Supplementary Information for

Coordination of Arenes and Phosphines by Charge Separated Alkaline Earth Cations

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Figure S1. ^{1}H NMR (500 MHz, tol-d_8, 298K) spectrum of compound **3**.

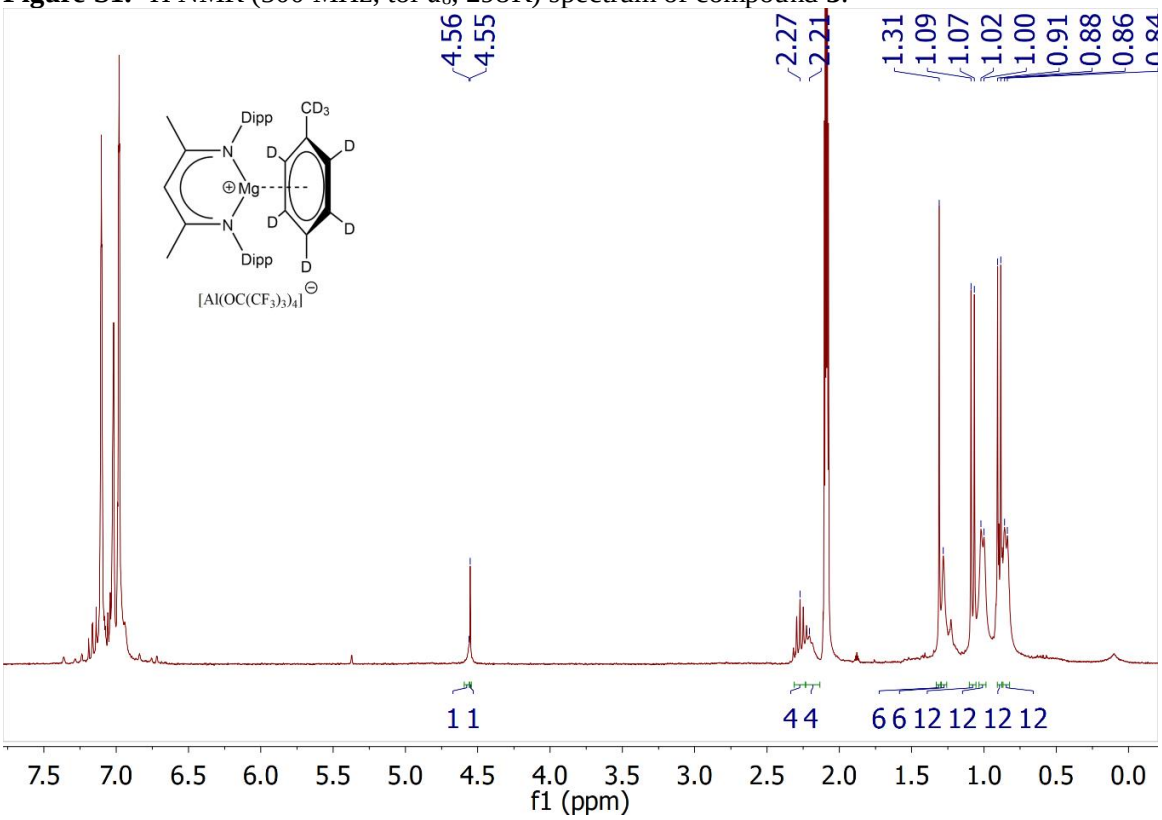


Figure S2. ^{19}F{^{1}H} NMR (470 MHz, tol-d_8, 298K) spectrum of compound **3**.

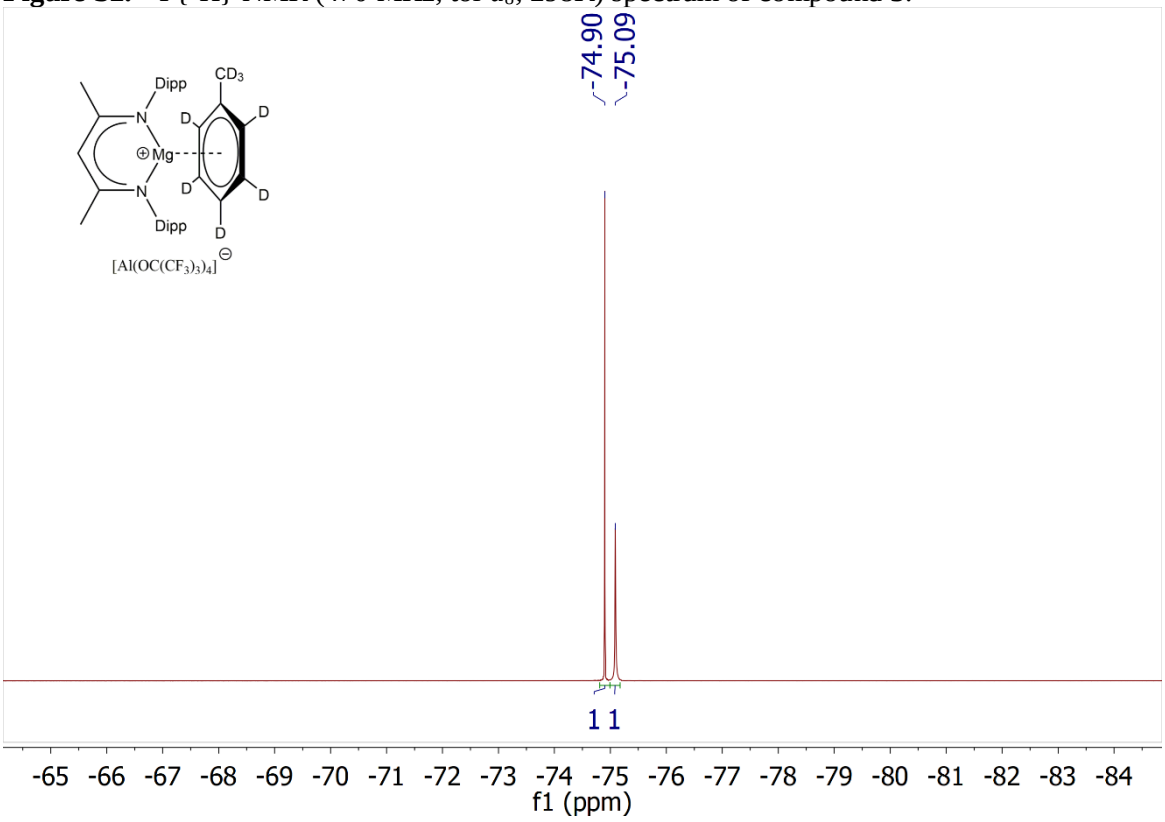


Figure S3. ^{1}H NMR (500 MHz, THF-d_8, 298K) spectrum of compound **3.THF**.

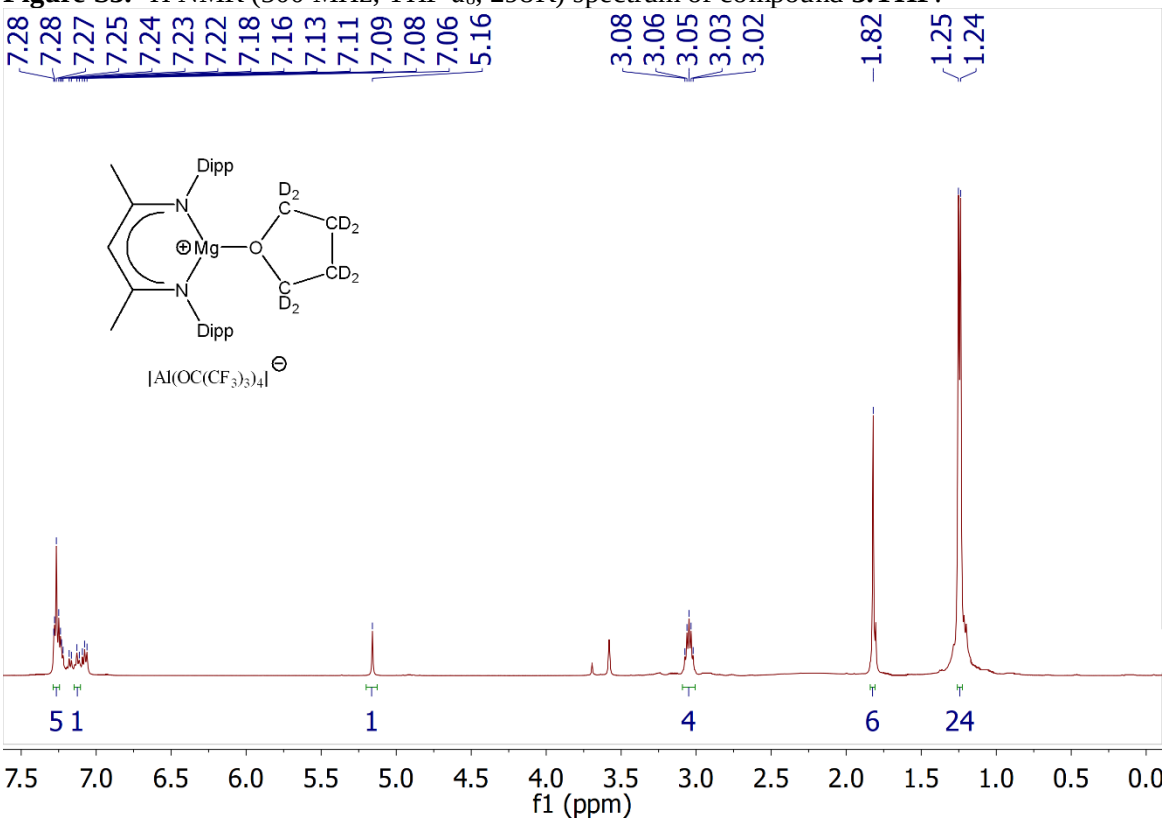


Figure S4. ^{13}C{^{1}H} NMR (126 MHz, THF-d_8, 298K) spectrum of compound **3**.**THF**.

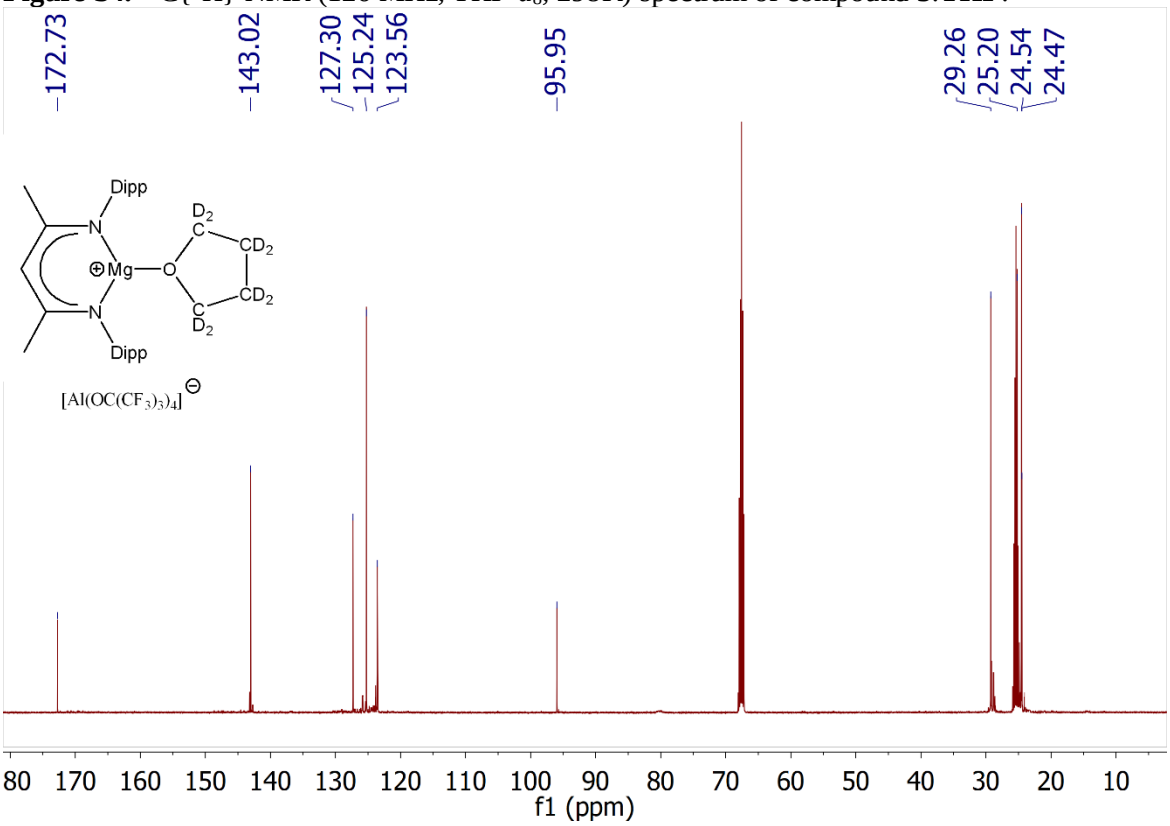


Figure S5. $^{19}F\{^{1}H\}$ NMR (470 MHz, THF-d_8, 298K) spectrum of compound **3.THF**.

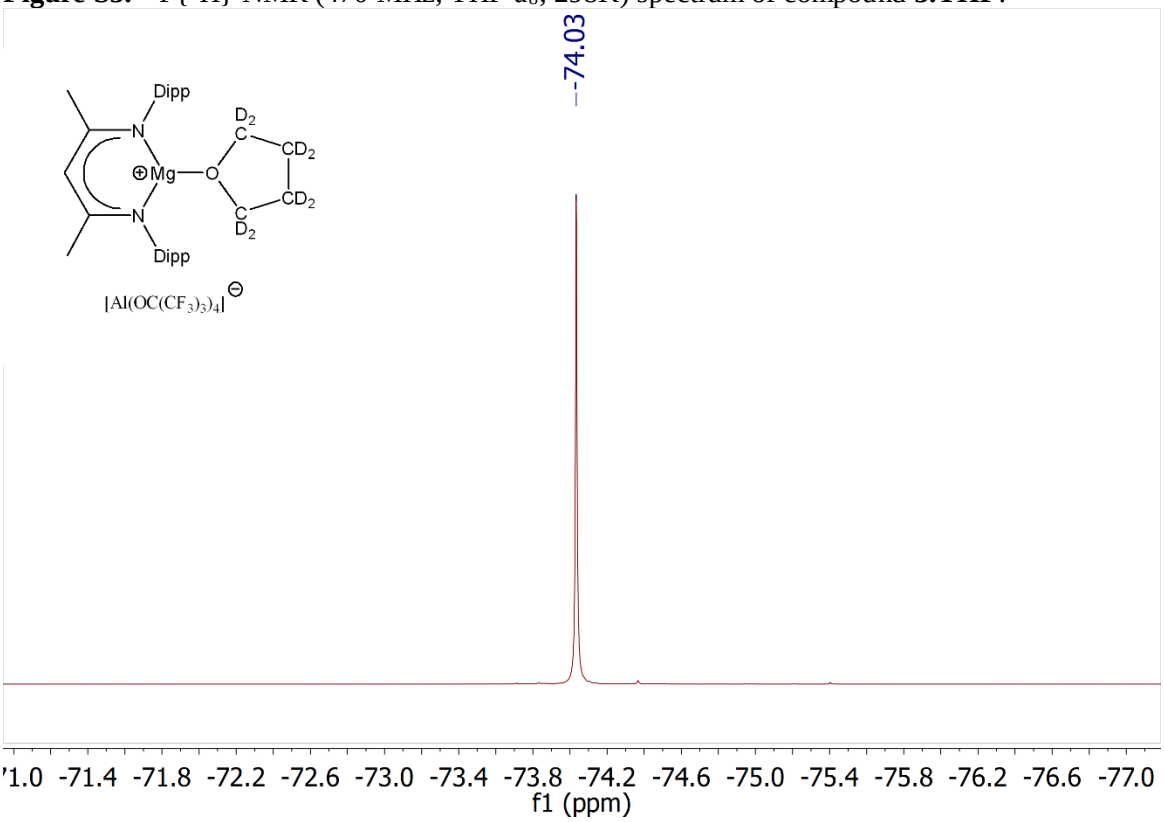


Figure S6. ^{1}H NMR (500 MHz, C_6D_6, 298K) spectrum of compound **4**.

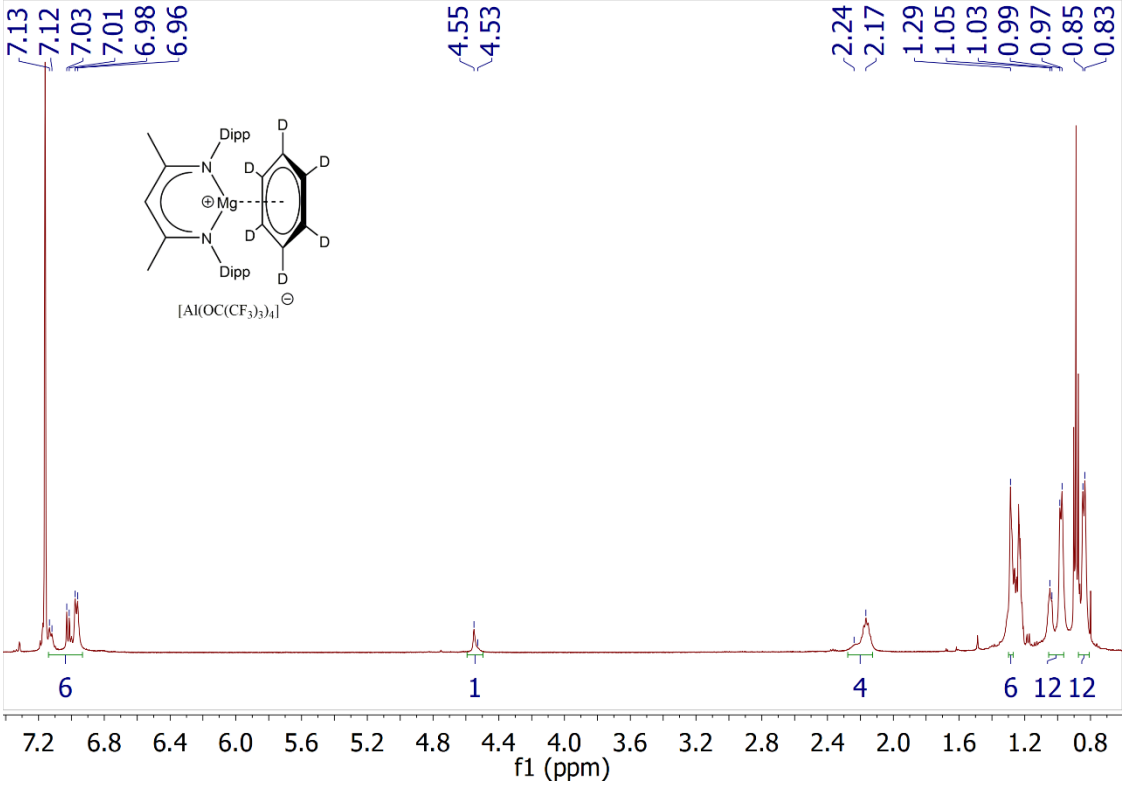


Figure S7. $^{19}F\{^{1}H\}$ NMR (470 MHz, C_6D_6, 298K) spectrum of compound **4**.

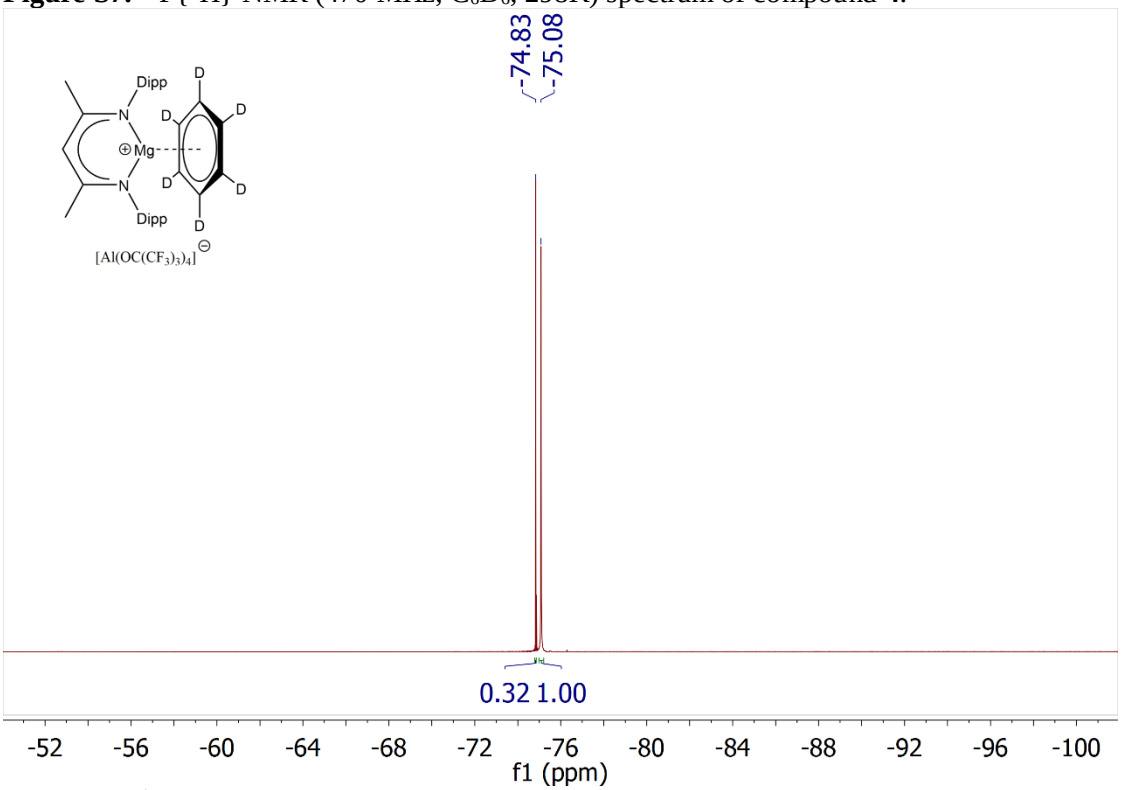


Figure S8. ^{1}H NMR (500 MHz, C_6D_6, 298K) spectrum of compound **5**.

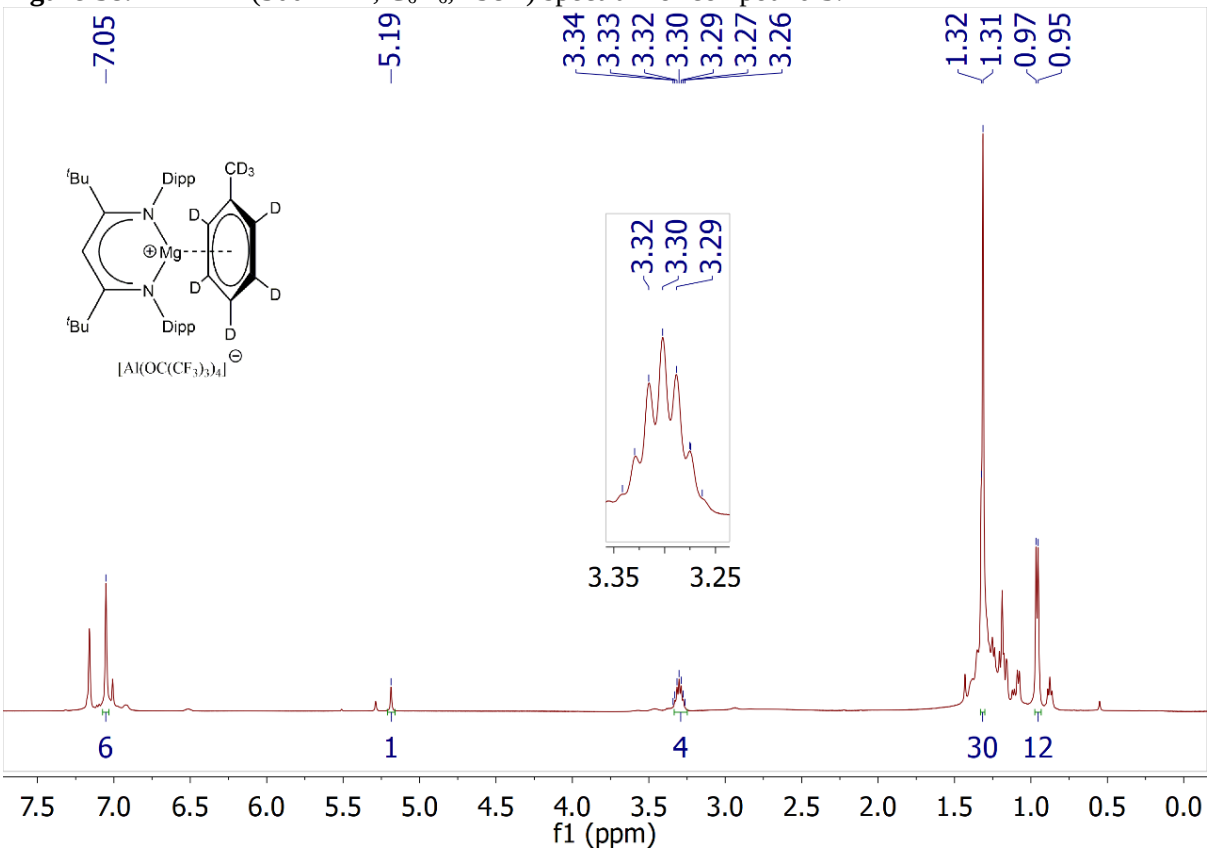


Figure S9. $^{19}F\{^{1}H\}$ NMR (470 MHz, tol-d_8, 298K) spectrum of compound **5**.

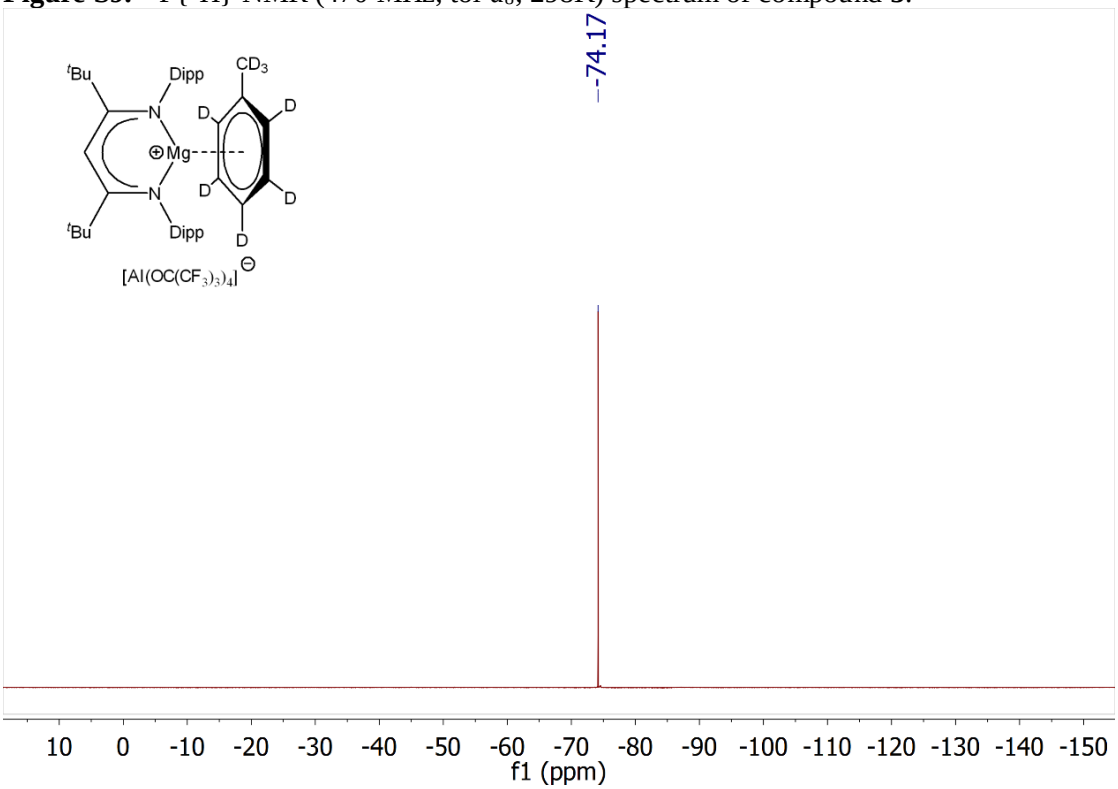


Figure S10. Ball and stick figure showing the connectivity of the cationic component of compound **5** from a preliminary X-ray diffraction analysis of a weakly diffracting sample (R_1 = 0.1769).

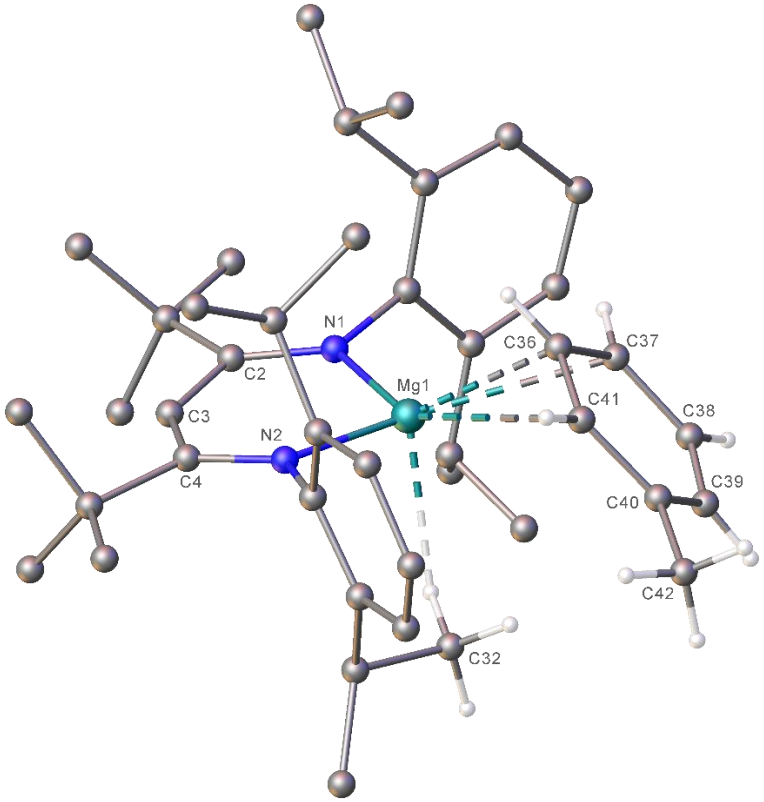


Figure S11. ^{1}H NMR (500 MHz, THF-d_8, 298K) spectrum of compound **5.THF**.

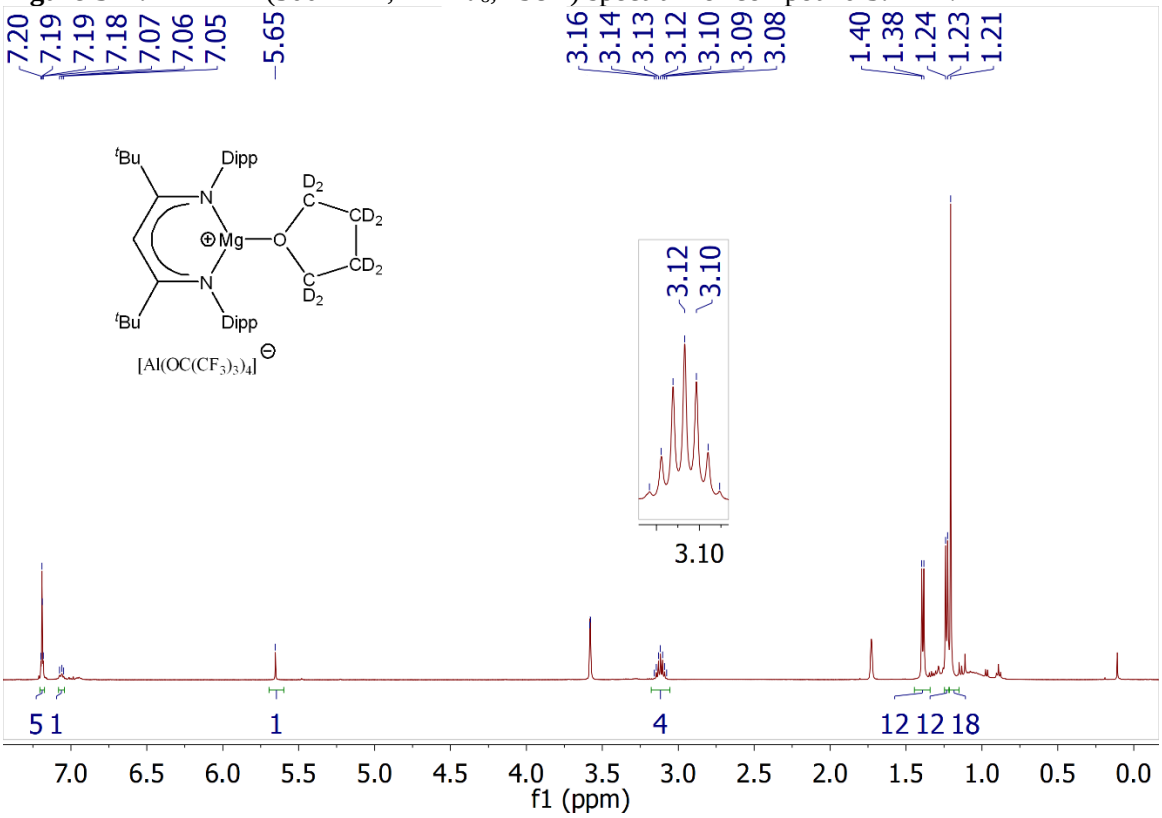


Figure S12. ^{13}C{^{1}H} NMR (126 MHz, THF-d_8, 298K) spectrum of compound **5.THF**.

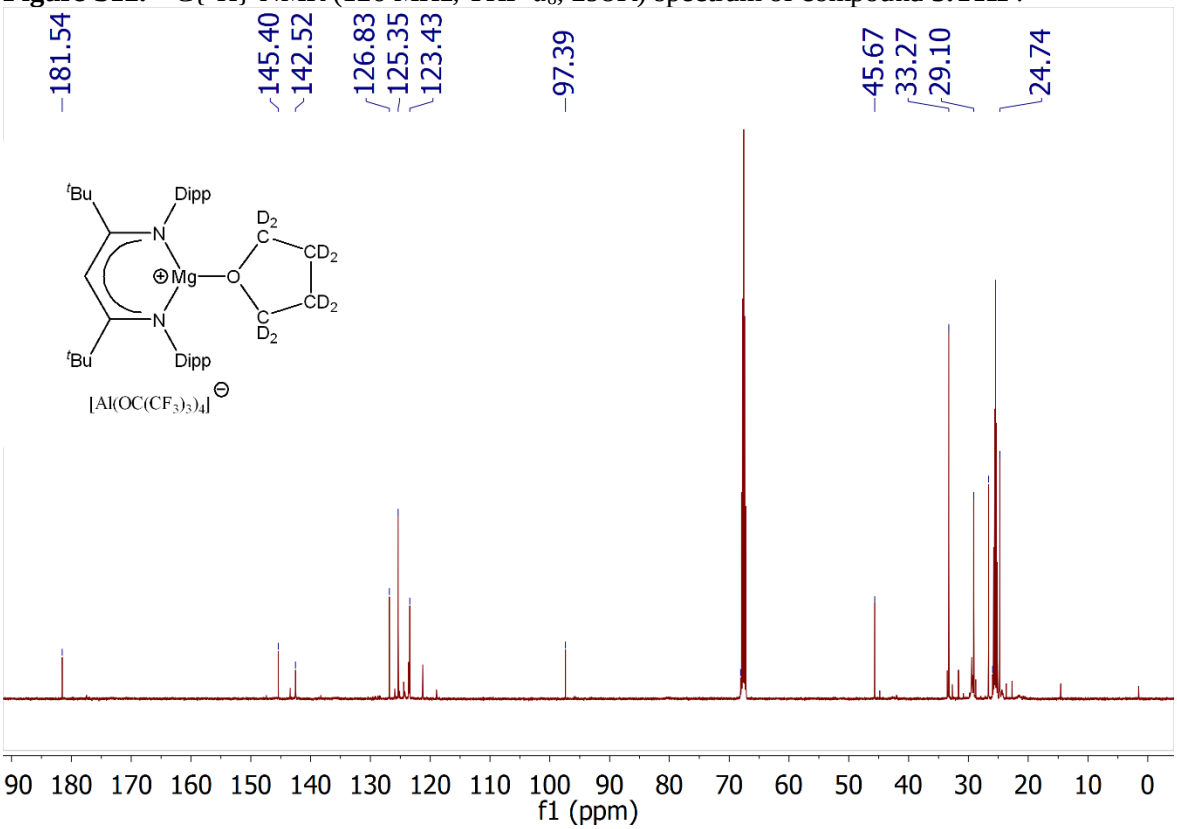


Figure S13. $^{19}F\{^{1}H\}$ NMR (470 MHz, THF-d_8, 298K) spectrum of compound **5.THF**.

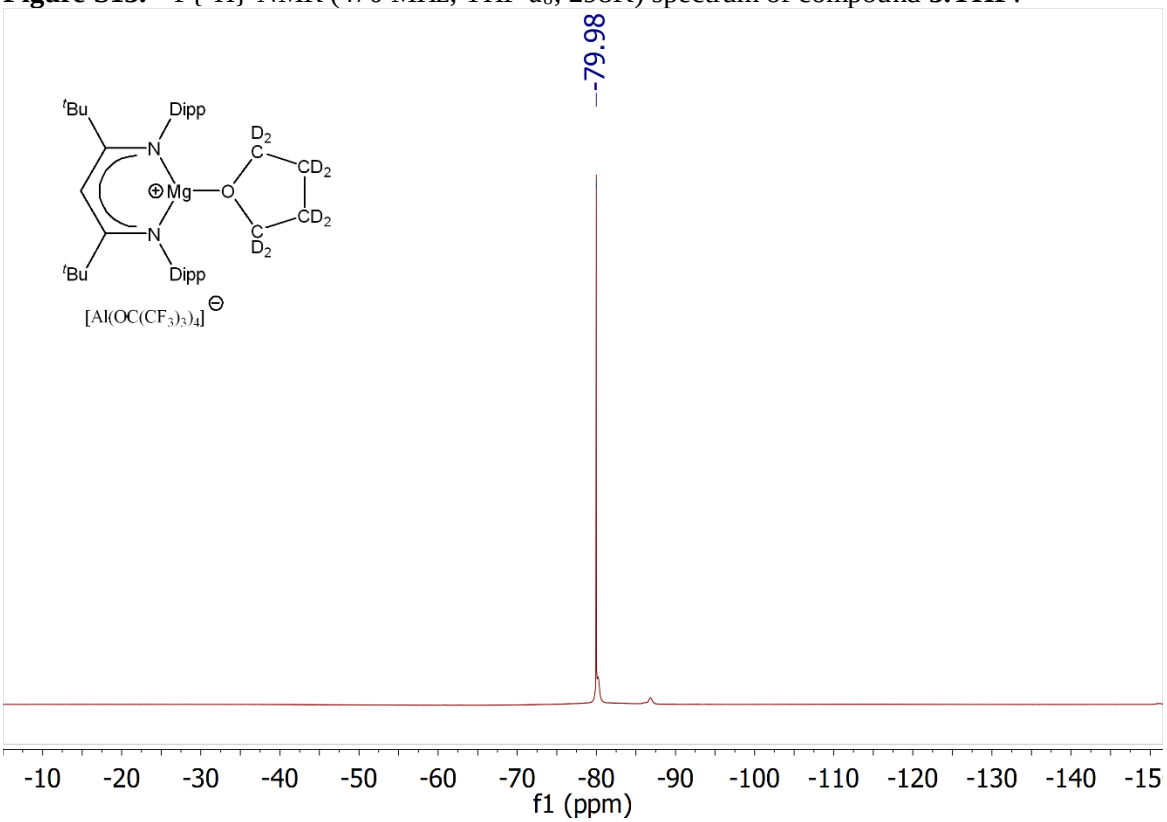


Figure S14. $^{19}F\{^{1}H\}$ NMR (470 MHz, C_6D_6-d_8, 298K) spectrum of compound **6**.

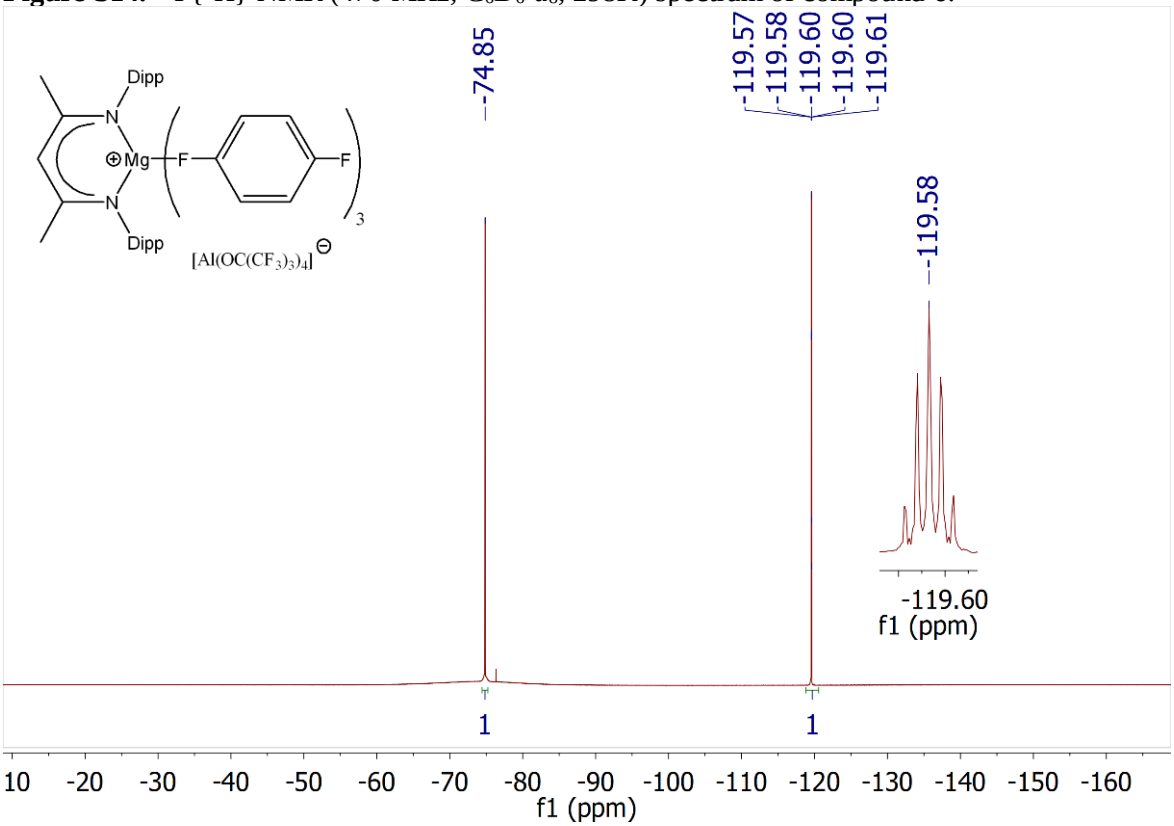


Figure S15. $^{19}F\{^{1}H\}$ NMR (470 MHz, C_6D_6, 298K) spectrum of compound **7**.

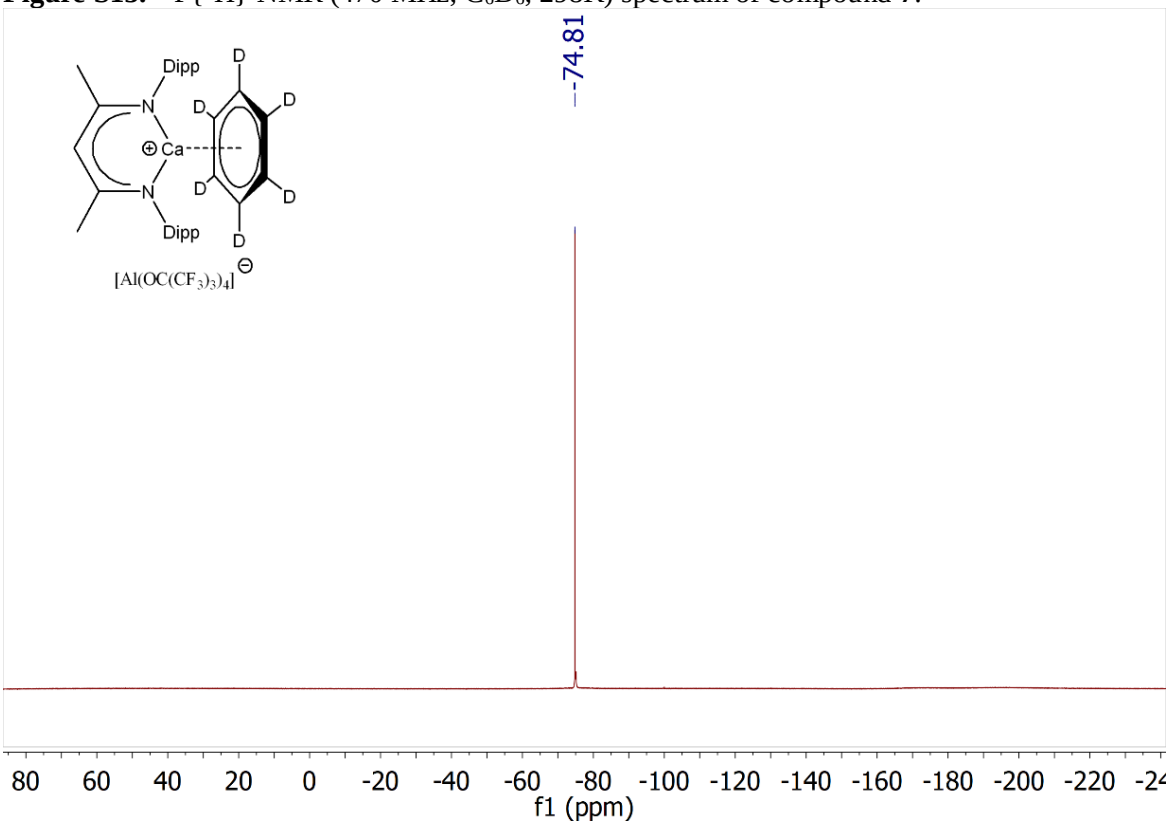


Figure S16. ^{1}H NMR (500 MHz, THF-d_8, 298K) spectrum of compound **7.THF**.

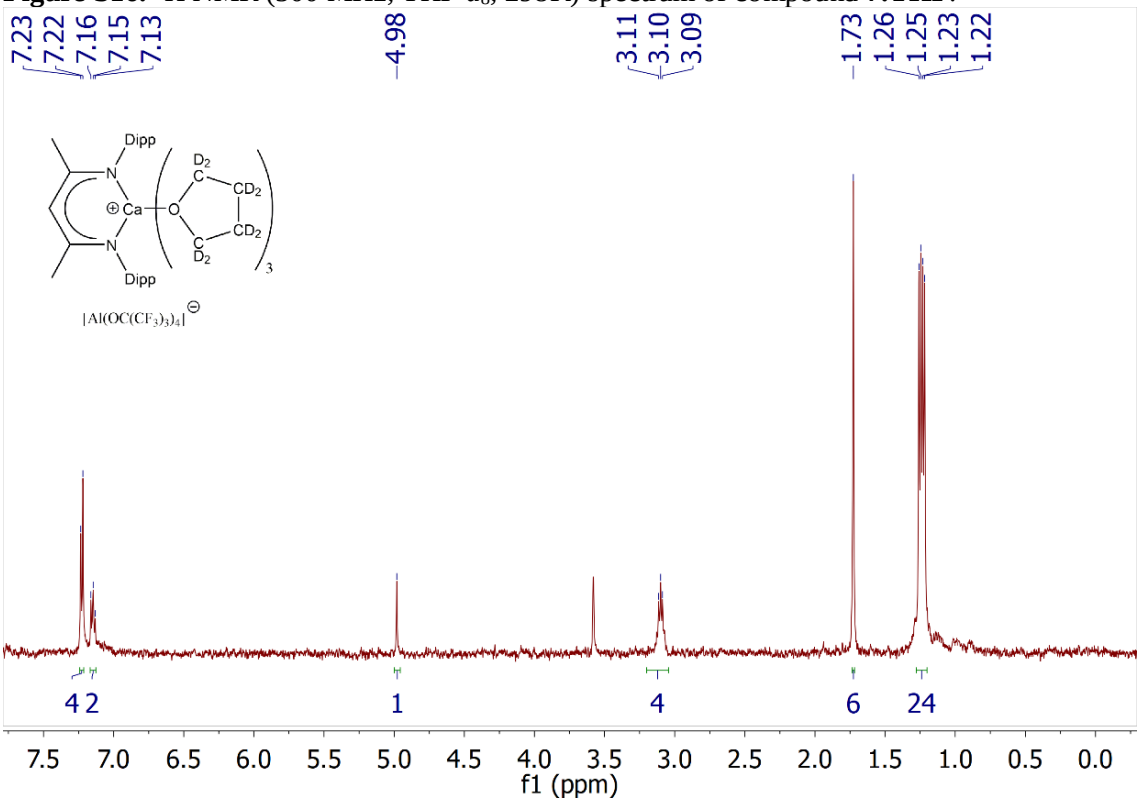


Figure S17. $^{13}C\{^{1}H\}$ NMR (126 MHz, THF-d_8, 298K) spectrum of compound **7.THF**.

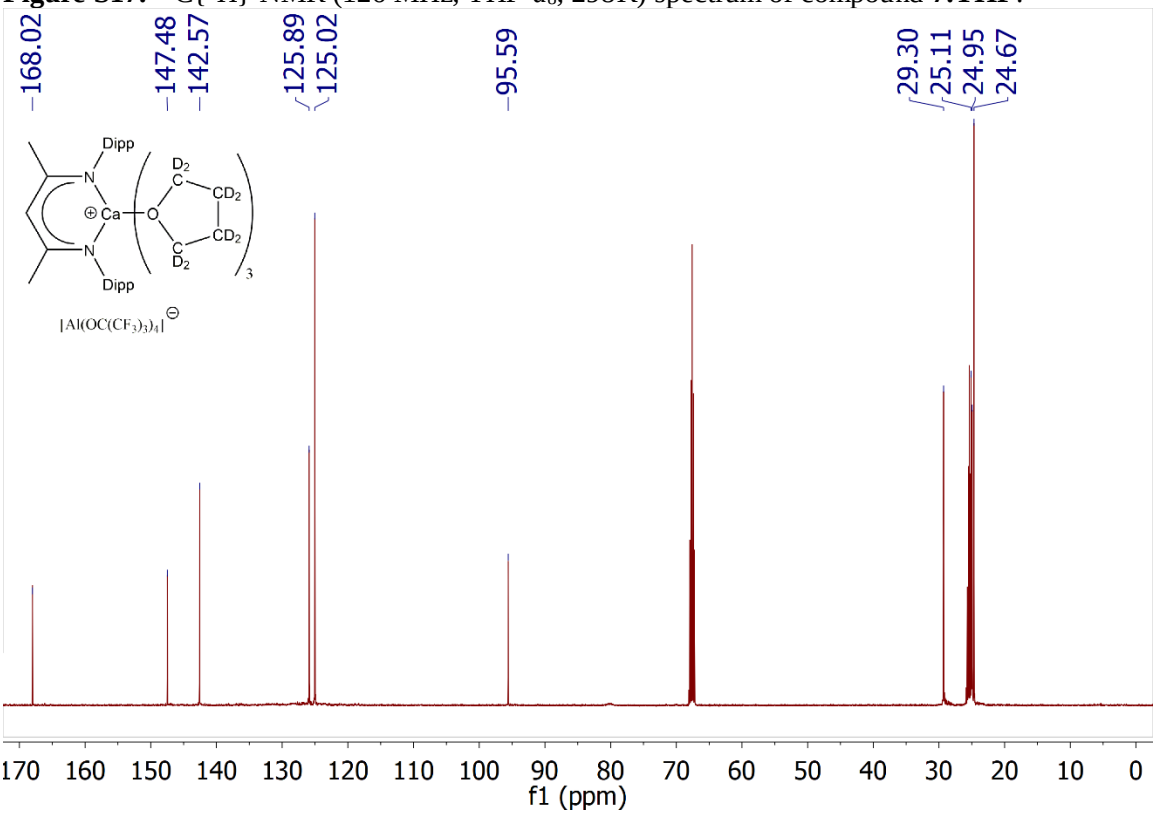


Figure S18. $^{19}F\{^{1}H\}$ NMR (470 MHz, THF-d_8, 298K) spectrum of compound **7.THF**.

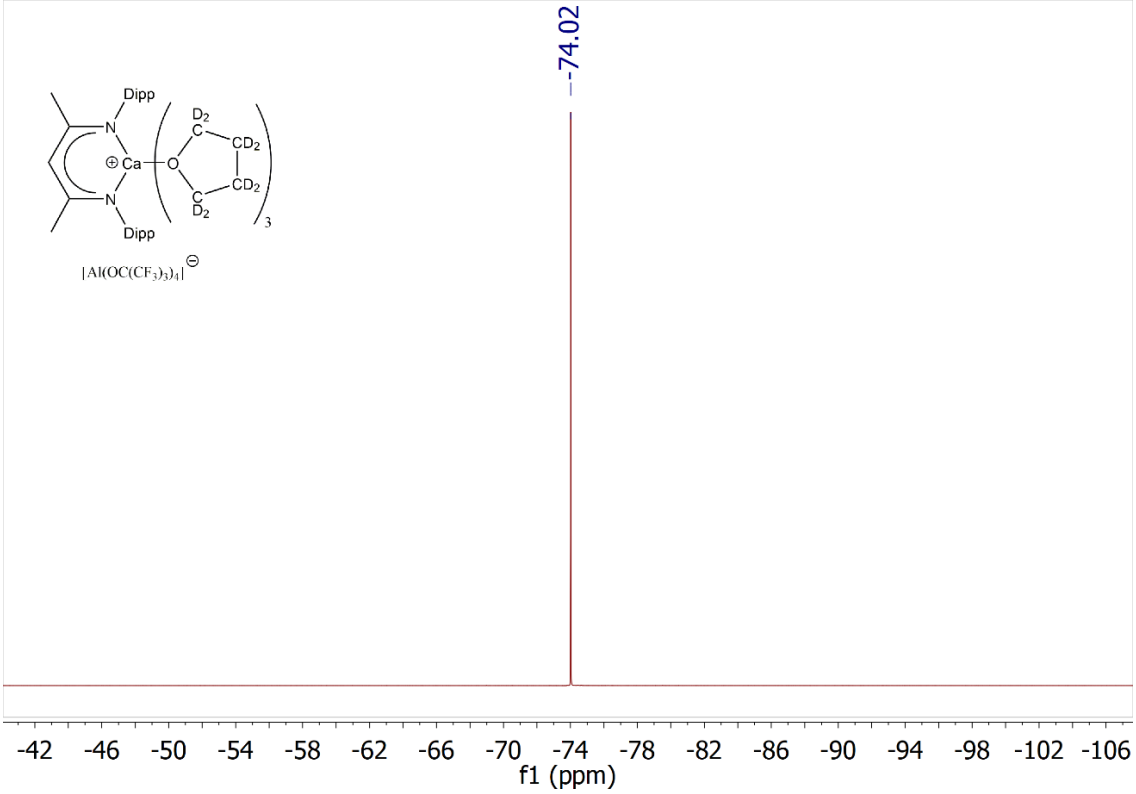


Figure S19. ORTEP representation (30% probability ellipsoids) of the cationic component of compound **7.THF**. Hydrogen atoms and the aluminate anion have been removed for clarity.

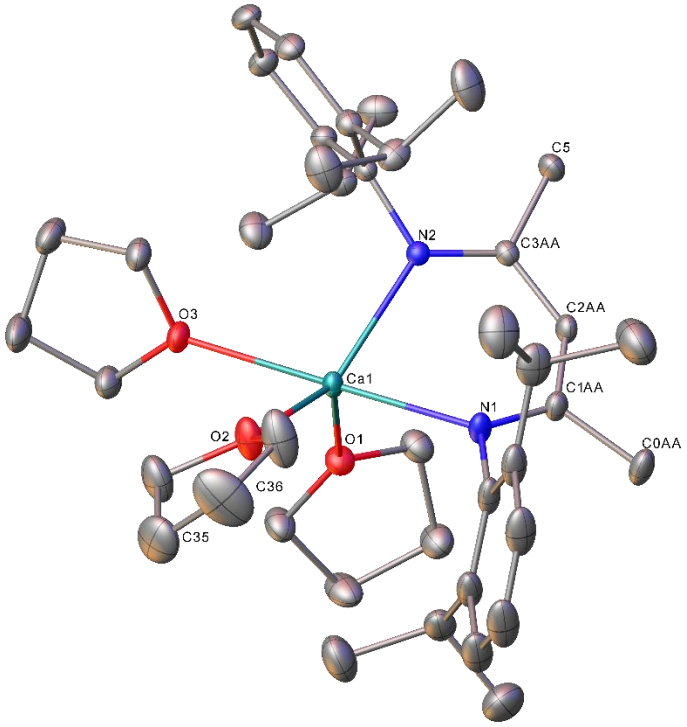


Figure S20. ^{1}H NMR (500 MHz, tol-d_8, 298K) spectrum of compound **9**.

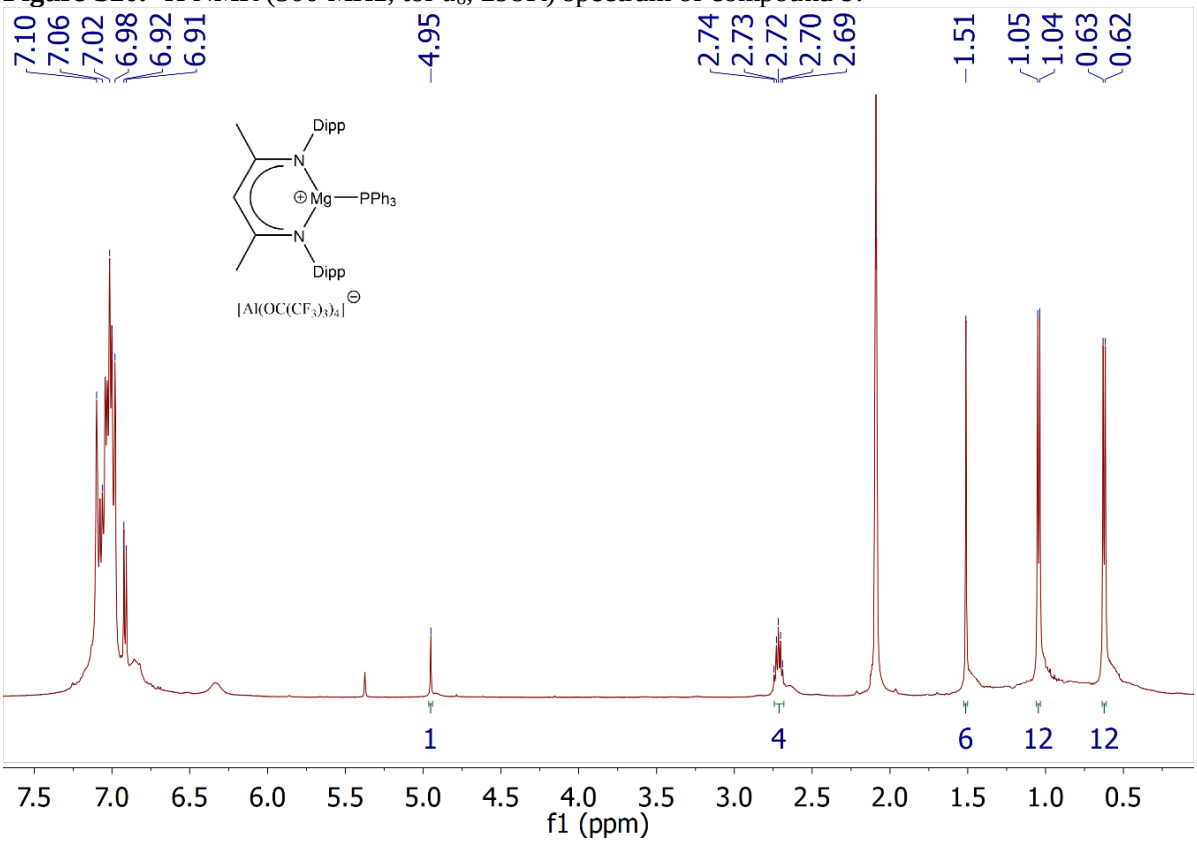


Figure S21. $^{13}C\{^{1}H\}$ NMR (126 MHz, tol-d_8, 298K) spectrum of compound **9**.

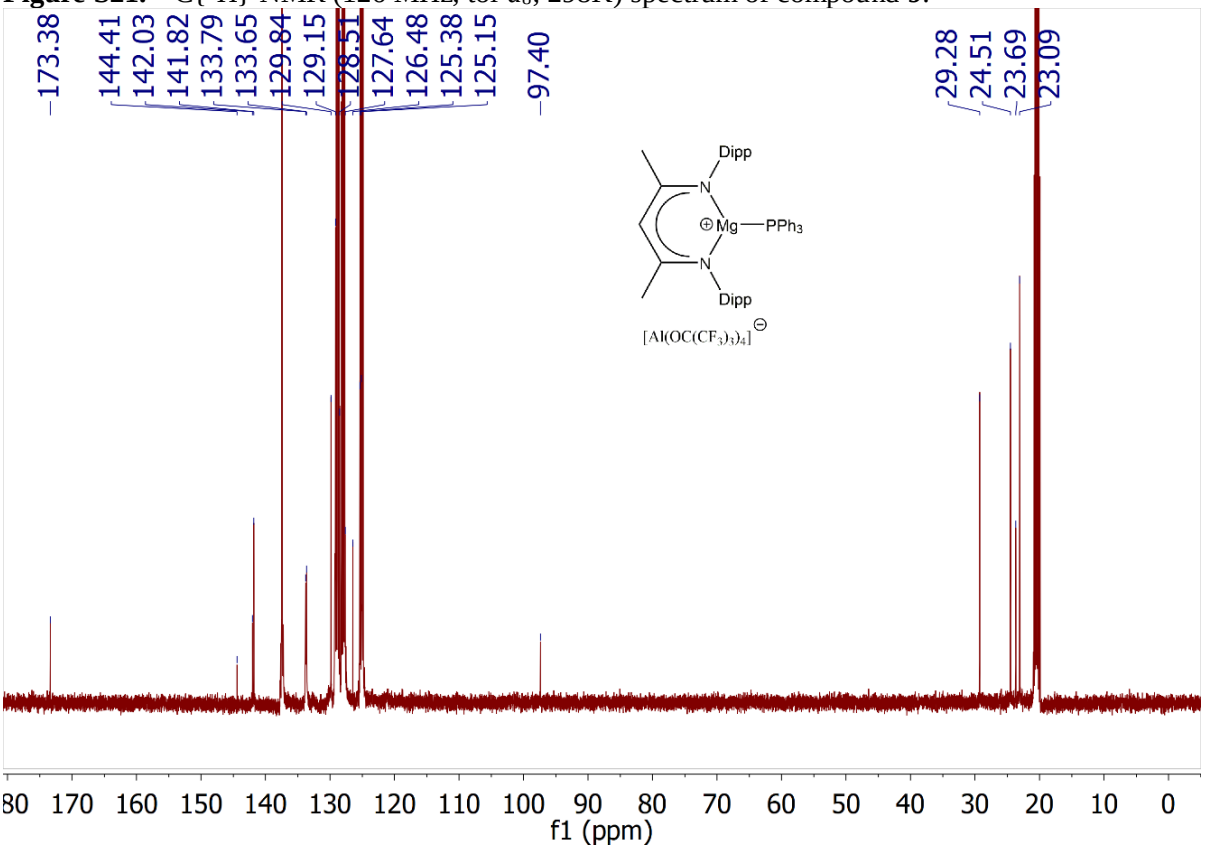


Figure S22. $^{31}P\{^{1}H\}$ NMR (125.8 MHz, tol-d_8, 298K) spectrum of compound **9**.

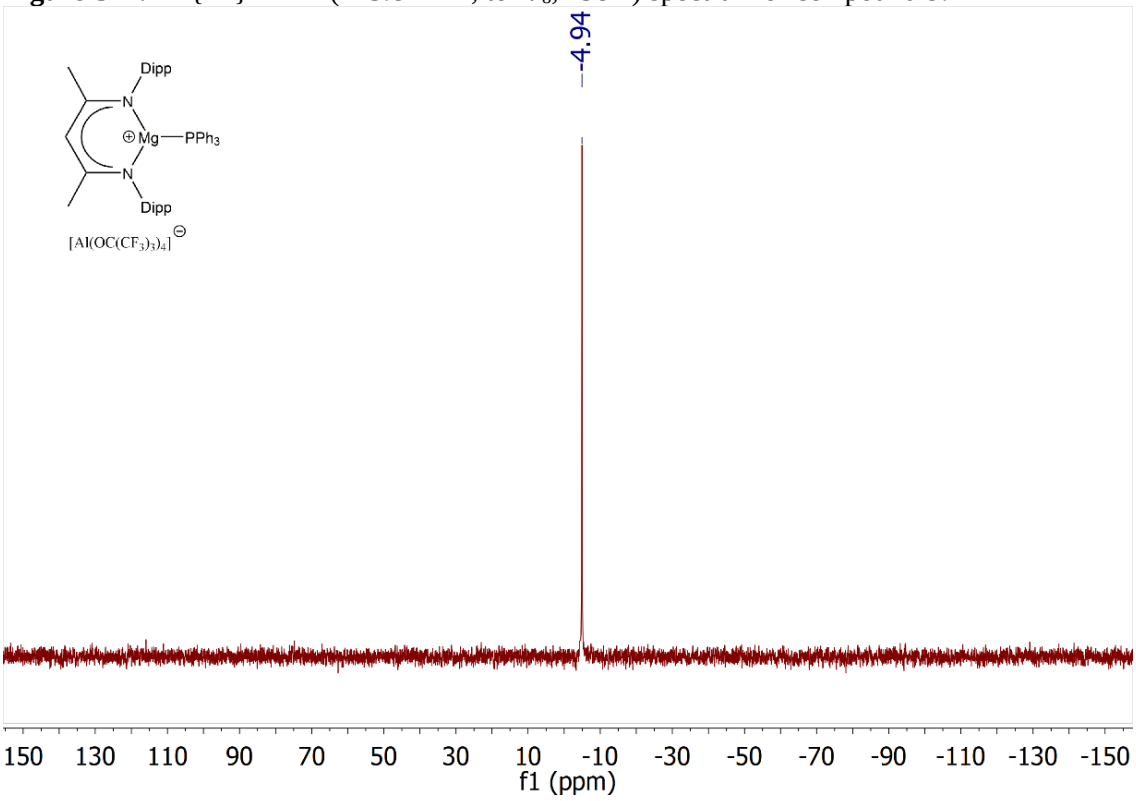


Figure S23. $^{19}F\{^{1}H\}$ NMR (470 MHz, tol-d_8, 298K) spectrum of compound **9**.

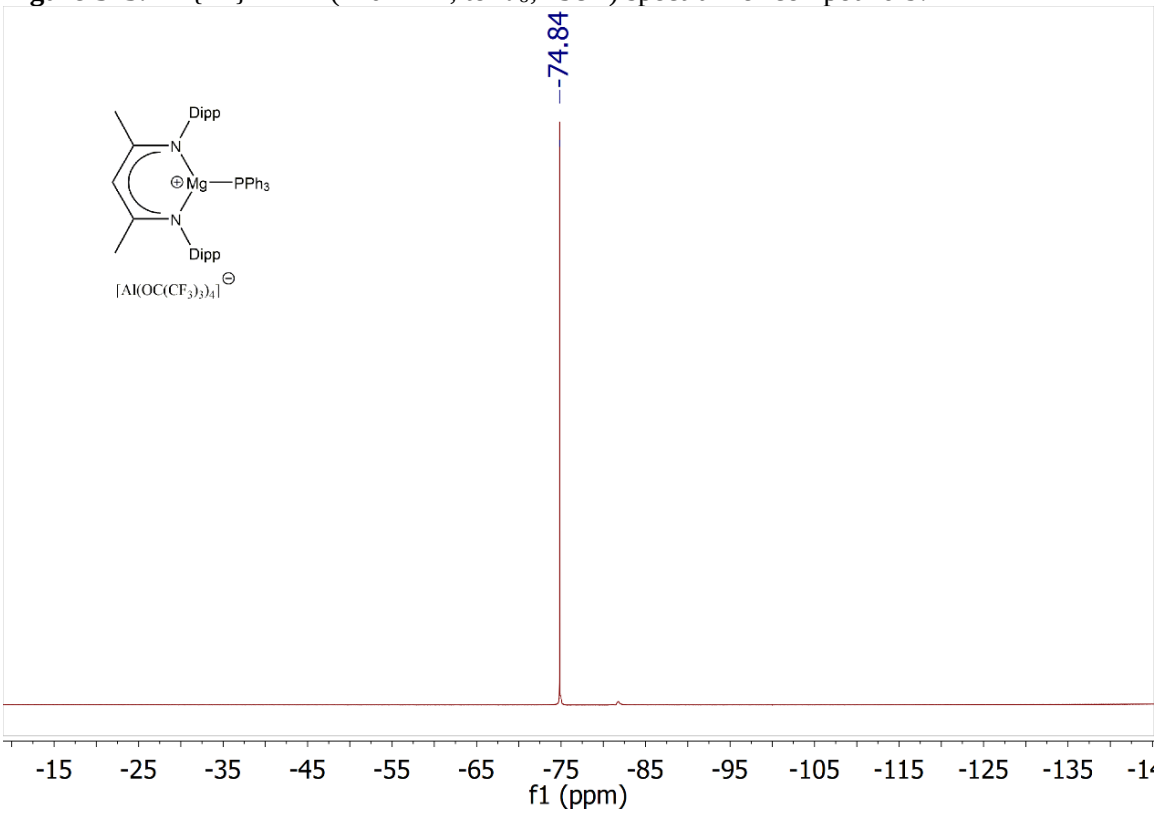


Figure S24. $^{31}P\{^{1}H\}$ NMR (125.8 MHz, tol-d_8, 298K) spectrum of compound **10**.

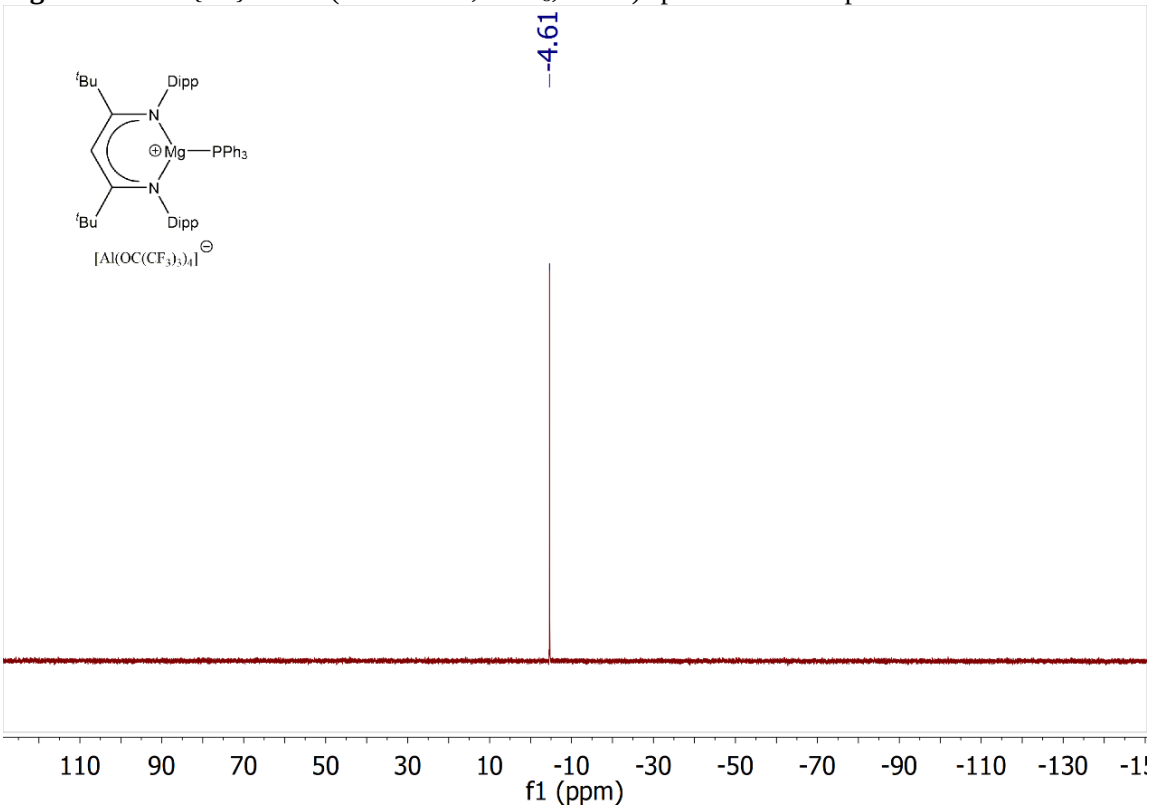


Figure S25. $^{19}F\{^{1}H\}$ NMR (470 MHz, tol-d_8, 298K) spectrum of compound **10**.

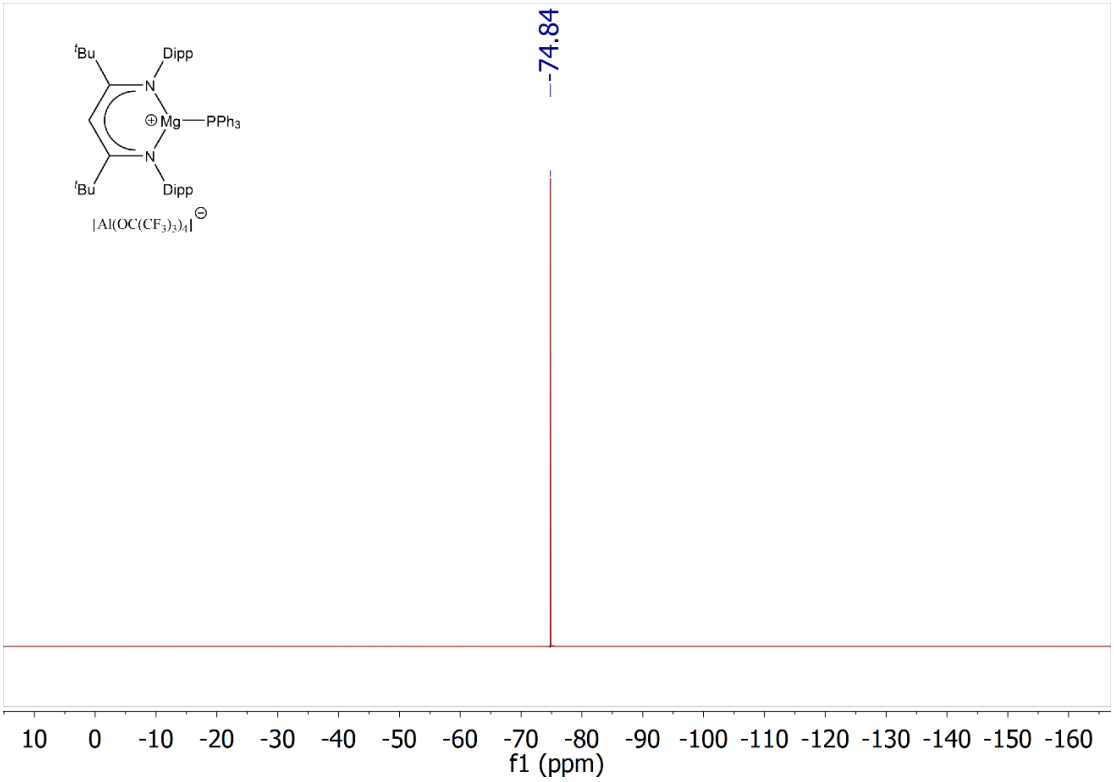


Figure S26. ^{1}H NMR (500 MHz, C_6D_6, 298K) spectrum of compound **8**.

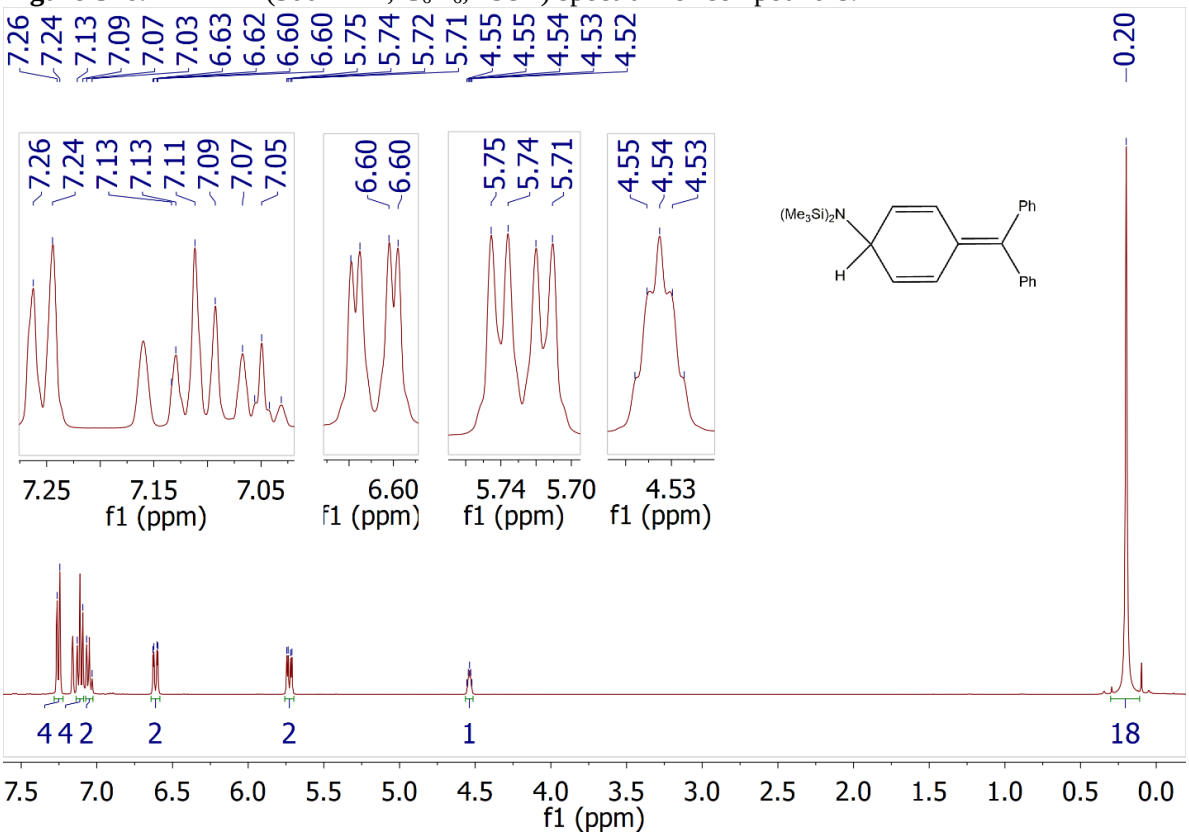


Figure S27. $^{12}C\{^{1}H\}$ NMR (126 MHz, C_6D_6, 298K) spectrum of compound **8**.

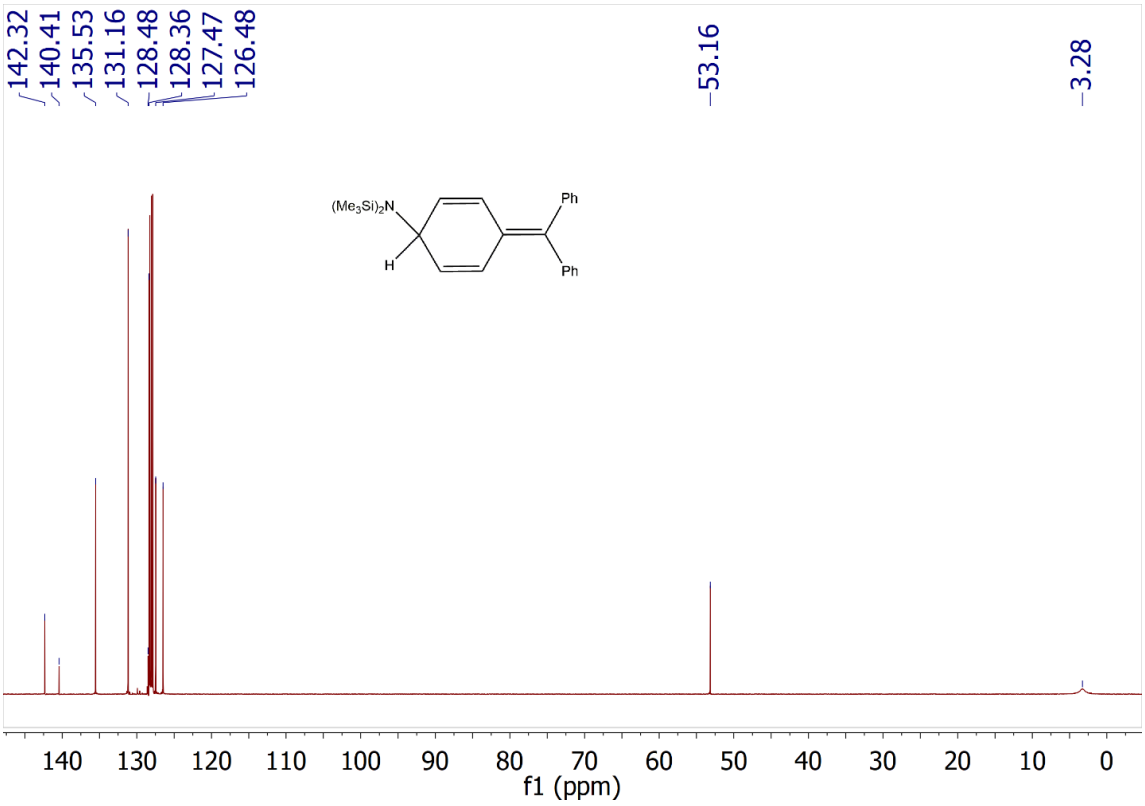
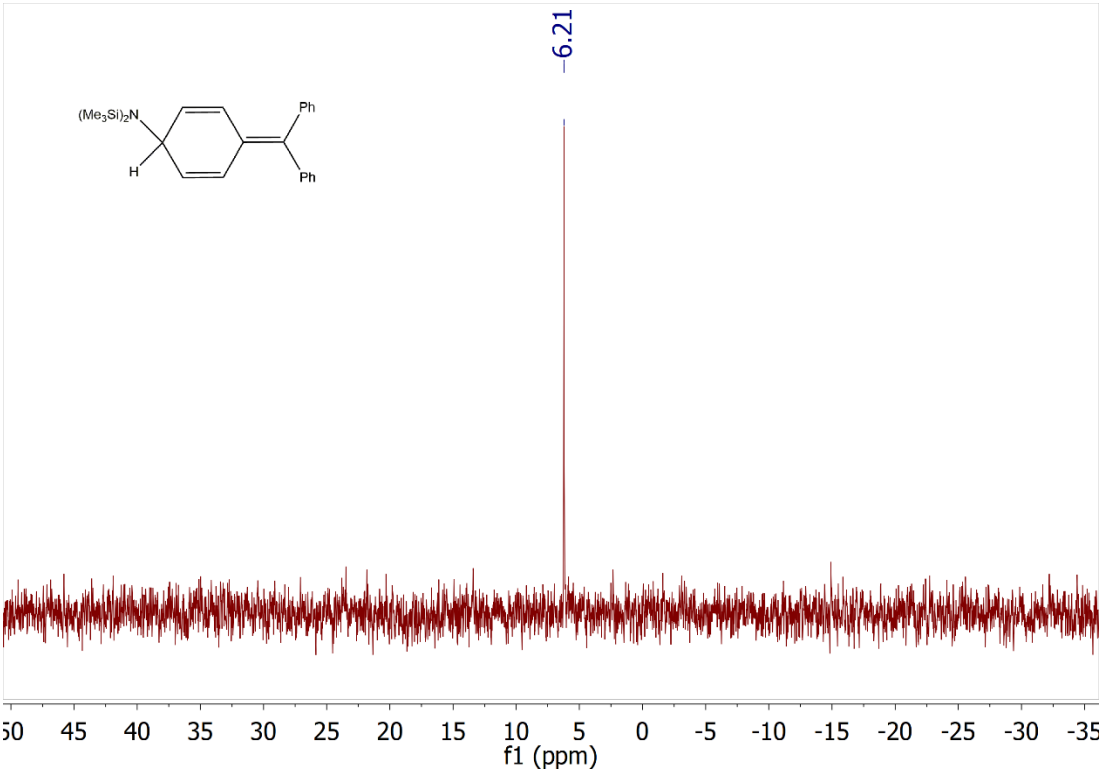


Figure S28. $^{29}Si\{^{1}H\}$ NMR (99.4 MHz, C_6D_6, 298K) spectrum of compound **8**.



Single Crystal X-Ray Diffraction Analysis

Data were collected for compounds **3**, **4**, **7**, **7.THF**, **9** and **10** on a SuperNova, Dual Cu at zero, EosS2 diffractometer, using CuKα radiation (λ = 1.54184 Å), while data for compound **6** were collected on a New Xcalibur, EosS2 diffractometer using MoKα radiation (λ = 0.71073 Å). The crystals were all kept at 150(2) K during data collection. Using Olex2,[1] the structures were solved via the olex2.solve[2] structure solution program using Charge Flipping and refined with the ShelXL[3] refinement package using Least Squares minimisation.

The asymmetric unit in **3** comprises one organometallic cation, one $[Al\{OC(CF_3)_3\}_4]^-$ anion and half of a molecule of hexane. The cation is entirely ordered, and the solvent moiety was easily modelled to take account of 50:50 disorder. Both solvent components are proximate to the crystallographic inversion center at ½, ½, ½ which serves to generate the complete hexane portions in each case. Unsurprisingly, the tert-butoxy groups in the aluminate were not immune to the disorder so typical of these large spherical anions. In this instance, the functionality based on O4 was found to be ordered, two of the $–OC(CF_3)_3$ moieties were completely disordered (60:40 ratio), and were modelled using the FragmentDB plugin for Olex2, which is a GUI-specific implementation of the invaluable DSR refinement package by Kratzert *et al*.[4]

The asymmetric unit in **4** comprises 2 cations and 2 $[Al\{OC(CF_3)_3\}_4]^-$ anions. The cations are entirely ordered. Unsurprisingly, all 8 $–OC(CF_3)_3$ moieties in the aluminates fell prey to the disorder so typical of these large spherical anions. Thus, the model incorporates 2 disordered residues per $–OC(CF_3)_3$ entity. The pairings and disorder ratios are, respectively, as follows: residues 1 and 10 (80:20 split), 2 and 15 (63:37 split), 3 and 16 (75:25 split), 4 and 11 (67:33 split), 5 and 13 (55:45 split), 6 and 9 (60:40 split), 7 and 14 (70:30 split) plus 8 and 12 (77:23 split). All were modelled using FragmentDB [4] Al-O distances were also restrained to being similar throughout. The asymmetric unit of **6** is composed of one magnesium based cation, one tetrakis perfluorobutoxy aluminum anion and one guest molecule of 1,4 difluorobenzene. Disorder is prevalent in all three moieties. It manifests in the cation as 50:50 disorder of the difluorobenzene based on F5. Mg-F and $F\text{-}C_{aromatic}$ distances affected by this disorder were restrained to being similar in the refinement and ADP similarity restraints were also included for each ligand component in addition to planarity restraints, to assist convergence. The guest solvent fluorines exhibited 65:35 disorder, and both O3 and O4 in the anion were modelled for 65:35 disorder. ADP restraints were included for O4/O4A. The residual electron density in this structure is in the anion region, and suggests, by its location that there is additional disorder in the perfluorobutoxy groups. Attempts were made to model this disorder, but they were abandoned as the level appeared to be in the region of 11% approximately and achievement of a stable model would have resulted in potential over-paramaterization.

The asymmetric unit in **7** comprises half of a cation and half of a $[Al\{OC(CF_3)_3\}_4]^-$ anion. The calcium centre, C3 C16, H3 and H16 in the former are coincident with a crystallographic 2-fold rotation axis. The orientation of the isopropyl group based on C10 is such that an interaction between Ca1 and H12C is facilitated. Although the hydrogen atoms attached to C12 have been included at calculated positions, their associated U_{iso} values indicate credibility with respect to their locations. However, a comparison between the C4-C5-C10-C12 and C4-C9-C13-C15 torsion angles [111.6 and 125.8° respectively] provides perhaps more solid proof of conformational adaptation to permit an agostic contact to H1C. Unsurprisingly, disorder was rampant in the half of the anion present in the asymmetric unit, which presents has an aluminium centre with half site-occupancy, one complete $–OC(CF_3)_3$ moiety, and two half $–OC(CF_3)_3$ fragments. The metal centre is coincident with a crystallographic mirror plane, as are the oxygen atoms and the carbons to which

they are bound in each of the two dendrite halves. All three $–CCF_3$ groups in residue 4 are disordered in a 50:50 ratio, either side of the mirror. In residue 3, one of the $–CCF_3$ units is bisected by the mirror and the fluorines therein are also disordered, while the other $–CCF_3$ moiety is disordered in a 55:45 ratio. The complete $–OC(CF_3)_3$ was also modelled for disorder, (55:45 ratio). Modelling of the Krossing moieties was achieved, as before, using FragmentDB.[4]

The structure of **7.THF** contains one cation, one anion and a small amount of diffuse solvent in the asymmetric unit. The hydrogen atoms attached to C34 in the former were located, and refined subject to being equidistant from the parent atom. The anion exhibited extensive 60:40 disorder pertaining to three of the $-OC(CF_3)_3$ groups, which was modelled using the excellent DSR (Disordered Structure Refinement) routine made available by Daniel Kratzert *et al.*[4] as Fragment DB for implementation in Olex2. Overall, the lattice contains some small voids, centered around the unit cell corners. These 'pockets' appear to contain a small amount of diffuse solvent, which was treated using the solvent mask algorithm in intrinsic to the software. Based on the electron density evident before employing the solvent mask, in addition to the analysis afforded by said algorithm, an allowance of one quarter of a molecule of THF has been made, per asymmetric unit, in the formula as presented herein. The asymmetric unit in **9** comprises one cationic magnesium complex, one one $[Al\{OC(CF_3)_3\}_4]^-$ anion and a portion of disordered solvent proximate to a crystallographic inversion centre. C29 in the cation was found to be disordered in a 65:35 ratio and, in the final least-squares, the distances of both associated fractional-occupancy carbons (from C27) were refined subject to being similar. The phenyl ring based on C42 exhibited disorder, in a similar ratio to C29. Both disordered rings were refined as rigid hexagons and with the inclusion of ADP restraints. P-C bond distances involving C42/C42A were refined with a restraint of being similar to each other. All four of the $–OC(CF_3)_3$ groups in the anion were bedeviled by disorder, and each ultimately refined over 2 positions. The associated disorder ratios (per dendrite) were 55:45, 65:35, 65:35 and 75:25. Residual electron density maxima are is in this region, and are probably indicative of disorder above that which has been (or could realistically be) modelled. The FragmentDB plugin for Olex2[4], once again proved its worth in this instance. The solvent was also disordered in this structure and there was evidence in the electron density of a portion of hexane overlaying with a toluene fragment. Ultimately, this region was treated using the solvent mask algorithm available on Olex2, after considering the data quality (from a plate-like crystal) and in preference to adding additional restraints to the existing model. Allowance for the presence of half of a molecule of toluene, per asymmetric unit, has been made in the formula as presented herein to account for solvent presence in the lattice. While the residuals for this structure are not the finest – but the model is unambiguous, and represents what can be achieved from a less than ideally shaped crystal using a modern diffractometer.

The structure of **10** contains one cation and one anion in the asymmetric unit. The hydrogen atoms attached to C34 in the former were located, and refined subject to being equidistant from the parent atom. The anion exhibited extensive 65:35 disorder of all atomic positions with the exception of the aluminium centre. As for previous structures, we are indebted to Kratzert's routine in achieving a credible disordered model for the anion.[4]

Table S1: Single Crystal X-ray Data Parameters for compounds **3**, **4**, **6**, **7** and **7**.THF.

Compound	**3**	**4**	**6**	**7**	**7.THF**
Empirical formula	$C_{55}H_{56}AlF_{36}MgN_2O_4$	$C_{102}H_{94}Al_2F_{71.98}Mg_2N_4O_8$	$C_{69}H_{57}AlF_{44}MgN_2O_4$	$C_{51}H_{47}AlCaF_{36}N_2O_4$	$C_{58}H_{66}AlCaF_{36}N_2O_{7.25}$
Formula weight	1544.30	2974.39	1865.45	1502.96	1658.18
Temperature/K	150.00(10)	150.01(10)	150.15	150.01(10)	150.00(10)
Crystal system	triclinic	monoclinic	monoclinic	monoclinic	triclinic
Space group	*P*-1	$P2_1/n$	$P2_1/n$	*C*2/*m*	*P*-1
a/Å	10.7692(2)	27.1738(4)	19.3502(3)	20.9248(10)	12.7913(3)
b/Å	15.7438(5)	16.4638(2)	21.2981(3)	24.8726(10)	15.0553(3)
c/Å	19.8667(4)	28.1140(4)	19.3981(4)	12.2476(6)	20.0086(4)
α/°	83.048(2)	90	90	90	73.743(2)
β/°	88.150(2)	103.064(2)	102.0273(16)	103.767(5)	72.551(2)
γ/°	74.609(2)	90	90	90	88.127(2)
Volume/Å^3	3223.69(14)	12252.2(3)	7818.9(2)	6191.2(5)	3523.38(14)
Z	2	4	4	4	2
ρ_{calc} g/cm^3	1.591	1.612	1.585	1.612	1.563
μ/mm^{-1}	1.756	1.824	0.187	2.431	2.228
F(000)	1562.0	5984.0	3752.0	3024.0	1686.0
Crystal size/mm^3	0.402 × 0.293 × 0.067	0.177 × 0.132 × 0.083	0.385 × 0.3555 × 0.1976	0.141 × 0.054 × 0.031	0.319 × 0.25 × 0.11
2Θ range, data collection/°	5.862 to 146.55	5.14 to 140.152	6.628 to 52.744	5.616 to 137.014	6.638 to 146.322
Reflections collected	41540	104604	62004	20064	48376
Independent reflections	12877 [R_{int} = 0.0336, R_{sigma} = 0.0319]	23244 [R_{int} = 0.0345, R_{sigma} = 0.0304]	15646 [R_{int} = 0.0438, R_{sigma} = 0.0542]	5829 [R_{int} = 0.0404, R_{sigma} = 0.0380]	14062 [R_{int}= 0.0326, R_{sigma} = 0.0302]
Data/restraints/parameters	12877/4327/1292	23244/11047/2741	15646/78/1178	5829/455/671	14062/1989/1348
Goodness-of-fit on F^2	1.206	1.239	1.049	1.027	1.016
Final R indexes [I>=2σ (I)]	R_1=0.0666, wR_2=0.1912	R_1=0.0984, wR_2=0.2891	R_1=0.0835, wR_2=0.2149	R_1=0.0764, wR_2=0.2013	R_1=0.0439, wR_2=0.1196
Final R indexes [all data]	R_1=0.0724, wR_2=0.1998	R_1=0.1327, wR_2=0.3292	R_1=0.1373, wR_2=0.2543	R_1=0.1024, wR_2=0.2255	R_1=0.0475, wR_2=0.1233
Largest peak/hole / e Å^{-3}	0.79/-0.47	1.06/-0.82	1.04/-0.52	0.53/-0.57	0.48/-0.34

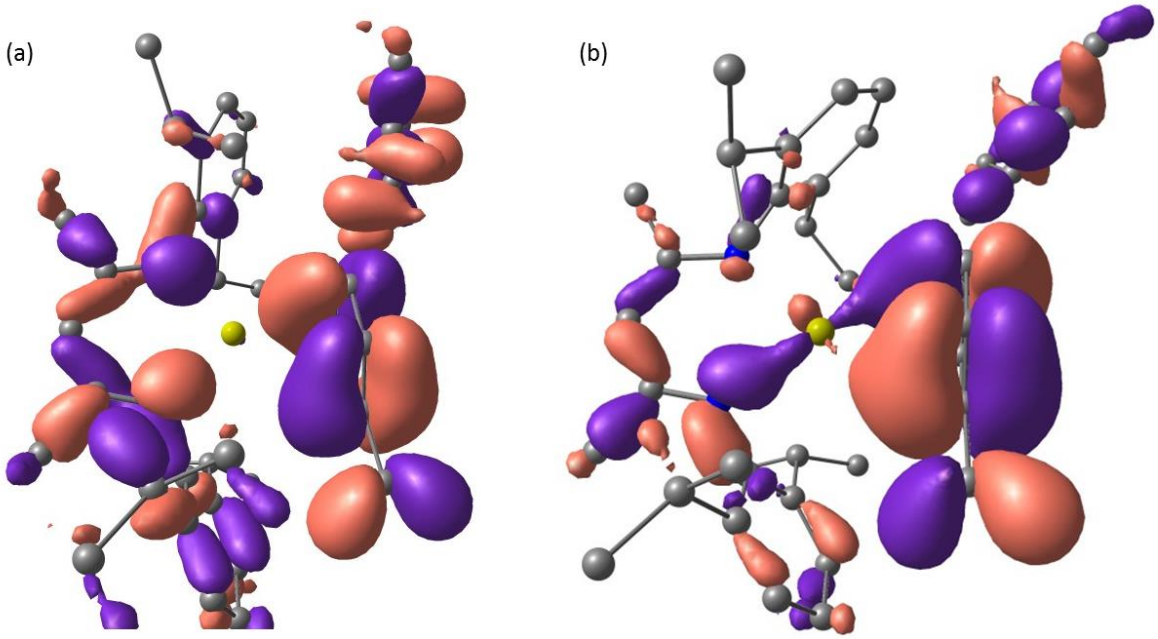
Table S2: Single Crystal X-ray Data Parameters for compounds **9** and **10**.

Compound	**9**	**10**
Empirical formula	$C_{66.5}H_{60}AlF_{36}MgN_2O_4P$	$C_{69}H_{68}AlF_{36}MgN_2O_4P$
Formula weight	1717.42	1755.51
Temperature/K	150.00(10)	150.00(10)
Crystal system	triclinic	Monoclinic
Space group	*P*-1	$P2_1/c$
a/Å	10.8232(3)	13.5387(2)
b/Å	18.2376(6)	35.7529(6)
c/Å	19.4282(4)	16.0778(3)
α/°	98.276(2)	90
β/°	93.426(2)	101.266(2)
γ/°	100.177(2)	90
Volume/Å^3	3720.95(17)	7632.5(2)
Z	2	4
ρ_{calc} g/cm^3	1.533	1.528
μ/mm^{-1}	1.785	1.753
F(000)	1738.0	3568.0
Crystal size/mm^3	0.229 × 0.111 × 0.052	0.164 × 0.107 × 0.081
2Θ range, data collection/°	6.238 to 133.2	6.126 to 146.362
Reflections collected	48476	54773
Independent reflections	13135 [R_{int} = 0.0502, R_{sigma} = 0.0408]	15127 [R_{int} = 0.0362, R_{sigma} = 0.0347]
Data/restraints/parameters	13135/3101/1512	15127/3635/1544
Goodness-of-fit on F^2	1.050	1.034
Final R indexes [I>=2σ (I)]	R_1=0.0904, wR_2=0.2642	R_1=0.0692, wR_2=0.1857
Final R indexes [all data]	R_1=0.1027, wR_2=0.2780	R_1=0.0878, wR_2=0.2017
Largest peak/hole / e Å^{-3}	0.72/-0.49	1.51/-0.61

Computational details:

Strontium, Barium and Fluorine were treated with a Stuttgart–Dresden pseudopotential in combination with their adapted basis set.[5-7] The basis set has been augmented by a set of polarization function (d for Sr and Ba).[8] For fluorine, a set of d polarization function was also added.[9] The 6-311+G(d) all-electron basis set was used for the magnesium and calcium atoms while all other atoms have been described with a 6–31G(d,p) double–ζ basis set.[10] Calculations were carried out at the DFT level of theory using the hybrid functional B3PW91.[11,12] Geometry optimisations were carried out without any symmetry restrictions, the nature of the *extrema* (*minimum* or *transition state*) was verified with analytical frequency calculations. All these computations have been performed with the Gaussian 09[13] suite of programs. Dispersion corrections were treated with the D3 version of Grimme's dispersion with Becke-Johnson damping.[14] The bonding situation was analysed using the NBO technique.[15]

Figure S29: (a) HOMO-8 of opt.**3**, the cation $[(^{Me}BDI)Mg(C_7H_8)]^+$, illustrating the electrostatic interaction between the Mg centre and the toluene π system; (b) HOMO-8 of the cation $[(^{Me}BDI)Ca(C_7H_8)]^+$, illustrating the π interaction between the toluene π-system and a 3d orbital of the calcium centre.



Cartesian coordinates of all optimised complexes:

Ca-Benzene adduct, opt.7

20	9.005087000	20.455703000	5.947888000
7	7.740448000	18.671956000	6.489435000
6	6.692458000	16.495764000	6.886169000
1	6.713523000	16.428536000	7.979969000
1	6.750444000	15.482936000	6.485071000
1	5.730075000	16.936966000	6.612702000
6	7.838891000	17.350478000	6.414398000
6	9.005014000	16.717809000	5.947738000
1	9.004985000	15.634324000	5.947680000
6	6.575076000	19.400534000	6.809832000

6	5.696858000	19.775784000	5.756453000
6	4.711945000	20.729459000	6.019403000
1	4.025059000	21.022566000	5.232530000
6	4.577906000	21.301799000	7.283737000
1	3.802701000	22.039944000	7.465752000
6	5.411674000	20.894217000	8.317745000
1	5.271671000	21.307980000	9.312881000
6	6.413794000	19.941166000	8.107260000
6	5.836103000	19.132086000	4.384183000
1	6.034559000	18.066163000	4.546505000
6	4.570751000	19.239431000	3.533537000
1	3.690214000	18.884056000	4.075816000
1	4.678937000	18.632642000	2.630349000
1	4.380731000	20.268962000	3.211332000
6	7.039126000	19.686895000	3.606879000
1	7.021895000	20.783058000	3.585093000
1	7.027445000	19.347093000	2.567202000
1	7.983203000	19.313670000	4.022779000
6	7.261169000	19.455567000	9.266805000
1	8.005602000	18.762766000	8.860098000
6	6.398758000	18.679044000	10.270414000
1	5.653298000	19.331627000	10.736172000
1	7.020026000	18.256523000	11.066099000
1	5.862532000	17.861442000	9.781326000
6	8.005881000	20.597553000	9.964165000
1	8.657227000	21.138762000	9.270043000
1	8.632134000	20.212996000	10.774509000
1	7.311474000	21.322880000	10.400704000
7	10.269666000	18.671945000	5.406211000
6	11.317542000	16.495738000	5.009242000
1	11.296446000	16.428633000	3.915435000
1	11.259509000	15.482869000	5.410229000
1	12.279959000	16.936854000	5.282730000
6	10.171169000	17.350465000	5.481138000
6	11.435079000	19.400499000	5.085909000
6	12.313289000	19.775759000	6.139304000
6	13.298175000	20.729459000	5.876361000
1	13.985038000	21.022590000	6.663246000
6	13.432238000	21.301770000	4.612016000
1	14.207446000	22.039911000	4.429998000
6	12.598516000	20.894140000	3.577990000
1	12.738565000	21.307854000	2.582840000
6	11.596390000	19.941096000	3.788477000
6	12.174102000	19.132093000	7.511594000
1	11.975885000	18.066118000	7.349335000
6	13.439412000	19.239777000	8.362252000
1	14.320035000	18.884572000	7.820000000
1	13.331351000	18.633016000	9.265472000
1	13.629199000	20.269371000	8.684394000
6	10.970948000	19.686691000	8.288849000
1	10.987882000	20.782861000	8.310518000

1	10.982732000	19.347004000	9.328562000
1	10.026963000	19.313160000	7.873014000
6	10.749114000	19.455352000	2.628917000
1	10.004718000	18.762519000	3.035638000
6	11.611636000	18.678805000	1.625422000
1	12.357076000	19.331402000	1.159653000
1	10.990446000	18.256170000	0.829738000
1	12.147890000	17.861284000	2.114614000
6	10.004343000	20.597210000	1.931413000
1	9.352867000	21.138380000	2.625440000
1	9.378211000	20.212533000	1.121033000
1	10.698709000	21.322591000	1.494901000
6	9.445940000	23.061898000	7.274656000
1	9.787348000	23.077873000	8.305135000
6	10.379394000	23.054006000	6.229244000
1	11.443747000	23.037383000	6.439498000
6	9.937885000	23.054838000	4.900675000
1	10.663237000	23.036837000	4.094584000
6	8.564360000	23.062025000	4.621450000
1	8.222954000	23.078095000	3.590973000
6	7.630905000	23.054084000	5.666859000
1	6.566553000	23.037513000	5.456598000
6	8.072413000	23.054789000	6.995429000
1	7.347055000	23.036758000	7.801515000

Mg-Toluene adduct

12	9.671131000	4.622868000	14.466311000
7	10.462564000	3.501836000	15.910841000
7	9.917066000	3.319338000	12.972126000
6	10.877540000	2.246287000	15.678793000
6	10.823777000	1.609293000	14.429293000
1	11.201834000	0.594590000	14.422361000
6	10.440517000	2.103833000	13.170172000
6	11.464272000	1.442448000	16.813073000
1	12.078646000	2.062654000	17.468646000
1	12.067234000	0.617506000	16.432618000
1	10.665776000	1.018009000	17.430195000
6	10.663826000	1.188861000	11.990804000
1	11.022487000	1.743020000	11.120830000
1	9.726562000	0.706324000	11.694200000
1	11.380732000	0.405161000	12.236819000
6	10.680721000	4.092408000	17.191497000
6	9.819835000	3.801139000	18.266798000
6	10.046534000	4.444611000	19.487545000
1	9.400808000	4.227854000	20.332670000
6	11.082328000	5.360193000	19.635571000
1	11.243939000	5.848629000	20.591580000
6	11.915678000	5.649841000	18.557587000
1	12.722922000	6.362367000	18.688606000
6	11.737736000	5.022215000	17.322186000
6	8.652380000	2.843446000	18.107475000

1	8.831574000	2.241190000	17.212775000
6	8.503999000	1.885827000	19.292424000
1	8.190446000	2.407876000	20.201783000
1	9.443793000	1.371056000	19.512724000
1	7.742969000	1.130651000	19.074801000
6	7.350772000	3.614580000	17.863727000
1	6.511921000	2.926450000	17.719335000
1	7.429658000	4.243301000	16.970548000
1	7.115363000	4.263925000	18.713168000
6	12.674895000	5.295142000	16.155470000
1	12.062115000	5.329328000	15.239527000
6	13.420717000	6.626194000	16.251997000
1	12.758861000	7.473968000	16.453272000
1	13.949578000	6.824421000	15.315163000
1	14.174951000	6.603456000	17.044643000
6	13.685387000	4.157363000	15.954598000
1	14.373875000	4.402985000	15.140028000
1	13.197688000	3.215204000	15.702523000
1	14.275983000	4.009230000	16.863959000
6	9.690128000	3.782032000	11.641614000
6	8.524947000	3.406493000	10.943999000
6	8.348549000	3.898875000	9.648120000
1	7.469268000	3.612453000	9.081920000
6	9.286177000	4.745345000	9.065721000
1	9.136679000	5.105365000	8.052948000
6	10.413368000	5.135128000	9.781020000
1	11.131306000	5.804246000	9.318855000
6	10.633955000	4.669030000	11.080168000
6	7.485455000	2.509093000	11.595951000
1	8.011467000	1.813766000	12.256882000
6	6.684542000	1.678285000	10.593591000
1	6.014479000	2.300316000	9.991545000
1	6.060557000	0.952934000	11.123421000
1	7.341113000	1.129798000	9.911899000
6	6.545383000	3.326112000	12.489035000
1	7.097325000	3.802905000	13.306065000
1	5.781127000	2.684917000	12.939309000
1	6.041001000	4.107522000	11.911872000
6	11.875012000	5.074412000	11.857907000
1	11.602509000	5.104895000	12.925774000
6	12.399595000	6.461872000	11.489541000
1	12.850637000	6.470655000	10.492694000
1	13.180833000	6.767504000	12.192505000
1	11.610185000	7.219837000	11.496706000
6	12.990134000	4.029076000	11.737668000
1	13.883295000	4.357699000	12.278337000
1	13.262046000	3.883381000	10.687567000
1	12.685986000	3.065325000	12.149761000
6	10.165839000	7.208676000	14.296503000
1	11.142414000	7.511501000	13.932462000
6	9.883756000	7.258080000	15.664874000

1	10.645885000	7.586977000	16.362296000
6	8.624000000	6.887485000	16.168792000
6	7.659490000	6.423569000	15.257286000
1	6.681391000	6.121944000	15.620363000
6	7.928903000	6.378545000	13.880318000
1	7.164527000	6.052627000	13.185006000
6	9.181056000	6.778537000	13.389100000
1	9.376150000	6.751219000	12.322887000
6	8.332899000	7.026919000	17.630334000
1	8.355230000	8.085733000	17.909924000
1	9.086743000	6.510562000	18.229995000
1	7.350376000	6.629210000	17.885998000

Ca Toluene adduct

20	9.508806000	4.573504000	14.522269000
7	10.784598000	3.197627000	15.778320000
7	10.283281000	3.047901000	13.062568000
6	11.438248000	2.055963000	15.581707000
6	11.519358000	1.440284000	14.319059000
1	12.076923000	0.512487000	14.268571000
6	10.969341000	1.913165000	13.116884000
6	12.098067000	1.352810000	16.740950000
1	12.367677000	2.049903000	17.537079000
1	12.989688000	0.811932000	16.417766000
1	11.406364000	0.617881000	17.168076000
6	11.190842000	1.124271000	11.853179000
1	11.892231000	1.654580000	11.198797000
1	10.259023000	1.015342000	11.290049000
1	11.599148000	0.134469000	12.060304000
6	10.728551000	3.871253000	17.019752000
6	9.788885000	3.501844000	18.009155000
6	9.682028000	4.290342000	19.158031000
1	8.975765000	4.006049000	19.933127000
6	10.458748000	5.431633000	19.326096000
1	10.362635000	6.028340000	20.228013000
6	11.362286000	5.806175000	18.334721000
1	11.967032000	6.696535000	18.473429000
6	11.514677000	5.044306000	17.175029000
6	8.890075000	2.294745000	17.827408000
1	9.205456000	1.780517000	16.914447000
6	9.011064000	1.305911000	18.991060000
1	8.643688000	1.739643000	19.926429000
1	10.050349000	1.006611000	19.150787000
1	8.421346000	0.406113000	18.791385000
6	7.433317000	2.730214000	17.631241000
1	6.788530000	1.865146000	17.447980000
1	7.328728000	3.412775000	16.779615000
1	7.054363000	3.251218000	18.516320000
6	12.533199000	5.417605000	16.112134000
1	12.129529000	5.097683000	15.139019000
6	12.831473000	6.914167000	16.034857000
1	11.919235000	7.515750000	15.976822000

1	13.438622000	7.129685000	15.150985000
1	13.399394000	7.258281000	16.904692000
6	13.831966000	4.621547000	16.297853000
1	14.562844000	4.893991000	15.530134000
1	13.653898000	3.547180000	16.228179000
1	14.269447000	4.833355000	17.278661000
6	9.608701000	3.539104000	11.926772000
6	8.241094000	3.202380000	11.748135000
6	7.509538000	3.900008000	10.783153000
1	6.464588000	3.659136000	10.620180000
6	8.104889000	4.888762000	10.003458000
1	7.519932000	5.413812000	9.255454000
6	9.456561000	5.178089000	10.157576000
1	9.917841000	5.920744000	9.515441000
6	10.229752000	4.515443000	11.113402000
6	7.620842000	2.076687000	12.569500000
1	8.326133000	1.236914000	12.538233000
6	6.292172000	1.579095000	12.001932000
1	5.499627000	2.329162000	12.101477000
1	5.967055000	0.687765000	12.545427000
1	6.379785000	1.314722000	10.944628000
6	7.447896000	2.436436000	14.055799000
1	8.404280000	2.389377000	14.591785000
1	6.797569000	1.716569000	14.560516000
1	6.966742000	3.417152000	14.172678000
6	11.704828000	4.826172000	11.290341000
1	12.163029000	3.958399000	11.774963000
6	11.915703000	6.022167000	12.223951000
1	11.431804000	6.921746000	11.831493000
1	12.980805000	6.237014000	12.353753000
1	11.514188000	5.834259000	13.227503000
6	12.422081000	5.061984000	9.959073000
1	13.500358000	5.148638000	10.121708000
1	12.091796000	5.987411000	9.477270000
1	12.245942000	4.237303000	9.263026000
6	9.381153000	7.450285000	14.409166000
1	10.322392000	7.964576000	14.241929000
6	8.941998000	7.210975000	15.715207000
1	9.549549000	7.525224000	16.558908000
6	7.713066000	6.568345000	15.961057000
6	6.962912000	6.137998000	14.852487000
1	6.013362000	5.636571000	15.019824000
6	7.402401000	6.368101000	13.541245000
1	6.814633000	6.023264000	12.696704000
6	8.610948000	7.031811000	13.315141000
1	8.947177000	7.212571000	12.300930000
6	7.220900000	6.384223000	17.366040000
1	6.910807000	7.350197000	17.779411000
1	8.008067000	5.985790000	18.011605000
1	6.362048000	5.711914000	17.406980000

Sr Toluene adduct

38	9.604885000	4.526500000	14.595120000
7	10.991813000	3.112534000	15.927772000
7	10.524475000	2.827706000	13.189629000
6	11.760067000	2.039405000	15.764214000
6	11.935581000	1.414714000	14.517113000
1	12.581313000	0.552576000	14.495500000
6	11.347264000	1.788129000	13.295433000
6	12.463310000	1.457845000	16.963289000
1	13.026636000	2.231858000	17.493254000
1	13.143254000	0.651442000	16.686094000
1	11.728513000	1.064497000	17.674544000
6	11.659669000	0.976233000	12.065953000
1	12.139530000	1.603209000	11.306878000
1	10.736050000	0.594012000	11.618092000
1	12.316545000	0.134362000	12.287997000
6	10.809404000	3.749526000	17.177716000
6	9.691546000	3.407465000	17.978793000
6	9.416407000	4.167504000	19.117170000
1	8.566897000	3.904332000	19.741238000
6	10.212803000	5.252276000	19.468856000
1	9.987114000	5.828713000	20.360987000
6	11.303520000	5.591528000	18.673364000
1	11.925863000	6.436349000	18.955279000
6	11.624291000	4.856707000	17.527457000
6	8.790330000	2.250084000	17.592737000
1	9.245251000	1.751386000	16.730603000
6	8.656236000	1.217793000	18.716577000
1	8.154880000	1.639950000	19.593431000
1	9.636477000	0.855073000	19.037538000
1	8.068536000	0.358346000	18.379907000
6	7.409559000	2.761798000	17.164054000
1	6.770908000	1.943566000	16.818412000
1	7.474938000	3.492697000	16.345179000
1	6.900532000	3.267115000	17.991148000
6	12.816137000	5.252335000	16.675959000
1	12.944280000	4.480730000	15.910081000
6	12.559941000	6.584452000	15.961285000
1	11.652440000	6.555942000	15.341173000
1	13.392248000	6.848146000	15.302087000
1	12.421450000	7.398904000	16.679873000
6	14.110868000	5.319881000	17.492007000
1	14.964918000	5.522541000	16.838778000
1	14.297455000	4.376548000	18.012370000
1	14.073906000	6.113677000	18.244939000
6	9.908308000	3.240068000	11.983893000
6	8.580245000	2.827390000	11.707781000
6	7.881911000	3.455030000	10.673491000
1	6.864320000	3.144245000	10.453645000
6	8.472327000	4.456402000	9.908743000
1	7.912948000	4.929672000	9.106093000
6	9.789936000	4.830185000	10.161899000

1	10.253407000	5.599005000	9.552212000
6	10.527951000	4.234308000	11.188213000
6	7.936751000	1.711225000	12.512650000
1	8.702657000	1.311248000	13.185271000
6	7.460784000	0.566477000	11.610615000
1	6.648574000	0.884427000	10.948474000
1	7.089624000	-0.267567000	12.214155000
1	8.275091000	0.196261000	10.981452000
6	6.782192000	2.226091000	13.380262000
1	7.104918000	3.008810000	14.080116000
1	6.350872000	1.418944000	13.980156000
1	5.983317000	2.655929000	12.766584000
6	11.957716000	4.663044000	11.452275000
1	12.381054000	3.968991000	12.184557000
6	12.005152000	6.065419000	12.066955000
1	11.554079000	6.804647000	11.397113000
1	13.034140000	6.373037000	12.275974000
1	11.456523000	6.116346000	13.017242000
6	12.818798000	4.599717000	10.187552000
1	13.863521000	4.822029000	10.425532000
1	12.488857000	5.323848000	9.436764000
1	12.776181000	3.606391000	9.731927000
6	8.903213000	7.446907000	13.526299000
1	9.658193000	8.002819000	12.977435000
6	8.830099000	7.552478000	14.918997000
1	9.530646000	8.192466000	15.447364000
6	7.847941000	6.857792000	15.651710000
6	6.938527000	6.061021000	14.934772000
1	6.156378000	5.533562000	15.474875000
6	7.013132000	5.949949000	13.539104000
1	6.301936000	5.327185000	13.006624000
6	8.002820000	6.632809000	12.828888000
1	8.074857000	6.532088000	11.752489000
6	7.788872000	6.964901000	17.150108000
1	7.522865000	7.983288000	17.452286000
1	8.755379000	6.729009000	17.608214000
1	7.045861000	6.283997000	17.569069000

Ba Toluene adduct

56	9.627588000	4.638601000	14.787051000
7	11.113011000	2.973860000	15.976087000
7	10.547913000	2.865520000	13.234993000
6	11.839670000	1.890358000	15.727524000
6	11.951199000	1.336691000	14.440405000
1	12.572267000	0.454110000	14.347746000
6	11.339863000	1.798397000	13.262303000
6	12.570639000	1.224892000	16.864138000
1	13.256918000	1.931324000	17.342460000
1	13.138495000	0.355385000	16.531745000
1	11.861196000	0.906960000	17.635310000
6	11.596892000	1.049813000	11.980490000
1	12.069701000	1.708785000	11.244709000

1	10.652980000	0.714969000	11.538747000
1	12.239117000	0.182353000	12.135476000
6	10.964973000	3.559810000	17.250212000
6	9.825738000	3.241094000	18.034143000
6	9.546430000	4.012675000	19.165710000
1	8.680789000	3.768641000	19.775736000
6	10.359887000	5.081035000	19.530402000
1	10.129234000	5.666374000	20.415087000
6	11.479155000	5.386096000	18.761502000
1	12.118413000	6.214175000	19.055689000
6	11.802664000	4.643507000	17.622864000
6	8.913495000	2.089837000	17.651087000
1	9.338929000	1.614342000	16.761269000
6	8.842660000	1.032358000	18.758482000
1	8.384898000	1.434854000	19.667854000
1	9.840344000	0.670862000	19.021832000
1	8.244270000	0.175338000	18.434634000
6	7.505550000	2.584877000	17.295136000
1	6.870961000	1.759797000	16.959017000
1	7.513067000	3.333021000	16.489102000
1	7.019928000	3.058433000	18.154084000
6	13.020363000	5.006437000	16.792070000
1	13.123605000	4.248354000	16.009360000
6	12.841203000	6.366511000	16.105144000
1	11.956845000	6.393176000	15.452208000
1	13.703944000	6.608077000	15.477328000
1	12.716953000	7.170096000	16.837985000
6	14.304435000	4.996261000	17.628632000
1	15.177377000	5.173185000	16.993110000
1	14.438597000	4.034976000	18.132018000
1	14.290318000	5.774856000	18.397910000
6	9.918871000	3.342048000	12.063086000
6	8.589656000	2.941277000	11.769916000
6	7.894205000	3.602893000	10.754261000
1	6.877677000	3.297794000	10.520195000
6	8.483052000	4.635064000	10.030148000
1	7.929552000	5.134061000	9.240582000
6	9.790187000	5.016372000	10.314428000
1	10.248687000	5.817389000	9.743272000
6	10.526382000	4.386338000	11.320538000
6	7.928230000	1.816672000	12.545282000
1	8.676433000	1.407004000	13.231494000
6	7.469012000	0.683236000	11.621812000
1	6.678722000	1.014355000	10.940384000
1	7.074371000	-0.152592000	12.207454000
1	8.296875000	0.310840000	11.012324000
6	6.753898000	2.330484000	13.386759000
1	7.056966000	3.121731000	14.085892000
1	6.313747000	1.524926000	13.981879000
1	5.966497000	2.753287000	12.754201000
6	11.950114000	4.825751000	11.609969000

1	12.354320000	4.152787000	12.373091000
6	11.990016000	6.252066000	12.171507000
1	11.575210000	6.970121000	11.457336000
1	13.014242000	6.556286000	12.406477000
1	11.403452000	6.354608000	13.094872000
6	12.839552000	4.717574000	10.366311000
1	13.877669000	4.958338000	10.614843000
1	12.516191000	5.407707000	9.581038000
1	12.814529000	3.706410000	9.950899000
6	8.665046000	7.709071000	13.521104000
1	9.408430000	8.213267000	12.910520000
6	8.626184000	7.937228000	14.902392000
1	9.338788000	8.623116000	15.354263000
6	7.665568000	7.309207000	15.715820000
6	6.734221000	6.455629000	15.096172000
1	5.963748000	5.981725000	15.699781000
6	6.771095000	6.225218000	13.715196000
1	6.039800000	5.566765000	13.256627000
6	7.744455000	6.842175000	12.921358000
1	7.786784000	6.648624000	11.854912000
6	7.654002000	7.518078000	17.206331000
1	8.063137000	8.495678000	17.472355000
1	8.259378000	6.760636000	17.721694000
1	6.639809000	7.450839000	17.607617000

Coordinates for 10

15	0.899511000	2.570620000	8.039876000
12	2.413993000	4.617649000	7.897972000
7	2.108238000	6.525398000	8.425777000
7	4.184071000	4.825130000	6.987456000
6	3.139395000	7.392655000	8.399697000
6	4.369888000	7.076741000	7.797384000
1	5.080994000	7.882371000	7.861611000
6	4.867427000	5.970620000	7.071143000
6	3.145978000	8.791083000	9.101638000
6	1.843398000	9.238734000	9.779329000
1	1.055648000	9.483622000	9.066977000
1	2.062000000	10.146182000	10.351205000
1	1.450223000	8.499190000	10.475954000
6	3.544788000	9.910033000	8.119421000
1	4.530062000	9.760007000	7.672902000
1	3.573618000	10.861259000	8.659839000
1	2.818955000	10.016328000	7.309390000
6	4.217638000	8.717965000	10.216043000
1	3.964398000	7.960869000	10.963155000
1	4.270320000	9.684445000	10.726841000
1	5.212157000	8.487514000	9.829097000
6	6.241025000	6.253301000	6.395598000
6	6.034558000	7.429225000	5.416731000
1	5.306730000	7.163240000	4.643349000

1	6.982346000	7.661998000	4.921492000
1	5.681040000	8.335163000	5.912617000
6	7.268370000	6.643311000	7.478603000
1	6.992930000	7.542029000	8.033785000
1	8.235546000	6.834503000	7.003914000
1	7.406649000	5.830573000	8.198627000
6	6.882635000	5.119542000	5.582716000
1	7.135280000	4.247498000	6.186232000
1	7.815892000	5.507104000	5.162059000
1	6.263634000	4.787148000	4.749707000
6	0.748005000	6.899225000	8.612786000
6	0.110356000	7.699646000	7.637219000
6	-1.226876000	8.047617000	7.833650000
1	-1.722957000	8.688796000	7.112807000
6	-1.931007000	7.598681000	8.945116000
1	-2.965201000	7.894321000	9.091667000
6	-1.317741000	6.741302000	9.849601000
1	-1.891008000	6.358477000	10.685307000
6	0.015836000	6.358978000	9.692948000
6	0.852589000	8.137203000	6.386522000
1	1.892935000	8.330646000	6.656680000
6	0.306080000	9.415388000	5.753786000
1	-0.686249000	9.265732000	5.315747000
1	0.967164000	9.744085000	4.946413000
1	0.233679000	10.226405000	6.484757000
6	0.881895000	6.994785000	5.367774000
1	1.386619000	6.117312000	5.784528000
1	1.431214000	7.283480000	4.466024000
1	-0.131071000	6.701364000	5.072282000
6	0.656087000	5.368229000	10.650421000
1	1.148602000	4.605648000	10.014810000
6	-0.351933000	4.615468000	11.515080000
1	-0.804143000	5.284188000	12.254493000
1	0.147117000	3.814828000	12.066946000
1	-1.149547000	4.170343000	10.917052000
6	1.748775000	5.977206000	11.532652000
1	2.544755000	6.420247000	10.934996000
1	2.189271000	5.210459000	12.179684000
1	1.327553000	6.753736000	12.178512000
6	4.624651000	3.623744000	6.356898000
6	4.211775000	3.328759000	5.044494000
6	4.618025000	2.118972000	4.477246000
1	4.322942000	1.883989000	3.459647000
6	5.392232000	1.213810000	5.192990000
1	5.713618000	0.285358000	4.730363000
6	5.754240000	1.497424000	6.507251000
1	6.357534000	0.785721000	7.060788000
6	5.379586000	2.699259000	7.110695000
6	3.348910000	4.298518000	4.260958000
1	3.404445000	5.269187000	4.765097000
6	1.887950000	3.836393000	4.288854000

1	1.783678000	2.827441000	3.878159000
1	1.246017000	4.515047000	3.719388000
1	1.497705000	3.790752000	5.312885000
6	3.825832000	4.498873000	2.820778000
1	4.879386000	4.790550000	2.785009000
1	3.238885000	5.285008000	2.336003000
1	3.708230000	3.590188000	2.222424000
6	5.781634000	3.029666000	8.536062000
1	5.895527000	4.116547000	8.600480000
6	4.664384000	2.633283000	9.503743000
6	7.107618000	2.402851000	8.966658000
1	7.038936000	1.313609000	9.052224000
1	7.402724000	2.785803000	9.948019000
1	7.906315000	2.636561000	8.256815000
6	-0.807593000	3.226354000	8.090483000
6	-1.101139000	4.323528000	7.272523000
1	-0.327901000	4.783835000	6.662941000
6	-2.393730000	4.832542000	7.229490000
1	-2.613252000	5.689096000	6.602555000
6	-3.390896000	4.258894000	8.017645000
1	-4.397849000	4.663630000	7.994327000
6	-3.097312000	3.173214000	8.840943000
1	-3.874696000	2.729657000	9.455327000
6	-1.806353000	2.648555000	8.877124000
1	-1.576082000	1.801645000	9.515612000
6	0.931876000	1.460864000	6.582238000
6	-0.212002000	1.244834000	5.809163000
1	-1.143705000	1.740594000	6.060211000
6	-0.148604000	0.386755000	4.713337000
1	-1.035513000	0.218972000	4.110220000
6	1.045680000	-0.260325000	4.400073000
1	1.090506000	-0.934194000	3.549990000
6	2.183784000	-0.042142000	5.176201000
1	3.117135000	-0.536583000	4.930755000
6	2.136340000	0.827160000	6.261213000
1	3.035296000	1.012498000	6.843298000
6	1.069348000	1.428392000	9.464469000
6	0.617346000	0.108554000	9.344380000
1	0.205214000	-0.240575000	8.403018000
6	0.705681000	-0.756298000	10.431882000
1	0.352717000	-1.778259000	10.335193000
6	1.706942000	0.997386000	11.756645000
1	2.137636000	1.343355000	12.691100000
6	1.618430000	1.866863000	10.673408000
1	1.982475000	2.882999000	10.776690000
6	1.249036000	-0.313735000	11.637395000
1	1.320624000	-0.992124000	12.481829000
1	4.898557000	2.918634000	10.533999000
1	3.713847000	3.118535000	9.242162000
1	4.472852000	1.556328000	9.474589000

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