Electronic Supplementary Material (ESI) for Chemical Science.

SUPPORTING INFORMATION

Contents

1. Supporting Experimental data

1.1. NMR spectra of synthesized compounds

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

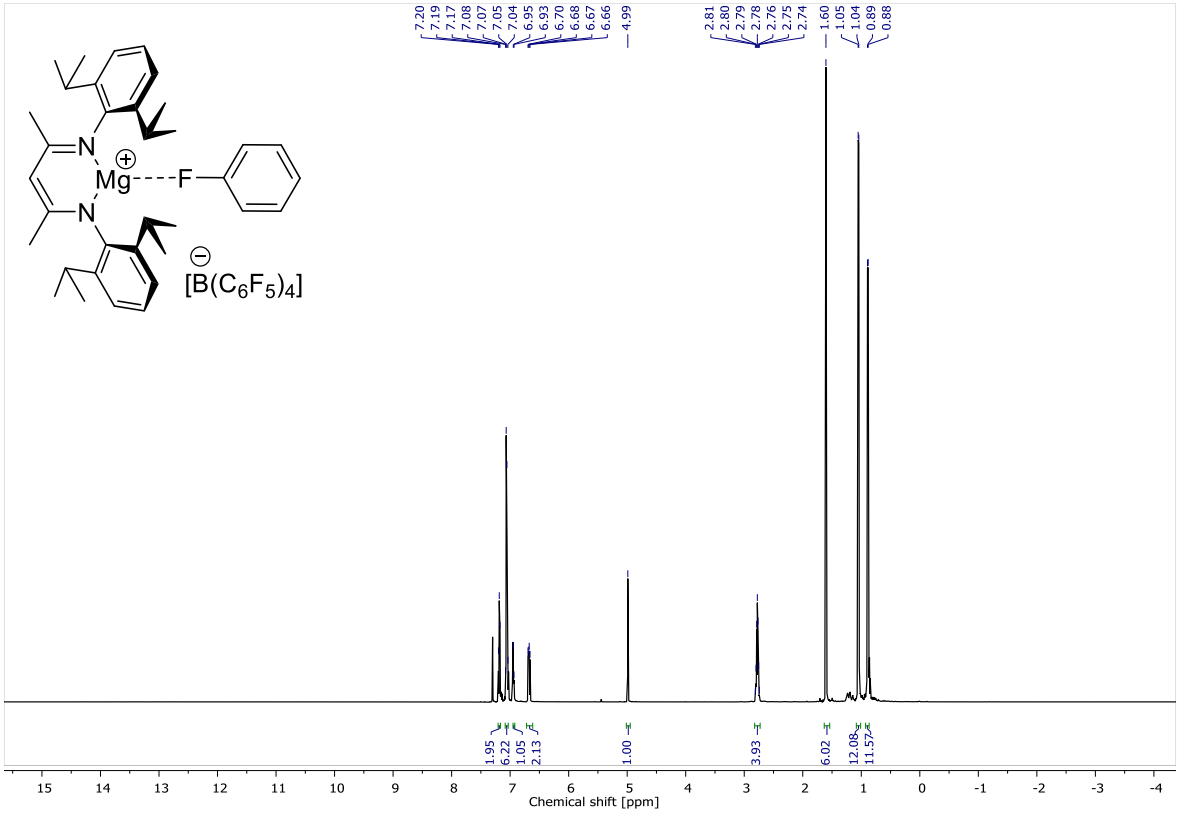

Figure S1: ^{1}H NMR spectrum of [(^{Me}BDI)Mg^{+}·PhF][B(C_6F_5)$_4^-$] in C_6D_5Br.

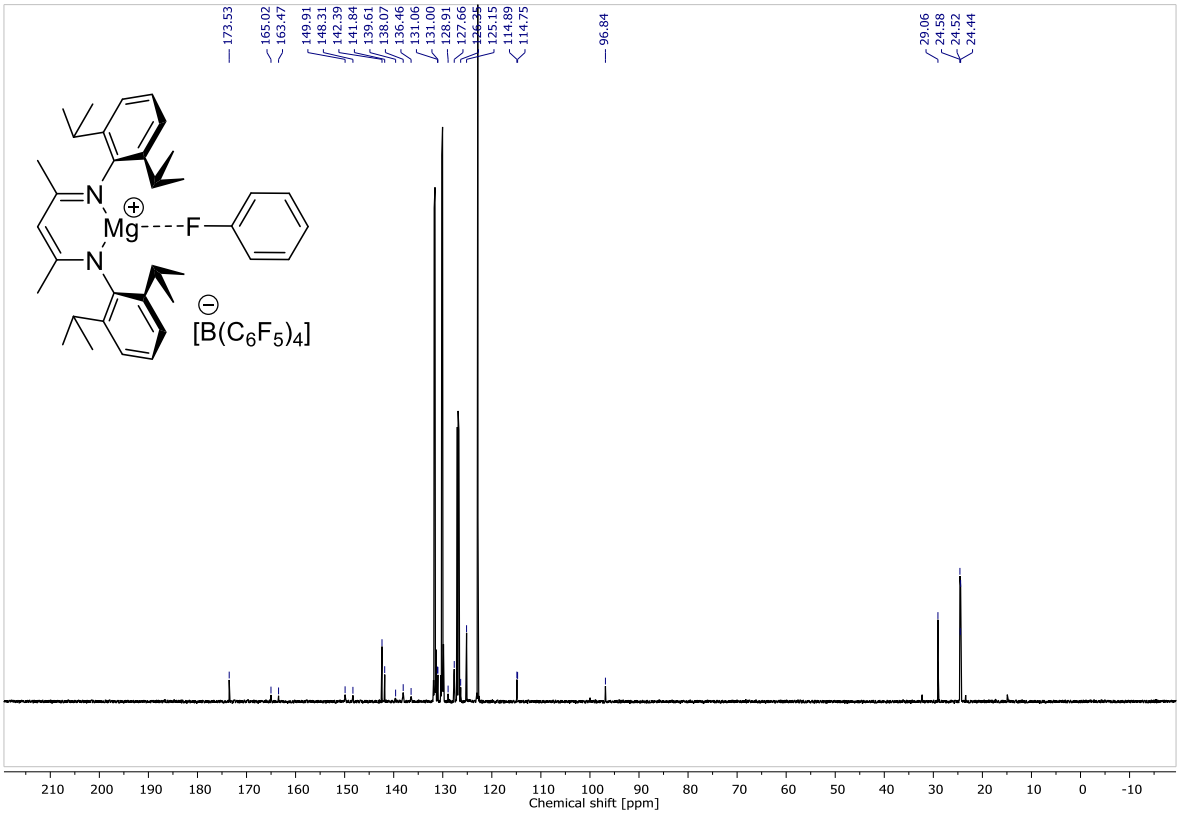

Figure S2: $^{13}C\{^{1}H\}$ NMR spectrum of $[(^{Me}BDI)Mg^{+}\cdot PhF][B(C_6F_5)_4^{-}]$ in C_6D_5Br.

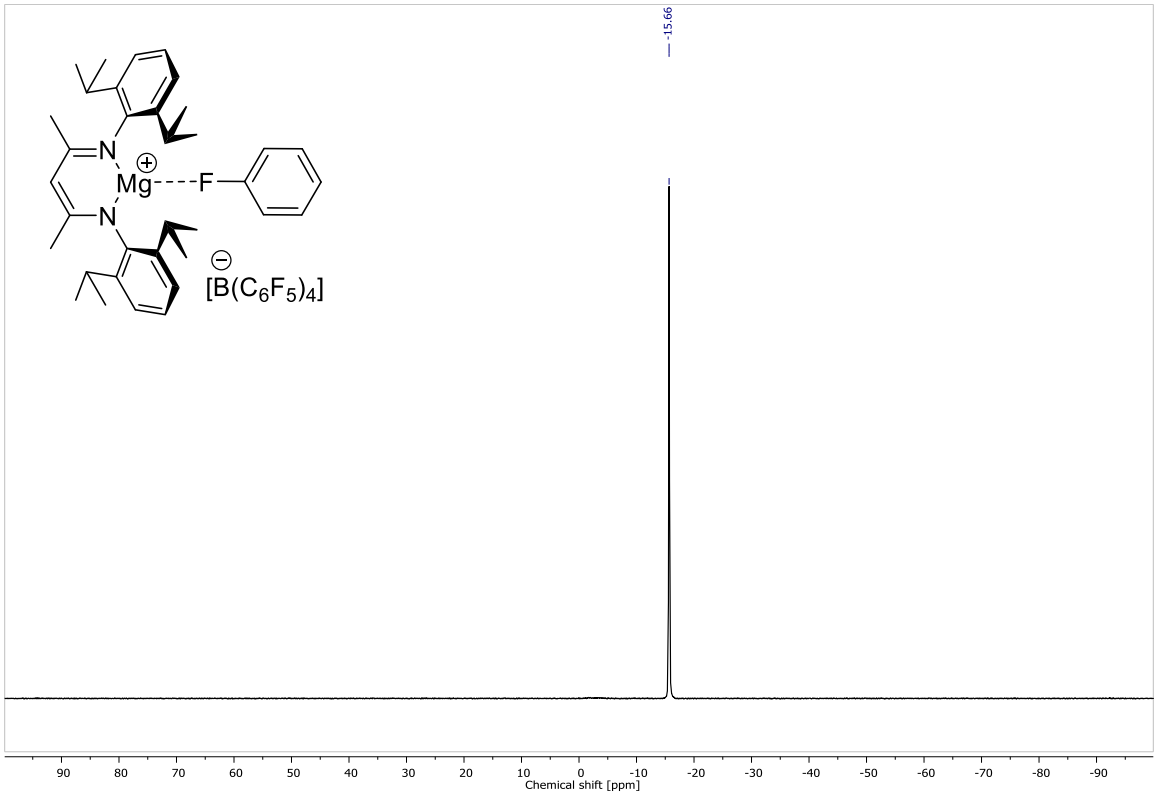

Figure S3: ^{11}B NMR spectrum of $[(^{Me}BDI)Mg^{+}\cdot PhF][B(C_6F_5)_4^{-}]$ in C_6D_5Br.

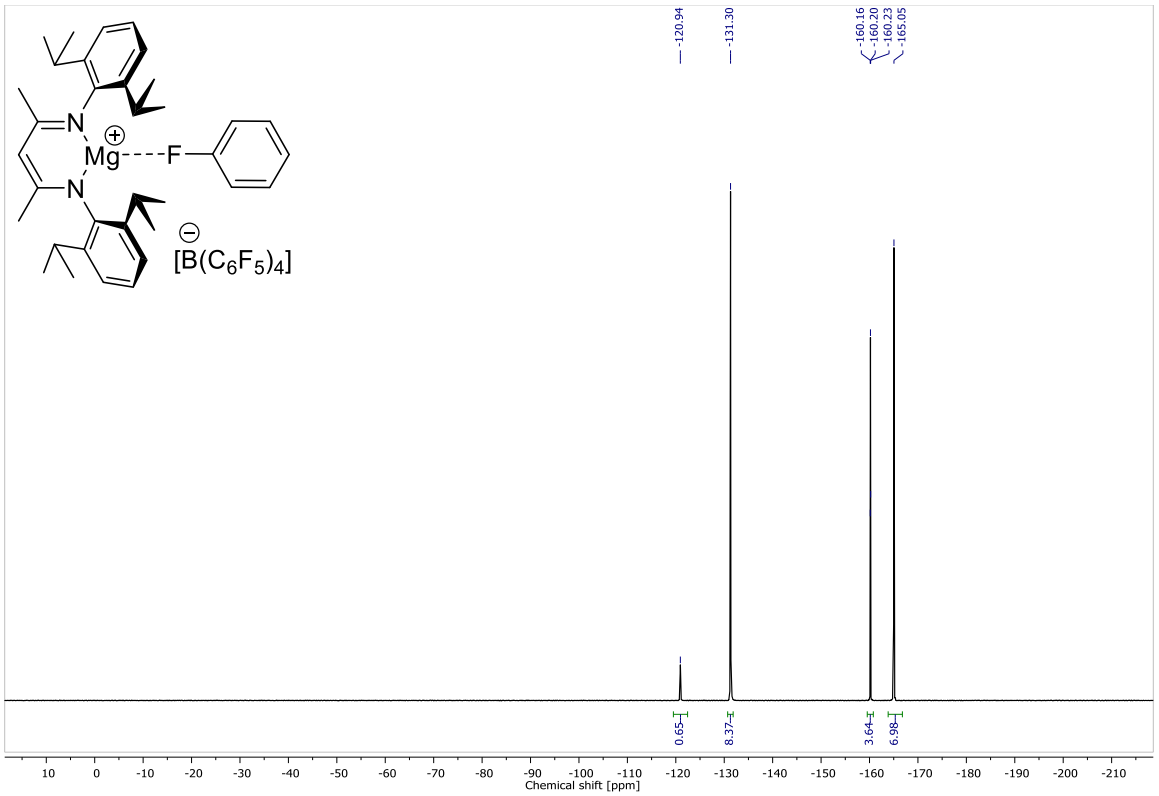

Figure S4: ^{19}F NMR spectrum of [(^{Me}BDI)Mg^{+}·PhF][B(C_6F_5)$_4^-$] in C_6D_5Br.

1.1.2. Spectra of [(^{tBu}BDI)Mg^{+}·(PhF)$_2$][B(C_6F_5)$_4^-$]

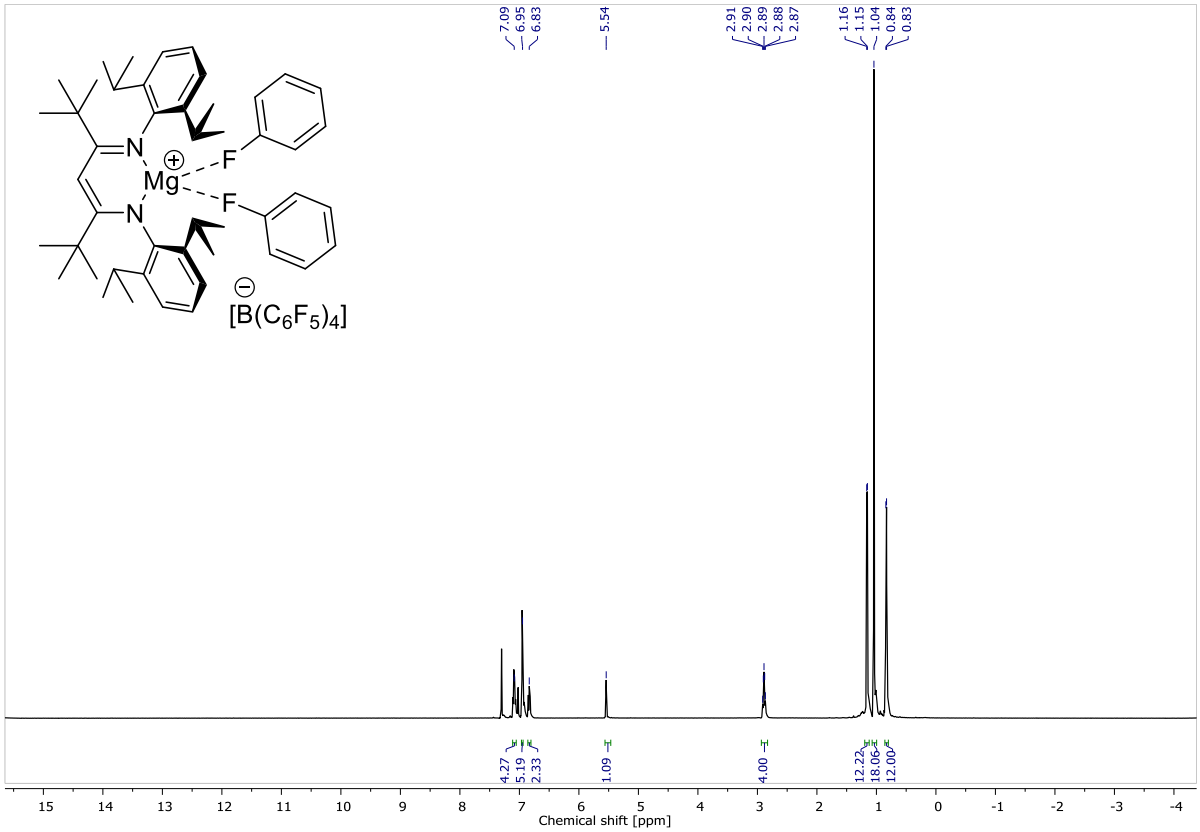

Figure S5: ^{1}H NMR spectrum of [(^{tBu}BDI)Mg^{+}·(PhF)$_2$][B(C_6F_5)$_4^-$] in C_6D_5Br.

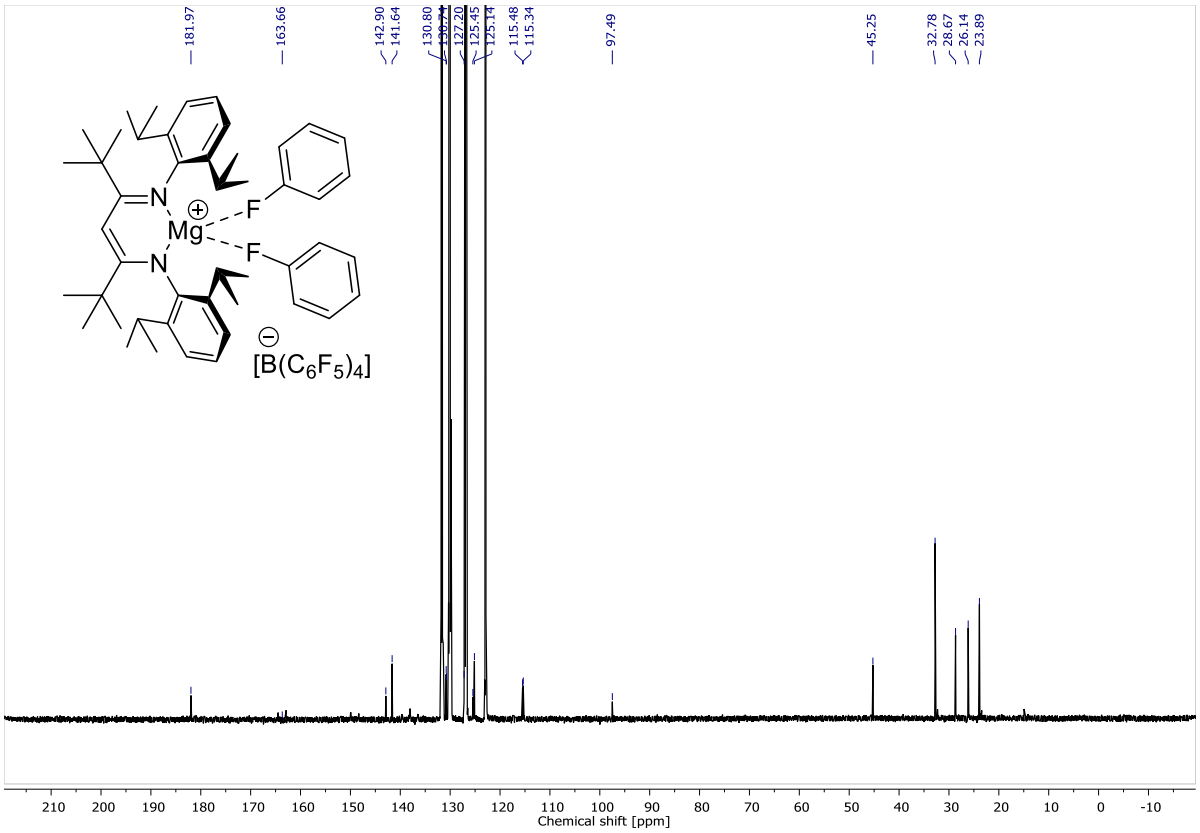

Figure S6: $^{13}C\{^{1}H\}$ NMR spectrum of $[(^{tBu}BDI)Mg^{+}\cdot(PhF)_2][B(C_6F_5)_4^{-}]$ in C_6D_5Br.

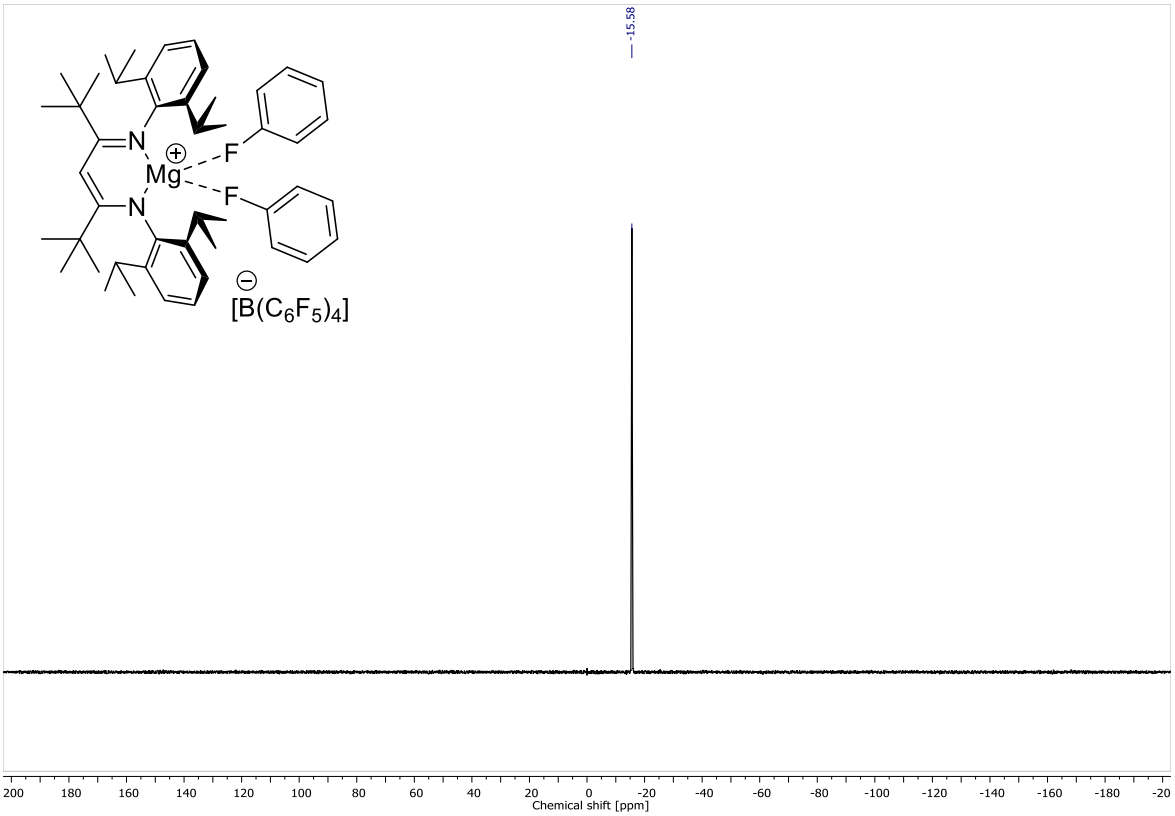

Figure S7: ^{11}B NMR spectrum of $[(^{tBu}BDI)Mg^{+}\cdot(PhF)_2][B(C_6F_5)_4^{-}]$ in C_6D_5Br.

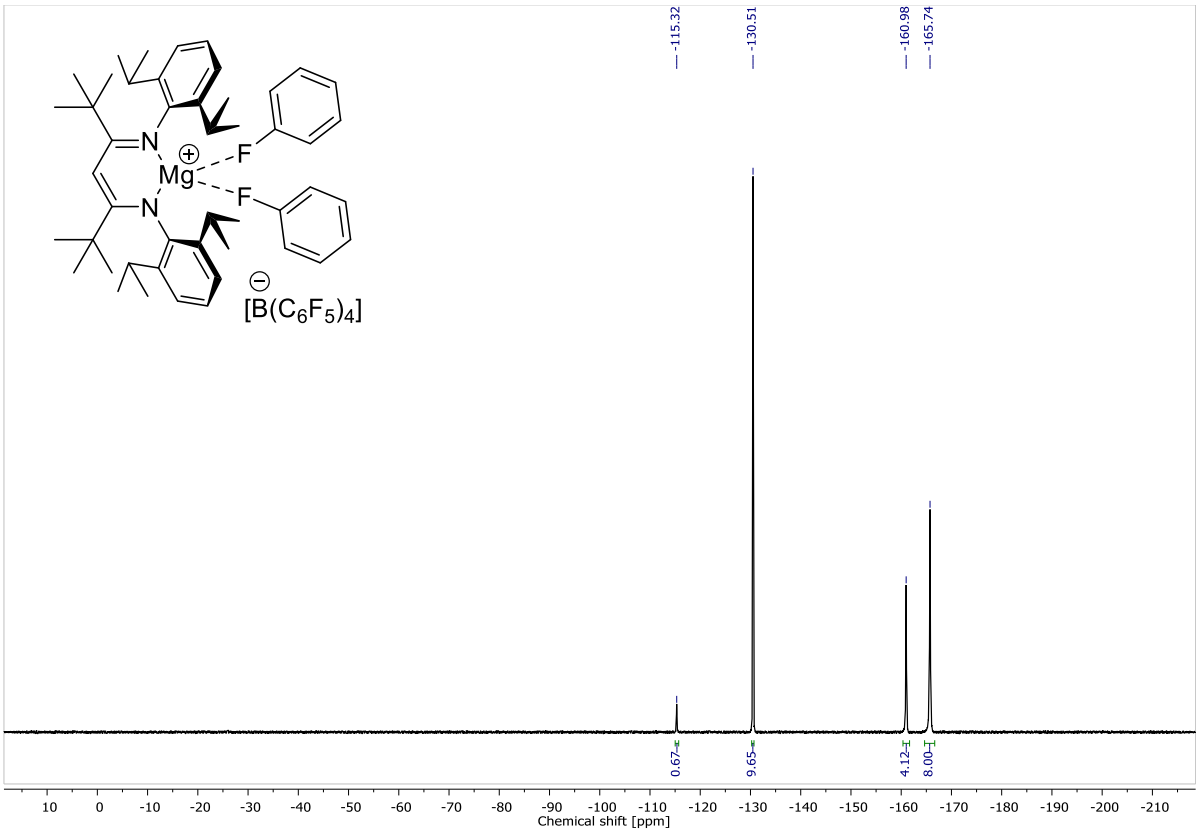

Figure S8: ^{19}F NMR spectrum of [($^{t\text{Bu}}$BDI)Mg^{+}·(PhF)$_2$][B(C$_6$F$_5$)$_4^{-}$] in C$_6$D$_5$Br.

1.1.3. Spectra of [($^{t\text{Bu}}$BDI)Mg^{+}·(PhF)$_2$][Al-F-Al^{-}]

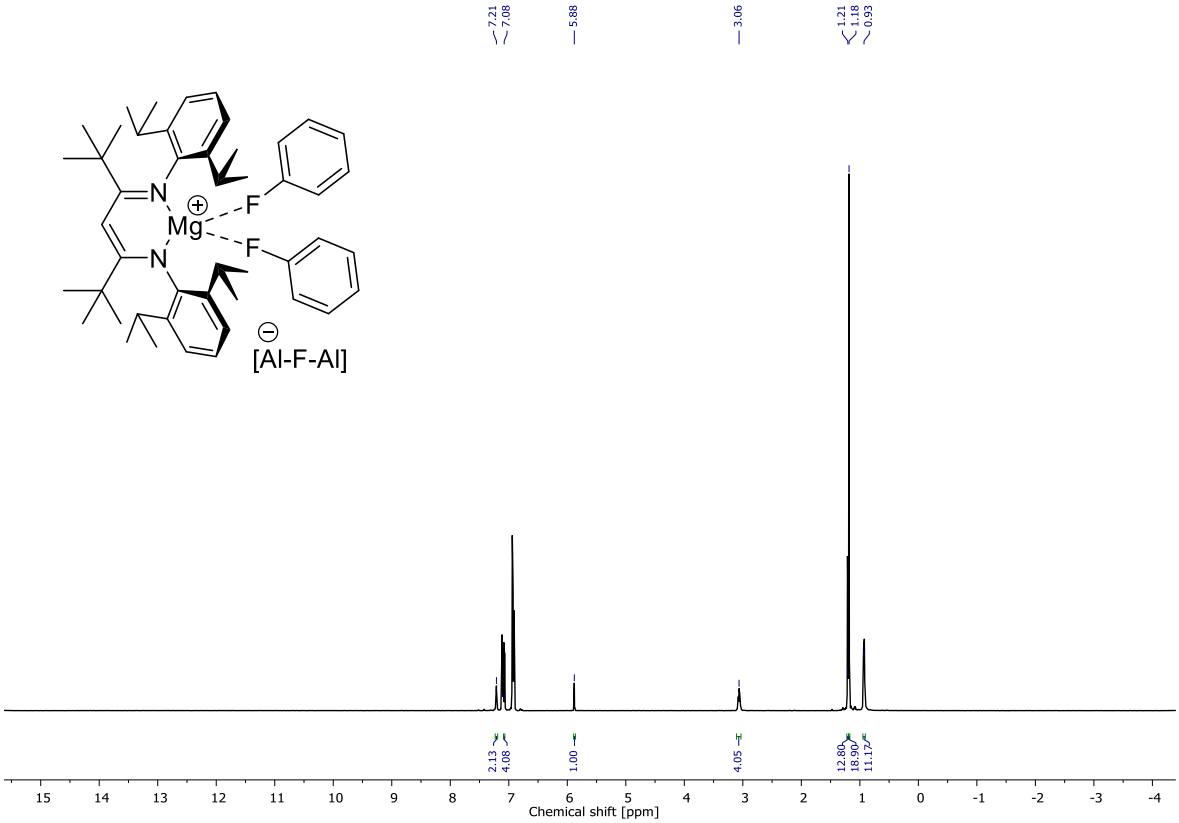

Figure S9: ^{1}H NMR spectrum of [($^{t\text{Bu}}$BDI)Mg^{+}·(PhF)$_2$][Al-F-Al^{-}] in C$_6$D$_5$F.

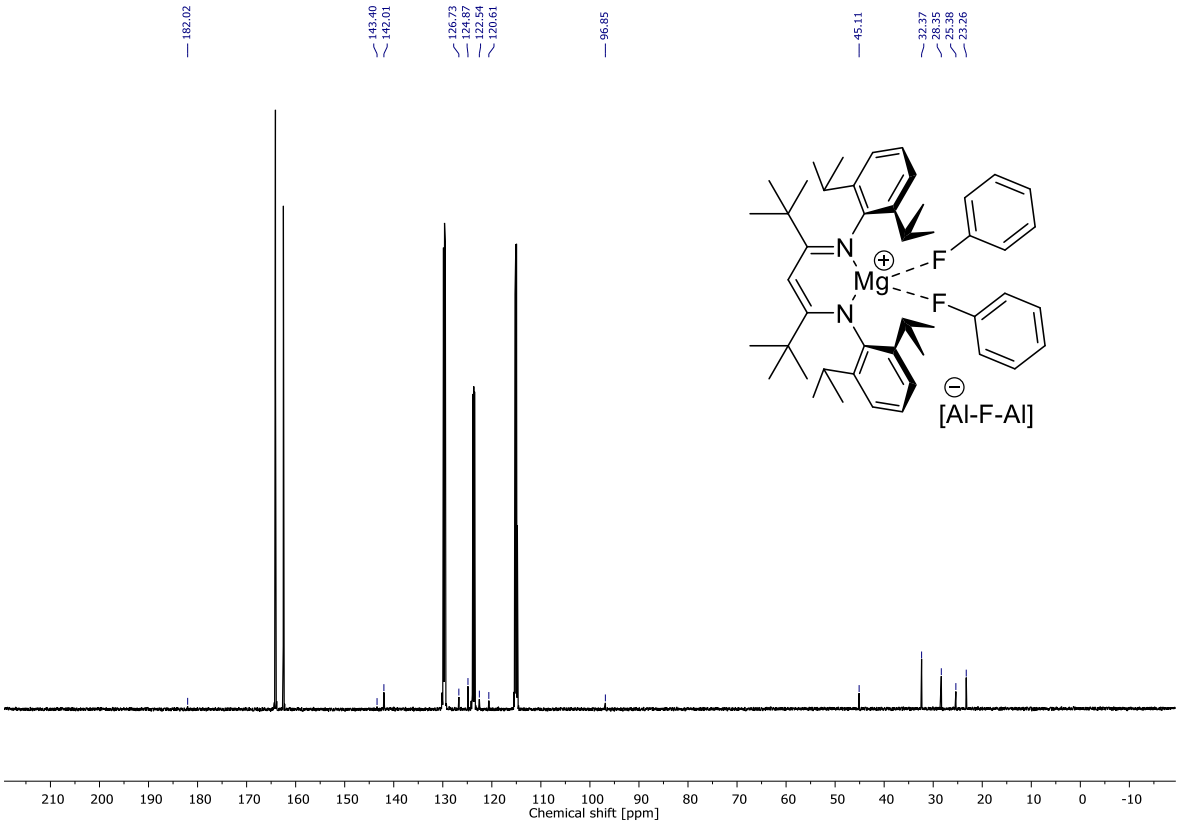

Figure S10: ^{13}C NMR spectrum of [($^{t\text{Bu}}$BDI)Mg^{+}·(PhF)$_2$][Al-F-Al^{-}] in C_6D_5F.

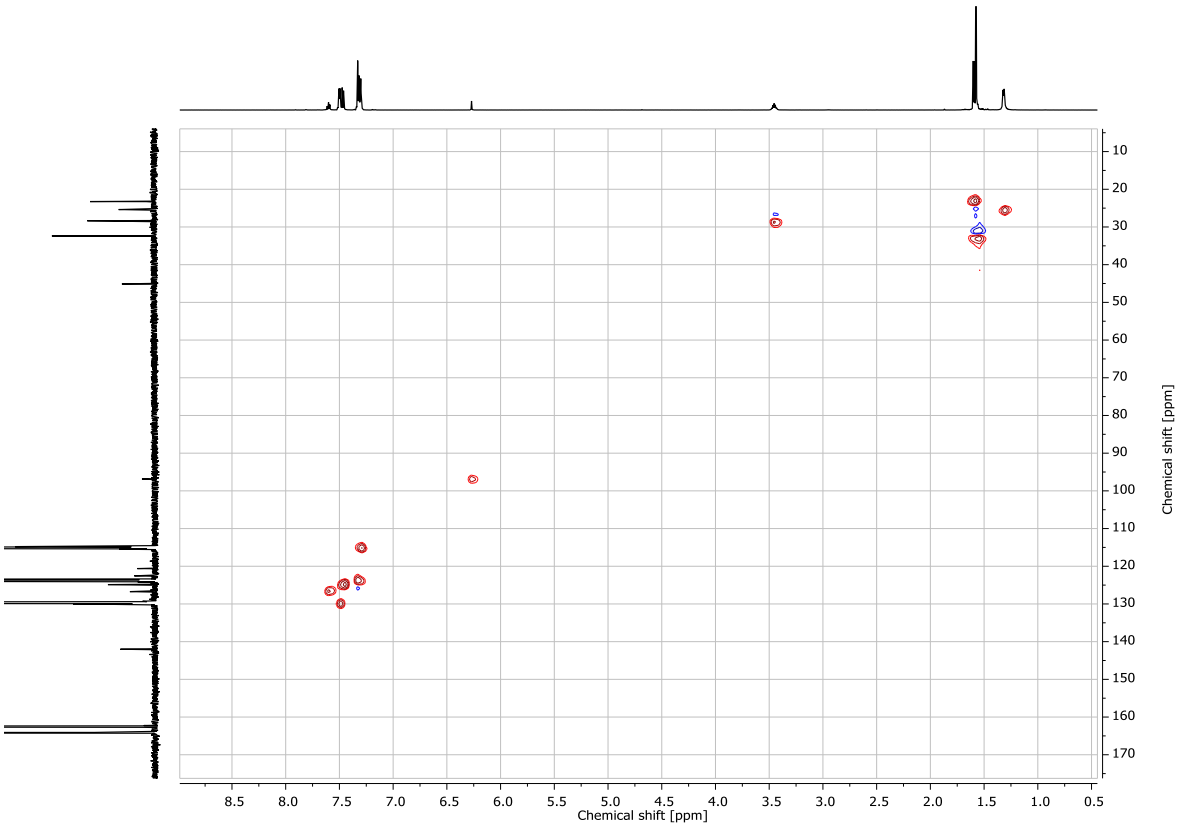

Figure S11: 2D HSQC NMR spectrum of [($^{t\text{Bu}}$BDI)Mg^{+}·(PhF)$_2$][Al-F-Al^{-}] in C_6D_5F.

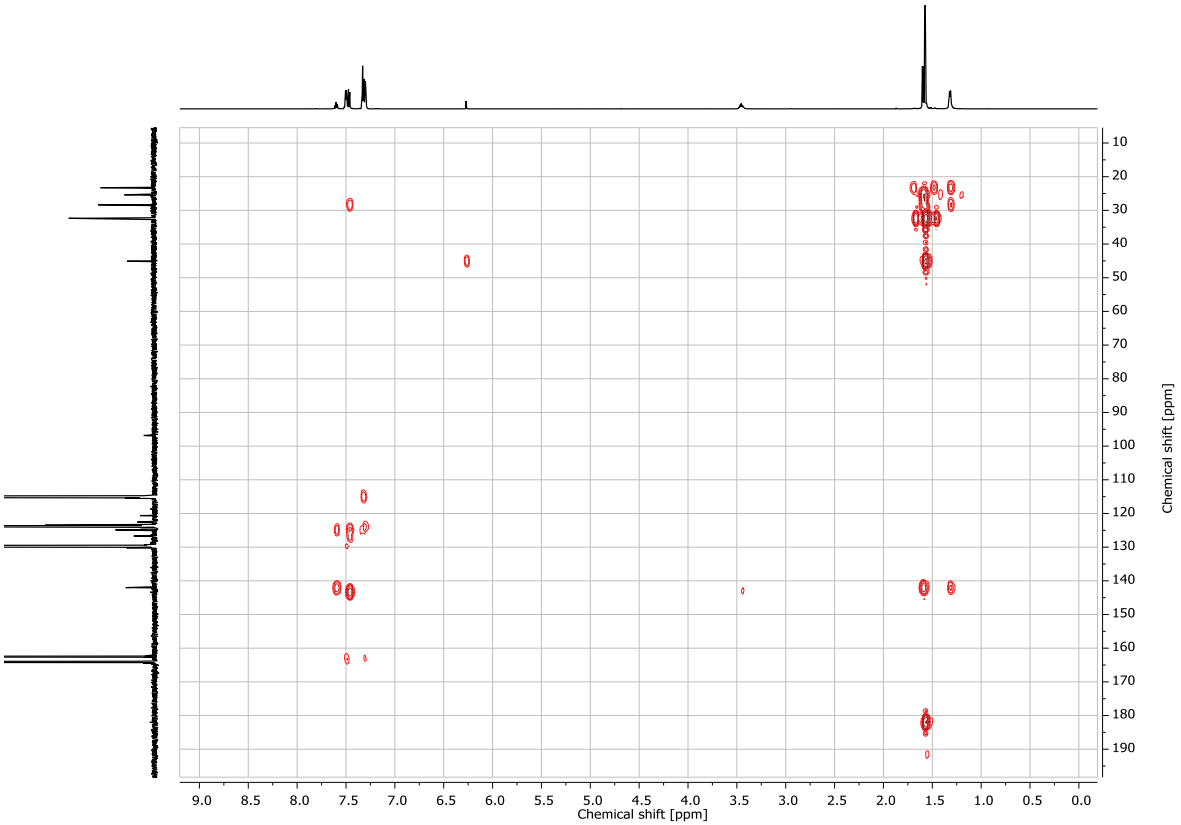

Figure S12: 2D HMBC NMR spectrum of [($^{t\text{Bu}}$BDI)Mg^{+}·(PhF)$_2$][Al-F-Al^{-}] in C_6D_5F.

Figure S13: ^{19}F NMR spectrum of [($^{t\text{Bu}}$BDI)Mg^{+}·(PhF)$_2$][Al-F-Al^{-}] in C_6D_5F.

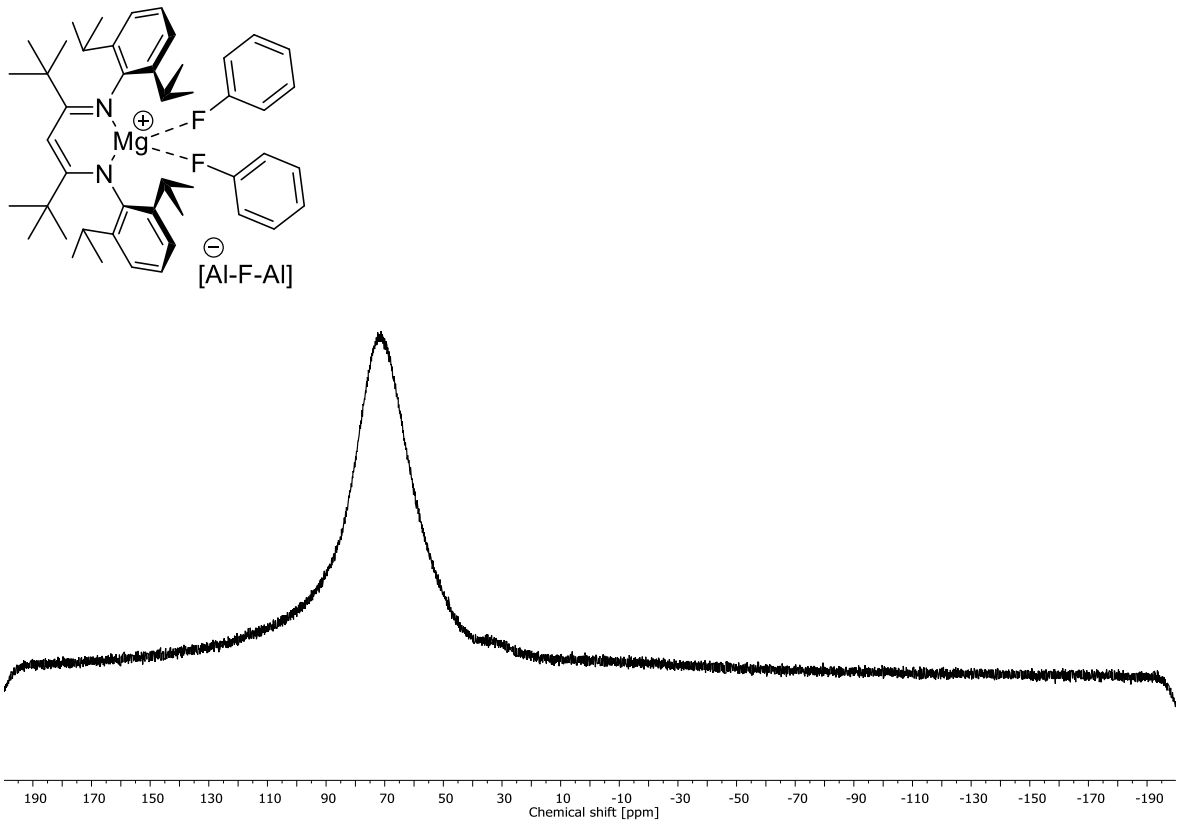

Figure S14: ^{27}Al NMR spectrum of [($^{t\text{Bu}}$BDI)Mg^{+}·(PhF)$_2$][Al-F-Al^{-}] in C_6D_5F.

1.1.4. Spectra of [($^{t\text{Bu}}$BDI)Mg^{+}·PhBr][B(C_6F_5)$_4^{-}$]

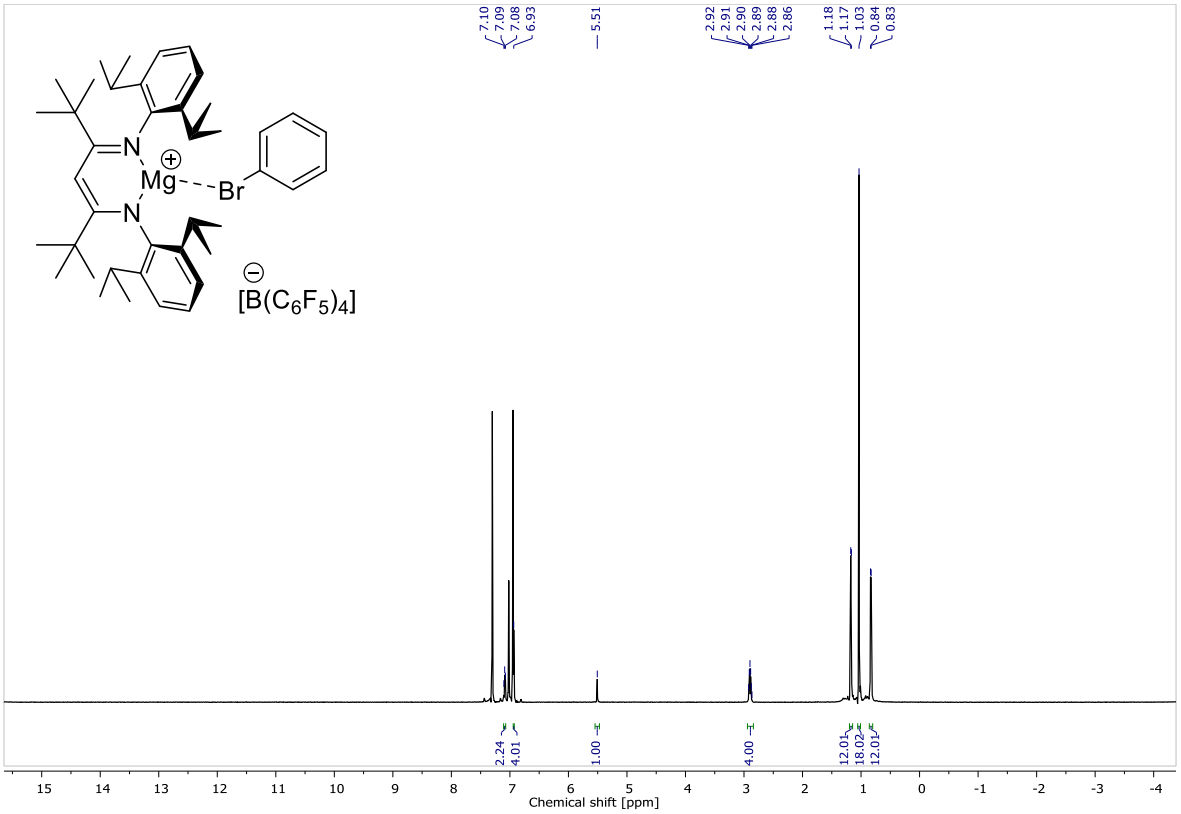

Figure S15: ^{1}H NMR spectrum of [($^{t\text{Bu}}$BDI)Mg^{+}·PhBr][B(C_6F_5)$_4^{-}$] in C_6D_5Br.

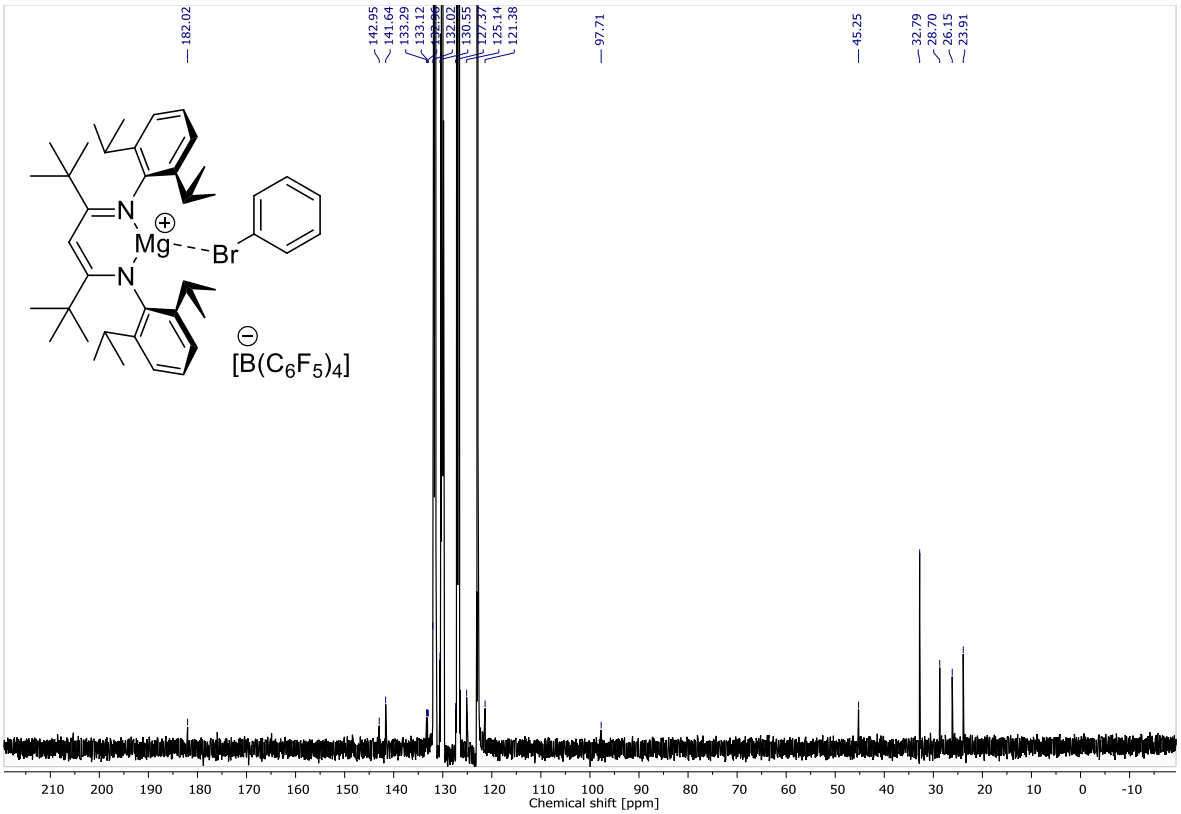

Figure S16: $^{13}C\{^{1}H\}$ NMR spectrum of [(^{tBu}BDI)Mg^{+}·PhBr][B(C$_6$F$_5$)$_4^{-}$] in C$_6$D$_5$Br.

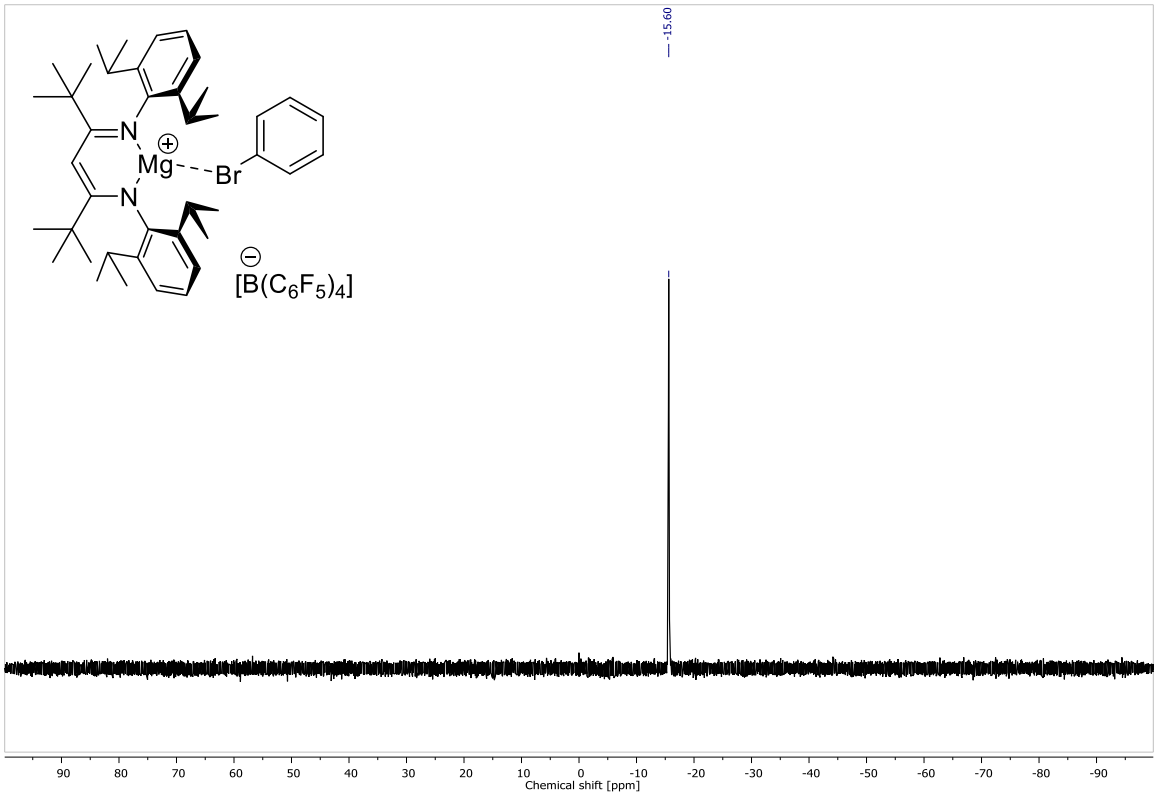

Figure S17: ^{11}B NMR spectrum of [(^{tBu}BDI)Mg^{+}·PhBr][B(C$_6$F$_5$)$_4^{-}$] in C$_6$D$_5$Br.

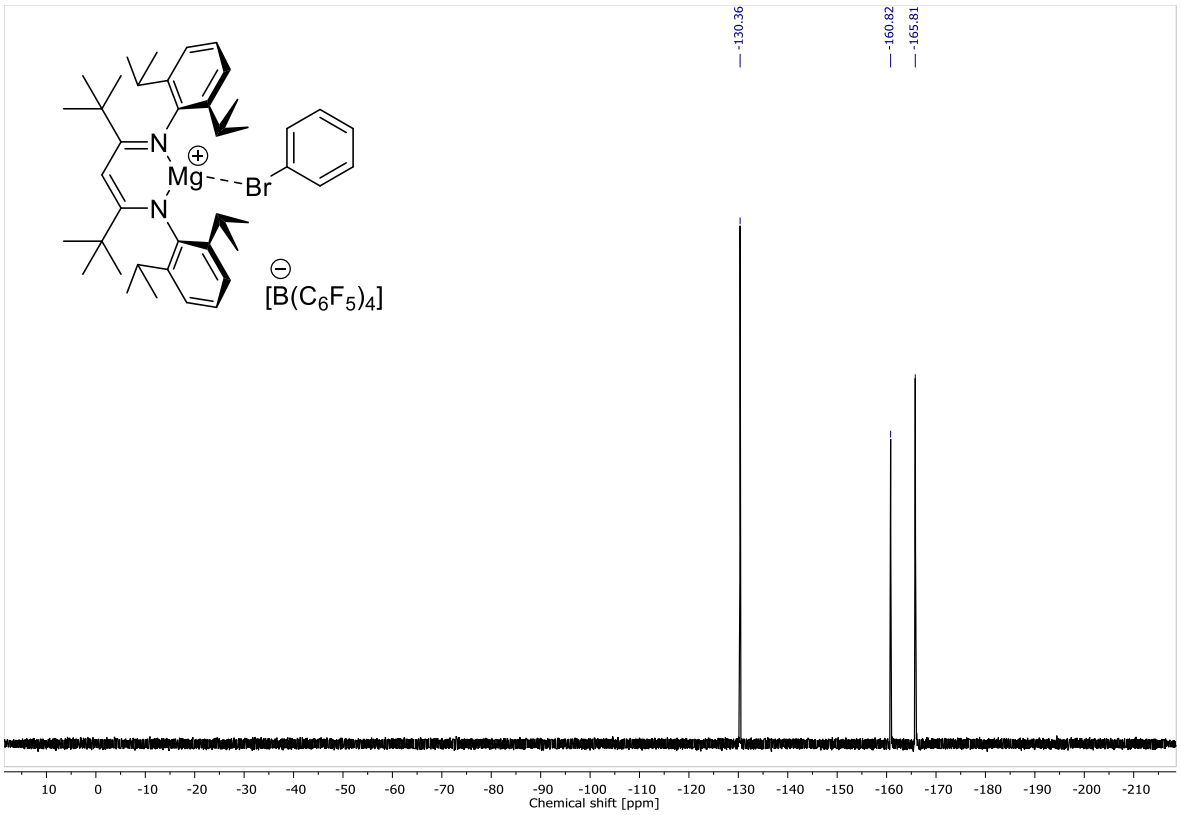

Figure S18: ^{19}F NMR spectrum of [($^{t\text{Bu}}$BDI)Mg^{+}·PhBr][B(C_6F_5)$_4^-$] in C_6D_5Br.

1.1.4 Spectra of [($^{t\text{Bu}}$BDI)Mg^{+}·PhI][B(C_6F_5)$_4^-$]

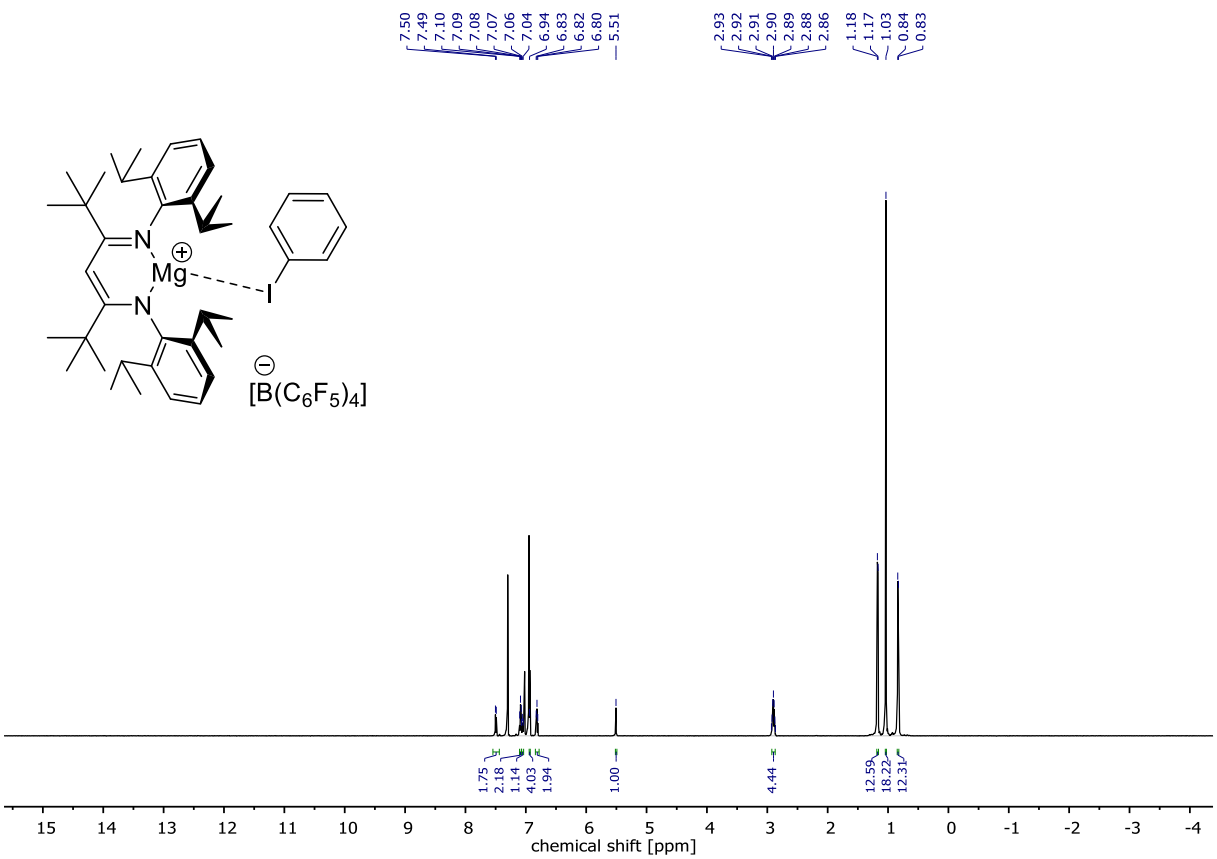

Figure S19: ^{1}H NMR spectrum of [($^{t\text{Bu}}$BDI)Mg^{+}·PhI][B(C_6F_5)$_4^-$] in C_6D_5Br.

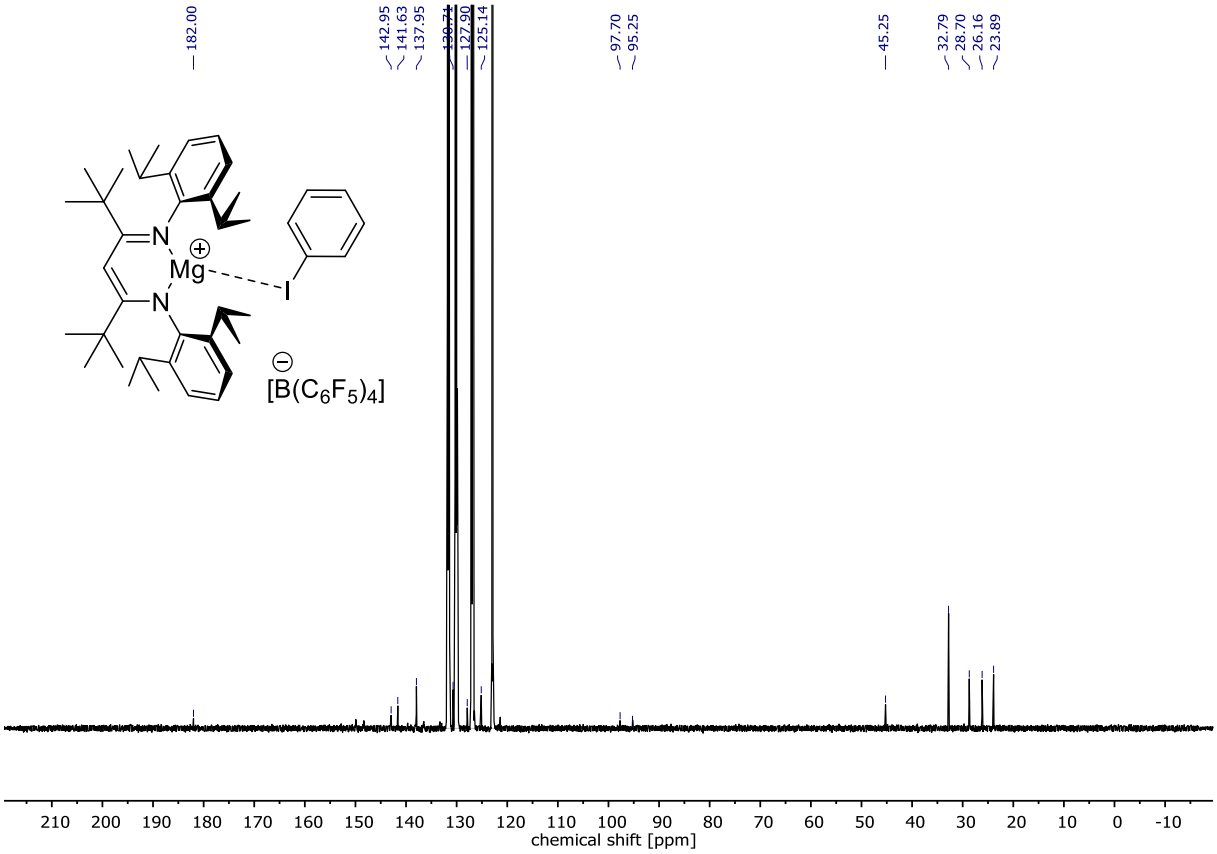

Figure S20: $^{13}C\{^{1}H\}$ NMR spectrum of [(^{tBu}BDI)Mg^{+}·PhI][B(C_6F_5)$_4^-$] in C_6D_5Br.

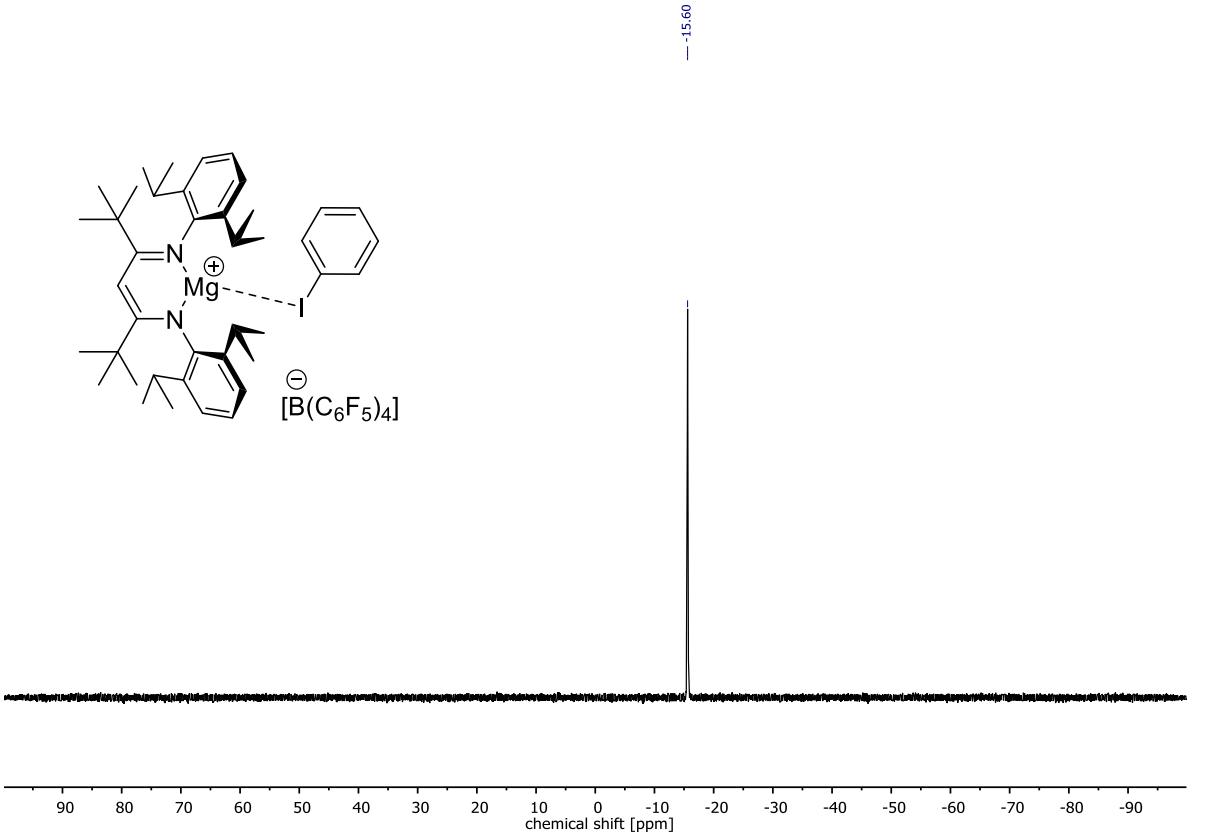

Figure S21: ^{11}B NMR spectrum of [(^{tBu}BDI)Mg^{+}·PhI][B(C_6F_5)$_4^-$] in C_6D_5Br.

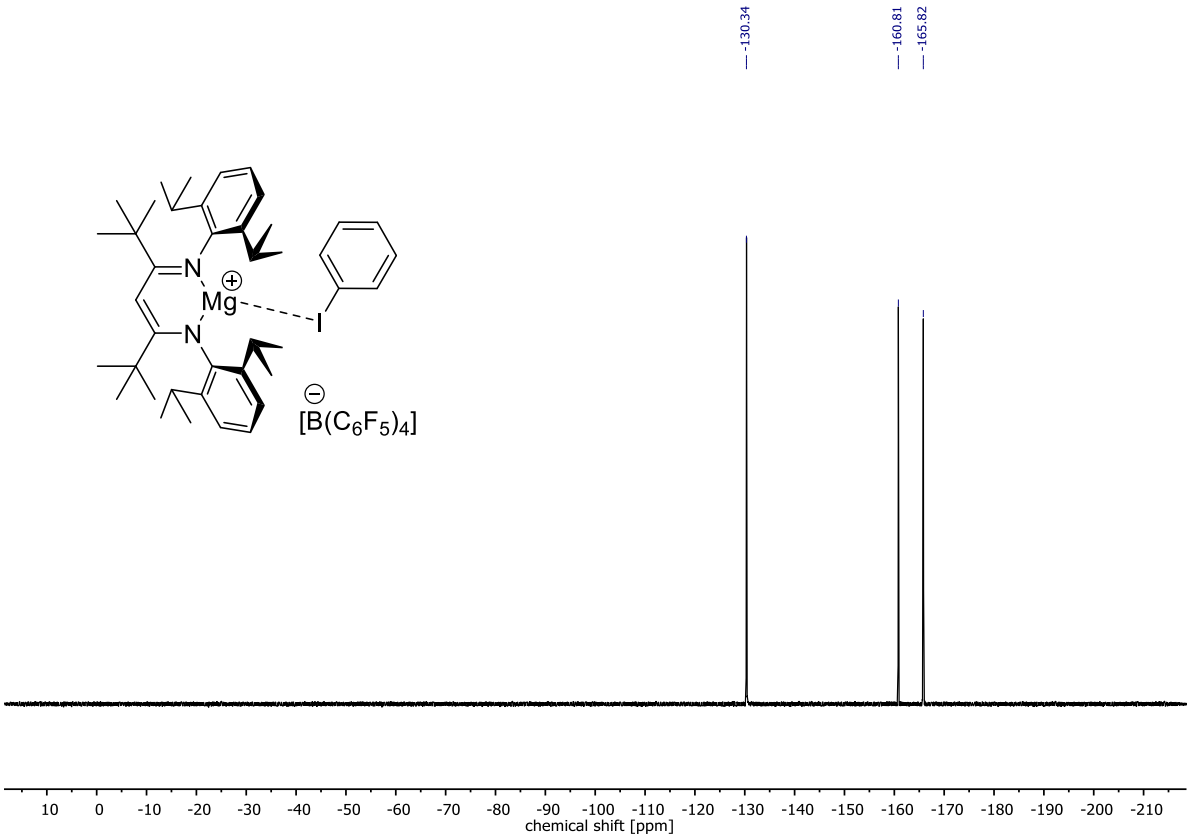

Figure S22: ^{19}F NMR spectrum of [($^{t\text{Bu}}$BDI)Mg^{+}·PhI][$B(C_6F_5)_4^{-}$] in C_6D_5Br.

1.2 Single Crystal X-Ray Diffraction

A crystal of the corresponding compound was embedded in inert perfluoropolyalkylether (viscosity 1800 cSt; ABCR GmbH) and mounted using a Hampton Research CryoLoop. The crystal was then flash cooled to 100.0(2) K in a nitrogen gas stream and kept at this temperature during the experiment. The crystal structure was measured on a SuperNova diffractometer with Atlas S2 detector using a CuKα microfocus source. The measured data was processed with the CrysAlisPro (v40.67a) software package.[S1] Using Olex2,[S2] the structure was solved with the ShelXT[S3A] structure solution program using Intrinsic Phasing and refined with the ShelXL[S3B] refinement package using Least Squares Minimization. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters.
[(^{Me}BDI)Mg^{+}·(PhF)$_3$][B(C$_6$F$_5$)$_4^{-}$]: Disorder of a *i*Pr group was observed and modeled with the help of similarity restraints (SADI). The relative occupancies of the two alternative orientations were refined to 0.57(3) and 0.43(3). [(^{tBu}BDI)Mg^{+}·(PhF)$_2$][B(C$_6$F$_5$)$_4^{-}$]: Disorder of a *t*Bu group was observed and modeled with the help of similarity restraints (SADI). The relative occupancies of the two alternative orientations were refined to 0.525(11) and 0.475(11). [(^{tBu}BDI)Mg^{+}·(PhF)$_2$][Al-F-Al^{-}]: Disorder of three perfluorinated *t*BuO groups and of one fluorobenzene ligand was observed. The disorder was modeled with the help of similarity restraints (SIMU, SADI). The relative occupancies of the two alternative orientations were refined to 0.916(3)/0.084(3) (F$_9$-*t*BuO 1), 0.721(8)/0.279(8) (F$_9$-*t*BuO 2), 0.607(16)/0.393(16) (F$_9$-*t*BuO 3), and 0.69(2)/0.31(2) (PhF), respectively.

Table S1. Crystal data.

Compound	$[(^{Me}BDI)Mg^{+}\cdot PhF][B(C_6F_5)_4^{-}]$	$[(^{Me}BDI)Mg^{+}\cdot(PhF)_3][B(C_6F_5)_4^{-}]$	$[(^{tBu}BDI)Mg^{+}\cdot(PhF)_2][B(C_6F_5)_4^{-}]$
Empirical formula	$C_{59}H_{46}BF_{21}MgN_2$	$C_{71}H_{56}BF_{23}MgN_2$	$C_{71}H_{63}BF_{22}MgN_2$
Formula weight	1217.10	1409.29	1397.35
Temperature/K	99.94(17)	100	100.0(1)
Crystal system	triclinic	triclinic	monoclinic
Space group	P-1	P-1	$P2_1/c$
a/Å	11.5834(5)	12.2177(3)	18.37340(10)
b/Å	12.7194(6)	15.9583(5)	18.09830(10)
c/Å	19.1287(8)	17.8965(5)	19.72950(10)
α/°	86.142(3)	102.494(3)	90
β/°	77.884(4)	106.268(3)	98.0610(10)
γ/°	80.927(4)	96.734(2)	90
Volume/Å^3	2719.3(2)	3210.88(17)	6495.77(6)
Z	2	2	4
ρ_{calc}g/cm^3	1.486	1.458	1.429
μ/mm^{-1}	0.147	1.238	1.193
F(000)	1240.0	1440.0	2872.0
Crystal size/mm^3	0.242 × 0.137 × 0.084	0.2647 × 0.1931 × 0.1823	0.273 × 0.193 × 0.155
Crystal color	colorless	colorless	colorless
Radiation	MoKα (λ = 0.71073)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.216 to 52.744	5.778 to 136.232	6.658 to 147.34
Index ranges	-14 ≤ h ≤ 14, -15 ≤ k ≤ 14, -23 ≤ l ≤ 23	-14 ≤ h ≤ 10, -18 ≤ k ≤ 19, -21 ≤ l ≤ 19	-22 ≤ h ≤ 22, -22 ≤ k ≤ 22, -24 ≤ l ≤ 23
Reflections collected	26778	19494	62369
Independent reflections	11109 [R_{int} = 0.0368, R_{sigma} = 0.0476]	11623 [R_{int} = 0.0354, R_{sigma} = 0.0436]	12980 [R_{int} = 0.0232, R_{sigma} = 0.0164]
Data/restraints/parameters	11109/0/767	11623/0/893	12980/15/919
Goodness-of-fit on F^2	1.044	1.046	1.022
Final R indexes [I>=2σ (I)]	R_1 = 0.0508, wR_2 = 0.1171	R_1 = 0.0417, wR_2 = 0.1066	R_1 = 0.0311, wR_2 = 0.0787
Final R indexes [all data]	R_1 = 0.0717, wR_2 = 0.1292	R_1 = 0.0474, wR_2 = 0.1117	R_1 = 0.0356, wR_2 = 0.0807
Largest diff. peak/hole / e Å^{-3}	0.41/-0.36	0.35/-0.32	0.26/-0.22

Table S1. Crystal data (continued).

Compound	[(^{tBu}BDI)Mg$^+$·(PhF)$_2$] [Al-F-Al$^-$]	[(^{tBu}BDI)Mg$^+$·PhBr] [B(C$_6$F$_5$)$_4^-$]	[(^{tBu}BDI)Mg$^+$·PhI] [B(C$_6$F$_5$)$_4^-$]
Empirical formula	$C_{71}H_{63}Al_2F_{57}MgN_2O_6$	$C_{65}H_{58}BBrF_{20}MgN_2$	$C_{65}H_{58}BF_{20}IMgN_2$
Formula weight	2201.50	1362.16	1409.15
Temperature/K	100.0(6)	100.0(3)	100.02(16)
Crystal system	triclinic	monoclinic	monoclinic
Space group	P-1	$P2_1/c$	$P2_1/c$
a/Å	11.3521(3)	18.6127(3)	18.7237(5)
b/Å	15.9191(5)	17.9643(2)	18.0226(4)
c/Å	24.7380(7)	18.7424(3)	18.7649(5)
α/°	74.924(3)	90	90
β/°	85.545(2)	102.9937(14)	102.692(3)
γ/°	89.290(2)	90	90
Volume/Å^3	4303.5(2)	6106.31(15)	6177.5(3)
Z	2	4	4
ρ_{calc}g/cm^3	1.699	1.482	1.515
μ/mm^{-1}	2.000	1.942	0.632
F(000)	2204.0	2776.0	2848.0
Crystal size/mm^3	0.295 × 0.249 × 0.1	0.339 × 0.26 × 0.16	0.175 × 0.123 × 0.067
Crystal color	colorless	colorless	colorless
Radiation	Cu Kα (λ = 1.54184)	CuKα (λ = 1.54184)	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	7.424 to 145.51	6.902 to 146.388	4.52 to 59.456
Index ranges	-13 ≤ h ≤ 10, -19 ≤ k ≤ 19, -30 ≤ l ≤ 29	-22 ≤ h ≤ 22, -20 ≤ k ≤ 21, -22 ≤ l ≤ 22	-25 ≤ h ≤ 25, -21 ≤ k ≤ 24, -25 ≤ l ≤ 25
Reflections collected	29394	21736	42831
Independent reflections	16538 [R_{int} = 0.0270, R_{sigma} = 0.0350]	11715 [R_{int} = 0.0179, R_{sigma} = 0.0233]	15163 [R_{int} = 0.0296, R_{sigma} = 0.0393]
Data/restraints/parameters	16538/6852/1633	11715/0/825	15163/0/825
Goodness-of-fit on F^2	1.023	1.027	1.021
Final R indexes [I>=2σ (I)]	R_1 = 0.0400, wR_2 = 0.1001	R_1 = 0.0304, wR_2 = 0.0750	R_1 = 0.0388, wR_2 = 0.0844
Final R indexes [all data]	R_1 = 0.0452, wR_2 = 0.1046	R_1 = 0.0326, wR_2 = 0.0767	R_1 = 0.0569, wR_2 = 0.0927
Largest diff. peak/hole / e Å^{-3}	0.48/-0.37	0.48/-0.62	0.57/-0.89

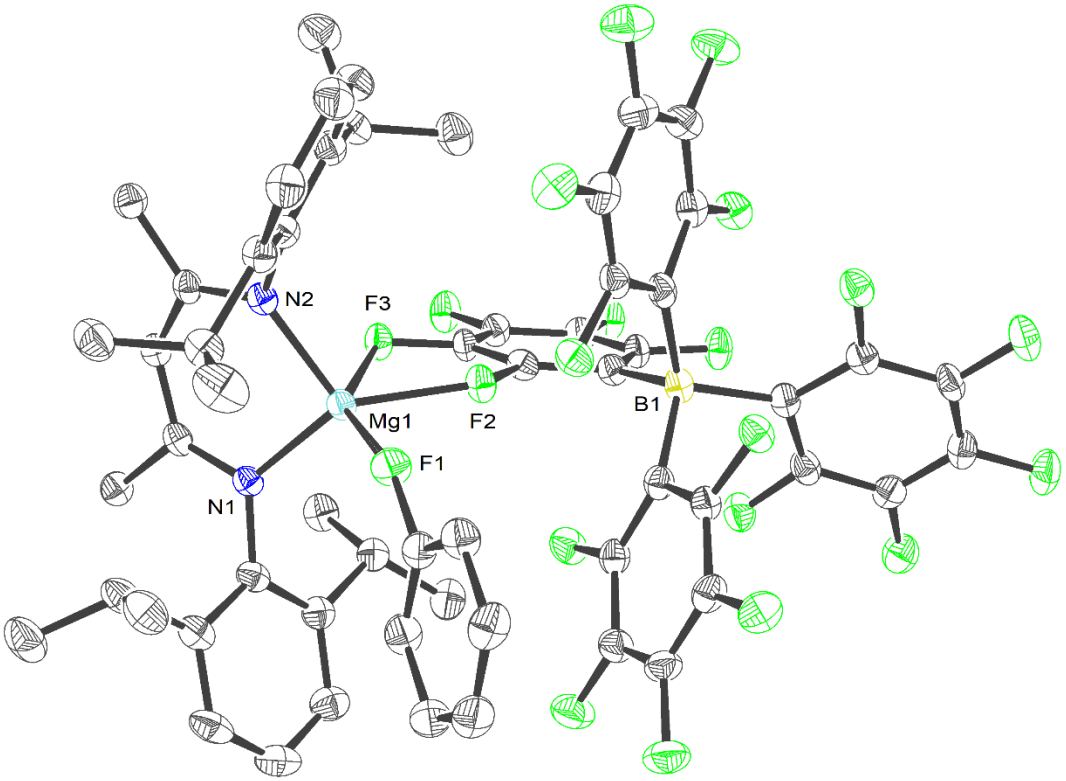

Figure S23: ORTEP representation of [(^{Me}BDI)Mg^{+}·(PhF)][B(C_6F_5)$_4^{-}$] (probability level 50%). Hydrogen atoms were emitted for clarity.

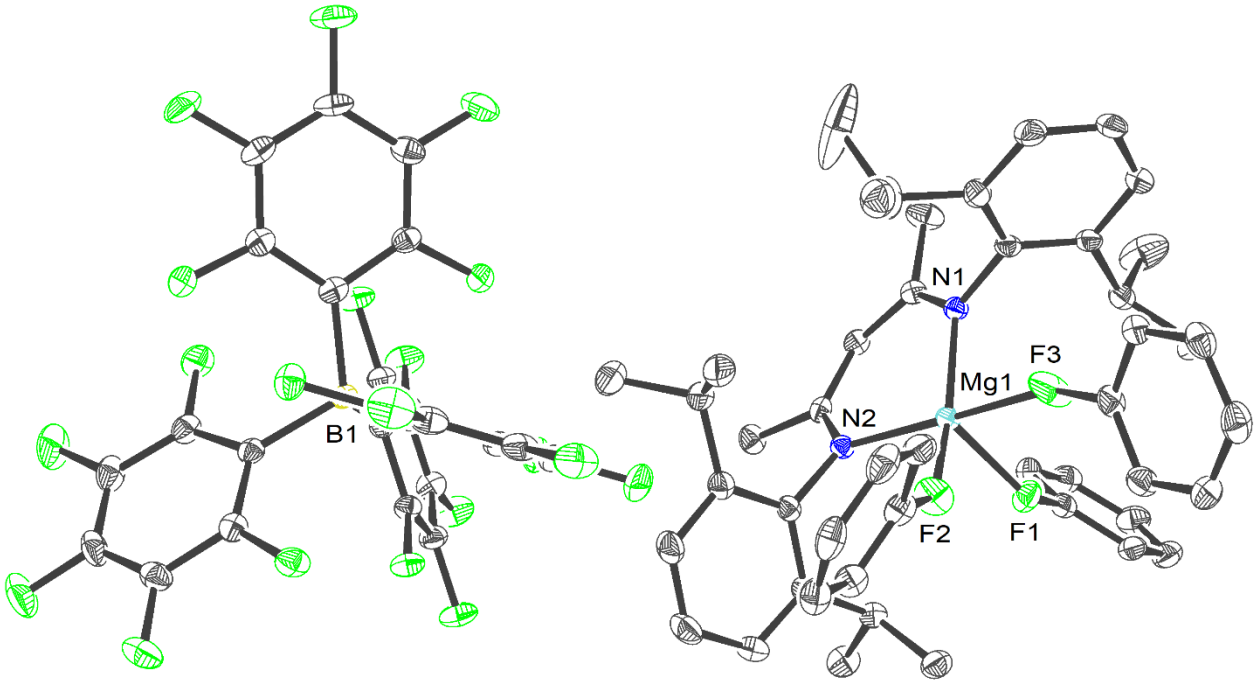

Figure S24: ORTEP representation of [(^{Me}BDI)Mg^{+}·(PhF)$_3$][B(C_6F_5)$_4^{-}$] (probability level 50%). Hydrogen atoms were emitted for clarity.

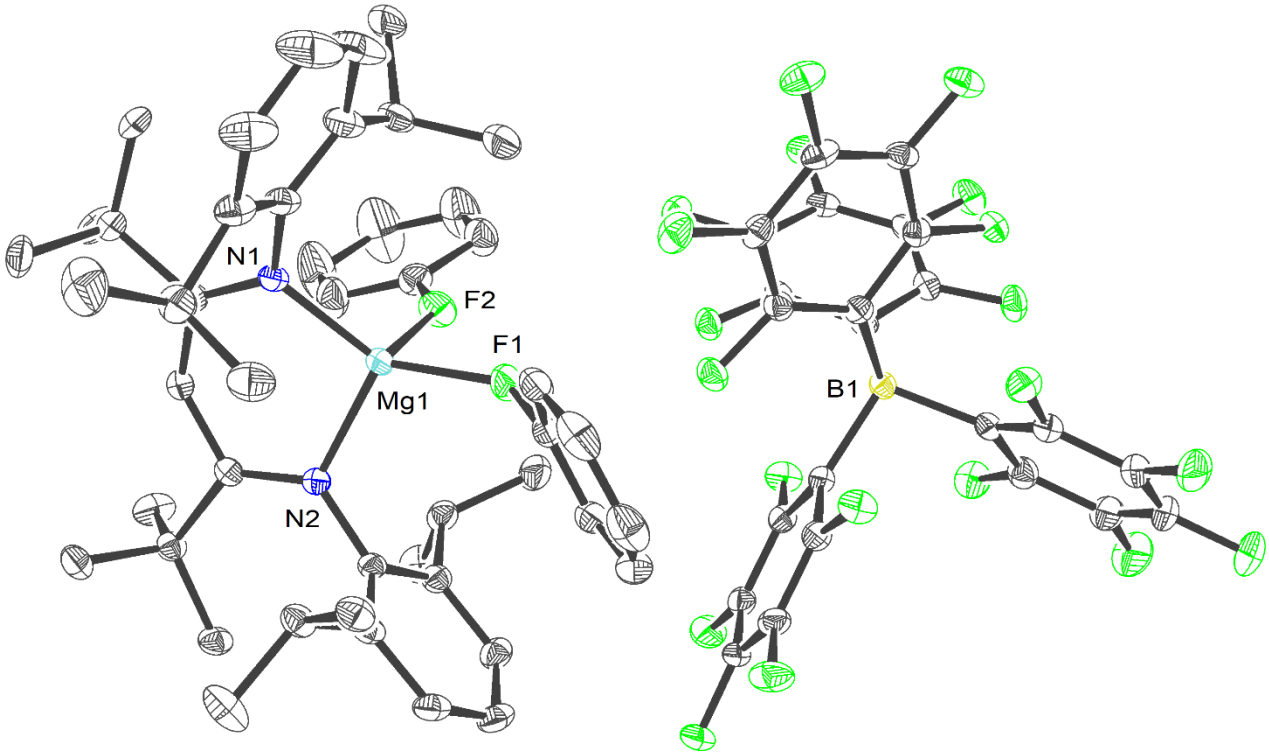

Figure S25: ORTEP representation of [(^{tBu}BDI)Mg^{+}·(PhF)$_2$][B(C$_6$F$_5$)$_4^{-}$] (probability level 50%). Hydrogen atoms were emitted for clarity.

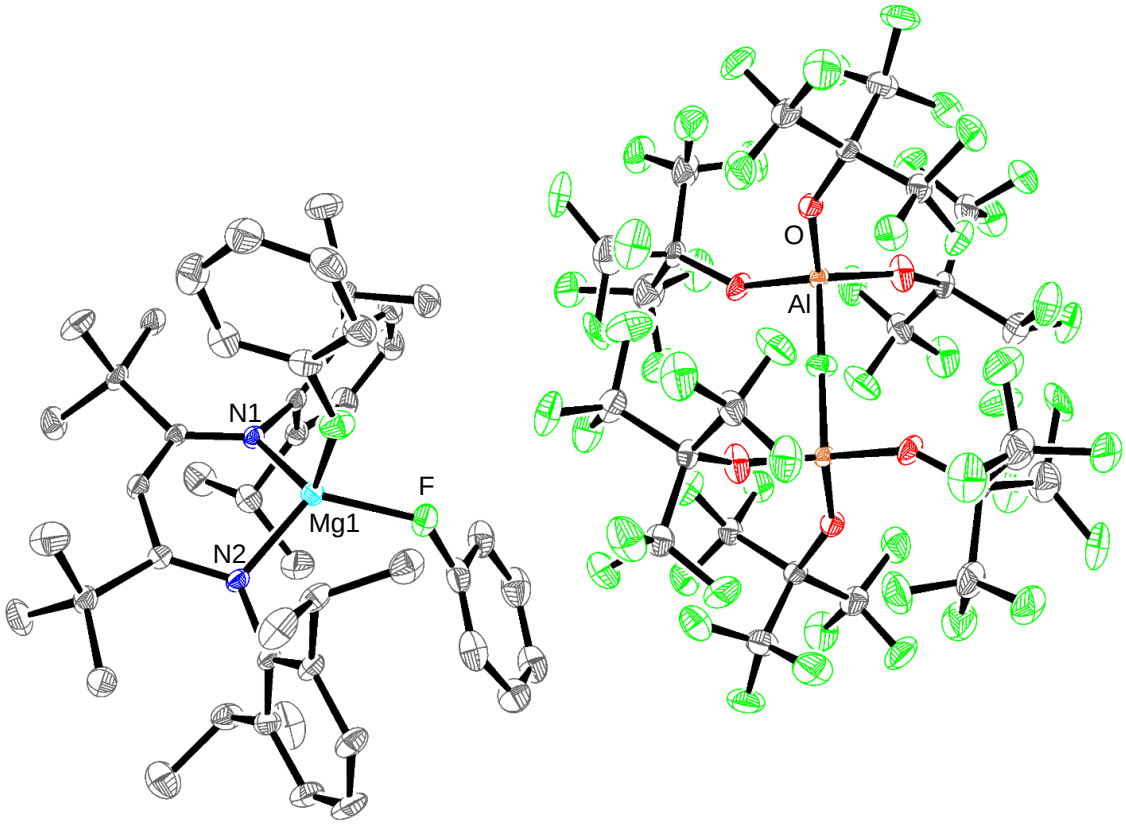

Figure S26: ORTEP representation of [(^{tBu}BDI)Mg^{+}·(PhF)$_2$][Al-F-Al^{-}] (probability level 50%). Hydrogen atoms were emitted for clarity.

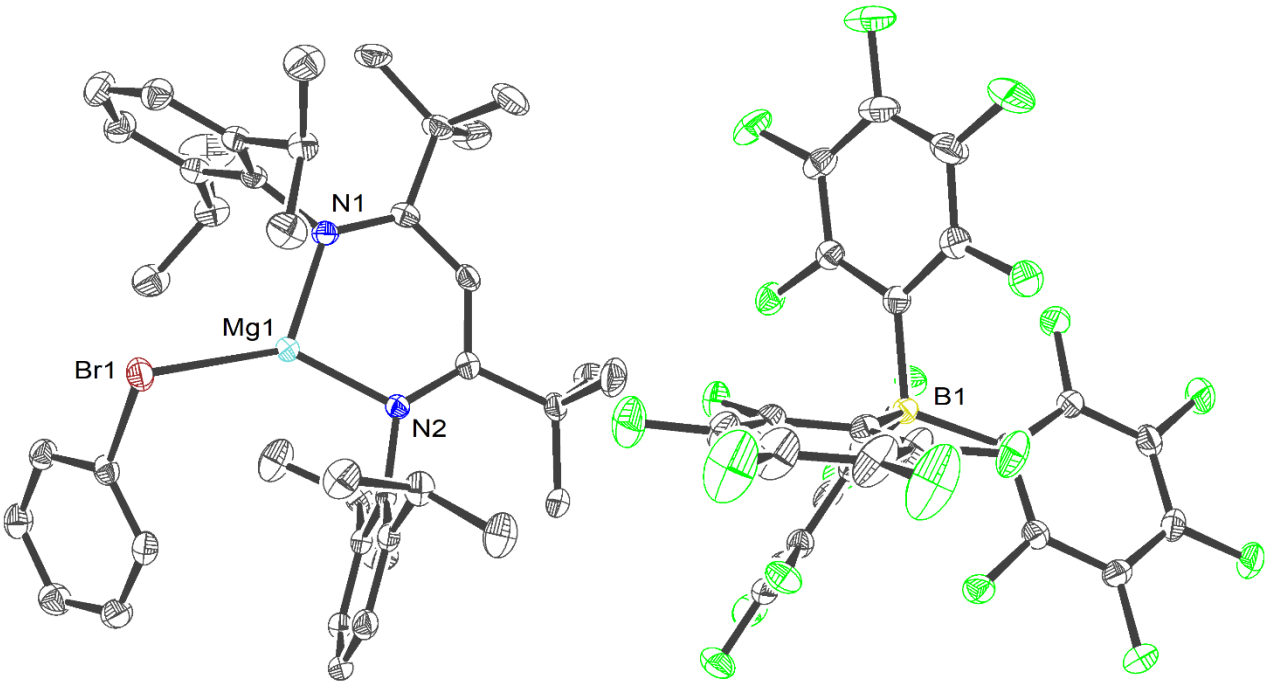

Figure S27: ORTEP representation of [(^{tBu}BDI)Mg^{+}·PhBr][B(C_6F_5)$_4^{-}$] (probability level 50%). Hydrogen atoms were emitted for clarity.

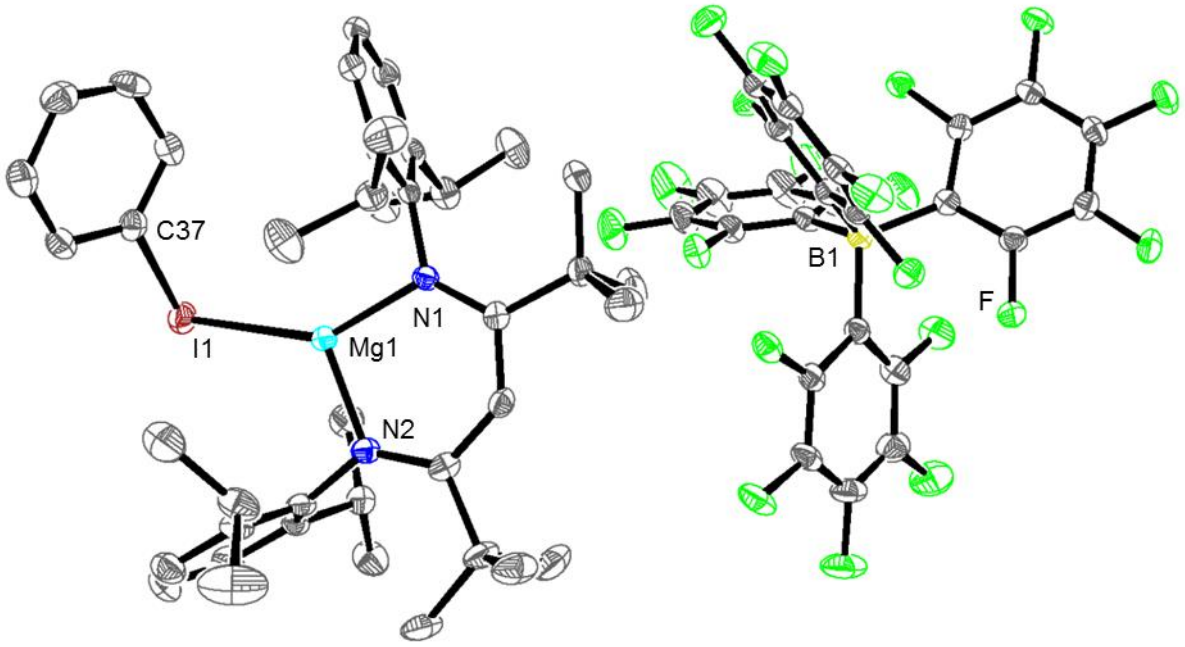

Figure S28: ORTEP representation of [(^{Me}BDI)Mg^{+}·PhI][B(C_6F_5)$_4^{-}$] (probability level 50%). Hydrogen atoms were emitted for clarity.

1.3. Literature known metal-halobenzene complexes

Table S2. Literature compilation of known metal halobenzene complexes.

PhF	**GEQJET**	**HOGHIV**	**NEBDAA**	**SAXSEQ**	**SAXSIU**	**UHAVUU**	**TOQQEV**	**UPAQAF**	**YAWNAO**
reference	[S4]	[S5]	[S6]	[S7]	[S7]	[S8]	[S9]	[S10]	[S11]
	M = Mg	M = Al	M = Ti	M = Sc	M = Ti	M = Ti	M = Li	M = Ru	M = Li
M-**F**(Ph)	2.098(4) 2.085(4)	1.8637(18)	2.1125(19)	2.2725(18) 2.2884(16)	2.166(6)	2.1512(15)	1.866(7)	1.998(5)	1.892(7)
C-**F**	1.346(5) 1.338(6)	1.447(4)	1.418(3)	1.408(3) 1.414(3)	1.406(10)	1.402(3)	(?)	1.328(8)	1.387(5)
angle M-**F**-C	134.7(3) 166.8(3)	129.98(15)	177.46(14)	172.21(16) 165.27(14)	157.3(7)	168.17(16)	180 (?)	134.9(4)	151.7(3)

PhCl	**EZEVOU**	**EZEVUA**	**KUNLAI**	**MAMFOY**	**ROWNIC**	**XIXBIP(01)**
reference	[S12]	[S12]	[S13]	[S14]	[S15]	[S16] ([S17])
	M = Re	M = Re	M = Zr	M = Zr	M = Rh	M = Al
M-**Cl**(Ph)	2.5613(12)	2.559(3)	2.7398(15)	2.6630(8)	2.5208(13)	2.540(3)
C-**Cl**	1.763(4)	1.690(12)	1.767(7)	1.775(3)	1.758(6)	1.774(7)
angle M-**Cl**-C	113.20(16)	114.2(4)	129.0(2)	120.66(10)	114.28(14)	102.7(2)

PhBr	**RAPVUZ**	**RUNWUU**
reference	[S18]	[S19]
	M = Pt	M = Pd
M-**Br**(Ph)	2.581(3)	2.5456(11)
C-**Br**	1.92(3)	1.922(2)
angle M-**Br**-C	116.4(6)	107.34(7)

PhI	**HAMRIW**	**HAMRIV01**	**PUDDEX**	**RAPVOT**
reference	[S20]	[S21]	[S21]	[S18]
	M = Ag	M = Ag	M = Ag	M = Pt
M-**I**(Ph)	2.929(3) 2.971(2)	2.927(2) 2.970(2)	2.853(1)	2.696(2)
C-**I**	(?)	2.093(26)	2.082(9)	2.123(8)
angle M-**I**-C	101.6(8) 93.9(7)	102.3(7) 94.4(7)	99.0(2)	114.8(3)

1.4. Computational details

All geometry optimizations were carried out using Gaussian 16 Rev. A.0.3.[S22] All structures were fully optimized on B3LYP/def2TZVP level of theory.[S23] In all cases dispersion correction Grimme`s third dispersion correction with Becke-Johnson damping (GD3BJ) was applied, unless indicated otherwise.[S24] In order to determine zero-point energies and to characterize the structures as minima, a frequency analysis has been calculated. Solvation effects were approximated using the PCM field of benzene.[S25] Molecules were drawn and evaluated using Molecules V2.311.[S26] Topological analyses were carried out using AIMAll V17 with the wavefunctions obtained from the B3LYP/def2TZVP calculations.[S27, S28]

1.4.1. Calculated structures (bond lengths, angles and energies)

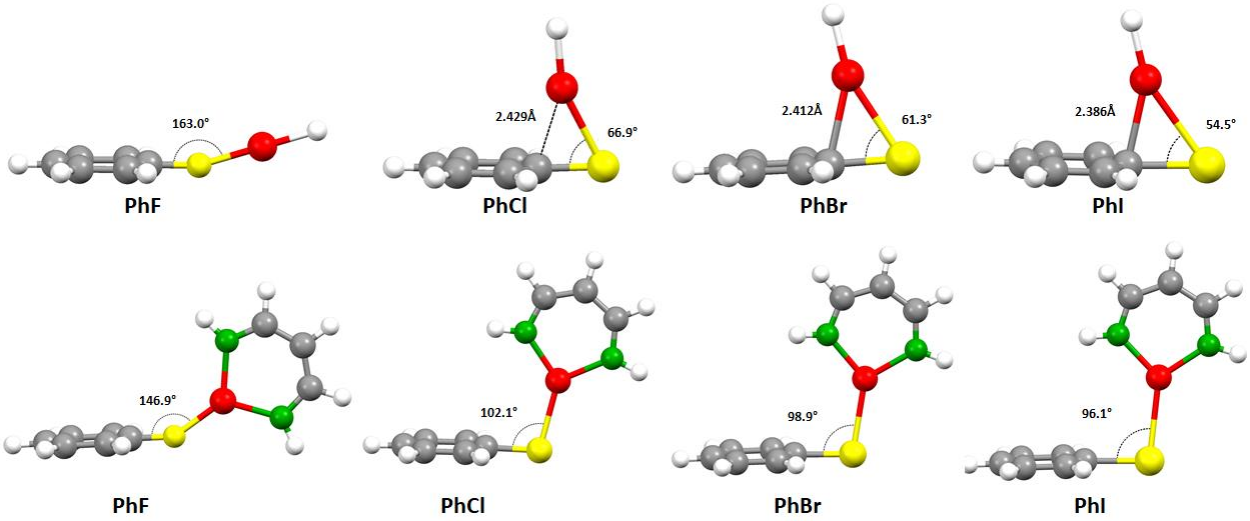

Figure S29: Calculated structures of $HMg^{+}\cdot PhX$ and ($^{mini}BDI)Mg^{+}\cdot PhX$, calculated without dispersion correction.

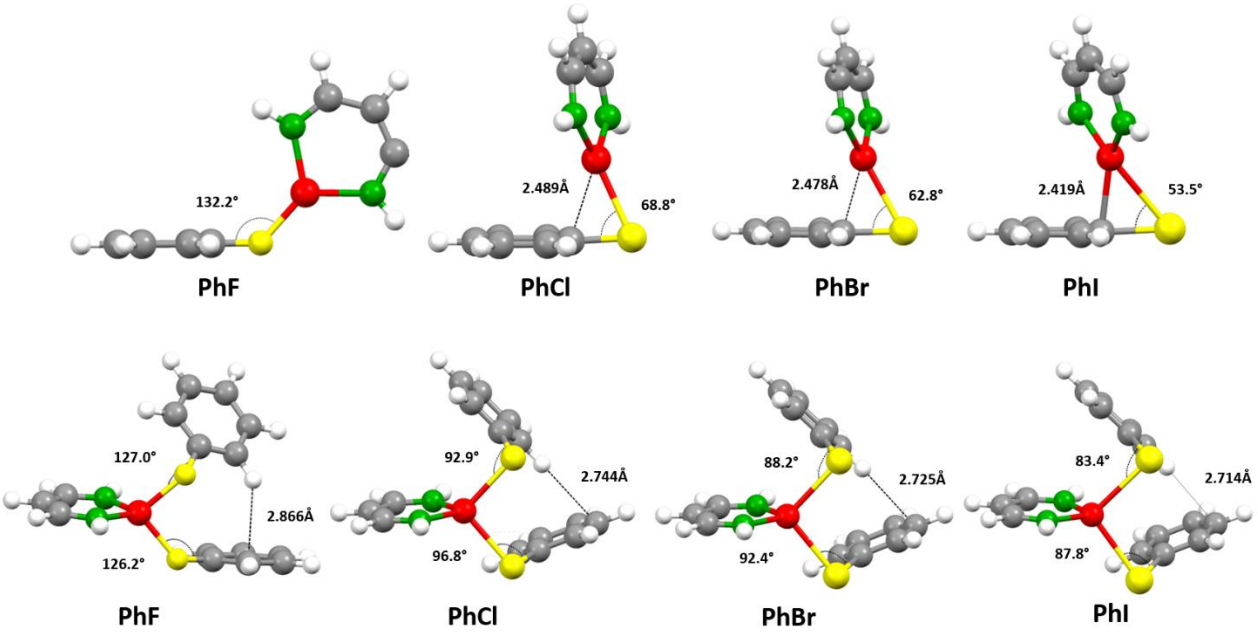

Figure S30: Calculated structures of (^{mini}BDI)Mg^{+}·PhX and (^{mini}BDI)Mg^{+}·(PhX)$_2$ with dispersion correction.

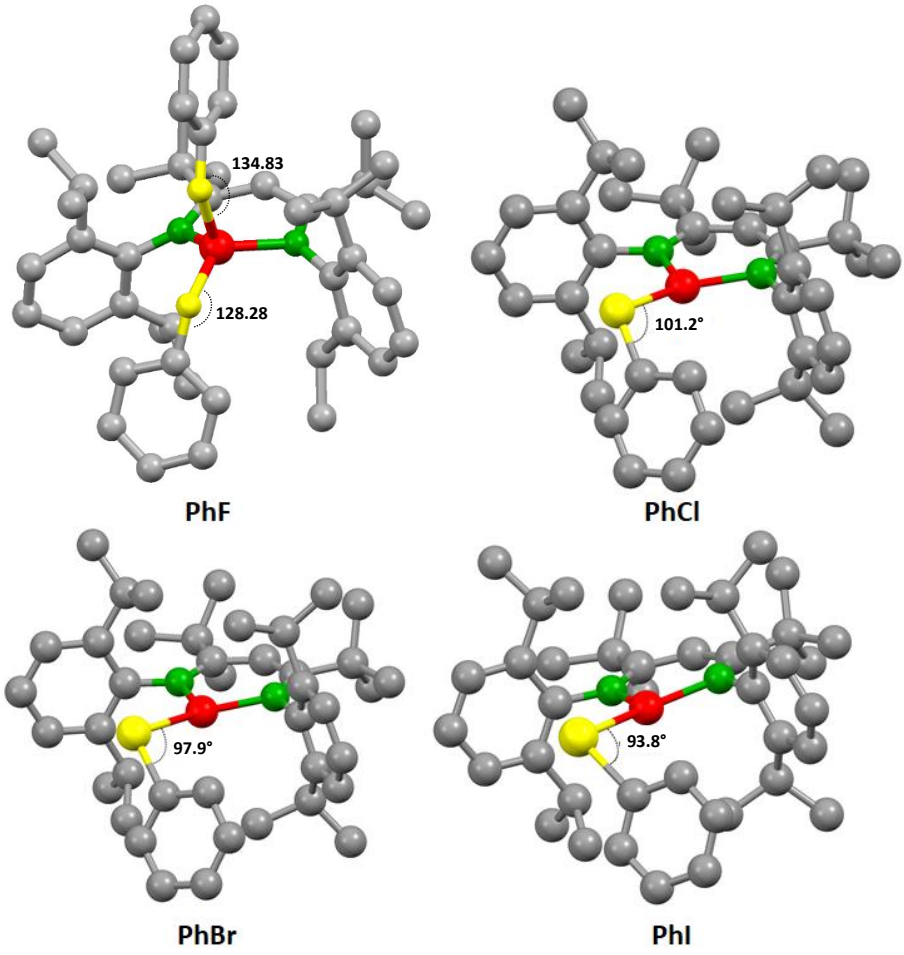

Figure S31: Calculated structures of ($^{t\text{Bu}}$BDI)Mg^{+}·PhX with dispersion correction.

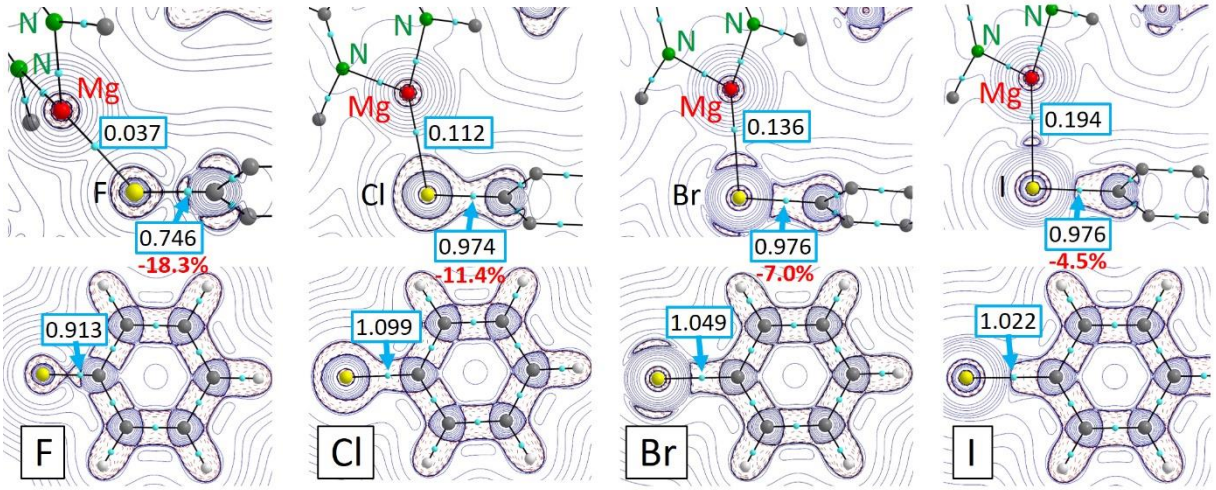

Figure S32: Contour plots of the negative Laplacian, $-\nabla^2\rho(r)$, for the cations (^{tBu}BDI)Mg$^+$···XPh (X = F, Cl, Br, I) in the Mg···X-C plane (top row) and for the free halobenzenes PhX in the molecule plane (middle row). Light-blue dots are bond-critical-points (BCP) and **boxed numbers show the Wiberg bond indices** calculated by the NBO program. (^{tBu}BDI)Mg$^+$···XPh coordination lead in all cases to weakening of the C-X bond. The percentage change (shown in red) is largest for C-F and gradually decreases down the group.

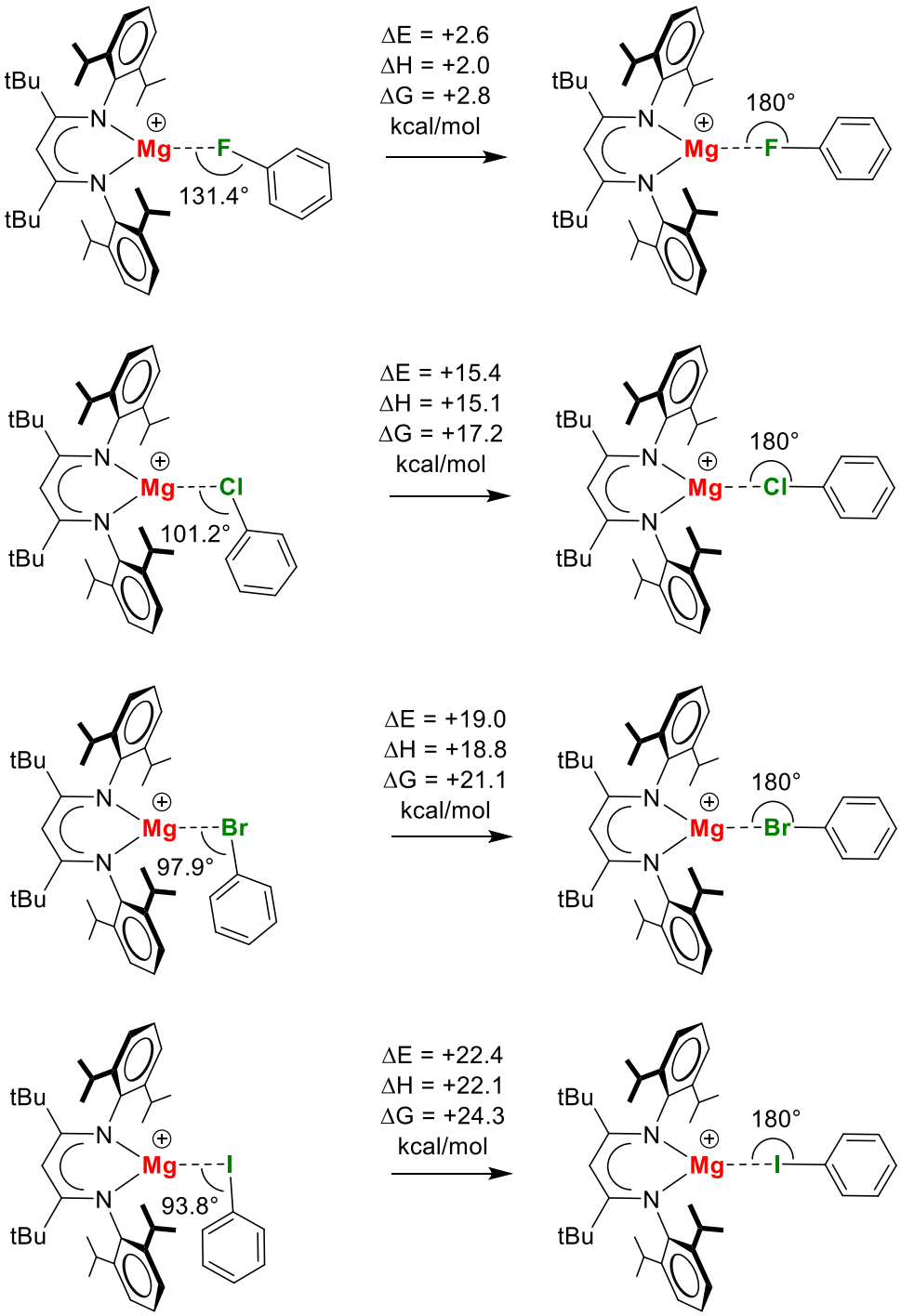

Figure S33: Energy needed for linearization of (^{tBu}BDI)Mg^{+}···XPh (X = F, Cl, Br, I) in kcal/mol, B3LYP/Def2TZVP GD3BJ; ΔG at 298 K.

Table 3: Calculated energies for complexation of (BDI)Mg^+ with ligands (B3LYP/def2TZVP with dispersion correction)

		ΔE [kcal mol^{-1}]	ΔH [kcal mol^{-1}]	ΔG [kcal mol^{-1}]
(^{mini}BDI)Mg^+	C_6H_6	–40.08	–39.07	–30.95
	C_6H_6 solvent correction PCM, benzene	–14.38	–13.37	–5.25
	PhF	–34.29	–33.84	–26.92
	PhF solvent correction PCM, benzene	–14.22	–13.78	–6.85
	2 PhF solvent correction PCM, benzene	–22.64	–21.31	–2.95
	PhCl	–35.44	–34.46	–26.54
	2 PhCl solvent correction PCM, benzene	–16.57	–15.15	4.30
	PhBr	–36.48	–35.90	–27.63
	2 PhBr solvent correction PCM, benzene	–16.02	–14.71	4.79
	PhI	–37.95	–37.33	–28.34
	2 PhI solvent correction PCM, benzene	–14.64	–13.37	6.99
(^{tBu}BDI)Mg^+	C_6H_6	–28.59	–27.25	–15.90
	C_6H_6 solvent correction PCM, benzene	–9.90	–8.56	2.78
	PhF	–22.95	–21.64	–9.04
	PhCl	–28.37	–27.96	–18.14
	PhBr	–29.59	–29.31	–19.46
	PhI	–30.98	–30.64	–20.06
	PhF solvent correction PCM, benzene	–13.02	–12.75	–2.65
	PhCl solvent correction PCM, benzene	–12.73	–12.32	–2.51
	PhBr solvent correction PCM, benzene	–12.09	–11.80	–1.95
	PhI solvent correction PCM, benzene	–11.24	–10.90	–0.33

Table 4: Calculated linearization energies for (^{mini}BDI)Mg^{+}·XPh and (^{tBu}BDI)Mg^{+}·XPh, *i.e.* the energy needed to convert the bent minimum in a linear structure (B3LYP/def2TZVP without dispersion correction).

complex	ΔE [kcal mol^{-1}]	ΔH [kcal mol^{-1}]	ΔG [kcal mol^{-1}]
(^{mini}BDI)Mg^{+}·FPh	0.19	0.07	4.53
(^{mini}BDI)Mg^{+}·ClPh	9.88	9.33	11.62
(^{mini}BDI)Mg^{+}·BrPh	12.49	11.94	14.68
(^{mini}BDI)Mg^{+}·IPh	16.21	15.62	21.34
(^{tBu}BDI)Mg^{+}·FPh	2.62	2.00	2.75
(^{tBu}BDI)Mg^{+}·ClPh	15.43	15.06	17.16
(^{tBu}BDI)Mg^{+}·BrPh	19.03	18.78	21.09
(^{tBui}BDI)Mg^{+}·IPh	22.44	22.06	24.34

1.4.2. XYZ coordinates

XYZ-Files:

```
        14
PhF—Mg+H, O.D.
C       0.115933        -0.024191       0.000000
F       0.122698        1.448319        0.000000
C       0.120297        -0.628384       1.227651
C       0.120297        -0.628384       -1.227651
C       0.120297        -2.023150       1.208828
C       0.120297        -2.023150       -1.208828
C       0.119554        -2.710955       0.000000
H       0.128668        -0.067861       2.151621
H       0.128668        -0.067861       -2.151621
H       0.123643        -2.561594       2.146678
H       0.123643        -2.561594       -2.146678
H       0.120945        -3.792343       0.000000
Mg      -0.427424       3.281642        0.000000
H       -0.900810       4.865959        0.000000

        14
PhCl—Mg+H, O.D.
C       -0.137176       -0.424540       -0.294938
Cl      -1.887391       -0.757923       -0.493315
C       0.599351        -1.185317       0.607549
C       1.943759        -0.867541       0.778270
C       2.520765        0.183491        0.069763
C       0.415528        0.630248        -1.025954
C       1.763525        0.929587        -0.825793
```

H	0.144105	-2.006083	1.144976
H	2.539219	-1.451310	1.467660
H	3.567136	0.417071	0.213172
H	-0.164889	1.155301	-1.775733
H	2.215047	1.735441	-1.388929
Mg	-1.426407	1.245670	0.909398
H	-1.732593	2.490668	1.959054

14

PhBr—Mg+H, O.D.

C	0.227843	-0.360651	-0.000393
Br	-1.725772	-0.463376	-0.000503
C	0.895396	-0.312720	1.224314
C	2.284331	-0.199386	1.207429
C	2.972845	-0.141905	-0.000173
C	0.895332	-0.309355	-1.225007
C	2.284271	-0.196057	-1.207891
H	0.356938	-0.393177	2.159391
H	2.821762	-0.168171	2.145977
H	4.051371	-0.058770	-0.000085
H	0.356830	-0.387315	-2.160273
H	2.821650	-0.162262	-2.146380
Mg	-0.580189	1.912281	0.002096
H	-0.404394	3.560920	0.004124

14

PhI—Mg+H, O.D.

C	-0.559277	-0.327943	0.001285
I	1.590634	-0.265061	0.001147
C	-1.241897	-0.324623	1.223412
C	-1.242148	-0.338569	-1.220762
C	-2.635964	-0.331625	1.208093
C	-2.636064	-0.345454	-1.205050
C	-3.328318	-0.342346	0.001642
H	-0.705673	-0.347593	2.163018
H	-0.705913	-0.371731	-2.160022
H	-3.173285	-0.337801	2.147388
H	-3.173701	-0.362381	-2.144040
H	-4.410041	-0.351038	0.001677
Mg	-0.141272	2.021597	-0.008619
H	-0.577741	3.622959	-0.017089

23

PhF—miniNacNacMg+, O.D., bent

C	1.969149	-0.359099	-0.042484
F	0.593522	-0.798033	-0.097739
C	2.559009	-0.335213	1.194961
C	3.889084	0.080009	1.230781
C	4.546493	0.436299	0.058108
C	2.559480	-0.029364	-1.235197
C	3.889599	0.381728	-1.166538
H	2.026891	-0.630446	2.088412

H	4.404936	0.117114	2.180518
H	5.579284	0.754332	0.098363
H	2.027680	-0.093928	-2.174128
H	4.405815	0.652907	-2.077289
Mg	-1.289796	-0.287845	-0.037109
N	-2.861747	-1.451254	-0.106126
N	-2.115072	1.481061	0.105551
C	-4.061921	-0.879107	-0.049880
C	-3.445363	1.545593	0.125216
C	-4.346392	0.483249	0.055466
H	-5.393130	0.747298	0.086886
H	-4.925582	-1.539466	-0.089814
H	-3.889258	2.535645	0.204579
H	-2.925220	-2.457787	-0.181098
H	-1.692658	2.397555	0.169957

23

PhCl—miniNacNacMg+, O.D., bent

C	1.960374	-0.595296	0.000199
Cl	0.667480	-1.856266	0.000589
C	2.440591	-0.160041	1.221813
C	3.462637	0.784833	1.206621
C	3.969027	1.254457	-0.000357
C	2.440933	-0.161146	-1.221675
C	3.462974	0.783744	-1.207051
H	2.052072	-0.547739	2.153011
H	3.864250	1.143040	2.145056
H	4.767032	1.984684	-0.000575
H	2.052672	-0.549682	-2.152631
H	3.864850	1.141102	-2.145698
Mg	-1.356452	-0.511588	-0.000147
N	-3.213612	-1.143514	-0.000243
N	-1.618311	1.430997	-0.000083
C	-4.185691	-0.235279	-0.000179
C	-2.865969	1.896329	-0.000047
C	-4.046336	1.153595	-0.000074
H	-4.964583	1.722156	-0.000028
H	-5.208450	-0.606444	-0.000214
H	-2.989263	2.977369	0.000010
H	-3.579063	-2.086626	-0.000332
H	-0.937047	2.178149	-0.000063

23

PhBr—miniNacNacMg+, O.D., bent

C	1.955973	-0.233929	-0.000060
Br	0.647115	-1.697603	-0.000257
C	2.406401	0.231476	1.221817
C	3.365166	1.241427	1.206587
C	3.839808	1.743839	0.000189
C	2.406034	0.232132	-1.221822
C	3.364803	1.242076	-1.206337
H	2.045110	-0.176433	2.155027

H	3.741951	1.624514	2.145652
H	4.588506	2.524600	0.000286
H	2.044462	-0.175274	-2.155143
H	3.741306	1.625667	-2.145309
Mg	-1.521820	-0.296835	0.000319
N	-3.379720	-0.933582	0.000312
N	-1.798285	1.646011	0.000080
C	-4.356669	-0.030806	0.000105
C	-3.047419	2.106435	-0.000086
C	-4.224634	1.358672	-0.000088
H	-5.145582	1.922859	-0.000245
H	-5.377502	-0.407377	0.000083
H	-3.175323	3.186999	-0.000235
H	-3.740681	-1.878438	0.000431
H	-1.120188	2.396087	0.000053

23

PhI—miniNacNacMg+, O.D.,bent

C	1.975122	0.110608	0.000044
I	0.662267	-1.591159	-0.000360
C	2.395445	0.614909	1.220302
C	3.279101	1.691318	1.206137
C	3.716989	2.227163	0.000547
C	2.394920	0.615920	-1.219975
C	3.278580	1.692320	-1.205299
H	2.066024	0.189356	2.157444
H	3.626209	2.100750	2.145718
H	4.407449	3.059979	0.000739
H	2.065112	0.191128	-2.157327
H	3.625288	2.102531	-2.144689
Mg	-1.719321	-0.129105	0.000138
N	-3.576162	-0.777668	0.000983
N	-2.021240	1.812955	-0.000658
C	-4.562277	0.114898	0.000806
C	-3.273425	2.263346	-0.000561
C	-4.444258	1.505412	0.000093
H	-5.370435	2.060965	0.000056
H	-5.579323	-0.271951	0.001267
H	-3.410498	3.342856	-0.001038
H	-3.928341	-1.725845	0.001562
H	-1.349157	2.568517	-0.001168

23

PhF—miniNacNacMg+, O.D., linear

C	0.000000	0.000000	-2.038537
F	0.000000	0.000000	-0.593762
C	0.000000	1.224774	-2.653856
C	0.000000	-1.224774	-2.653856
C	0.000000	1.208126	-4.047664
C	0.000000	-1.208126	-4.047664
C	0.000000	0.000000	-4.736785
H	0.000000	2.148134	-2.091964

H	0.000000	-2.148134	-2.091964
H	0.000000	2.145851	-4.586409
H	0.000000	-2.145851	-4.586409
H	0.000000	0.000000	-5.818220
Mg	0.000000	0.000000	1.347364
N	1.515493	0.000000	2.585561
N	-1.515493	0.000000	2.585561
C	1.253799	0.000000	3.890967
C	-1.253799	0.000000	3.890967
C	0.000000	0.000000	4.503156
H	0.000000	0.000000	5.583199
H	2.107849	0.000000	4.564934
H	-2.107849	0.000000	4.564934
H	2.509528	0.000000	2.399581
H	-2.509528	0.000000	2.399581

23

PhCl—miniNacNacMg+, O.D., linear

C	0.000000	0.000000	2.444348
Cl	0.000000	0.000000	0.620200
C	0.000000	1.225471	3.074041
C	0.000000	-1.225471	3.074041
C	0.000000	1.206743	4.466918
C	0.000000	-1.206743	4.466918
C	0.000000	0.000000	5.157112
H	0.000000	2.153787	2.522595
H	0.000000	-2.153787	2.522595
H	0.000000	2.146044	5.003612
H	0.000000	-2.146044	5.003612
H	0.000000	0.000000	6.238699
Mg	0.000000	0.000000	-1.805041
N	-1.515383	0.000000	-3.041353
N	1.515383	0.000000	-3.041353
C	-1.253742	0.000000	-4.346553
C	1.253742	0.000000	-4.346553
C	0.000000	0.000000	-4.958757
H	0.000000	0.000000	-6.038768
H	-2.108139	0.000000	-5.020118
H	2.108139	0.000000	-5.020118
H	-2.508818	0.000000	-2.852582
H	2.508818	0.000000	-2.852582

23

PhBr—miniNacNacMg+, O.D., linear

C	0.000000	0.000000	2.527066
Br	0.000000	0.000000	0.541332
C	0.000000	1.226726	3.152234
C	0.000000	-1.226726	3.152234
C	0.000000	1.206490	4.546162
C	0.000000	-1.206490	4.546162
C	0.000000	0.000000	5.236215
H	0.000000	2.156803	2.604338

H	0.000000	-2.156803	2.604338
H	0.000000	2.146592	5.081743
H	0.000000	-2.146592	5.081743
H	0.000000	0.000000	6.317820
Mg	0.000000	0.000000	-2.042777
N	-1.515283	0.000000	-3.279529
N	1.515283	0.000000	-3.279529
C	-1.253777	0.000000	-4.584678
C	1.253777	0.000000	-4.584678
C	0.000000	0.000000	-5.196931
H	0.000000	0.000000	-6.276948
H	-2.108364	0.000000	-5.258034
H	2.108364	0.000000	-5.258034
H	-2.508501	0.000000	-3.089782
H	2.508501	0.000000	-3.089782

23

PhI—miniNacNacMg+, O.D., linear

I	0.000000	0.000000	0.494692
Mg	0.000000	0.000000	-2.314501
N	0.000000	1.514976	-3.552441
N	0.000000	-1.514976	-3.552441
C	0.000000	0.000000	2.671214
C	1.226403	0.000000	3.300501
C	-1.226403	0.000000	3.300501
C	1.205814	0.000000	4.695101
C	-1.205814	0.000000	4.695101
C	0.000000	0.000000	5.385403
C	0.000000	1.253625	-4.857411
C	0.000000	-1.253625	-4.857411
C	0.000000	0.000000	-5.469852
H	2.159959	0.000000	2.758825
H	-2.159959	0.000000	2.758825
H	2.146583	0.000000	5.229936
H	-2.146583	0.000000	5.229936
H	0.000000	0.000000	6.467089
H	0.000000	0.000000	-6.549849
H	0.000000	2.108436	-5.530564
H	0.000000	-2.108436	-5.530564
H	0.000000	2.507984	-3.361503
H	0.000000	-2.507984	-3.361503

23

PhF—miniNacNacMg+, Dispersion, bent

C	1.881337	-0.543510	0.000031
F	0.589998	-1.187430	0.000066
C	2.435813	-0.273101	1.224332
C	3.682577	0.349061	1.208122
C	4.297895	0.657754	-0.000035
C	2.435843	-0.273294	-1.224300
C	3.682606	0.348870	-1.208158
H	1.939569	-0.540086	2.146666

H	4.168136	0.583279	2.145176
H	5.266736	1.137370	-0.000061
H	1.939621	-0.540425	-2.146603
H	4.168187	0.582941	-2.145237
Mg	-1.228399	-0.478767	0.000023
N	-2.961858	-1.383082	0.000052
N	-1.769198	1.400457	-0.000057
C	-4.058756	-0.629478	0.000017
C	-3.072326	1.675073	-0.000074
C	-4.127696	0.763973	-0.000041
H	-5.120311	1.188785	-0.000063
H	-5.014111	-1.149273	0.000034
H	-3.355205	2.725258	-0.000118
H	-3.181377	-2.370089	0.000092
H	-1.206814	2.240591	-0.000089

23

PhCl—miniNacNacMg+, Dispersion, bent

C	-1.741188	0.588300	-0.097091
Cl	-1.082057	2.175934	-0.592358
C	-1.758679	0.272376	1.259516
C	-2.206738	-0.993712	1.627754
C	-2.630586	-1.896887	0.660621
C	-2.166446	-0.293347	-1.084280
C	-2.614242	-1.547244	-0.686247
H	-1.460141	0.998791	2.003484
H	-2.232742	-1.260822	2.675250
H	-2.980938	-2.875905	0.957050
H	-2.155219	-0.004131	-2.125678
H	-2.956165	-2.248514	-1.435135
Mg	0.746461	0.530232	-0.168573
N	2.163405	0.811041	1.161822
N	1.594576	-0.827634	-1.304644
C	3.290657	0.114244	1.052348
C	2.818515	-1.246872	-0.995644
C	3.606282	-0.832238	0.077592
H	4.579069	-1.293383	0.159818
H	4.059790	0.296181	1.799825
H	3.264000	-1.996519	-1.646017
H	2.187796	1.441772	1.951704
H	1.240672	-1.282708	-2.135005

23

PhBr—miniNacNacMg+, Dispersion, bent

C	1.601352	0.092692	0.055677
Br	1.390776	-1.829115	-0.192456
C	1.490679	0.616286	1.343333
C	1.582308	1.997599	1.497621
C	1.790667	2.815823	0.393984
C	1.819106	0.890541	-1.064075
C	1.911852	2.265176	-0.877962
H	1.360173	-0.031432	2.199462

H	1.500653	2.424266	2.487983
H	1.864413	3.886554	0.525306
H	1.920809	0.452191	-2.046710
H	2.085944	2.903196	-1.733746
Mg	-0.830685	-0.366033	-0.059603
N	-2.207326	-0.650238	1.314714
N	-1.897129	0.556281	-1.428014
C	-3.444411	-0.221799	1.084009
C	-3.187126	0.780876	-1.195297
C	-3.910088	0.437740	-0.053499
H	-4.955592	0.707286	-0.052960
H	-4.184276	-0.401881	1.860986
H	-3.750410	1.288001	-1.975720
H	-2.130875	-1.108839	2.212589
H	-1.614614	0.900177	-2.335652

23

PhI—miniNacNacMg+, Dispersion, bent

I	-1.852232	-1.212406	-0.138539
Mg	0.962262	-0.264999	0.021945
N	2.234530	0.365842	-1.338619
N	2.198749	-1.232062	1.209913
C	-0.719713	2.967566	-0.794057
H	-0.725496	3.652763	-1.631202
C	-0.729243	1.208878	1.373573
H	-0.776498	0.541997	2.224767
C	4.115663	-0.687840	-0.198010
H	5.182682	-0.834098	-0.274202
C	-0.235205	2.505175	1.521007
H	0.132609	2.823372	2.487056
C	3.521514	0.055247	-1.217281
C	-1.206613	1.677334	-0.970799
H	-1.581922	1.357672	-1.932547
C	-0.230058	3.379036	0.441941
H	0.150717	4.383656	0.563719
C	3.491001	-1.273878	0.903289
C	-1.204921	0.805722	0.119283
H	4.194401	0.414974	-1.992863
H	2.056608	0.910942	-2.171079
H	1.997198	-1.748709	2.055420
H	4.143332	-1.824957	1.577439

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(PhF)2—miniNacNacMg+, Dispersion

C	-0.522347	1.633201	-0.783372
F	0.193092	0.534426	-1.334826
C	0.196982	2.762044	-0.476052
C	-0.516921	3.826781	0.068033
C	-1.887755	3.719615	0.275881
C	-1.873431	1.470307	-0.603037
C	-2.562489	2.550499	-0.057925
H	1.261390	2.816572	-0.654343

H	0.004529	4.739181	0.322065
H	-2.433295	4.553442	0.695462
H	-2.368986	0.550480	-0.875395
H	-3.629348	2.472264	0.099213
Mg	1.537680	-0.631921	-0.393655
N	3.297836	-1.063495	-1.173153
N	2.129844	0.191039	1.302608
C	4.398547	-0.789307	-0.484372
C	3.430008	0.257932	1.573266
C	4.480765	-0.188018	0.773448
H	5.475139	-0.048706	1.170463
H	5.349833	-1.056012	-0.940407
H	3.718919	0.712239	2.518963
H	3.511799	-1.498638	-2.060564
H	1.575368	0.604009	2.040362
C	-1.172471	-2.020843	0.025853
F	0.194775	-2.137355	-0.319360
C	-1.467838	-1.620808	1.306615
C	-2.816423	-1.480652	1.624424
C	-3.792431	-1.744765	0.670164
C	-2.093141	-2.300826	-0.953860
C	-3.434963	-2.156222	-0.610062
H	-0.686148	-1.439102	2.031228
H	-3.096917	-1.172062	2.621866
H	-4.837244	-1.639373	0.927479
H	-1.781781	-2.620529	-1.938072
H	-4.196524	-2.370777	-1.346997

35

(PhCl)2—miniNacNacMg+, Dispersion

C	0.113007	1.848878	-1.045882
Cl	0.226932	0.458512	-2.164177
C	1.176678	2.729618	-0.986361
C	1.091795	3.784661	-0.084794
C	-0.030463	3.930829	0.723055
C	-1.021585	1.964927	-0.264650
C	-1.082473	3.026347	0.631813
H	2.044416	2.599639	-1.616596
H	1.907746	4.491278	-0.018852
H	-0.087428	4.755314	1.420503
H	-1.832299	1.257825	-0.349803
H	-1.960438	3.144291	1.252378
Mg	1.220247	-1.021994	-0.423118
N	3.031940	-1.785247	-0.643670
N	1.495662	-0.087645	1.299342
C	3.948843	-1.581098	0.294103
C	2.673599	-0.154467	1.906544
C	3.804748	-0.844709	1.471288
H	4.673529	-0.791597	2.110203
H	4.928514	-2.028352	0.137450
H	2.784158	0.387721	2.843899
H	3.395103	-2.346593	-1.402458

H	0.845875	0.507775	1.794709
C	-1.897486	-1.698884	0.102940
Cl	-0.581879	-2.747457	-0.482815
C	-1.884612	-1.305258	1.430167
C	-2.922130	-0.493942	1.877734
C	-3.935299	-0.105490	1.008834
C	-2.888900	-1.329493	-0.789037
C	-3.919386	-0.522945	-0.317985
H	-1.099127	-1.629652	2.097388
H	-2.939785	-0.179575	2.912428
H	-4.744239	0.516275	1.367345
H	-2.865066	-1.664546	-1.815765
H	-4.711072	-0.227393	-0.992870

35

(PhBr)2—miniNacNacMg+, Dispersion

C	1.051140	1.847044	-0.822276
Br	0.570783	0.472639	-2.112737
C	2.385015	2.185732	-0.691094
C	2.718761	3.135012	0.269265
C	1.732796	3.710028	1.063147
C	0.041931	2.401961	-0.057454
C	0.400984	3.346597	0.898684
H	3.144342	1.727159	-1.307348
H	3.754516	3.421248	0.391687
H	2.002757	4.447636	1.806523
H	-0.989012	2.114597	-0.193984
H	-0.369394	3.799447	1.508196
Mg	0.821560	-1.314790	-0.173094
N	2.189543	-2.743369	-0.273003
N	1.393320	-0.481524	1.531107
C	3.082404	-2.870509	0.700659
C	2.428003	-0.975658	2.197477
C	3.205780	-2.078153	1.843199
H	4.004009	-2.339609	2.521636
H	3.808820	-3.675564	0.607475
H	2.715449	-0.472835	3.119212
H	2.324552	-3.439657	-0.993908
H	1.018034	0.347914	1.970856
C	-2.386784	-0.517558	0.369111
Br	-1.668342	-2.221348	-0.217447
C	-2.179472	-0.133165	1.683026
C	-2.716035	1.082037	2.097569
C	-3.439954	1.870317	1.210715
C	-3.098403	0.244552	-0.541121
C	-3.630497	1.453077	-0.102265
H	-1.629006	-0.761296	2.368112
H	-2.575489	1.400147	3.121824
H	-3.864042	2.807615	1.544264
H	-3.244740	-0.090269	-1.557538
H	-4.198991	2.062140	-0.791999

35

(PhI)2—miniNacNacMg+, Dispersion

C	-2.232113	-0.897706	-0.536523
I	-1.041153	-0.055510	-2.094930
C	-3.473744	-0.342465	-0.274224
C	-4.209766	-0.858716	0.787349
C	-3.700825	-1.898164	1.557439
C	-1.700283	-1.938366	0.207235
C	-2.452739	-2.436775	1.266070
H	-3.863225	0.471766	-0.867683
H	-5.183219	-0.441692	1.007768
H	-4.280861	-2.293171	2.380416
H	-0.730228	-2.353309	-0.018957
H	-2.056475	-3.251745	1.856961
Mg	0.000298	1.566523	0.029642
N	-0.306259	3.525076	0.067874
N	-0.883698	1.108447	1.745406
C	-0.936996	4.077098	1.096944
C	-1.432230	2.058518	2.488483
C	-1.454534	3.427427	2.218362
H	-1.940373	4.053562	2.951681
H	-1.077704	5.156131	1.073488
H	-1.926775	1.751350	3.408481
H	-0.043805	4.217224	-0.621139
H	-1.035237	0.186258	2.131220
C	2.102892	-1.193585	0.502229
I	2.738820	0.744223	-0.116707
C	1.717668	-1.376767	1.822364
C	1.333024	-2.652082	2.225124
C	1.343335	-3.708268	1.321831
C	2.114840	-2.227501	-0.422055
C	1.731526	-3.495962	0.003671
H	1.725418	-0.557130	2.526126
H	1.039068	-2.815580	3.253399
H	1.055722	-4.699338	1.645720
H	2.421912	-2.062225	-1.444433
H	1.745233	-4.316914	-0.700704

11

miniNacNacMg+_nackt, Dispersion

Mg	0.000000	0.000000	1.576089
N	0.000000	1.536791	0.399662
N	0.000000	-1.536791	0.399662
C	0.000000	1.257865	-0.905705
C	0.000000	-1.257865	-0.905705
C	0.000000	0.000000	-1.508670
H	0.000000	0.000000	-2.588425
H	0.000000	2.107663	-1.583815
H	0.000000	-2.107663	-1.583815
H	0.000000	2.530606	0.584103
H	0.000000	-2.530606	0.584103

23

miniNacNacMg+--Benzene, Dispersion

C	-2.002663	1.233998	0.707455
Mg	0.176186	0.135064	-0.000016
N	1.302376	-1.479343	-0.000063
N	1.599262	1.497945	0.000002
C	2.627134	-1.362969	-0.000022
C	2.874987	1.123177	-0.000027
C	3.366457	-0.181446	-0.000010
H	-1.916698	2.164241	1.253083
H	4.440764	-0.288663	-0.000002
C	-2.128517	0.023875	1.399466
C	-2.256049	-1.174491	0.691339
C	-2.255341	-1.167056	-0.704221
C	-2.002058	1.241488	-0.694431
C	-2.127160	0.038826	-1.399441
H	-2.132675	0.018493	2.481239
H	-2.352931	-2.108808	1.227461
H	-2.351674	-2.095596	-1.250390
H	-1.915612	2.177481	-1.230059
H	-2.130384	0.044989	-2.481217
H	3.206237	-2.283950	-0.000046
H	1.013463	-2.448341	-0.000161
H	3.624725	1.911505	-0.000009
H	1.508343	2.505245	0.000069

12

Benzene, Dispersion

H	0.000000	0.000000	2.473025
C	0.000000	0.000000	1.390436
C	0.000000	1.204158	0.695218
C	0.000000	1.204158	-0.695218
C	0.000000	0.000000	-1.390436
C	0.000000	-1.204158	0.695218
C	0.000000	-1.204158	-0.695218
H	0.000000	2.141706	1.236519
H	0.000000	2.141706	-1.236518
H	0.000000	0.000000	-2.473025
H	0.000000	-2.141706	1.236519
H	0.000000	-2.141706	-1.236518

12

PhF, Dispersion

F	0.000000	0.000000	2.276125
C	0.000000	0.000000	0.925138
C	0.000000	1.212373	0.258992
C	0.000000	1.203258	-1.131240
C	0.000000	0.000000	-1.828077
C	0.000000	-1.212373	0.258992
C	0.000000	-1.203258	-1.131240
H	0.000000	2.134308	0.823871
H	0.000000	2.142197	-1.669243

H	0.000000	0.000000	-2.909774
H	0.000000	-2.134308	0.823871
H	0.000000	-2.142197	-1.669243

12
PhCl, Dispersion

Cl	0.000000	0.000000	2.250381
C	0.000000	0.000000	0.504683
C	0.000000	1.209727	-0.176324
C	0.000000	1.202052	-1.565790
C	0.000000	0.000000	-2.263509
C	0.000000	-1.209727	-0.176324
C	0.000000	-1.202052	-1.565790
H	0.000000	2.139096	0.375356
H	0.000000	2.142278	-2.101751
H	0.000000	0.000000	-3.345352
H	0.000000	-2.139096	0.375356
H	0.000000	-2.142278	-2.101751

12
PhBr, Dispersion

Br	0.000000	0.000000	1.805198
C	0.000000	0.000000	-0.104504
C	0.000000	1.210317	-0.783526
C	0.000000	1.202140	-2.173605
C	0.000000	0.000000	-2.870918
C	0.000000	-1.210317	-0.783526
C	0.000000	-1.202140	-2.173605
H	0.000000	2.141960	-0.236035
H	0.000000	2.142482	-2.709477
H	0.000000	0.000000	-3.952796
H	0.000000	-2.141960	-0.236035
H	0.000000	-2.142482	-2.709477

12
PhI, Dispersion

I	1.549383	0.000000	-0.000007
C	-0.561437	0.000021	0.000019
C	-1.245595	-1.209496	0.000033
C	-2.635979	-1.201835	0.000000
C	-3.333662	-0.000015	-0.000043
C	-1.245620	1.209510	0.000033
C	-2.636011	1.201816	0.000000
H	-0.704556	-2.145103	0.000090
H	-3.171323	-2.142602	0.000004
H	-4.415592	-0.000027	-0.000092
H	-0.704608	2.145135	0.000090
H	-3.171372	2.142573	0.000004

103
tBuBDIMg+--Benzene, Dispersion

Mg	0.003002	-0.672579	0.180759

N	1.507980	0.582423	-0.111186
N	-1.487255	0.596849	-0.110556
C	-1.277454	1.852498	-0.508768
C	1.314592	1.860515	-0.435861
C	2.719440	-0.108288	0.198768
C	-2.717555	-0.115317	0.034579
C	0.021265	2.384818	-0.622624
H	0.026478	3.412102	-0.924453
C	3.173448	-0.112337	1.534314
C	3.307196	-0.938377	-0.772539
C	-3.174615	-0.883002	-1.055765
C	-3.329654	-0.211740	1.296438
C	2.454018	2.884880	-0.716345
C	2.900078	-0.872052	-2.236165
H	2.102279	-0.133396	-2.323139
C	-2.401992	2.872514	-0.857746
C	2.586630	0.852020	2.556221
H	2.299946	1.755133	2.017308
C	4.323337	-1.806330	-0.374037
H	4.793237	-2.447281	-1.108777
C	-2.515210	-0.739359	-2.418783
H	-2.102492	0.267562	-2.474225
C	4.188259	-0.998537	1.882260
H	4.557545	-1.018063	2.897763
C	-3.834842	2.323264	-0.912022
H	-3.961232	1.563507	-1.679493
H	-4.497330	3.151829	-1.165096
H	-4.176172	1.912679	0.031449
C	4.752000	-1.852901	0.942019
H	5.540081	-2.534046	1.234192
C	3.882796	2.433545	-0.380351
H	4.025113	2.246010	0.680739
H	4.559169	3.242689	-0.658322
H	4.194005	1.550299	-0.926405
C	2.418787	3.202900	-2.227351
H	2.594477	2.303887	-2.819582
H	3.204646	3.920970	-2.466635
H	1.465721	3.627900	-2.536079
C	-4.399089	-1.094806	1.445452
H	-4.891155	-1.174680	2.405972
C	-4.239295	-1.755055	-0.856350
H	-4.612451	-2.344383	-1.682464
C	4.064931	-0.401988	-3.118933
H	4.460916	0.557821	-2.790215
H	3.735318	-0.294367	-4.153649
H	4.884610	-1.121965	-3.103921
C	2.210009	4.177607	0.090832
H	1.298060	4.696898	-0.193906
H	3.041602	4.863470	-0.074749
H	2.157789	3.968599	1.160639
C	-4.847552	-1.868584	0.387081
H	-5.679038	-2.546988	0.524275

C	-2.128837	3.481292	-2.250822
H	-1.208128	4.057805	-2.295375
H	-2.947976	4.151573	-2.513753
H	-2.076032	2.703071	-3.014238
C	2.358879	-2.208090	-2.756337
H	3.119531	-2.989111	-2.705344
H	2.051391	-2.114158	-3.798986
H	1.498362	-2.551194	-2.183356
C	-2.872342	0.622846	2.480718
H	-2.026585	1.228022	2.152485
C	-0.069756	-2.621605	1.525545
H	-0.073634	-1.968902	2.391874
C	-1.346571	-1.713503	-2.594133
H	-0.576695	-1.603758	-1.817868
H	-0.834571	-1.551020	-3.542834
H	-1.681770	-2.749080	-2.551169
C	-2.372347	3.987018	0.209550
H	-2.559691	3.581435	1.204252
H	-3.151820	4.719257	-0.006769
H	-1.416974	4.507618	0.234335
C	-1.284330	-3.111543	1.019562
H	-2.224517	-2.752170	1.414456
C	1.309082	0.312873	3.210486
H	0.490651	0.232693	2.490569
H	0.957736	0.991376	3.988907
H	1.478121	-0.664335	3.666826
C	1.155166	-3.093639	1.024601
H	2.089345	-2.727619	1.429615
C	3.590155	1.270437	3.633278
H	3.823880	0.451262	4.315131
H	3.173526	2.081018	4.232186
H	4.524733	1.619546	3.193351
C	-1.265423	-4.072294	0.017208
H	-2.198343	-4.454592	-0.372957
C	-0.051951	-4.545050	-0.473642
H	-0.044408	-5.299793	-1.248981
C	1.152954	-4.053696	0.019327
H	2.091856	-4.422114	-0.368632
C	-3.492157	-0.892313	-3.587094
H	-3.864907	-1.913456	-3.678887
H	-2.995184	-0.642072	-4.525257
H	-4.350624	-0.230502	-3.471244
C	-3.973592	1.578841	2.959716
H	-4.321834	2.229402	2.158858
H	-3.601669	2.209395	3.768939
H	-4.835656	1.027063	3.337725
C	-2.400092	-0.251589	3.648949
H	-3.216190	-0.857947	4.044439
H	-2.022442	0.368489	4.463063
H	-1.601891	-0.932566	3.353097

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tBuBDIMg+_nackt, Dispersion

Mg	-0.033119	-1.096179	0.522602
N	-1.525640	0.156018	0.369247
N	1.442893	0.026788	-0.138154
C	1.176159	1.228914	-0.658888
C	-1.323018	1.429688	0.008350
C	-2.738549	-0.583419	0.453961
C	2.706040	-0.630254	-0.027377
C	-0.072235	1.860679	-0.464341
H	-0.077426	2.880854	-0.795919
C	-3.503602	-0.823020	-0.709950
C	-3.037322	-1.259000	1.655036
C	3.665700	-0.192291	0.901126
C	2.887496	-1.836744	-0.734348
C	-2.380519	2.563892	0.161937
C	-2.215365	-1.140662	2.933779
H	-2.697099	-1.819367	3.639092
C	2.139566	2.024603	-1.589421
C	-3.096805	-0.223914	-2.046499
H	-2.688368	0.765590	-1.860951
C	-4.153735	-2.095019	1.692293
H	-4.403012	-2.596529	2.619145
C	3.421633	1.020051	1.780932
H	2.647118	1.625871	1.315535
C	-4.606910	-1.664780	-0.617459
H	-5.214416	-1.842175	-1.493038
C	3.467695	1.337867	-1.937517
H	4.142592	1.253483	-1.092177
H	3.966948	1.943841	-2.694337
H	3.324406	0.344511	-2.358861
C	-4.945592	-2.288906	0.574408
H	-5.812159	-2.933950	0.624847
C	-3.773895	2.110482	0.617093
H	-4.299629	1.537623	-0.141920
H	-4.368353	3.001364	0.822511
H	-3.745454	1.520399	1.529040
C	-1.834453	3.518996	1.250760
H	-1.712807	3.005169	2.204484
H	-2.541621	4.336115	1.399729
H	-0.873018	3.946982	0.973812
C	4.070252	-2.547494	-0.569136
H	4.236242	-3.459096	-1.125458
C	4.833575	-0.940367	1.041014
H	5.591129	-0.612537	1.739397
C	-0.764277	-1.656000	2.812715
H	-0.689636	-2.510544	2.118889
H	-0.391811	-2.044977	3.760231
H	-0.059718	-0.839943	2.584286
C	-2.558683	3.368837	-1.140709
H	-1.644825	3.865526	-1.460406
H	-3.307941	4.143953	-0.975406
H	-2.909043	2.744422	-1.962034

C	5.048699	-2.094390	0.304767
H	5.969516	-2.649472	0.422117
C	2.468024	3.404338	-0.987486
H	1.581254	4.013283	-0.821788
H	3.116843	3.948153	-1.675416
H	2.995611	3.310272	-0.039166
C	-2.221399	0.250614	3.571907
H	-1.714939	0.974809	2.936904
H	-1.713648	0.230801	4.538171
H	-3.241864	0.593394	3.737244
C	1.752628	-2.356700	-1.600041
H	1.263475	-1.488437	-2.043743
C	2.879123	0.573385	3.146092
H	1.963539	-0.012103	3.035314
H	2.651354	1.435692	3.774764
H	3.606824	-0.048943	3.669744
C	1.394203	2.217612	-2.932944
H	1.130379	1.252918	-3.370909
H	2.047632	2.737533	-3.634480
H	0.481179	2.798291	-2.827105
C	-1.969340	-1.042784	-2.691500
H	-1.062498	-1.007960	-2.084464
H	-1.710040	-0.636848	-3.670360
H	-2.266663	-2.085064	-2.822479
C	-4.256926	-0.046913	-3.026377
H	-4.638279	-1.002907	-3.388365
H	-3.920793	0.516634	-3.897511
H	-5.085402	0.497278	-2.571402
C	4.656218	1.908411	1.953182
H	5.439275	1.410873	2.526450
H	4.389446	2.818423	2.492459
H	5.079082	2.197377	0.990453
C	2.176633	-3.266966	-2.750441
H	2.899824	-2.764743	-3.392298
H	1.311093	-3.532632	-3.359285
H	2.625011	-4.194453	-2.392451
C	0.703304	-3.084194	-0.706435
H	0.762816	-4.167595	-0.810683
H	-0.338656	-2.838912	-0.963099
H	0.917244	-2.955063	0.371116

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tBuBDIMg+--PhI, Dispersion

I	0.273494	-2.637216	1.144085
Mg	-0.084924	-0.121411	0.070138
N	0.797577	1.628504	-0.068882
N	-1.937355	0.412446	-0.306912
C	2.201634	1.482723	0.157569
C	3.031089	1.138031	-0.929277
C	4.394421	-2.526272	-0.284512
H	5.290788	-1.981185	-0.025853
C	-3.239004	-0.947838	1.246819

C	2.704954	1.511919	1.469326
C	-3.130857	0.140346	2.303604
H	-3.139011	1.099426	1.786181
C	4.061886	1.250440	1.663867
H	4.471497	1.291005	2.664659
C	-2.758477	-0.729086	-0.061020
C	4.378314	0.899492	-0.687932
H	5.035611	0.661511	-1.512137
C	2.067642	-3.917029	-0.950896
H	1.164558	-4.452030	-1.205995
C	-1.275915	2.679695	-0.667495
H	-1.677739	3.632241	-0.947495
C	3.246835	-4.144493	-1.652301
H	3.252903	-4.866952	-2.457404
C	0.113804	2.717058	-0.434005
C	3.226832	-2.278820	0.430680
H	3.220339	-1.544755	1.223406
C	-2.863414	-1.724973	-1.047119
C	4.406220	-3.453551	-1.318565
H	5.320304	-3.639553	-1.865954
C	1.823997	1.837223	2.662503
H	0.818201	2.031583	2.288025
C	-2.257134	1.668848	-0.605090
C	2.259478	4.248476	-0.482618
H	2.637931	3.933575	0.484254
H	2.524070	5.299013	-0.609123
H	2.783671	3.688253	-1.252650
C	2.091195	-2.988661	0.078640
C	-3.689383	2.144465	-0.977864
C	2.444458	1.009153	-2.324273
H	1.607043	1.702973	-2.397317
C	-3.456091	-2.939166	-0.704745
H	-3.555638	-3.712268	-1.455529
C	4.897684	0.963261	0.598315
H	5.951927	0.787036	0.767629
C	0.732634	4.137225	-0.605257
C	-2.346903	-1.508310	-2.459009
H	-1.935839	-0.499058	-2.509901
C	-3.811564	-2.181490	1.542994
H	-4.193262	-2.368335	2.536989
C	-3.918837	-3.175130	0.578591
H	-4.372399	-4.125074	0.827874
C	1.747624	0.651567	3.633129
H	1.399657	-0.256821	3.137471
H	1.062966	0.868536	4.454222
H	2.725843	0.433626	4.064555
C	-1.802893	0.058842	3.065015
H	-1.681177	-0.912702	3.547531
H	-1.745403	0.829705	3.834724
H	-0.943529	0.220645	2.408567
C	-4.303846	0.147867	3.286633
H	-5.260290	0.160817	2.763183

H	-4.251808	1.034017	3.920419
H	-4.292263	-0.722178	3.944746
C	2.291542	3.100522	3.395972
H	3.283478	2.962686	3.828891
H	1.605118	3.342547	4.208986
H	2.337702	3.958909	2.726423
C	0.376469	4.688472	-2.002992
H	0.750382	4.029894	-2.788944
H	0.847761	5.663465	-2.132765
H	-0.692323	4.818734	-2.154542
C	3.423773	1.359011	-3.445817
H	3.865455	2.343696	-3.290683
H	2.905043	1.368202	-4.405238
H	4.234946	0.633466	-3.522353
C	-4.810991	1.113966	-0.789938
H	-4.667961	0.216841	-1.383599
H	-5.744841	1.574477	-1.114632
H	-4.939785	0.818370	0.248345
C	-4.076497	3.375262	-0.132569
H	-4.038677	3.146524	0.933795
H	-5.098876	3.667913	-0.374741
H	-3.438523	4.237178	-0.313838
C	-3.666080	2.526149	-2.474158
H	-2.956564	3.324097	-2.684730
H	-4.657853	2.863267	-2.779533
H	-3.399311	1.665791	-3.090264
C	1.888694	-0.403594	-2.542519
H	2.674295	-1.155220	-2.468520
H	1.401727	-0.496045	-3.513559
H	1.132208	-0.679567	-1.795169
C	0.122411	5.044128	0.485282
H	-0.959820	5.120310	0.402953
H	0.540674	6.048202	0.399568
H	0.357373	4.666089	1.481268
C	-1.220891	-2.492142	-2.802996
H	-0.396530	-2.434277	-2.089659
H	-0.817994	-2.286759	-3.795913
H	-1.582962	-3.521466	-2.794807
C	-3.470855	-1.597476	-3.498807
H	-3.912815	-2.594777	-3.519058
H	-3.083636	-1.384191	-4.496565
H	-4.268007	-0.885319	-3.286765

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tBuBDIMg+--PhBr, Dispersion

Br	0.203715	-2.538405	1.290532
Mg	-0.074018	-0.264052	0.141439
N	0.909117	1.418522	-0.104929
N	-1.894657	0.348209	-0.256600
C	2.305568	1.210596	0.118832
C	3.106042	0.767186	-0.953861
C	4.141414	-2.916876	-0.042204

H	5.087322	-2.433542	0.154813
C	-3.281749	-0.833453	1.370245
C	2.821796	1.282548	1.423881
C	-3.079702	0.295271	2.368928
H	-3.039369	1.227778	1.805937
C	4.164700	0.959832	1.623835
H	4.584883	1.031220	2.618485
C	-2.785228	-0.724548	0.055266
C	4.440668	0.468775	-0.708144
H	5.077588	0.154193	-1.522622
C	1.687130	-4.150625	-0.550409
H	0.732695	-4.620469	-0.735824
C	-1.107875	2.549667	-0.751138
H	-1.457470	3.506099	-1.083080
C	2.834126	-4.567631	-1.216696
H	2.766192	-5.376596	-1.931342
C	0.282859	2.522181	-0.526655
C	3.008825	-2.478084	0.636713
H	3.072651	-1.662313	1.341983
C	-2.960335	-1.763013	-0.874539
C	4.055855	-3.954159	-0.961998
H	4.943628	-4.287863	-1.481727
C	1.969097	1.713891	2.603858
H	0.972914	1.945552	2.225151
C	-2.144743	1.601279	-0.626859
C	2.509062	3.929959	-0.666762
H	2.875753	3.647417	0.314556
H	2.828497	4.956540	-0.850217
H	2.998178	3.302390	-1.407302
C	1.815258	-3.115704	0.358688
C	-3.549460	2.137841	-1.021872
C	2.503003	0.604709	-2.338561
H	1.715374	1.350473	-2.446289
C	-3.645087	-2.907817	-0.470206
H	-3.800579	-3.712169	-1.177453
C	4.974146	0.571365	0.569914
H	6.018919	0.347619	0.741693
C	0.977699	3.894808	-0.778236
C	-2.424634	-1.662767	-2.292134
H	-1.961244	-0.681289	-2.402460
C	-3.953399	-1.998286	1.727950
H	-4.351957	-2.100165	2.727472
C	-4.134275	-3.032359	0.818928
H	-4.663064	-3.928054	1.116216
C	1.834262	0.582243	3.631110
H	1.429509	-0.327594	3.183415
H	1.170931	0.877293	4.445248
H	2.802364	0.329201	4.066185
C	-1.740429	0.160516	3.103397
H	-1.665892	-0.797971	3.619712
H	-1.615732	0.955509	3.839879
H	-0.889041	0.246285	2.421814

C	-4.222407	0.426904	3.378045
H	-5.189796	0.478384	2.877578
H	-4.095761	1.336834	3.965931
H	-4.249251	-0.409736	4.077702
C	2.510741	2.983430	3.272702
H	3.496309	2.812373	3.708280
H	1.843976	3.302559	4.075354
H	2.599674	3.804127	2.561421
C	0.642855	4.387652	-2.202793
H	0.974607	3.667494	-2.952827
H	1.165981	5.326603	-2.387873
H	-0.418181	4.568111	-2.357187
C	3.497302	0.826213	-3.479458
H	4.008967	1.783481	-3.376682
H	2.973879	0.823467	-4.436312
H	4.254190	0.041543	-3.521310
C	-4.729708	1.187288	-0.778447
H	-4.642673	0.252675	-1.323265
H	-5.635234	1.685177	-1.127296
H	-4.872409	0.955767	0.274119
C	-3.859870	3.432378	-0.242405
H	-3.830827	3.258364	0.834497
H	-4.864418	3.771354	-0.498303
H	-3.173282	4.244599	-0.469771
C	-3.511443	2.437632	-2.536523
H	-2.759758	3.182291	-2.791108
H	-4.484330	2.812916	-2.857599
H	-3.296179	1.532052	-3.106231
C	1.848212	-0.774740	-2.482004
H	2.576129	-1.575935	-2.355945
H	1.363841	-0.887490	-3.452206
H	1.064807	-0.948075	-1.732129
C	0.425198	4.892262	0.263047
H	-0.651878	5.022403	0.181390
H	0.896380	5.865876	0.119857
H	0.646917	4.557682	1.277487
C	-1.347879	-2.722802	-2.556936
H	-0.529065	-2.659463	-1.837376
H	-0.923720	-2.605380	-3.555310
H	-1.762802	-3.729476	-2.484571
C	-3.542224	-1.759806	-3.337609
H	-4.034339	-2.732867	-3.303258
H	-3.136199	-1.627301	-4.341882
H	-4.303857	-0.996802	-3.177958

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tBuBDIMg+--PhCl, Dispersion

Cl	-0.197957	2.451096	1.484172
Mg	0.067835	0.379535	0.258683
N	-0.985170	-1.234580	-0.121121
N	1.862005	-0.269655	-0.189934
C	2.797715	0.744128	0.183745

C	-0.400419	-2.330674	-0.616642
C	0.989576	-2.399503	-0.834309
C	-2.374864	-0.984433	0.100855
C	-3.142074	-0.436986	-0.947747
C	-2.910520	-1.122421	1.392712
C	3.295743	0.754561	1.502316
C	2.063187	-1.504397	-0.642942
C	-4.464980	-0.095139	-0.694552
H	-5.077535	0.301210	-1.491844
C	-1.147816	-3.653888	-0.964779
C	-2.516632	-0.213532	-2.314021
H	-1.764465	-0.988081	-2.464077
C	3.028736	1.820876	-0.688053
C	-2.857884	2.626622	0.860039
H	-2.997796	1.744796	1.468245
C	-5.017963	-0.257800	0.568931
H	-6.053397	0.002252	0.745857
C	-1.382343	4.312049	-0.107456
H	-0.388505	4.719721	-0.217976
C	-2.091792	-1.669902	2.548417
H	-1.104903	-1.927190	2.161964
C	-2.680574	-3.633729	-0.868921
H	-3.046655	-3.403496	0.126193
H	-3.038840	-4.631776	-1.124062
H	-3.136023	-2.938459	-1.569363
C	-4.240180	-0.753791	1.601548
H	-4.675642	-0.872810	2.584982
C	3.025431	-0.412340	2.439114
H	2.953904	-1.313408	1.829457
C	-1.612457	3.193107	0.672288
C	-3.936377	3.228429	0.220290
H	-4.921603	2.803796	0.347377
C	3.447331	-2.072264	-1.066820
C	-2.476700	4.892322	-0.737655
H	-2.329870	5.769600	-1.352700
C	-3.748154	4.352813	-0.573412
H	-4.594589	4.813024	-1.064635
C	3.774421	2.902982	-0.222907
H	3.974292	3.735158	-0.885395
C	2.492199	1.826257	-2.108755
H	1.986634	0.874182	-2.276004
C	4.032245	1.857949	1.920963
H	4.435083	1.883240	2.923525
C	4.271059	2.928190	1.069076
H	4.849486	3.775114	1.413203
C	-1.910575	-0.612989	3.645911
H	-1.455488	0.301609	3.260229
H	-1.271851	-0.991772	4.444911
H	-2.869333	-0.338307	4.088479
C	1.680122	-0.251744	3.157970
H	1.633261	0.689426	3.707796
H	1.510823	-1.068257	3.861195

H	0.836145	-0.281403	2.461404
C	4.140582	-0.646151	3.460318
H	5.114410	-0.716131	2.974870
H	3.962104	-1.577913	3.998401
H	4.190425	0.152208	4.202199
C	4.666641	-1.195005	-0.750371
H	4.628578	-0.222880	-1.231211
H	5.552220	-1.709699	-1.125074
H	4.808204	-1.042002	0.316645
C	1.462186	2.945014	-2.307813
H	0.638572	2.869746	-1.594835
H	1.036589	2.908999	-3.311838
H	1.918543	3.926813	-2.171270
C	3.694577	-3.430162	-0.377262
H	3.657121	-3.330919	0.708845
H	4.688317	-3.790894	-0.645152
H	2.979898	-4.196142	-0.669265
C	-2.702328	-2.950099	3.131829
H	-3.682185	-2.757866	3.571375
H	-2.059829	-3.352426	3.916668
H	-2.825084	-3.718643	2.369110
C	-3.508050	-0.312201	-3.474478
H	-4.066754	-1.247767	-3.438015
H	-2.974579	-0.273665	-4.424971
H	-4.225404	0.509838	-3.471459
C	-0.817083	-4.067288	-2.415251
H	-1.110142	-3.287010	-3.119871
H	-1.376271	-4.969594	-2.665567
H	0.237239	-4.281907	-2.571869
C	-0.647973	-4.738201	0.014633
H	0.423855	-4.906842	-0.065848
H	-1.156448	-5.680421	-0.195378
H	-0.867685	-4.460687	1.046629
C	3.409774	-2.264566	-2.598774
H	2.626281	-2.953272	-2.908975
H	4.366997	-2.662612	-2.938986
H	3.242899	-1.312687	-3.105674
C	-1.793768	1.138120	-2.362634
H	-2.481500	1.964723	-2.185036
H	-1.299315	1.290805	-3.322199
H	-1.005881	1.219255	-1.602332
C	3.613889	1.936630	-3.148410
H	4.145175	2.885429	-3.060596
H	3.203755	1.877261	-4.157988
H	4.343779	1.135580	-3.032849
H	1.302954	-3.345313	-1.226952

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tBuBDIMg+--PhF, Dispersion

N	1.662096	-0.631703	0.004818
N	-1.310396	-1.016315	0.066548
C	1.623334	-1.874684	-0.464043

C	0.394916	-2.552220	-0.638183
H	0.518063	-3.551109	-1.005033
C	-0.955424	-2.193695	-0.460632
C	2.754122	0.247523	0.268728
C	3.221693	0.321738	1.599726
C	2.872832	-2.702781	-0.871271
C	3.184514	1.167180	-0.703160
C	-2.592361	-0.388596	0.084996
C	4.100109	2.147903	-0.321132
H	4.455835	2.854562	-1.059524
C	4.228761	-2.074665	-0.520906
H	4.404483	-1.126526	-1.015807
H	5.010918	-2.761862	-0.845393
H	4.353150	-1.926422	0.550105
C	4.568703	2.232319	0.978394
H	5.280443	2.999665	1.252070
C	2.700035	1.115867	-2.141627
H	1.973954	0.306023	-2.219224
C	1.281198	-0.449189	3.078920
H	1.023699	0.615627	3.066702
H	1.111643	-0.776166	4.104727
H	0.568749	-1.055564	2.501332
C	-3.246323	-0.210815	1.317277
C	-1.959690	-3.331420	-0.814011
C	4.130912	1.320755	1.930434
H	4.515286	1.389639	2.937343
C	-2.733002	-0.857692	2.592556
H	-1.859867	-1.457357	2.327370
C	2.745210	-0.692506	2.635090
H	2.766103	-1.673098	2.155947
C	-2.350615	0.059879	-2.408368
H	-1.880232	-0.922692	-2.413950
C	-3.092254	0.209418	-1.091336
C	2.824658	-2.916595	-2.398053
H	1.929224	-3.453744	-2.705807
H	3.693860	-3.495936	-2.713550
H	2.844672	-1.964589	-2.928701
C	2.838242	-4.072093	-0.157456
H	2.790897	-3.948899	0.926163
H	3.752638	-4.618297	-0.391547
H	2.000166	-4.694488	-0.461864
C	-2.300311	0.192085	3.624901
H	-1.568052	0.896173	3.221006
H	-1.861478	-0.284146	4.503078
H	-3.152304	0.785632	3.959164
C	3.846916	0.818811	-3.118022
H	4.584805	1.622612	-3.111569
H	3.462528	0.729586	-4.135465
H	4.364601	-0.107007	-2.872020
C	1.997177	2.417078	-2.547222
H	1.156734	2.645781	-1.894037
H	1.618625	2.343544	-3.567596

H	2.685477	3.263171	-2.510972
C	3.644910	-0.774943	3.868859
H	4.685537	-0.937790	3.589473
H	3.331078	-1.607423	4.499433
H	3.593110	0.132296	4.473365
C	-3.255792	0.129868	-3.638589
H	-4.090830	-0.567592	-3.561758
H	-2.684648	-0.123774	-4.532451
H	-3.664080	1.130416	-3.789932
C	-4.409627	0.558782	1.353205
H	-4.930453	0.692925	2.292224
C	-1.222589	1.092054	-2.513059
H	-1.613694	2.109284	-2.469199
H	-0.675281	0.974434	-3.448965
H	-0.498076	0.972414	-1.705879
C	-4.260986	0.957898	-1.007355
H	-4.668720	1.410509	-1.899911
C	-3.760231	-1.819871	3.201616
H	-4.661748	-1.290959	3.513709
H	-3.343644	-2.315151	4.080215
H	-4.055030	-2.588512	2.487346
C	-4.919478	1.136916	0.203026
H	-5.829611	1.720370	0.244893
C	-1.686646	-3.882646	-2.227569
H	-1.782044	-3.099583	-2.981127
H	-2.420603	-4.656034	-2.457215
H	-0.700112	-4.328661	-2.330668
C	-1.736607	-4.448954	0.231418
H	-0.722292	-4.842071	0.206774
H	-2.425790	-5.271912	0.036299
H	-1.932169	-4.079491	1.239898
C	-3.451051	-2.971385	-0.761127
H	-3.763744	-2.602585	0.211053
H	-4.018485	-3.880822	-0.962325
H	-3.736341	-2.239075	-1.511493
C	-0.598710	3.194613	0.648742
F	-0.149369	2.043158	1.369860
C	-1.942488	3.282624	0.394848
C	-2.355099	4.400560	-0.325557
C	-1.429138	5.351020	-0.741843
C	0.365678	4.093378	0.271117
C	-0.078020	5.201656	-0.445718
H	-2.637321	2.524253	0.725791
H	-3.404520	4.517737	-0.557355
H	-1.761989	6.215323	-1.299790
H	1.407463	3.933099	0.510883
H	0.638350	5.942596	-0.772091
Mg	0.064884	0.171527	0.823490

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tBuBDIMg-FPh linear geometry, Dispersion

Mg	0.004113	-0.310537	0.350696
F	0.783420	-2.050886	0.175199
C	1.363039	-3.345292	0.044671
C	2.471339	-5.787129	-0.216949
N	-1.769405	0.413836	-0.009482
N	1.092463	1.298416	0.115444
C	-1.960972	1.721469	-0.178194
C	-0.878506	2.627557	-0.191028
H	-1.187880	3.645436	-0.318523
C	0.520373	2.488787	-0.075585
C	-2.698903	-0.666077	0.102305
C	-3.153554	-1.028898	1.387176
C	-3.348568	2.381854	-0.408141
C	-2.966717	-1.476330	-1.014458
C	2.465550	0.911015	0.050531
C	-3.733761	-2.626256	-0.828606
H	-3.966423	-3.250967	-1.681129
C	-4.565167	1.457918	-0.260243
H	-4.562506	0.631644	-0.963768
H	-5.459632	2.050272	-0.456436
H	-4.660280	1.050108	0.743561
C	-4.209425	-2.980014	0.422706
H	-4.810041	-3.871566	0.544439
C	-2.441360	-1.136521	-2.397514
H	-1.878085	-0.205881	-2.319188
C	-1.448672	-0.639827	3.190291
H	-1.488081	-1.683736	3.502921
H	-1.159458	-0.028110	4.045526
H	-0.612863	-0.555145	2.479339
C	3.123087	0.529884	1.233206
C	1.295518	3.837324	-0.095872
C	-3.912976	-2.185827	1.522512
H	-4.286841	-2.471042	2.495814
C	2.480981	0.709446	2.597811
H	1.504239	1.173088	2.445553
C	-2.786593	-0.182816	2.594825
H	-2.655928	0.844236	2.254124
C	2.317270	1.046061	-2.486471
H	1.659119	1.886867	-2.270748
C	3.065343	0.703744	-1.209498
C	-3.363497	2.941506	-1.846465
H	-2.584445	3.684513	-2.006463
H	-4.328008	3.411627	-2.044714
H	-3.222405	2.142933	-2.576330
C	-3.551802	3.531968	0.601069
H	-3.476340	3.169624	1.627839
H	-4.549613	3.951579	0.467747
H	-2.837582	4.342656	0.477303
C	2.265879	-0.641844	3.293419
H	1.696643	-1.340489	2.673285
H	1.728427	-0.514363	4.234116
H	3.218233	-1.125050	3.515414

C	-3.574806	-0.904835	-3.404263
H	-4.163998	-1.810994	-3.552824
H	-3.167501	-0.610596	-4.372934
H	-4.252378	-0.119267	-3.070459
C	-1.485726	-2.224577	-2.905433
H	-0.660926	-2.397858	-2.211220
H	-1.057446	-1.943706	-3.868418
H	-2.006083	-3.174583	-3.035794
C	-3.858817	-0.166140	3.686421
H	-4.829850	0.113338	3.277259
H	-3.595258	0.557653	4.458623
H	-3.964916	-1.136730	4.172795
C	3.227908	1.471552	-3.639132
H	3.905763	2.270755	-3.337144
H	2.625546	1.835560	-4.472353
H	3.829714	0.642213	-4.013840
C	4.399591	-0.024628	1.138989
H	4.925751	-0.304326	2.042407
C	1.421567	-0.122984	-2.914699
H	2.009041	-1.026409	-3.086184
H	0.880798	0.114523	-3.831877
H	0.667516	-0.350695	-2.158188
C	4.338768	0.146748	-1.252643
H	4.822148	-0.005651	-2.207233
C	3.288527	1.655921	3.494059
H	4.279775	1.251752	3.704377
H	2.779673	1.805063	4.447808
H	3.419099	2.630601	3.023916
C	5.008914	-0.213006	-0.089691
H	6.003987	-0.634244	-0.145458
C	0.923500	4.655814	-1.348350
H	1.164643	4.109816	-2.261631
H	1.498520	5.582630	-1.353342
H	-0.129860	4.924296	-1.385945
C	0.875148	4.610896	1.174637
H	-0.193307	4.815029	1.200243
H	1.404896	5.563954	1.211678
H	1.133123	4.047782	2.073474
C	2.826826	3.738199	-0.068542
H	3.200231	3.201465	0.798719
H	3.225223	4.752371	-0.020940
H	3.235989	3.271032	-0.960434
C	0.501093	-4.410570	0.018376
C	2.729404	-3.390789	-0.052054
C	1.089323	-5.666159	-0.116458
C	3.286580	-4.660311	-0.185688
H	-0.568600	-4.273404	0.093044
H	3.326043	-2.488915	-0.025596
H	0.460550	-6.545204	-0.143686
H	4.360098	-4.760767	-0.265909
H	2.915989	-6.767073	-0.321646

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tBuBDIMg-ClPh linear geometry, Dispersion

Mg	0.091908	-0.129208	-0.725828
Cl	-1.804770	-1.626223	-0.331883
C	-3.192771	-2.721748	-0.043590
C	-5.316629	-4.355922	0.419851
N	1.937202	-0.293559	-0.078634
N	-0.317655	1.707106	-0.150803
C	2.630908	0.804660	0.218750
C	2.009179	2.070882	0.305474
H	2.701162	2.858871	0.523475
C	0.680644	2.526360	0.191878
C	2.367273	-1.649173	-0.209870
C	2.617760	-2.128947	-1.513386
C	4.161080	0.835172	0.497425
C	2.343832	-2.522846	0.887927
C	-1.729628	1.899425	-0.049384
C	2.644637	-3.866974	0.666032
H	2.650566	-4.551932	1.503691
C	4.918426	-0.479172	0.260295
H	4.598794	-1.283607	0.913329
H	5.974399	-0.295653	0.461891
H	4.840598	-0.825613	-0.768364
C	2.937442	-4.342201	-0.600079
H	3.176747	-5.386828	-0.747535
C	1.982700	-2.054845	2.285242
H	1.818603	-0.977948	2.243816
C	1.083771	-0.732329	-2.985380
H	0.358133	-1.422316	-2.523856
H	0.843027	-0.778492	-4.047038
H	0.898460	0.316384	-2.715723
C	-2.492956	1.939408	-1.228748
C	0.521203	4.065365	0.369672
C	2.913000	-3.475828	-1.685863
H	3.133127	-3.860063	-2.671028
C	-1.841010	2.043324	-2.597163
H	-0.760973	2.097683	-2.442837
C	2.548197	-1.165463	-2.690181
H	3.089055	-0.263145	-2.400154
C	-1.527159	1.758111	2.487857
H	-0.608192	2.316297	2.314647
C	-2.352604	1.823417	1.213566
C	4.369403	1.239700	1.971278
H	3.955993	2.222711	2.189186
H	5.436998	1.263039	2.195715
H	3.900092	0.521286	2.643907
C	4.825367	1.880331	-0.426556
H	4.631322	1.653684	-1.476700
H	5.904885	1.855122	-0.274077
H	4.492547	2.897623	-0.235528
C	-2.142767	0.814094	-3.464762
H	-1.875766	-0.122181	-2.966973

H	-1.601526	0.862967	-4.411085
H	-3.207337	0.749119	-3.693299
C	3.103003	-2.319024	3.298574
H	3.283156	-3.388116	3.420860
H	2.830943	-1.916155	4.275567
H	4.041754	-1.857560	2.993605
C	0.675947	-2.711596	2.751896
H	-0.138470	-2.527569	2.050195
H	0.376625	-2.322879	3.726109
H	0.795232	-3.792244	2.845397
C	3.199649	-1.692041	-3.968119
H	4.232617	-1.989368	-3.788833
H	3.201973	-0.913523	-4.731993
H	2.663623	-2.551374	-4.374472
C	-2.214972	2.397559	3.695258
H	-2.558523	3.408557	3.472501
H	-1.516581	2.453713	4.531196
H	-3.074467	1.815858	4.032185
C	-3.883175	1.898927	-1.129557
H	-4.483008	1.942753	-2.029363
C	-1.113688	0.316830	2.804430
H	-1.987880	-0.325885	2.922012
H	-0.533831	0.277008	3.727802
H	-0.489868	-0.100629	2.014910
C	-3.741932	1.786622	1.261841
H	-4.239696	1.738472	2.219996
C	-2.246868	3.328892	-3.328465
H	-3.318301	3.344802	-3.532777
H	-1.723728	3.406998	-4.283077
H	-2.007517	4.212711	-2.737379
C	-4.508063	1.819576	0.102902
H	-5.588289	1.800697	0.165901
C	1.185671	4.542406	1.675978
H	0.742756	4.054976	2.545506
H	1.031673	5.616861	1.782902
H	2.258203	4.363203	1.701142
C	1.231877	4.715694	-0.840309
H	2.290006	4.465089	-0.881583
H	1.140833	5.800945	-0.774863
H	0.770888	4.396083	-1.776866
C	-0.916033	4.603747	0.378009
H	-1.466639	4.351177	-0.523159
H	-0.862931	5.691694	0.434040
H	-1.490520	4.262255	1.234683
C	-4.422537	-2.128300	0.155229
C	-2.958790	-4.080789	-0.022001
C	-5.498843	-2.977984	0.390390
C	-4.055412	-4.903748	0.215802
H	-4.534648	-1.053786	0.131353
H	-1.970048	-4.485056	-0.179361
H	-6.480333	-2.552946	0.550990
H	-3.914234	-5.975691	0.240812

H	-6.160897	-5.006039	0.603737

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tBuBDIMg-BrPh linear geometry, Dispersion

Mg	-0.224957	-0.075490	-0.816729
Br	2.130612	-1.215552	-0.355014
C	3.858664	-2.051905	-0.016299
C	6.283466	-3.179308	0.483818
N	-0.148964	1.773274	-0.107422
N	-2.014171	-0.598341	-0.200371
C	-1.294296	2.411629	0.120166
C	-2.530067	1.724016	0.141038
H	-3.365171	2.376337	0.297781
C	-2.903027	0.369375	0.062210
C	1.188125	2.271989	-0.166023
C	1.712082	2.565911	-1.443300
C	-1.424480	3.940584	0.378988
C	2.014996	2.253744	0.968791
C	-2.158403	-2.004474	0.014433
C	3.364316	2.568096	0.803132
H	4.013073	2.579152	1.669145
C	-0.140312	4.767218	0.221272
H	0.645955	4.479835	0.909315
H	-0.388714	5.809315	0.425728
H	0.261594	4.723653	-0.788746
C	3.890442	2.867134	-0.441370
H	4.939138	3.112626	-0.545514
C	1.496908	1.909817	2.354700
H	0.454299	1.605415	2.254000
C	0.323726	1.138546	-3.044808
H	1.046596	0.378254	-2.717987
H	0.256726	1.008090	-4.124852
H	-0.695420	0.930278	-2.690205
C	-2.182056	-2.860800	-1.100241
C	-4.437158	0.131341	0.209348
C	3.064865	2.863150	-1.558615
H	3.485735	3.106160	-2.522998
C	-2.195910	-2.287825	-2.505542
H	-2.556933	-1.260118	-2.433159
C	0.790784	2.565781	-2.658399
H	-0.106321	3.121083	-2.378901
C	-2.015019	-1.605589	2.528398
H	-2.395044	-0.627550	2.240048
C	-2.108496	-2.521832	1.321921
C	-1.941767	4.138081	1.818922
H	-2.918947	3.683010	1.968895
H	-2.028676	5.204565	2.032476
H	-1.255134	3.703799	2.545480
C	-2.438955	4.540224	-0.620544
H	-2.133359	4.350512	-1.651256
H	-2.480715	5.620783	-0.479262
H	-3.447725	4.155157	-0.493572

C	-0.771865	-2.254457	-3.075867
H	-0.044826	-1.794721	-2.389150
H	-0.721075	-1.716017	-4.023119
H	-0.393354	-3.265896	-3.230433
C	1.550503	3.119919	3.298556
H	2.580638	3.443137	3.458050
H	1.129869	2.858862	4.271127
H	0.994074	3.970665	2.909681
C	2.272954	0.741743	2.977702
H	2.251284	-0.143404	2.344593
H	1.843923	0.475578	3.944269
H	3.317549	1.008246	3.145193
C	1.385138	3.260546	-3.883411
H	1.713959	4.271423	-3.643651
H	0.633362	3.329812	-4.670415
H	2.237388	2.712588	-4.289250
C	-2.849673	-2.079513	3.720226
H	-3.887079	-2.259062	3.435111
H	-2.840537	-1.322506	4.505951
H	-2.457463	-3.000246	4.154015
C	-2.170464	-4.236941	-0.890818
H	-2.203908	-4.909003	-1.737526
C	-0.548510	-1.410672	2.929155
H	-0.095934	-2.358565	3.226346
H	-0.463438	-0.714414	3.764807
H	0.038407	-1.009579	2.102199
C	-2.101032	-3.904808	1.483538
H	-2.071787	-4.322527	2.480413
C	-3.131727	-3.025290	-3.465865
H	-2.797562	-4.045676	-3.656557
H	-3.171987	-2.509332	-4.426547
H	-4.143698	-3.073090	-3.063606
C	-2.133329	-4.760084	0.392161
H	-2.133119	-5.831490	0.542120
C	-4.940739	0.688326	1.554617
H	-4.474551	0.172505	2.394130
H	-6.018331	0.534172	1.626630
H	-4.750335	1.753699	1.666969
C	-5.123674	0.888017	-0.952958
H	-4.952950	1.961522	-0.918248
H	-6.200026	0.717534	-0.906095
H	-4.767988	0.520172	-1.917353
C	-4.914931	-1.323995	0.107933
H	-4.619878	-1.794718	-0.826820
H	-6.005186	-1.317706	0.139912
H	-4.568201	-1.946867	0.926702
C	4.932444	-1.203438	0.160204
C	3.921057	-3.428126	0.044360
C	6.166008	-1.796066	0.414722
C	5.169251	-3.989507	0.300402
H	4.817476	-0.130760	0.105184
H	3.045205	-4.043052	-0.096838

H	7.032986	-1.165428	0.558615
H	5.260026	-5.065902	0.355760
H	7.247099	-3.627969	0.682305

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tBuBDIMg-IPh linear geometry, Dispersion

Mg	-0.377908	0.060890	-0.668325
I	2.379671	0.816540	-0.239628
C	4.423065	1.376482	0.078040
C	7.033679	2.044754	0.505829
N	-2.058943	0.884769	-0.080402
N	-0.698162	-1.802560	-0.136941
C	-3.117510	0.113661	0.169723
C	-3.005571	-1.292044	0.260162
H	-3.944508	-1.772202	0.447841
C	-1.932863	-2.201570	0.177811
C	-1.961090	2.306465	-0.188732
C	-1.949181	2.859387	-1.487194
C	-4.566093	0.641823	0.379878
C	-1.687743	3.100095	0.935603
C	0.549514	-2.489997	-0.015741
C	-1.471482	4.464508	0.740583
H	-1.276663	5.095745	1.597490
C	-4.782718	2.142273	0.136527
H	-4.229764	2.774017	0.822534
H	-5.842935	2.352619	0.281941
H	-4.529479	2.440904	-0.878807
C	-1.501094	5.027596	-0.522825
H	-1.338144	6.089507	-0.649279
C	-1.599088	2.519181	2.334527
H	-1.829942	1.455693	2.269249
C	-0.941418	1.023549	-2.931374
H	-0.046591	1.387576	-2.396885
H	-0.624879	1.016427	-3.973966
H	-1.164676	-0.029991	-2.713911
C	1.262809	-2.807727	-1.184811
C	-2.346998	-3.691989	0.352275
C	-1.729261	4.223551	-1.632414
H	-1.739983	4.672360	-2.614809
C	0.625940	-2.708627	-2.560999
H	-0.399326	-2.357618	-2.423838
C	-2.167668	1.949121	-2.687630
H	-3.009290	1.297250	-2.447730
C	0.365677	-2.287189	2.518386
H	-0.685654	-2.494446	2.323735
C	1.141496	-2.628991	1.256829
C	-4.983747	0.334295	1.832409
H	-4.970343	-0.732819	2.046313
H	-5.996282	0.702090	2.006141
H	-4.320486	0.827557	2.543151
C	-5.515239	-0.086805	-0.598063
H	-5.199825	0.061664	-1.632604

H	-6.519259	0.325753	-0.493203
H	-5.581076	-1.156921	-0.417510
C	1.360083	-1.708494	-3.463271
H	1.449820	-0.721555	-3.002783
H	0.841601	-1.594299	-4.416723
H	2.375865	-2.044453	-3.675583
C	-2.605346	3.159425	3.298719
H	-2.393492	4.219556	3.445518
H	-2.553571	2.674378	4.274896
H	-3.628367	3.073635	2.933862
C	-0.172989	2.657540	2.885203
H	0.561423	2.205350	2.217807
H	-0.088908	2.174265	3.859559
H	0.096062	3.707823	3.008643
C	-2.521373	2.688361	-3.977308
H	-3.388582	3.332781	-3.835028
H	-2.761038	1.971118	-4.763315
H	-1.694076	3.304311	-4.333642
C	0.768695	-3.132206	3.728303
H	0.746277	-4.198158	3.498198
H	0.079197	-2.948930	4.553352
H	1.770113	-2.885026	4.084096
C	2.580876	-3.245543	-1.064540
H	3.139917	-3.502419	-1.954868
C	0.465072	-0.794977	2.849783
H	1.502156	-0.492831	3.002031
H	-0.096167	-0.564396	3.756493
H	0.048837	-0.179598	2.051775
C	2.458789	-3.067478	1.324584
H	2.931600	-3.184848	2.289413
C	0.537810	-4.079148	-3.244846
H	1.531165	-4.492356	-3.425436
H	0.031052	-3.993536	-4.207622
H	-0.013660	-4.793635	-2.634176
C	3.181736	-3.366853	0.176065
H	4.203480	-3.714981	0.254250
C	-3.178752	-3.886126	1.635251
H	-2.616514	-3.584012	2.519911
H	-3.426457	-4.942789	1.743388
H	-4.114362	-3.331591	1.627069
C	-3.207102	-4.049347	-0.882174
H	-4.100873	-3.432719	-0.954475
H	-3.517393	-5.093410	-0.818906
H	-2.633653	-3.924624	-1.802622
C	-1.201831	-4.712422	0.405090
H	-0.570216	-4.684372	-0.477353
H	-1.645274	-5.707507	0.457663
H	-0.569215	-4.592773	1.280375
C	5.322159	0.351624	0.304270
C	4.757167	2.716479	0.054348
C	6.650401	0.709171	0.520840
C	6.093481	3.041275	0.274400

H	5.011645	-0.682885	0.314328
H	4.020271	3.484593	-0.124817
H	7.380927	-0.068167	0.701208
H	6.389559	4.081738	0.262871
H	8.068276	2.309919	0.675244

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Author Contributions

A.F. and J.P. conducted the experimental work. DFT calculations were done by J.E.; crystal structure determination was done by J.P and J.L. The manuscript was written by S.H. and A.F. while S.H., A.G and N.v.E.-H. were responsible for supervision and discussion.