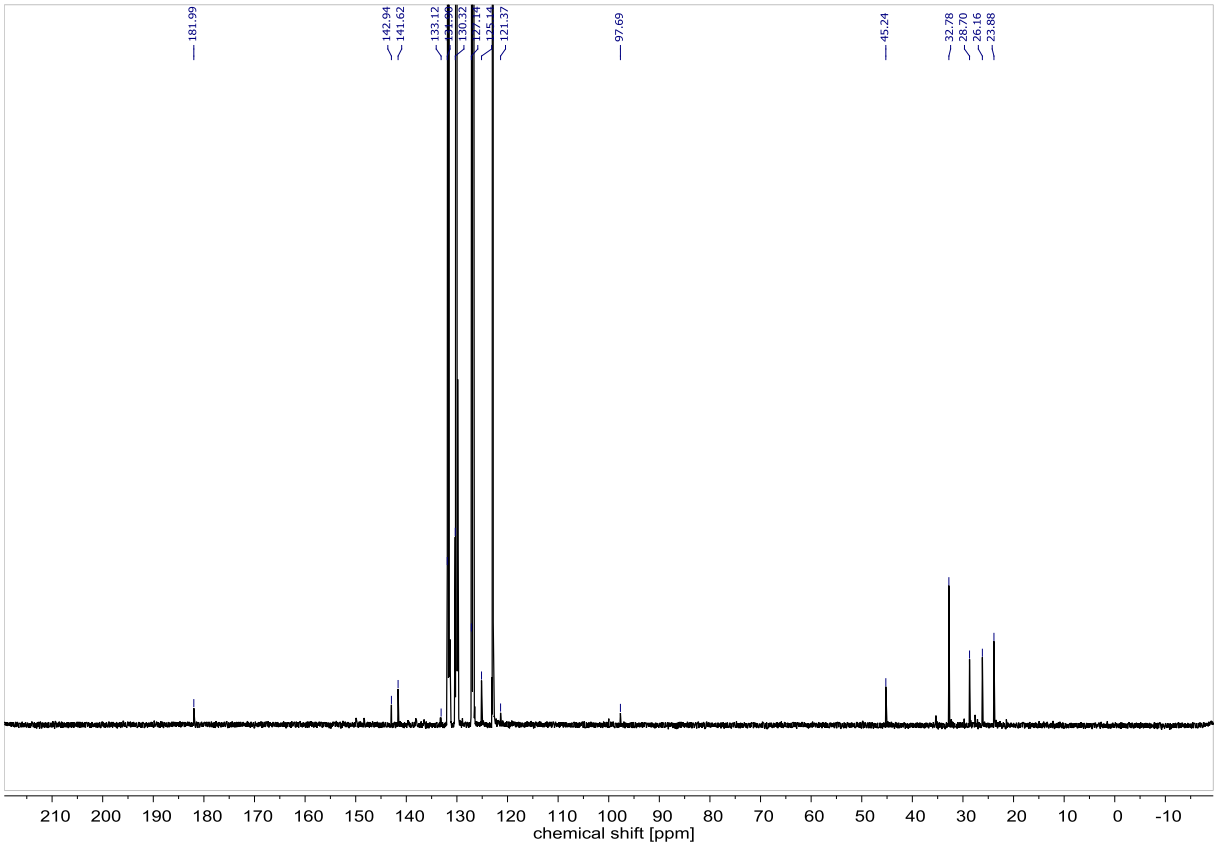

Figure S17: $^{13}C\{^{1}H\}$ NMR spectrum of $[(^{tBu}BDI)Mg\cdot(PhCl)]^+[B(C_6F_5)_4]^-$ in C_6D_5Br.

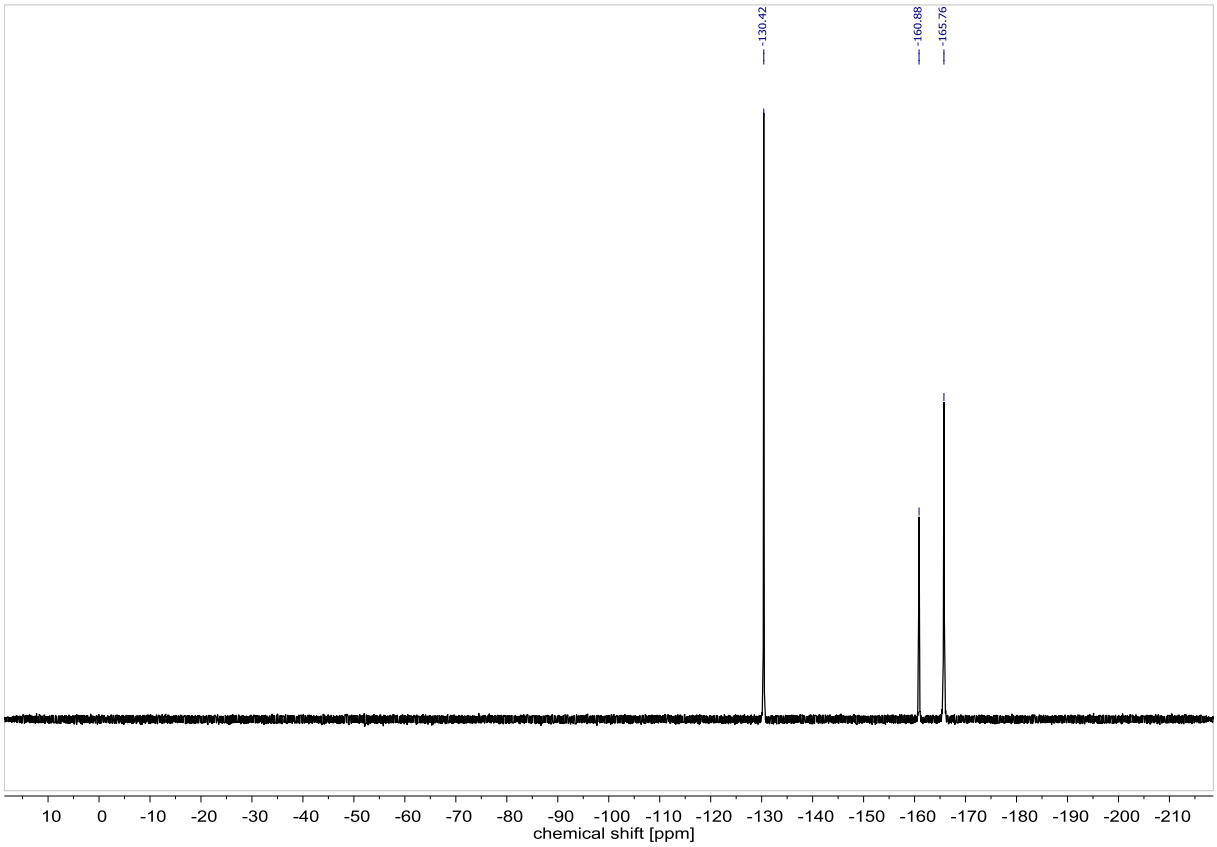

Figure S18: ^{19}F NMR spectrum of $[(^{tBu}BDI)Mg{\cdot}(PhCl)]^{+}[B(C_6F_5)_4]^{-}$ in C_6D_5Br.

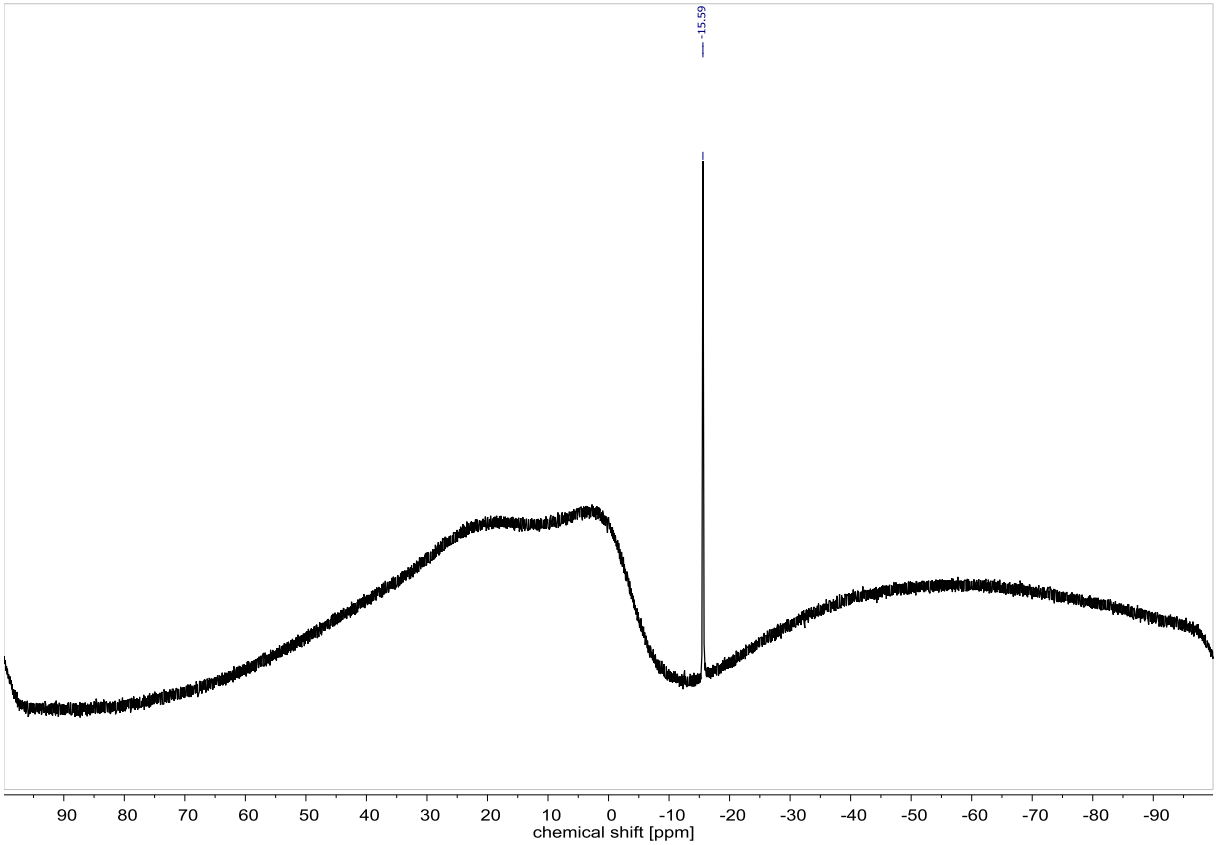

Figure S19: ^{11}B NMR spectrum of $[(^{tBu}BDI)Mg{\cdot}(PhCl)]^{+}[B(C_6F_5)_4]^{-}$ in C_6D_5Br.

1.2 Single Crystal X-Ray Diffraction

Single crystal X–ray diffraction data for all compounds were collected on a SuperNova diffractometer (Rigaku Oxford diffraction) with Atlas S2 detector using a CuK_α or MoK_α microfocus source. All crystals were maintained at 100 K during data collection. Using Olex2[S1] the structures were solved by Direct Methods (ShelXT)[S2] and refined with ShelXL[S3] using Least Squares minimization. The hydrogen atoms have been placed on calculated positions and were refined isotropically in a riding model. All presented structures had the complete molecule in their respective asymmetric units without any cocrystallized solvents. For the solution of $[(^{tBu}BDI)Mg\cdot(PhCl)]^+[B(C_6F_5)_4]^-$ five reflexes were omitted for error minimization.

The crystal structure of $[(^{tBu}BDI)Mg\cdot toluene]^+[B(C_6F_5)_4]^-$ was of poor quality but we give the cell parameters for identification: a = 17.765(2) Å, b = 18.283(3) Å, c = 18.738(3) Å, α = 98.377(14)°, β = 90.344(13)°, γ = 95.415(14)°, V = 5993.0(16) $Å^3$, space group: P-1.

Table S1. *Crystal data.*

Identification code	[(^{tBu}BDI)Mg·benzene]$^+$ [B(C_6F_5)$_4$]$^-$	[(^{tBu}BDI)Mg·*m*–xylene]$^+$ [B(C_6F_5)$_4$]$^-$	[(^{tBu}BDI)Mg·PhCl]$^+$ [B(C_6F_5)$_4$]$^-$
Empirical formula	$C_{65}H_{59}BF_{20}MgN_2$	$C_{67}H_{63}BF_{20}MgN_2$	$C_{65}H_{58}BClF_{20}MgN_2$
Formula weight	1283.26	1311.31	1317.70
Temperature/K	200.00(10)	99.98(16)	100
Crystal system	monoclinic	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$
a/Å	17.6212(4)	18.3516(3)	18.5500(2)
b/Å	17.7017(5)	17.6435(3)	17.9339(2)
c/Å	19.0530(4)	18.8442(3)	18.7239(2)
α/°	90	90	90
β/°	90.265(2)	93.9920(14)	103.2360(10)
γ/°	90	90	90
Volume/Å^3	5943.1(2)	6086.70(16)	6063.48(12)
Z	4	4	4
ρ_{calc}g/cm^3	1.434	1.431	1.443
μ/mm^{-1}	1.201	1.184	1.588
F(000)	2640.0	2704.0	2704.0
Crystal size/mm^3	0.1684 × 0.1292 × 0.0797	0.334 × 0.238 × 0.068	0.568 × 0.33 × 0.274
Crystal color	colorless	colorless	colorless
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.816 to 148.33	6.87 to 145.646	6.914 to 136.216
Index ranges	-21 ≤ h ≤ 21, -15 ≤ k ≤ 21, -23 ≤ l ≤ 21	-22 ≤ h ≤ 20, -21 ≤ k ≤ 19, -14 ≤ l ≤ 22	-20 ≤ h ≤ 22, -21 ≤ k ≤ 21, -22 ≤ l ≤ 22
Reflections collected	33902	21338	33397
Independent reflections	11638 [R_{int} = 0.0340, R_{sigma} = 0.0306]	11659 [R_{int} = 0.0321, R_{sigma} = 0.0424]	11056 [R_{int} = 0.0301, R_{sigma} = 0.0269]
Data/restraints/parameters	11638/0/816	11659/0/836	11056/0/829
Goodness-of-fit on F^2	1.030	1.017	1.030
Final R indexes [I>=2σ (I)]	R_1 = 0.0479, wR_2 = 0.1287	R_1 = 0.0490, wR_2 = 0.1286	R_1 = 0.0427, wR_2 = 0.1155
Final R indexes [all data]	R_1 = 0.0605, wR_2 = 0.1426	R_1 = 0.0558, wR_2 = 0.1363	R_1 = 0.0456, wR_2 = 0.1188
Largest diff. peak/hole / e Å^{-3}	0.45/-0.37	0.98/-0.54	0.59/-0.36

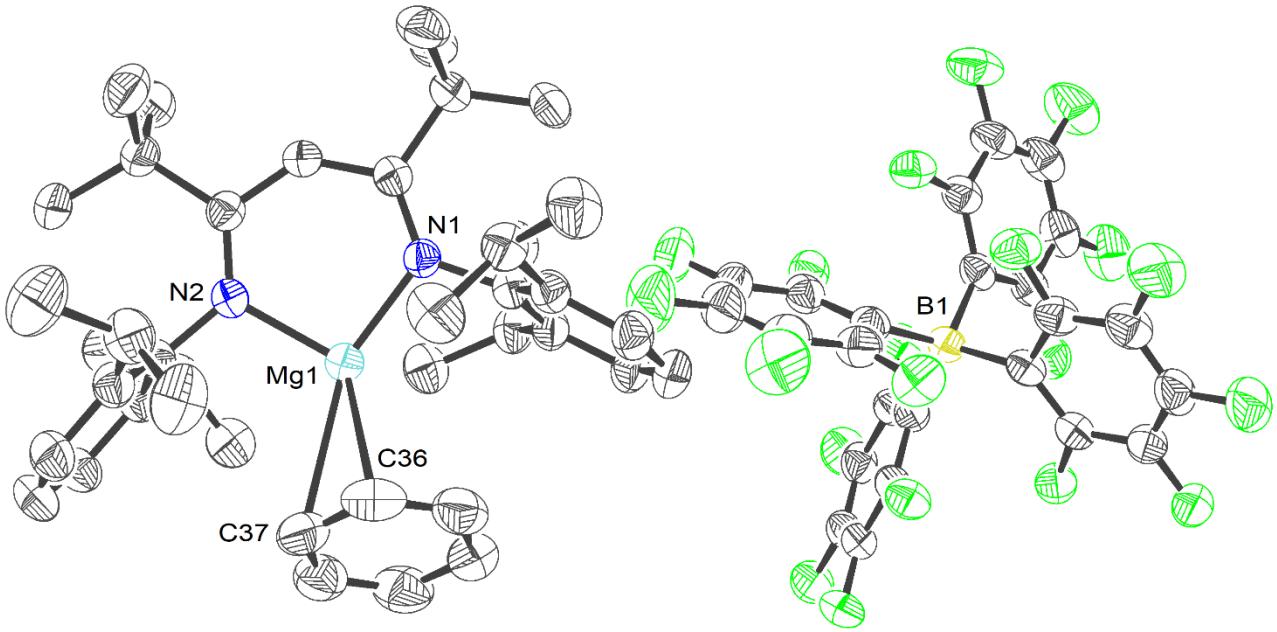

Figure S20: ORTEP representation of [(^{tBu}BDI)Mg·benzene]$^{+}$[B(C_6F_5)$_4$]$^{-}$ (probability level 50%). Hydrogen atoms were omitted for clarity.

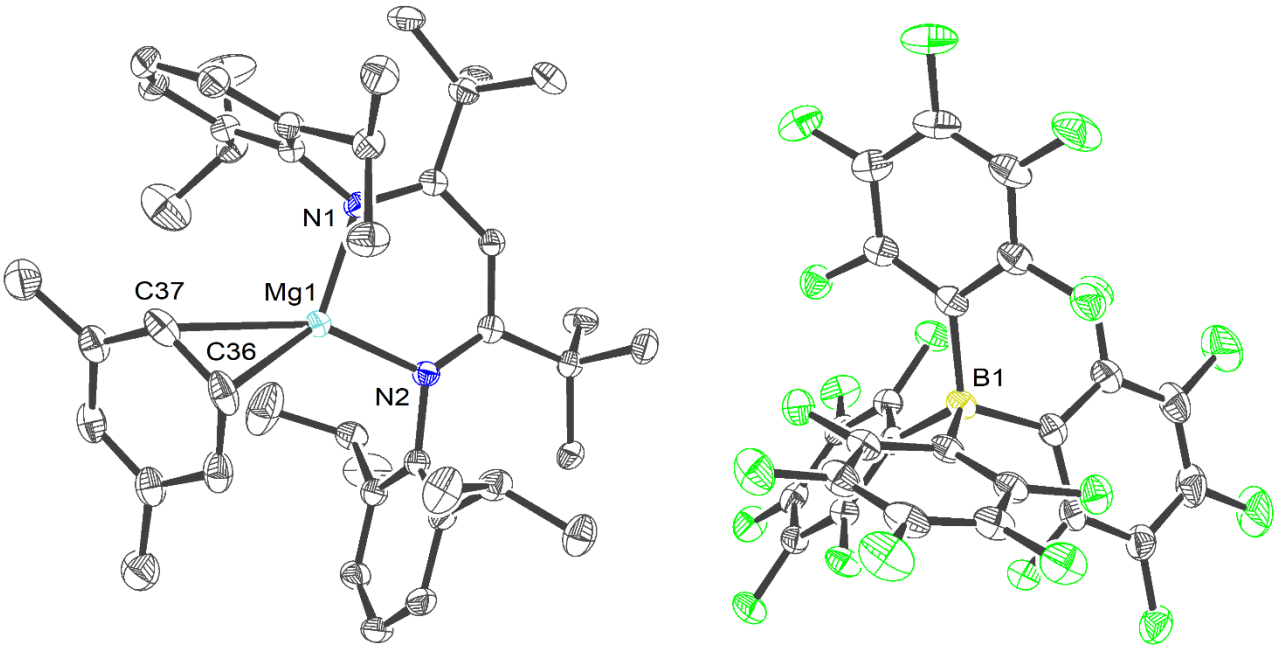

Figure S21: ORTEP representation of [(^{tBu}BDI)Mg·*m*-xylene]$^{+}$[B(C_6F_5)$_4$]$^{-}$ (probability level 50%). Hydrogen atoms were omitted for clarity.

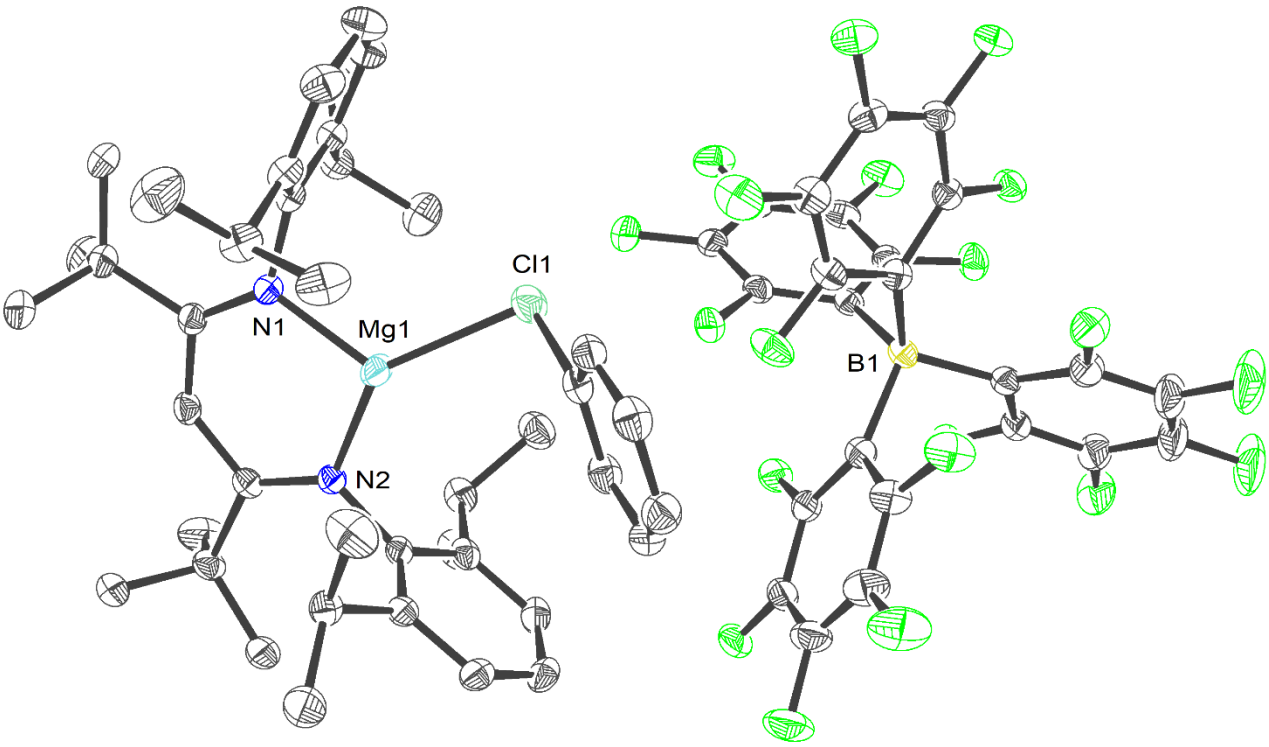

Figure S22: ORTEP representation of $[(^{tBu}BDI)Mg{\cdot}(PhCl)]^{+}[B(C_6F_5)_4]^{-}$ (probability level 50%). Hydrogen atoms were emitted for clarity.

2. DFT calculations

General

All calculations were carried out using Gaussian 16 A.[S4] All methods were used as implemented. All structures were fully optimized on a ωB97XD/6-31+G** level of theory. In order to determine zero point energies and to characterize the structures as minima frequency analysis has been applied.[S5-8] Energies were calculated on ωB97XD/6-311+G** level of theory. Charges were calculated via NBO analysis.[S9] Molecules were drawn and evaluated using Molecule V2.3.[S10] Topological analyses were carried out using AIMAll V17 using the wavefunctions of the geometry optimizations.[S11-12]

Table S2. Complexation energies of cations with benzene calculated at the ωB97XD/6-311+G**//ωB97XD/6-31+G** level. ΔH and ΔG (298 K, 1 atm) given in kcal/mol.

Reaction	dE	dH	dG (298K, 1 atm)
$(^{Me}BDI)Mg^+ + C_6H_6 \rightarrow (^{Me}BDI)Mg^+ \cdot C_6H_6$	-36.06	-33.62	-18.75
$(^{tBu}BDI)Mg^+ + C_6H_6 \rightarrow (^{tBu}BDI)Mg^+ \cdot C_6H_6$	-33.45	-31.49	-16.64
$[(^{Me}BDI)Mg^+] + C_6H_6 \rightarrow [(^{Me}BDI)Mg^+ \cdot C_6H_6]$ $[B(C_6F_5)_4^-]$ $[B(C_6F_5)_4^-]$	-6.03	-3.75[a]	+8.83[a]

[a] Calculated at ωB97XD/6-311+G**//6-31G*.[S13]

XYZ Coordinates

103
tBu C6H6

Mg	0.003548	-0.756033	-0.205419
N	1.504420	0.543605	-0.327563
N	-1.446133	0.591420	-0.031094
C	-1.254877	1.897379	-0.243491
C	1.328931	1.854343	-0.494192
C	2.697940	-0.220141	-0.197973
C	-2.632409	-0.095108	0.365272
C	0.032269	2.415417	-0.503662
H	0.030937	3.472614	-0.695243
C	3.343971	-0.310694	1.054164
C	3.072470	-1.063192	-1.266280
C	-3.491789	-0.631979	-0.614642
C	-2.797056	-0.416214	1.732177
C	2.471419	2.902737	-0.675984
C	2.380790	-1.089273	-2.630070
H	2.800980	-1.961970	-3.142253
C	-2.388914	2.970942	-0.315796

C	2.870301	0.500315	2.251788
H	2.177958	1.263121	1.889021
C	4.152493	-1.929916	-1.078136
H	4.468578	-2.565822	-1.901107
C	-3.258963	-0.388357	-2.098935
H	-2.475899	0.369463	-2.191376
C	4.408745	-1.200810	1.193863
H	4.922434	-1.273691	2.147798
C	-3.773103	2.542345	0.203401
H	-4.221043	1.744106	-0.384584
H	-4.440539	3.406227	0.132573
H	-3.760285	2.225149	1.247180
C	4.825037	-1.999813	0.135215
H	5.662726	-2.678298	0.258034
C	3.893514	2.332606	-0.804453
H	4.242904	1.851687	0.107889
H	4.574190	3.164077	-1.010099
H	3.993480	1.619697	-1.623793
C	2.212675	3.737522	-1.953119
H	2.162765	3.108799	-2.846355
H	3.038623	4.441742	-2.089641
H	1.293783	4.324627	-1.905245
C	-3.893779	-1.199351	2.098221
H	-4.056040	-1.443015	3.142635
C	-4.563713	-1.423474	-0.199721
H	-5.244616	-1.833651	-0.939792
C	0.857962	-1.322706	-2.610162
H	0.579153	-2.125841	-1.905552
H	0.510969	-1.691709	-3.579143
H	0.299857	-0.390098	-2.445176
C	2.460149	3.854051	0.541775
H	1.505363	4.373190	0.652817
H	3.243216	4.608743	0.417253
H	2.663409	3.317301	1.472659
C	-4.779166	-1.693039	1.145990
H	-5.625520	-2.298516	1.452936
C	-2.551441	3.355939	-1.804861
H	-1.622963	3.745563	-2.229986
H	-3.318951	4.131150	-1.896710
H	-2.869720	2.501044	-2.408099
C	2.694607	0.133886	-3.497757
H	2.244708	1.034381	-3.073494
H	2.291604	-0.000161	-4.506652
H	3.772812	0.291107	-3.582144
C	-1.792658	0.048442	2.782364
H	-0.807813	0.092810	2.294806
C	-0.112555	-2.774351	1.074158
H	-0.304854	-2.159814	1.952857
C	-2.747744	-1.663837	-2.784376
H	-1.833889	-2.040334	-2.312103
H	-2.529160	-1.476614	-3.840435
H	-3.493945	-2.463916	-2.729950

C	-1.992963	4.241347	0.474699
H	-1.713849	4.012342	1.506660
H	-2.848085	4.922489	0.503448
H	-1.166876	4.791493	0.019760
C	-1.198383	-3.258164	0.322720
H	-2.209875	-2.945256	0.567142
C	2.084877	-0.388750	3.226708
H	1.219511	-0.849352	2.738494
H	1.709943	0.198631	4.070644
H	2.712635	-1.193244	3.624846
C	1.196286	-3.191423	0.781887
H	2.034480	-2.816740	1.361593
C	4.010705	1.217840	2.984371
H	4.687280	0.511903	3.476013
H	3.603042	1.872520	3.760631
H	4.605797	1.832838	2.303717
C	-0.966471	-4.167373	-0.708271
H	-1.800956	-4.550289	-1.285622
C	0.332949	-4.596715	-0.981788
H	0.504919	-5.316705	-1.775354
C	1.412470	-4.104720	-0.248348
H	2.422285	-4.430603	-0.470935
C	-4.504041	0.139925	-2.823120
H	-5.304027	-0.606562	-2.847458
H	-4.258100	0.390737	-3.859541
H	-4.900994	1.038937	-2.344361
C	-2.071211	1.472268	3.280381
H	-1.968708	2.201464	2.476714
H	-1.363124	1.743242	4.069710
H	-3.084038	1.548582	3.689462
C	-1.679913	-0.903160	3.979814
H	-2.547602	-0.820186	4.641629
H	-0.798582	-0.646957	4.574979
H	-1.597340	-1.953675	3.680957

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tBu

Mg	-0.058719	-1.067664	0.566781
N	-1.527066	0.211166	0.414841
N	1.412635	0.043522	-0.123300
C	1.160604	1.240247	-0.662586
C	-1.334610	1.475989	0.017956
C	-2.705576	-0.583652	0.463059
C	2.661537	-0.642379	-0.010682
C	-0.081501	1.895732	-0.464267
H	-0.078260	2.916282	-0.809135
C	-3.419134	-0.867162	-0.728184
C	-2.999976	-1.279037	1.657590
C	3.627221	-0.220525	0.921609
C	2.819931	-1.853836	-0.718357
C	-2.404736	2.600163	0.144221
C	-2.240800	-1.093324	2.971208

H	-2.715576	-1.785458	3.673754
C	2.132546	2.010052	-1.606022
C	-3.023563	-0.216713	-2.048752
H	-2.754076	0.819865	-1.843070
C	-4.060363	-2.192002	1.656316
H	-4.310400	-2.712939	2.576430
C	3.415593	1.008621	1.791497
H	2.608572	1.602062	1.355722
C	-4.468331	-1.782534	-0.670962
H	-5.040468	-1.996290	-1.566760
C	3.443938	1.288758	-1.958546
H	4.127564	1.197829	-1.114933
H	3.954160	1.877149	-2.726792
H	3.274480	0.291451	-2.372085
C	-4.800086	-2.437886	0.510205
H	-5.623959	-3.142940	0.530972
C	-3.803049	2.115461	0.557212
H	-4.299596	1.540627	-0.227146
H	-4.424615	2.992546	0.759621
H	-3.785904	1.510485	1.465100
C	-1.897659	3.555518	1.252202
H	-1.807427	3.042822	2.214064
H	-2.611248	4.375709	1.377994
H	-0.924416	3.987040	1.006435
C	3.989643	-2.590077	-0.546267
H	4.141483	-3.508752	-1.102663
C	4.781025	-0.993987	1.068428
H	5.545116	-0.680783	1.772864
C	-0.756472	-1.523611	2.929384
H	-0.603087	-2.428031	2.309217
H	-0.395508	-1.816669	3.918400
H	-0.094977	-0.681189	2.660110
C	-2.555378	3.413444	-1.159024
H	-1.647526	3.957257	-1.429617
H	-3.345859	4.157111	-1.021301
H	-2.839675	2.786639	-2.008924
C	4.975077	-2.156750	0.334606
H	5.885592	-2.733253	0.458043
C	2.497489	3.384568	-1.009005
H	1.625790	4.021920	-0.843839
H	3.161719	3.910263	-1.701703
H	3.026554	3.279789	-0.057883
C	-2.356977	0.310489	3.572725
H	-1.863746	1.048056	2.935624
H	-1.890203	0.344911	4.562218
H	-3.405429	0.596659	3.684954
C	1.680662	-2.348868	-1.598091
H	1.205224	-1.464418	-2.034405
C	2.953561	0.582865	3.193401
H	2.042404	-0.024579	3.142733
H	2.742517	1.457482	3.816167
H	3.721697	-0.016137	3.693511

C	1.380053	2.210109	-2.945600
H	1.086710	1.245034	-3.373256
H	2.041057	2.708190	-3.661154
H	0.479828	2.818224	-2.840891
C	-1.772135	-0.878091	-2.646593
H	-0.896554	-0.712299	-2.008487
H	-1.535482	-0.440603	-3.621111
H	-1.923503	-1.954520	-2.786294
C	-4.151351	-0.175238	-3.082805
H	-4.386338	-1.169143	-3.477612
H	-3.848901	0.444920	-3.931387
H	-5.066824	0.251800	-2.662744
C	4.652226	1.910862	1.876514
H	5.469301	1.434458	2.426850
H	4.404003	2.837341	2.402987
H	5.027002	2.175003	0.883134
C	2.104450	-3.241321	-2.765993
H	2.852151	-2.738144	-3.384102
H	1.240375	-3.469817	-3.396859
H	2.525229	-4.192682	-2.426616
C	0.617683	-3.083964	-0.723569
H	0.653340	-4.167011	-0.868371
H	-0.423735	-2.811391	-0.968371
H	0.837828	-3.004245	0.361454

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BDI C6H6

C	-1.421359	-0.878093	-2.721556
Mg	0.050330	-0.191623	-0.481621
N	1.559817	0.083817	0.793263
N	-1.417792	0.117088	0.829316
C	2.565351	0.652989	2.969590
C	-2.331854	0.525702	3.081900
C	1.378343	0.371585	2.079416
C	-1.175727	0.343118	2.124372
C	0.109802	0.457116	2.684970
C	2.852530	-0.116109	0.216009
C	-2.754823	0.080746	0.322740
C	3.576429	0.981846	-0.288862
C	-3.447352	1.280278	0.071135
C	4.727211	0.732262	-1.041880
C	-4.697433	1.203034	-0.549441
C	5.160831	-0.563997	-1.282994
C	-5.254720	-0.018986	-0.899804
C	3.307468	-1.440560	0.029808
C	-3.303080	-1.170769	-0.035038
C	4.462620	-1.633890	-0.733233
C	-4.561452	-1.196251	-0.637447
H	-2.422567	-1.290803	-2.682116
H	2.402881	0.256494	3.973519
H	-2.579013	1.589352	3.163564
H	0.125812	0.666078	3.748136

H	2.689291	1.737604	3.059819
H	-3.229534	0.004066	2.746757
H	3.491531	0.240503	2.567592
H	-2.062986	0.172410	4.078443
C	3.170550	2.420496	0.001954
C	-2.878698	2.644692	0.441963
H	5.297881	1.566875	-1.439124
H	-5.248404	2.115575	-0.756763
H	6.053232	-0.741599	-1.873998
H	-6.230887	-0.057319	-1.371972
C	2.698579	-2.677950	0.695006
C	-2.533448	-2.459224	0.228922
H	4.831233	-2.644818	-0.886251
H	-5.010736	-2.144221	-0.913065
C	-0.305016	-1.719289	-2.681578
C	0.987563	-1.176681	-2.711357
C	1.160980	0.211001	-2.779135
C	-1.250295	0.507913	-2.778996
C	0.038974	1.052383	-2.807067
H	-0.442336	-2.794169	-2.620924
H	1.858499	-1.821815	-2.664897
H	2.163458	0.625982	-2.783850
H	-2.120458	1.154969	-2.779977
H	0.169106	2.128637	-2.853902
C	-2.415170	3.420913	-0.798982
C	-3.877874	3.478200	1.256859
H	-1.994453	2.491556	1.065303
C	-2.941972	-3.629384	-0.670909
H	-1.473122	-2.259066	0.018315
C	-2.607964	-2.880730	1.703781
C	2.871702	3.221916	-1.271847
H	2.253069	2.401117	0.597369
C	4.252806	3.129995	0.831253
H	3.173907	-3.529052	0.193625
C	3.094628	-2.763429	2.177371
C	1.185646	-2.898821	0.553772
H	2.589269	4.248089	-1.018714
H	3.743857	3.271424	-1.931623
H	2.046900	2.782585	-1.840047
H	3.907397	4.120618	1.142332
H	4.511186	2.558733	1.726768
H	5.170319	3.265214	0.249491
H	2.831360	-3.745306	2.582991
H	4.170041	-2.617391	2.308602
H	2.569295	-2.010352	2.771058
H	0.934765	-3.923088	0.846645
H	0.605991	-2.236446	1.204888
H	0.855161	-2.792043	-0.486425
H	-2.061064	-3.815600	1.861731
H	-2.177063	-2.126572	2.365243
H	-3.649308	-3.041500	2.000299
H	-2.236714	-4.456138	-0.543529

H	-3.933453	-4.013100	-0.411805
H	-2.959117	-3.357206	-1.731691
H	-3.393613	4.382449	1.637295
H	-4.731209	3.795528	0.649352
H	-4.269488	2.913933	2.108190
H	-2.056693	4.415690	-0.517601
H	-1.592188	2.904786	-1.303990
H	-3.231834	3.548342	-1.517823

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BDI

Mg	-0.000045	-0.001639	-0.704801
N	-1.505358	-0.136778	0.545784
N	1.505619	0.134208	0.545425
C	-2.817446	-0.362181	0.019409
C	-1.257923	-0.247343	1.856981
C	3.820618	-0.614135	0.145177
C	0.000397	-0.002095	2.443017
H	0.000589	-0.002501	3.525692
C	1.258436	0.244147	1.856715
C	2.817149	0.362156	0.018733
C	-3.818941	0.616115	0.146238
C	5.071712	-0.338780	-0.412314
H	5.872285	-1.064410	-0.318189
C	-3.032620	-1.540120	-0.725067
C	3.029844	1.540643	-0.725606
C	1.849155	2.466409	-0.985334
H	1.245415	2.490690	-0.071348
C	-3.512778	1.969045	0.774762
H	-2.747504	1.830759	1.543398
C	4.292233	1.774497	-1.267388
H	4.487610	2.683745	-1.825554
C	5.314214	0.846898	-1.095396
H	6.297194	1.040966	-1.511221
C	3.517138	-1.967977	0.772993
H	2.750939	-1.831730	1.541075
C	-2.906132	2.898615	-0.288840
H	-1.992827	2.462107	-0.713193
H	-2.643144	3.868423	0.144441
H	-3.611222	3.066963	-1.109195
C	-5.070617	0.343455	-0.411274
H	-5.869735	1.070650	-0.316915
C	2.378630	0.653969	2.782493
H	3.148919	-0.119433	2.848626
H	2.004243	0.854832	3.785616
H	2.868689	1.554335	2.399798
C	-4.295525	-1.771253	-1.266825
H	-4.492860	-2.680008	-1.825095
C	-1.853948	-2.468557	-0.984463
H	-1.251238	-2.495150	-0.069900
C	-2.378213	-0.656757	2.782812
H	-3.148370	0.116787	2.848738

H	-2.003934	-0.857551	3.785988
H	-2.868420	-1.557094	2.400213
C	0.973567	1.879517	-2.130575
H	1.262835	2.292440	-3.101160
H	-0.097989	2.116259	-2.024816
H	1.154401	0.796721	-2.300483
C	-5.315554	-0.841550	-1.094661
H	-6.298942	-1.033495	-1.510508
C	2.214393	3.915557	-1.310480
H	2.829833	4.346079	-0.516852
H	1.308601	4.521997	-1.403053
H	2.763464	3.998853	-2.253334
C	4.724112	-2.625542	1.447684
H	5.476286	-2.947568	0.720667
H	4.404214	-3.516229	1.995602
H	5.206650	-1.945933	2.156508
C	-4.718718	2.629171	1.448815
H	-5.469535	2.953351	0.721352
H	-4.397118	3.518822	1.997421
H	-5.203439	1.950382	2.156932
C	-0.975348	-1.882879	-2.128135
H	-1.261292	-2.297340	-3.099041
H	0.096034	-2.119187	-2.018989
H	-1.156320	-0.800425	-2.299789
C	2.913443	-2.898422	-0.291537
H	1.999766	-2.463528	-0.716763
H	2.651937	-3.868894	0.141147
H	3.619723	-3.065100	-1.111205
C	-2.222593	-3.916462	-1.311327
H	-2.839968	-4.346162	-0.518753
H	-1.318270	-4.525152	-1.403490
H	-2.770869	-3.997465	-2.254846

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