Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information for

Crystalline Radicals Derived from the Boron-Dipyrromethene and Its Heavier Analogues

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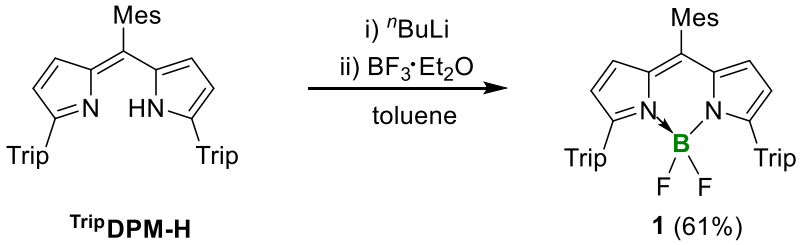
1. Synthesis and spectral data of compounds 1–6

General considerations: All experiments were carried out under an argon or nitrogen atmosphere using standard Schlenk or dry glovebox techniques. Solvents were dried over Na metal and were distilled under nitrogen prior to use. Commercially available reagents were purchased from Energy Chemical and used as received. ^{1}H、^{13}C{^{1}H}、^{1}B{^{1}H} and ^{19}F NMR were obtained with a Bruker AVIII 400 MHz BBFO1 spectrometer at 298K. Chemical shifts (δ) are given in p.p.m. Coupling constants *J* are given in Hz. NMR multiplicities are abbreviated as follows: s = singlet, d = doublet, t = triplet, m = multiplet, br = broad signal. UV-vis spectra were recorded on the UH5300 Spectrophotometer at room temperature. EPR spectra were obtained using JEOL JES-X320 X-band variable-temperature apparatus. Element analyses were performed on an ElementarVario EL III instrument. **^{Trip}DPM-H** was synthesized according to the literature procedures.[S1]

Synthesis of 1

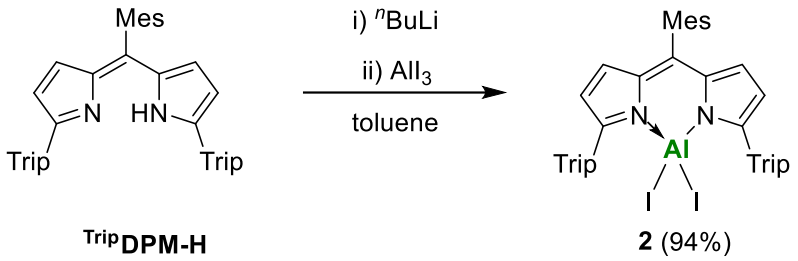


^{Trip}DPM-H　　**1** (61%)

A hexane solution of ^{n}BuLi (2.1 ml, 1.6 M, 3.3 mmol) was added dropwise to a toluene (50 ml) solution of **^{Trip}DPM-H** (2.0 g, 3.0 mmol) at -78 °C. After warming up to ambient temperature and stirring for 2 hours, BF_3·Et_2O(0.45 ml, 3.6 mmol) was added dropwise to the reaction solution at -35 °C. Then the reaction solution was warmed to ambient temperature and stirred overnight. After filtration and removal of the solvent under vacuum, an orange solid was afforded, which was washed with hexane (3 × 3 ml) and dried to give **1** as a red powder (1.3 g, 61%).

^{1}H NMR (C_6D_6, 400 MHz, 298 K): δ 7.07 (s, 4H, Ar-*H*), 6.70 (s, 2H, Ar-*H*), 6.48 (d, *J* = 4.0 Hz, 2H, Ar-*H*), 6.20 (d, *J* = 4.0 Hz, 2H, Ar-*H*), 3.06 (sept, *J* = 8.0 Hz, 4H, $(CH_3)_2CH$), 2.67 (sept, *J* = 8 Hz, 2H, $(CH_3)_2CH$), 2.12 (s, 3 H, CH_3), 2.03 (s, 3H, CH_3), 1.49 (d, *J* = 4 Hz, 12H, $(CH_3)_2CH$), 1.19 (d, *J* = 8 Hz, 12H, $(CH_3)_2CH$), 1.06 (d, *J* = 4 Hz, 12H, $(CH_3)_2CH$); ^{13}C NMR (C_6D_6, 400 MHz, 298 K): δ 159.58 (Ar-*C*), 149.90 (Ar-*C*), 148.04 (Ar-*C*), 144.64 (Ar-*C*), 138.59 (Ar-*C*), 136.91 (Ar-*C*), 135.61 (Ar-*C*), 130.97 (Ar-*C*), 128.44 (Ar-*C*H), 128.23 (Ar-*C*), 122.38 (Ar-*C*H), 120.98 (Ar-*C*H), 120.74 (Ar-*C*H), 34.51 (*C*H$(CH_3)_2$), 31.98 (*C*H$(CH_3)_2$), 26.27 (*C*H_3), 23.95 (*C*H_3), 23.01 (*C*H_3), 21.11 (*C*H_3), 20.14 (*C*H_3); ^{19}F NMR (C_6D_6, 377 MHz, 298 K): δ -143.41 (q, *J* = 30.2 Hz, 2F, BF_2); ^{11}B NMR (C_6D_6, 128 MHz, 298 K): δ 1.08 (t, *J* = 30.2 Hz, 1B, BF_2); UV-vis (hexane): λ_{max} = 519 nm; Elemental analysis for $C_{48}H_{61}BF_2N_2$ (%): Calculated: C 80.65, H 8.60, N 3.92; Found: C 80.35, H 8.26, N 4.14.

Synthesis of 2

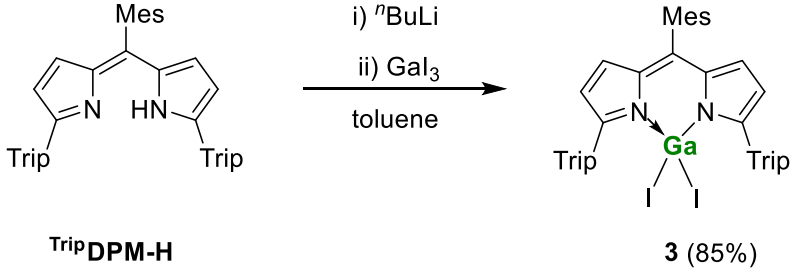


^{Trip}**DPM-H** **2** (94%)

A hexane solution of ^{n}BuLi (3.4 ml, 1.6 M, 5.5 mmol) was added dropwise to a toluene (50 ml) solution of ^{Trip}**DPM-H** (3.3 g, 5.0 mmol) at -78 °C. After warming up to ambient temperature and stirring for one hour, the reaction solution was transferred to a suspension of AlI_3 (2.2 g, 5.5 mmol) in toluene (10 mL) at -35 °C. Then the reaction mixture was warmed to room temperature and stirred overnight. After filtration and removal of the solvent under vacuum, the residue was washed with hexane (3 × 3 ml) and dried to give **2** as a red powder (4.5 g, 94%).

^{1}H NMR (C_6D_6, 400 MHz, 298 K): δ 7.16 (s, 4H, Ar-H), 6.74 (s, 2H, Ar-*H*), 6.68 (d, *J* = 4.0 Hz, 2H, Ar-*H*), 6.34 (d, *J* = 4.0 Hz, 2H, Ar-*H*), 3.06 (sept, *J* = 8.0 Hz, 4H, $(CH_3)_2CH$), 2.78 (sept, *J* = 8 Hz, 2H, $(CH_3)_2CH$), 2.23 (s, 6 H, CH_3), 2.18 (s, 3H, CH_3), 1.52 (d, *J* = 4 Hz, 12H, $(CH_3)_2CH$), 1.21 (d, *J* = 8 Hz, 12H, $(CH_3)_2CH$), 1.12 (d, *J* = 4 Hz, 12H, $(CH_3)_2CH$); ^{13}C NMR (C_6D_6, 400 MHz, 298 K): δ 164.19 (Ar-*C*), 151.42 (Ar-*C*), 148.39 (Ar-*C*), 146.95 (Ar-*C*), 139.28 (Ar-*C*), 138.53 (Ar-*C*), 137.16 (Ar-*C*), 134.38 (Ar-*C*H), 133.26 (Ar-*C*), 128.63 (Ar-*C*), 128.39 (Ar-*C*H), 123.82 (Ar-*C*H), 121.22 (Ar-*C*H), 34.99 ($CH(CH_3)_2$), 31.69 ($CH(CH_3)_2$), 26.39 (CH_3), 24.34 (CH_3), 23.66 (CH_3), 21.15 (CH_3), 20.37 (CH_3); UV-vis (hexane): λ_{max} = 514 nm; Elemental analysis for $C_{48}H_{61}AlI_2N_2$ (%): Calculated: C 60.89, H 6.49, N 2.96; Found: C 60.56, H 6.22, N 3.13.

Synthesis of 3



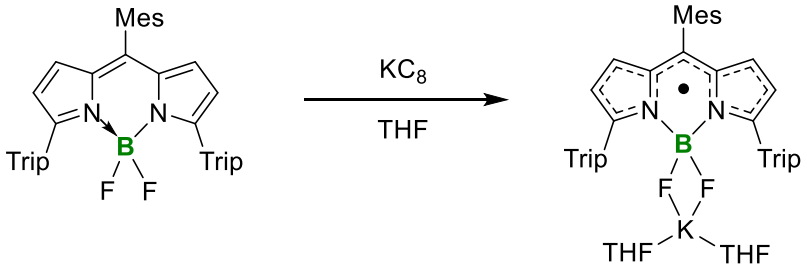
^{Trip}**DPM-H** **3** (85%)

A hexane solution of ^{n}BuLi (0.85 ml, 2.5 M, 2.1 mmol) was added dropwise to a toluene (50 ml) solution of ^{Trip}**DPM-H** (1.34 g, 2.0 mmol) at -78 °C. After warming up to ambient temperature and stirring for one hour, GaI_3(0.9 g, 2.0 mmol) was added at -35 °C. Then the reaction mixture was warmed to room temperature and stirred overnight. After filtration and removal of the solvent under vacuum, the residue

was washed with hexane (3 × 3 ml) and dried to give **3** as a red powder (1.7 g, 85%).

^{1}H NMR (C_6D_6, 400 MHz, 298 K): δ 7.16 (s, 4H, Ar-*H*), 6.75 (s, 2H, Ar-*H*), 6.70 (d, *J* = 4.0 Hz, 2H, Ar-*H*), 6.34 (d, *J* = 4.0 Hz, 2H, Ar-*H*), 3.05 (sept, *J* = 8.0 Hz, 4H, $(CH_3)_2CH$), 2.79 (sept, *J* = 8 Hz, 2H, $(CH_3)_2CH$), 2.24 (s, 6 H, CH_3), 2.18 (s, 3H, CH_3), 1.51 (d, *J* = 8 Hz, 12H, $(CH_3)_2CH$), 1.21 (d, *J* = 8 Hz, 12H, $(CH_3)_2CH$), 1.13 (d, *J* = 4 Hz, 12H, $(CH_3)_2CH$); ^{13}C NMR (C_6D_6, 400 MHz, 298 K): δ 163.10 (Ar-C), 151.33 (Ar-C), 148.52 (Ar-*C*), 146.23 (Ar-C), 138.43 (Ar-C), 137.17 (Ar-C), 133.57 (Ar-C), 133.51 (Ar-CH), 128.37 (Ar-CH), 128.18 (Ar-*C*), 127.95 (Ar-*C*), 123.02 (Ar-CH), 121.17 (Ar-CH), 35.00 ($CH(CH_3)_2$), 31.63 ($CH(CH_3)_2$), 26.35 (CH_3), 24.35 (CH_3), 23.74 (CH_3), 21.16 (CH_3), 20.42 (CH_3); UV-vis (hexane): λ_{max} = 516 nm; Elemental analysis for $C_{48}H_{61}GaI_2N_2$ (%): Calculated: C 58.26, H 6.21, N 2.83; Found: C 58.01, H 5.98, N 3.09.

Synthesis of 4

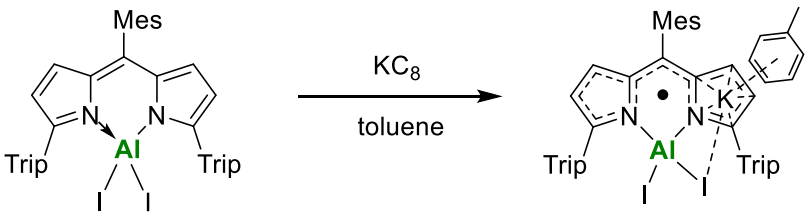


1 **4** (55%)

To a tetrahydrofuran solution of **1** (0.72 g, 1.0 mmol) was added KC_8 (0.17 g, 1.25 mmol) in three portions at room temperature and the reaction mixture was stirred overnight. After filtration and removal of the solvent under vacuum, the residue was washed with hexane (3 × 3 ml) and dried to give **4** as a red powder (0.49 g, 55%).

UV-vis (hexane): λ_{max} = 520 nm; Elemental analysis for $C_{56}H_{77}BF_2KN_2O_2$ (%): Calculated: C 74.89, H 8.64, N 3.12, O 3.56; Found: C 74.56, H 8.36, N 3.40, O 3.81.

Synthesis of 5



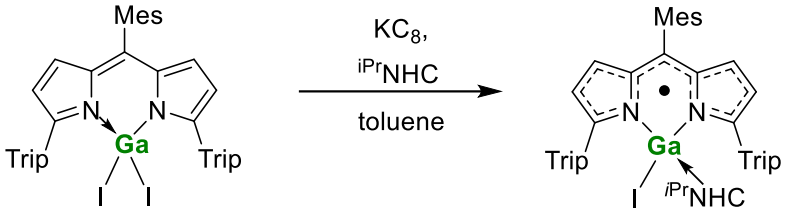
2 **5** (62%)

To a toluene solution of **2** (0.95 g, 1.0 mmol) was added KC_8 (0.15 g, 1.1 mmol) in three portions at -35 ^{o}C and the reaction mixture was warmed up to room temperature and stirred overnight. After filtration and removal of the solvent under vacuum, the residue was washed with hexane (3 × 3 ml) and dried to

give **5** as a red powder (0.67 g, 62%).

UV-vis (hexane): λ_{max} = 513 nm; Elemental analysis for $C_{55}H_{69}AlI_2KN_2$ (%): Calculated: C 61.28, H 6.45, N 2.60; Found: C 60.97, H 6.19, N 2.96.

Synthesis of 6



3 **6** (74%)

^{ipr}NHC (0.11 g, 0.60 mmol) and KC_8 (0.09 g, 0.66 mmol) was added in sequence to a toluene solution of **3** (0.59 g, 0.60 mmol) at -35 ºC and the reaction mixture was warmed up to room temperature and stirred overnight. After filtration and removal of the solvent under vacuum, the residue was washed with hexane (3 × 3 ml) and dried to give **6** as a red powder (0.46 g, 74%).

UV-vis (hexane): λ_{max} = 508 nm; Elemental analysis for $C_{59}H_{81}GaIN_4$ (%): Calculated: C 67.95, H 7.83, N 5.37; Found: C 67.69, H 7.58, N 5.62.

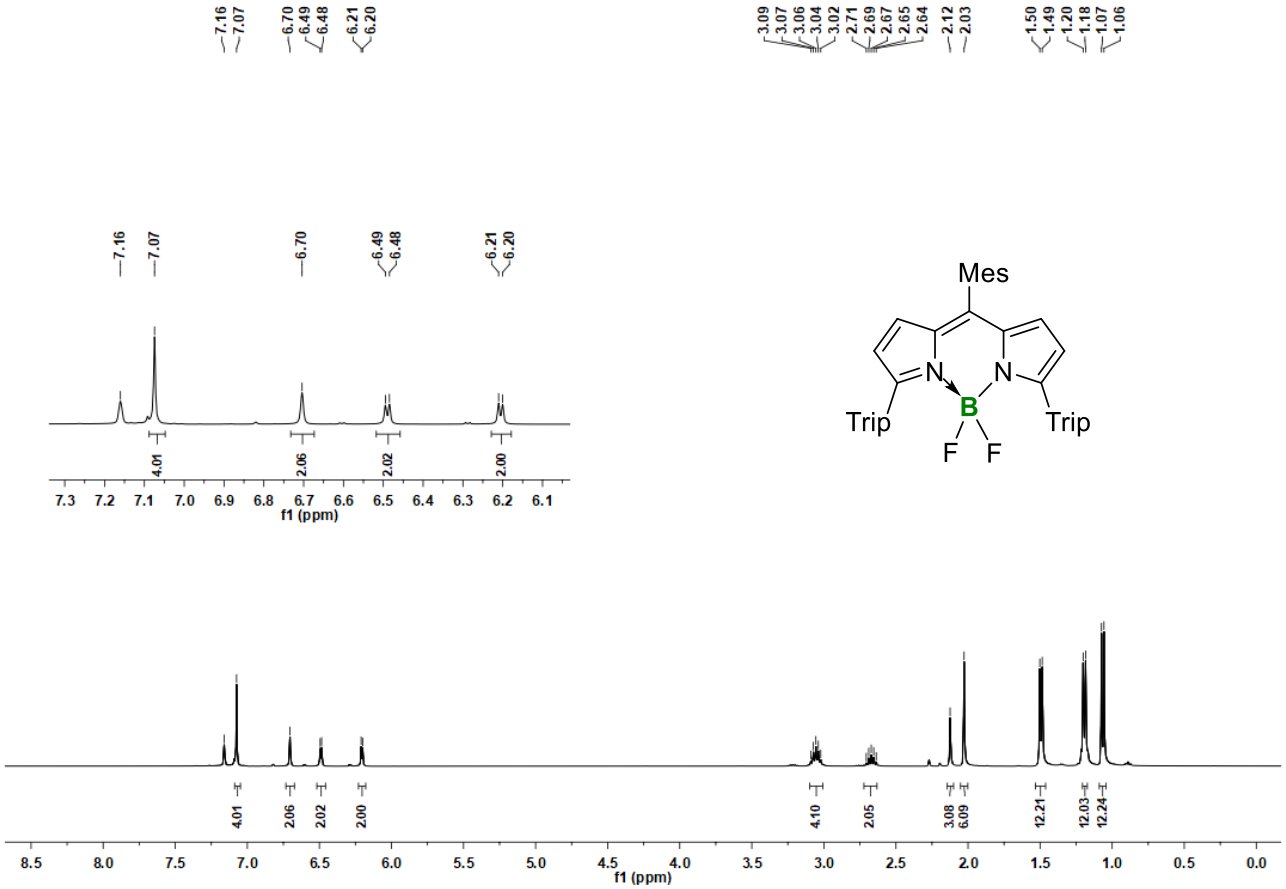


Fig. S1 ^{1}H NMR spectrum of **1** in C_6D_6.

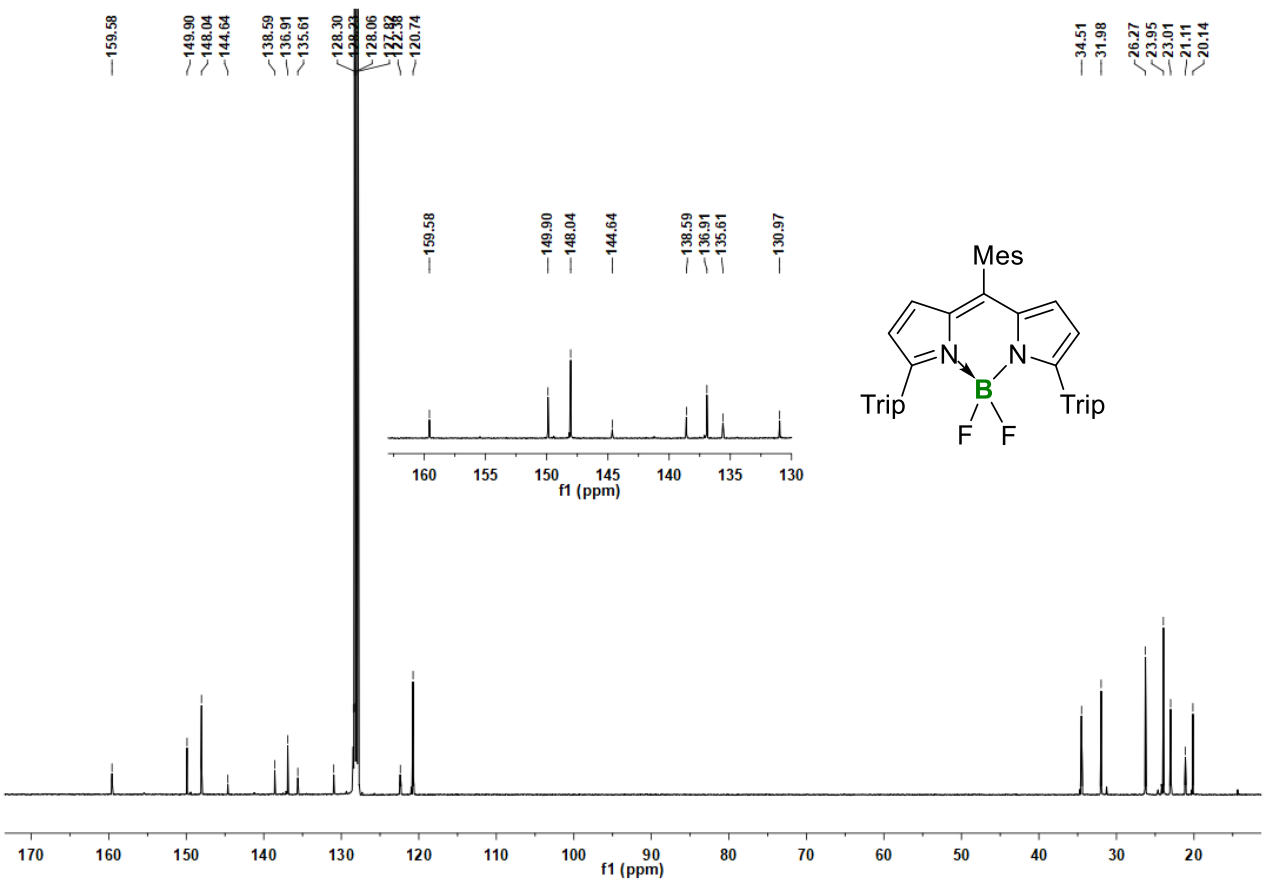


Fig. S2 $^{13}C\{^{1}H\}$ NMR spectrum of **1** in C_6D_6.

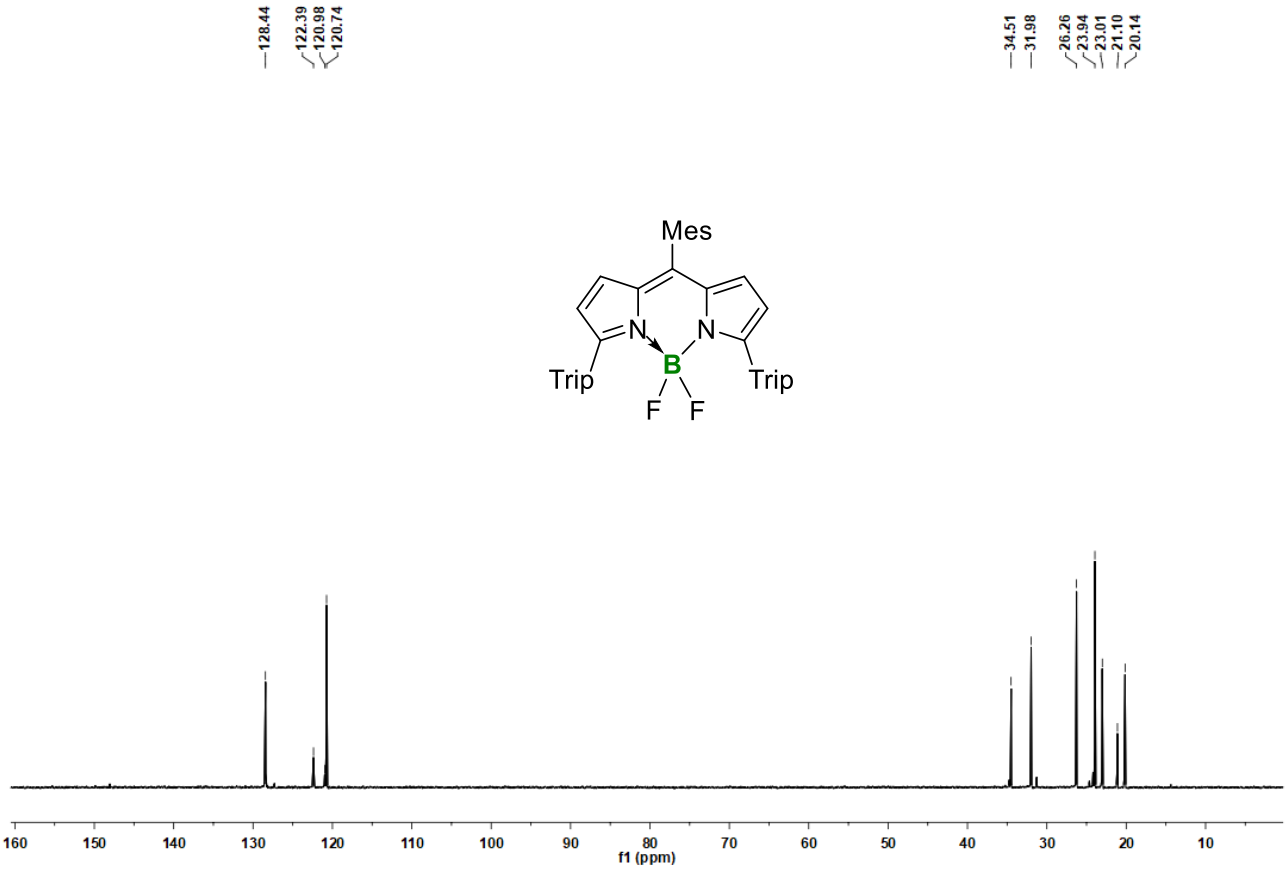


Fig. S3 ^{13}C (DEPT135) NMR spectrum of **1** in C_6D_6.

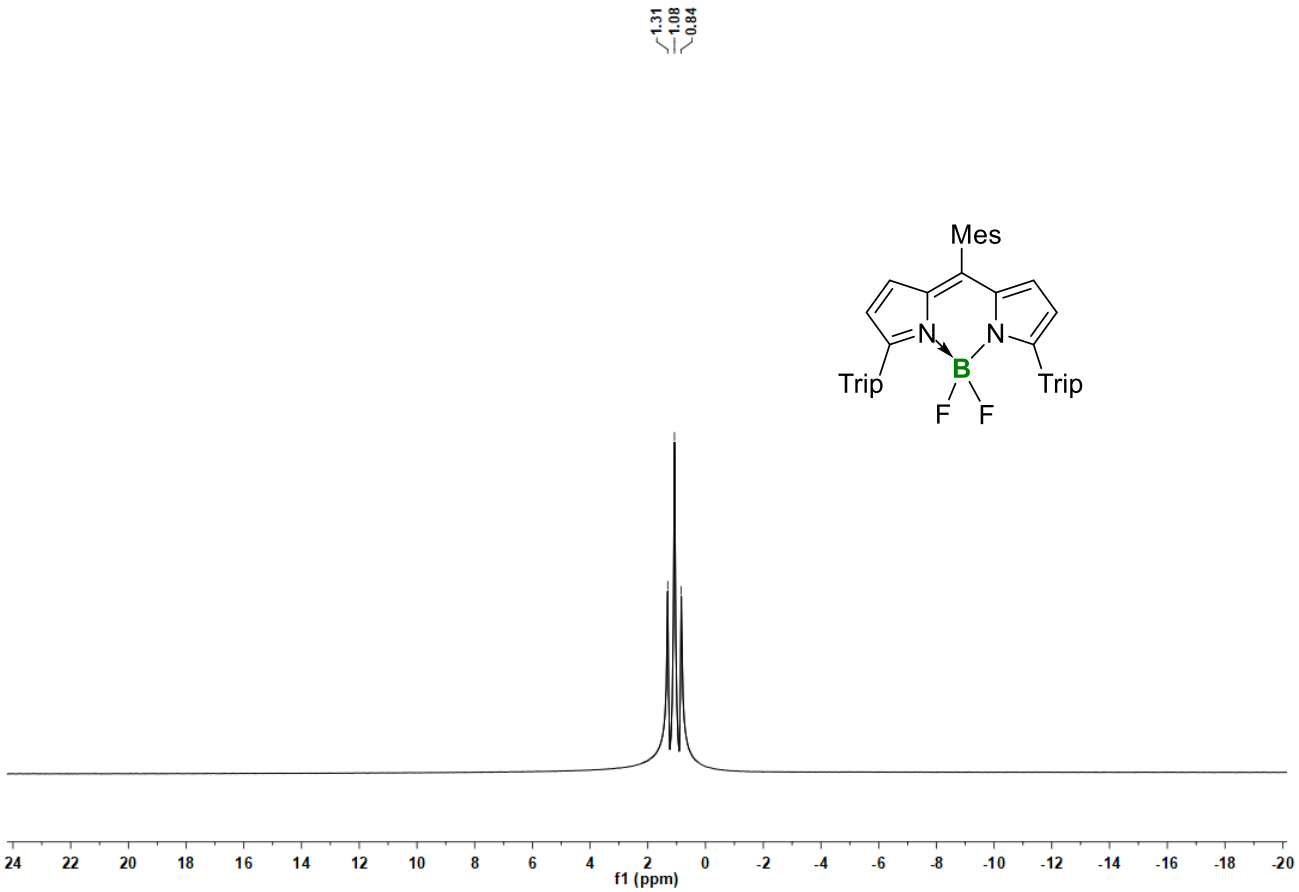


Fig. S4 $^{11}B\{^{1}H\}$ NMR spectrum of **1** in C_6D_6.

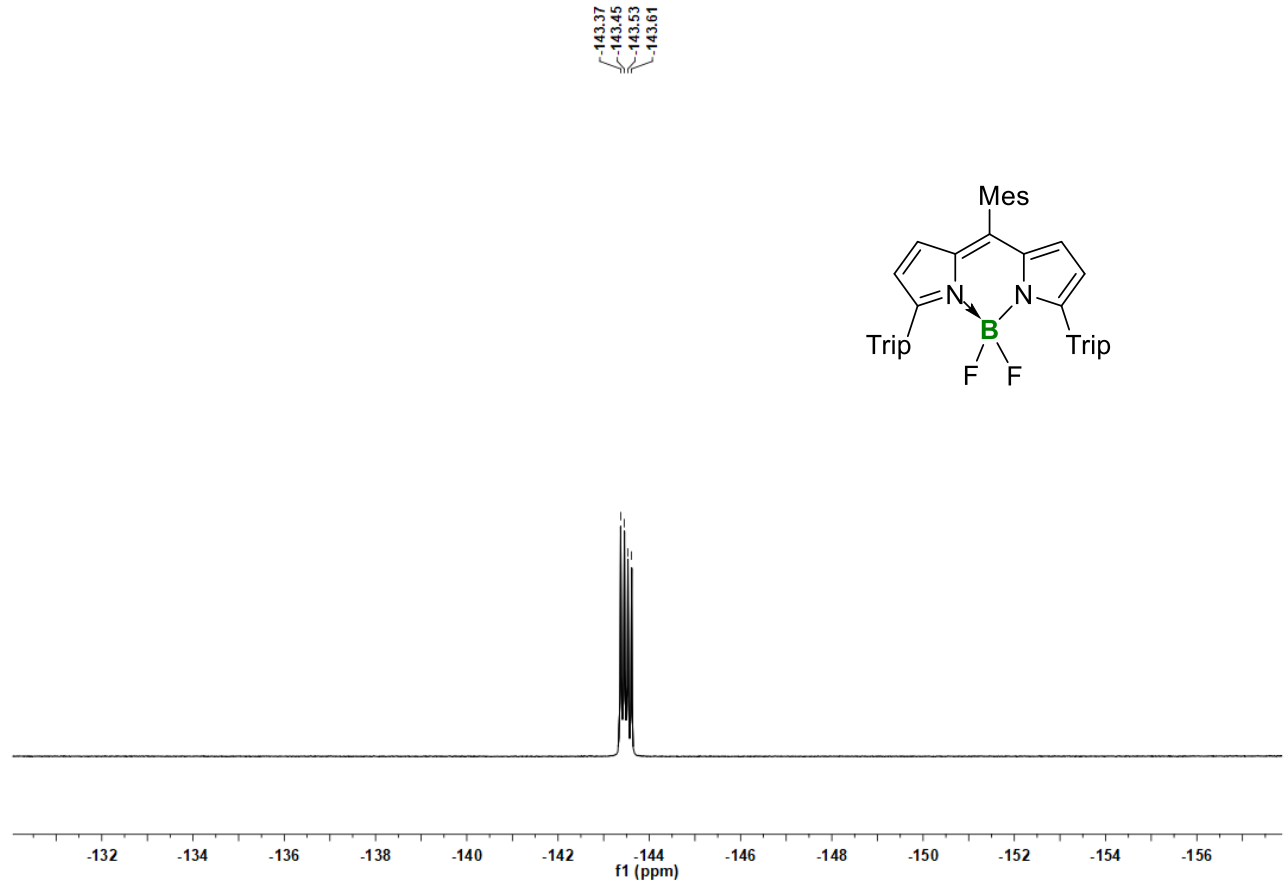


Fig. S5 ^{19}F NMR spectrum of **1** in C_6D_6.

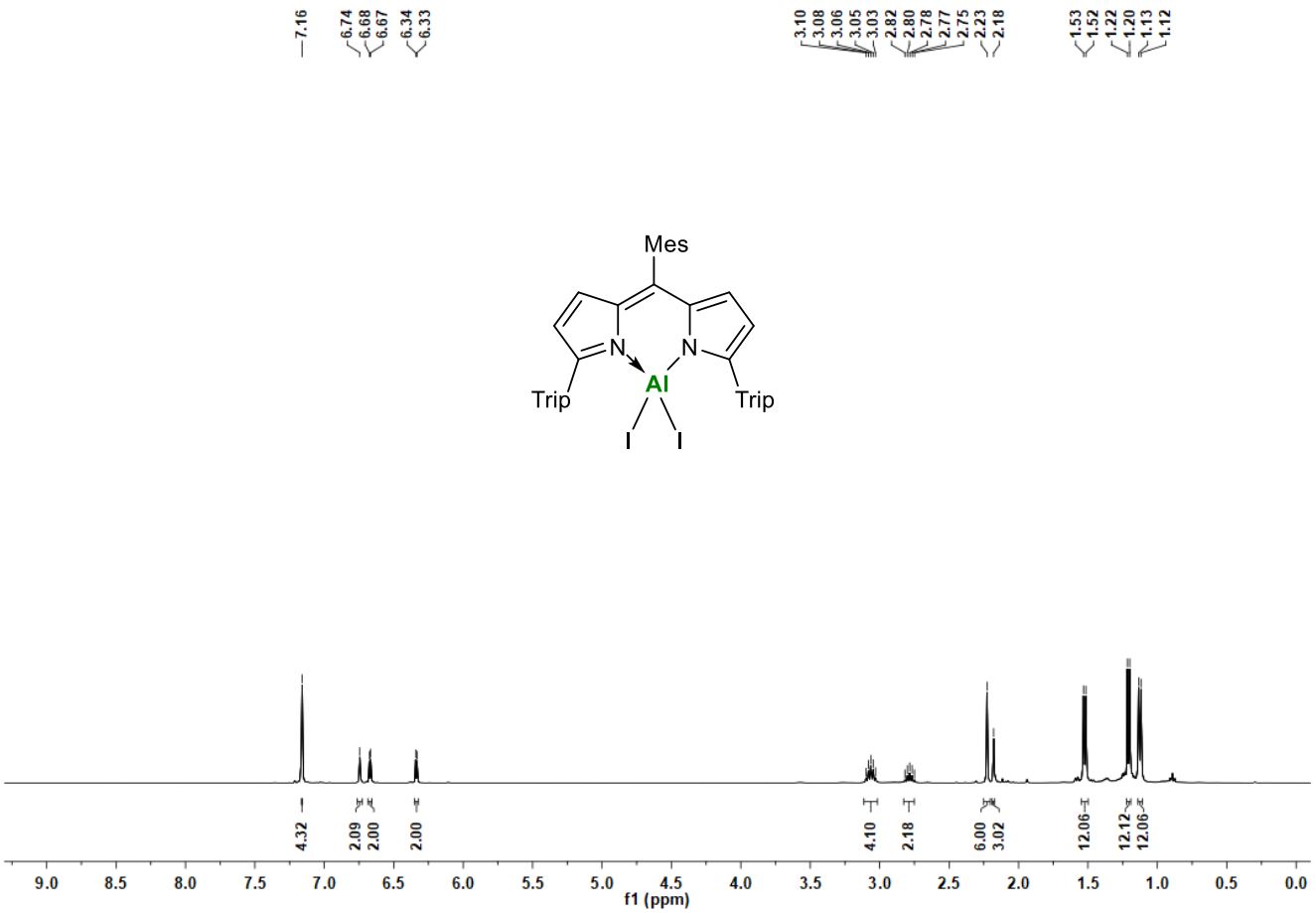


Fig. S6 ^{1}H NMR spectrum of **2** in C_6D_6.

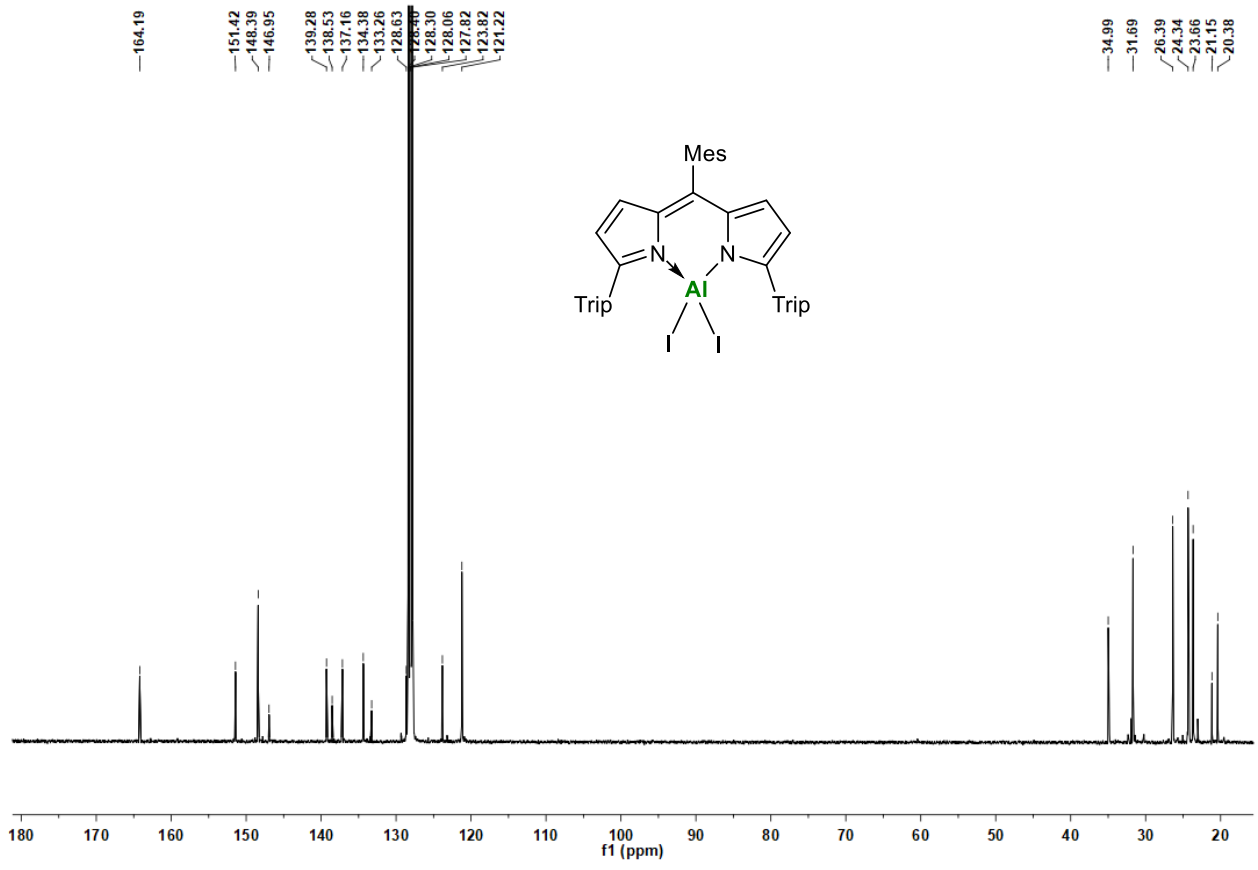


Fig. S7 ^{13}C{^{1}H} NMR spectrum of **2** in C_6D_6.

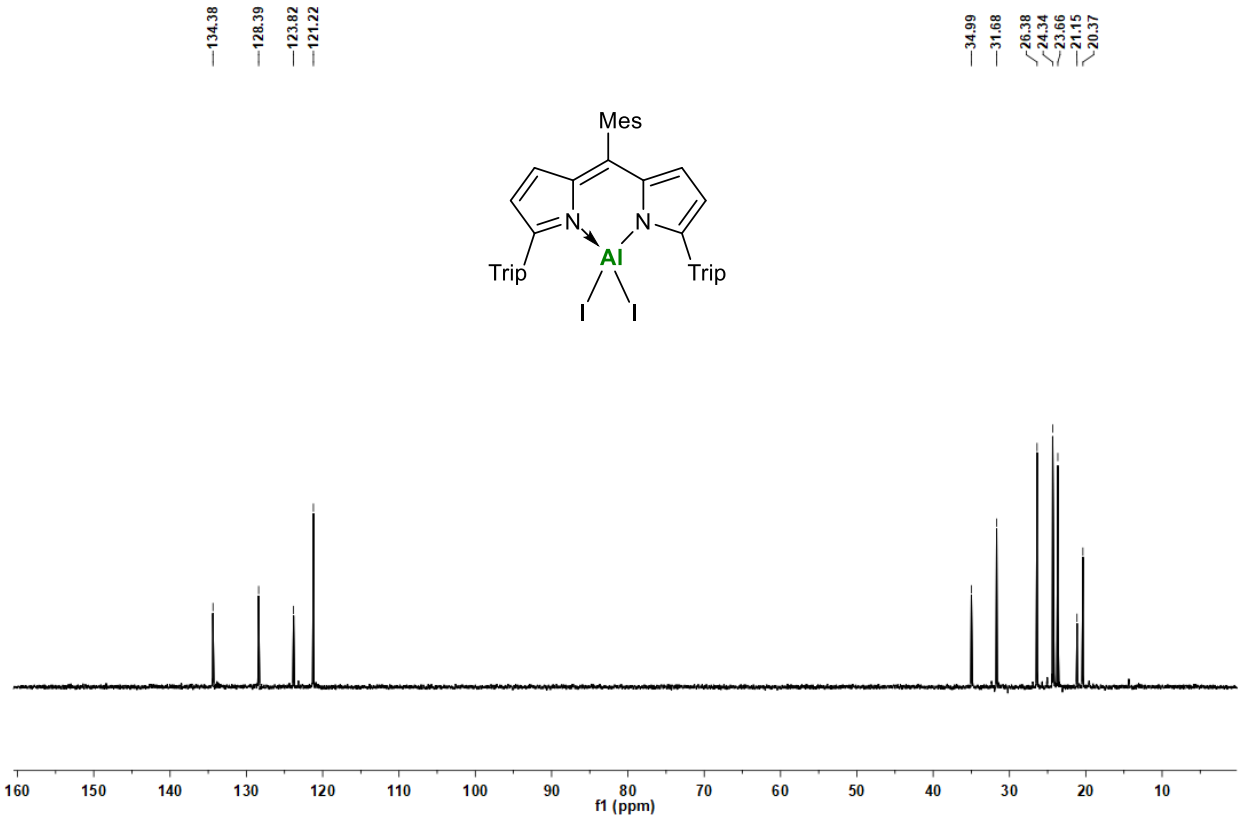


Fig. S8 ^{13}C (DEPT135) NMR spectrum of **2** in C_6D_6.

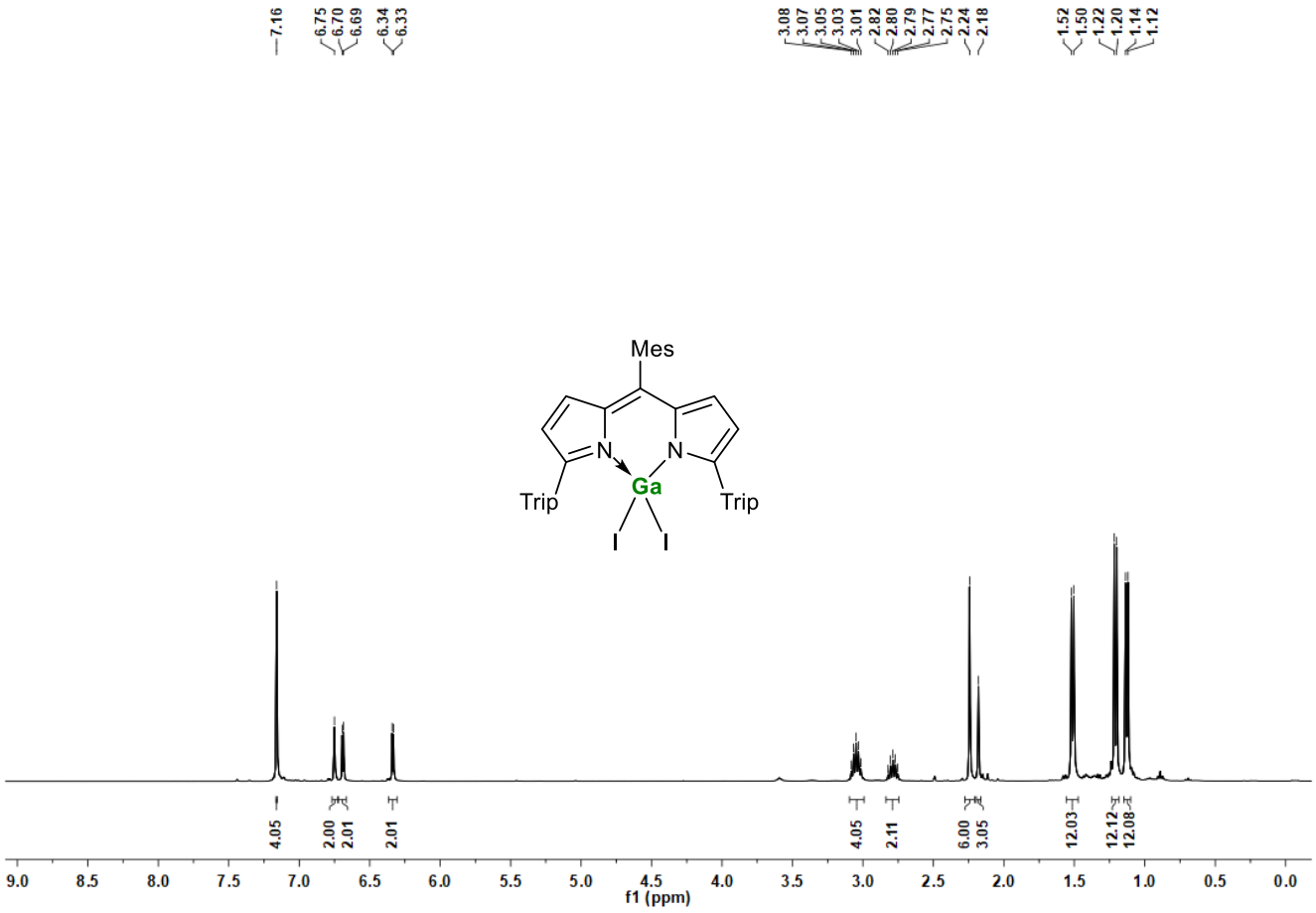


Fig. S9 ^{1}H NMR spectrum of **3** in C_6D_6.

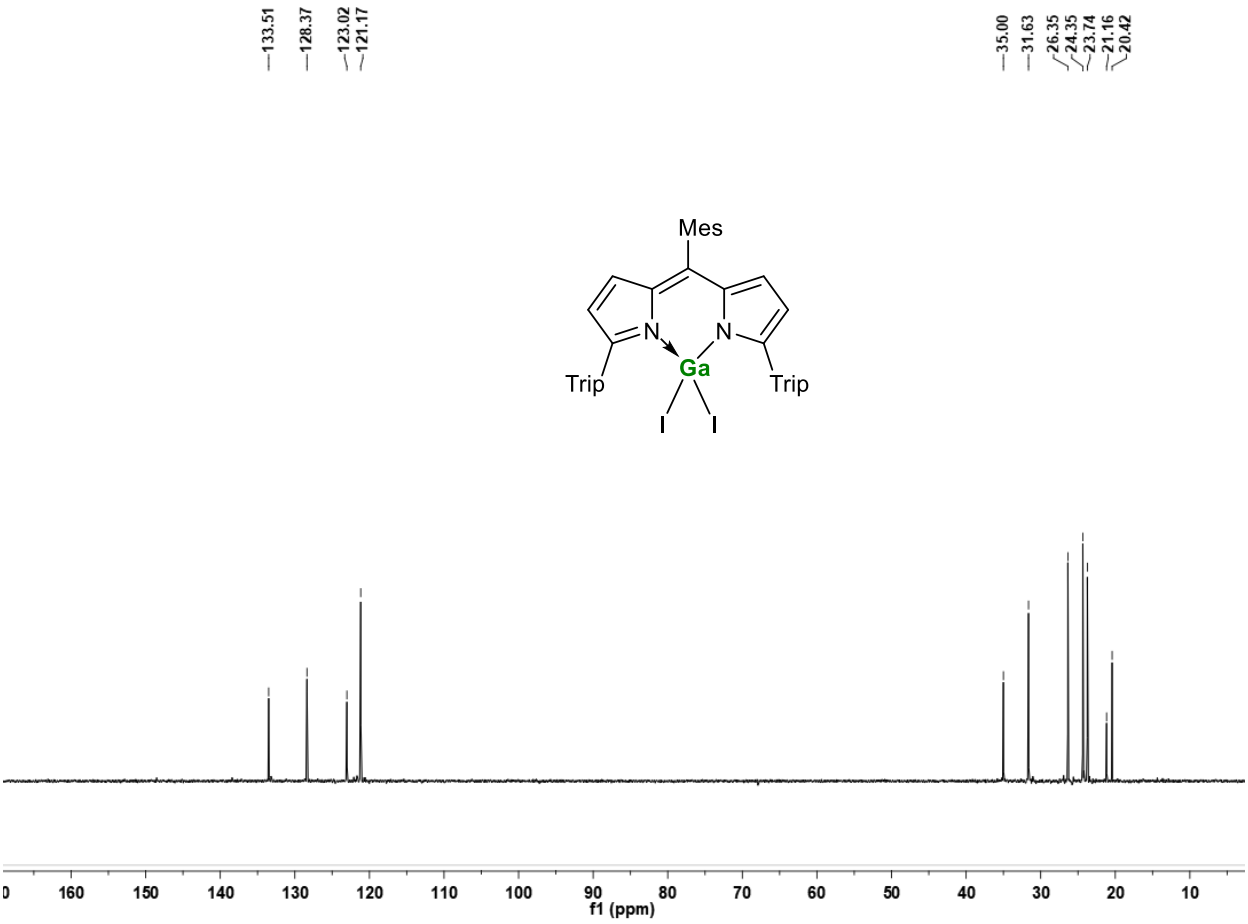


Fig. S10 ^{13}C (DEPT135) NMR spectrum of **3** in C_6D_6.

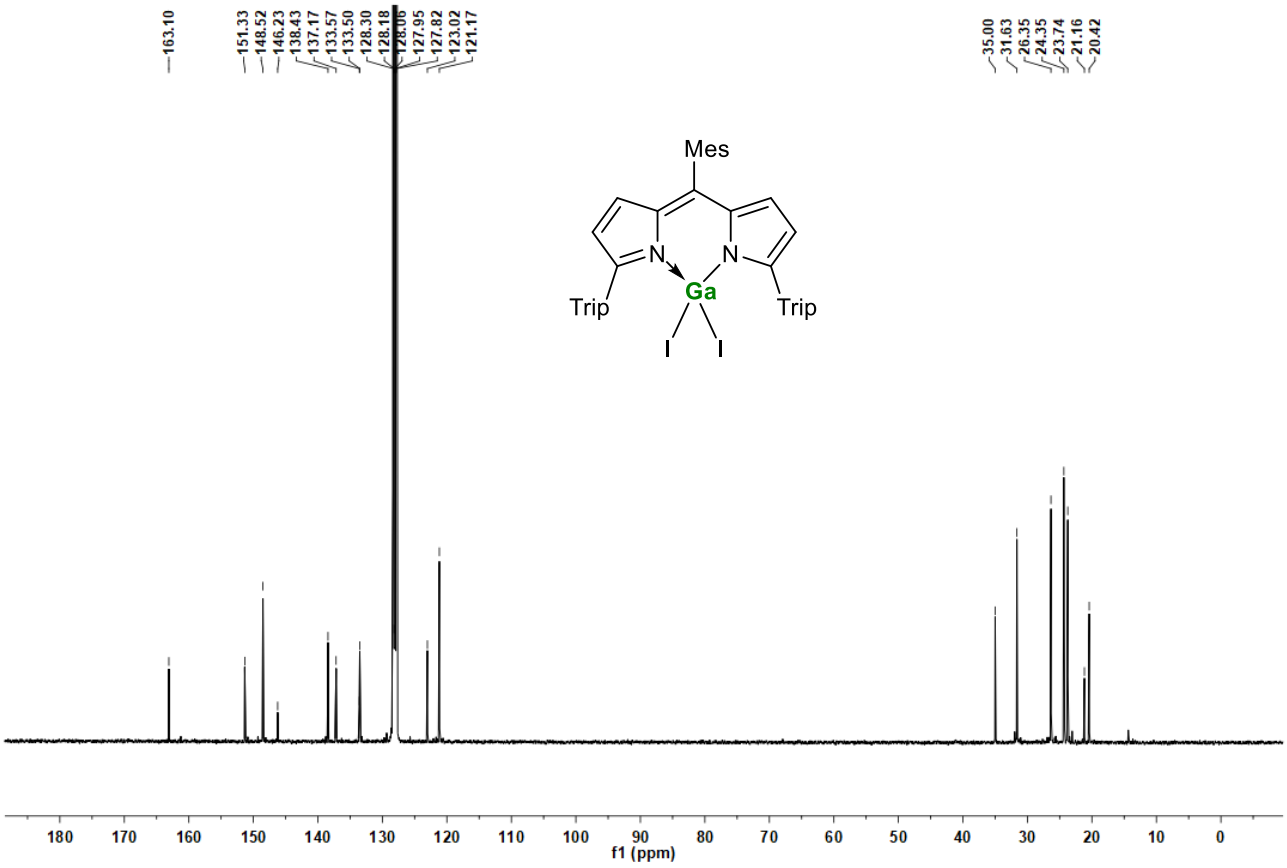


Fig. S11 $^{13}C\{^1H\}$ NMR spectrum of **3** in C_6D_6.

2. Crystal structural parameters for 1–6

For the single crystal X-ray structure analyses the crystals were each mounted on a glass capillary in perfluorinated oil and measured in a cold N_2 flow. The data for all compounds were collected on a Bruker D8 CMOS detector at low temperatures. The structures were solved by direct methods and all refined on F^2 with the SHELX-2018/3 software package. The positions of the H atoms were calculated and considered isotropically according to a riding model. CCDC: 2241367–2241372 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from the Cambridge Crystallography Data Center via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Summary of Data Collection and Structure Refinement.

Compounds	**1**	**2·0.5(C_6H_{14})**	**3·0.5(C_6H_{14})**	**4·C_6H_6**	**5**	**6**
CCDC	2241367	2241368	2241369	2241370	2241371	2241372
Formula	$C_{48}H_{61}BF_2N_2$	$C_{51}H_{68}AlI_2N_2$	$C_{51}H_{68}GaI_2N_2$	$C_{65}H_{86}BF_2KN_2O_2$	$C_{55}H_{69}AlI_2KN_2$	$C_{118}H_{162}Ga_2I_2N_8$
Fw	714.79	989.85	1032.59	1015.26	1078.00	2086.79
Crystal syst	monoclinic	triclinic	triclinic	monoclinic	triclinic	triclinic
Space group	P21/n	P-1	P-1	P21/c	P-1	P-1
Size, mm^3	0.22 × 0.16 × 0.06	0.16 × 0.1 × 0.08	0.16 × 0.14 × 0.12	0.28× 0.16 × 0.06	0.16× 0.12 × 0.08	0.2× 0.1 × 0.08
T, K	120.0	120.0	120.0	120.0	120.00	124.0
a, Å	12.4314(16)	11.2036(7)	11.1958(5)	19.1056(10)	12.5089(11)	10.9371(8)
b, Å	21.814(3)	13.6054(9)	13.6099(5)	15.0657(8)	14.5593(14)	15.3779(13)
c, Å	16.532(2)	18.1906(12)	18.1749(8)	22.8381(12)	15.7688(16)	38.663(3)
α, deg	90	83.321(2)	83.433(2)	90	71.708(4)	96.760(4)
β, deg	106.318(7)	72.994(2)	73.031(2)	113.478(2)	85.718(4)	94.073(4)
γ, deg	90	70.360(2)	70.377(2)	90	77.831(3)	98.626(4)
V, $Å^3$	4302.6(10)	2496.8(3)	2494.6(2)	6029.5(6)	2665.3(4)	6358.4(9)
Z	4	2	2	4	2	2
d_{calcd}, $g•cm^{-1}$	1.103	1.317	1.375	1.118	1.343	1.090
μ, mm^{-1}	0.340	6.896	7.334	0.749	7.107	3.120
Reflections collected	37880	43502	53886	88416	8591	132763
Independent reflections	7694	9066	10737	10954	8591	23205
[R_{int}]	0.0878	0.0539	0.0688	0.0487	--[a]	0.0732
R_1[I>2sigma(I)]	0.0701	0.0322	0.0446	0.0623	0.0433	0.0436
wR_2[I>2sigma(I)]	0.1771	0.0838	0.1180	0.1619	0.1089	0.1189
R_1[all data]	0.1114	0.0340	0.0564	0.0642	0.0488	0.0650
wR_2[all data]	0.2036	0.0848	0.1247	0.1635	0.1125	0.1273
GOF	1.021	1.070	1.071	1.019	1.051	1.114
Largest diff. Peak/hole, e•$Å^{-3}$	0.30/-0.37	0.68/-0.69	0.97/-2.25	0.85/-0.63	1.22/-1.02	0.92/-1.32

[a] The Rint value is of no meaning after handling twinning by using CELL NOW subprogram in APEX3.

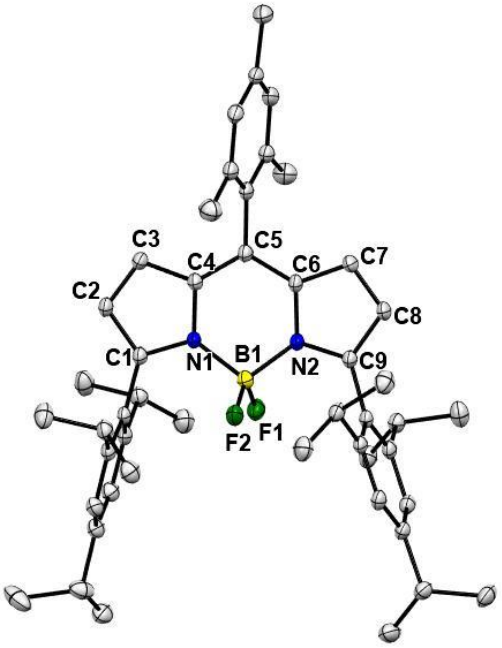


Fig. S12 Molecular structure of **1.** Hydrogen atoms are omitted for clarity. Thermal ellipsoids are set at the 30% probability level. Selected bond distances (Å) and angles (º): B1–N1 1.559(4), B1–N2 1.553(4), B1–F1 1.382(4), B1–F2 1.388(4), N1–C1 1.358(3), N2–C9 1.349(3), C1–C2 1.412(4), C2–C3 1.381(4), C3–C4 1.412(3), C4–C5 1.404(3), C5–C6 1.399(3), C6–C7 1.417(3), C7–C8 1.380(4), C8–C9 1.416(4), N1–B1–N2 107.4(2), N1–B1–F1 109.8(2), N1–B1–F2 109.3(2), F1–B1–F2 111.4(3).

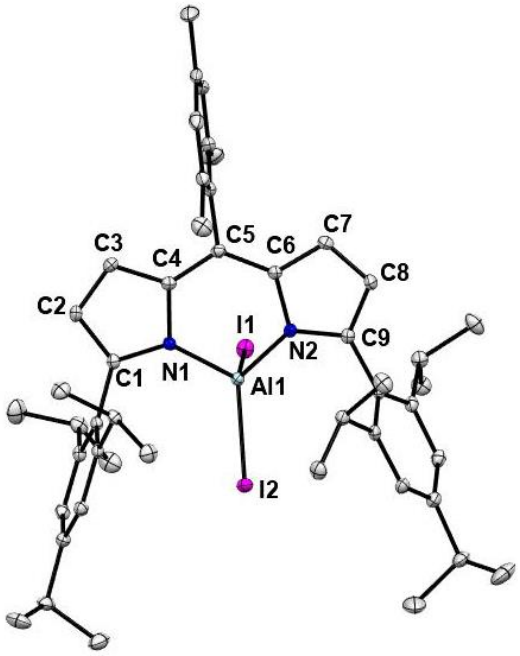


Fig. S13 Molecular structure of **2**. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are set at the 30% probability level. Selected bond distances (Å) and angles (º): Al1–N1 1.882(3), Al1–N2 1.886(2), Al1–I1 2.5304(9), Al1–I2 2.4847(8), N1–C1 1.361(4), N2–C9 1.356(4), C1–C2 1.411(4), C2–C3 1.388(4), C3–C4 1.411(4), C4–C5 1.397(4), C5–C6 1.398(4), C6–C7 1.415(4), C7–C8 1.377(4), C8–C9 1.413(4), N1–Al1–N2 96.64(11), N1–Al1–I1 105.46(8), N1–Al1–I2 115.94(8), I1–Al1–I2 112.91(3).

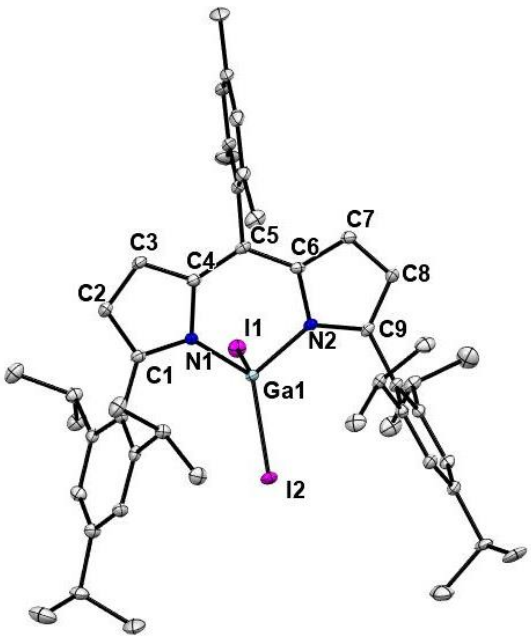


Fig. S14 Molecular structure of **3**. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are set at the 30% probability level. Selected bond distances (Å) and angles (º): Ga1–N1 1.936(3), Ga1–N2 1.938(3), Ga1–I1 2.5375(5), Ga1–I2 2.4874(5), N1–C1 1.346(4), N2–C9 1.358(4), C1–C2 1.414(5), C2–C3 1.367(5), C3–C4 1.416(5), C4–C5 1.388(5), C5–C6 1.411(5), C6–C7 1.403(5), C7–C8 1.380(5), C8–C9 1.410(5), N1–Ga1–N2 94.87(11), N1–Ga1–I1 104.58(8), N1–Ga1–I2 119.16(8), I1–Ga1–I2 114.411(17).

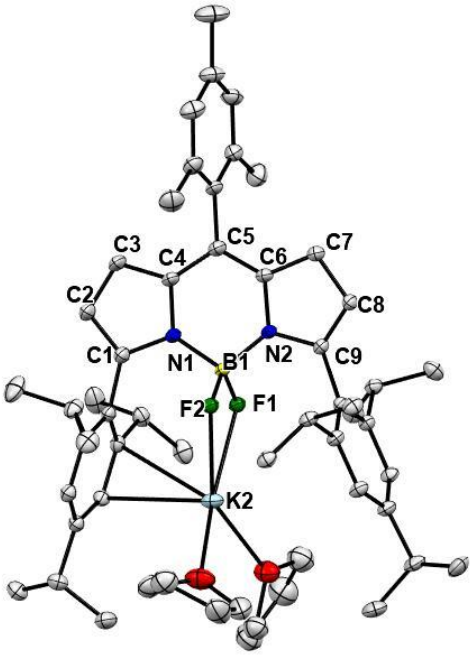


Fig. S15 Molecular structure of **4**. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are set at the 30% probability level. Selected bond distances (Å) and angles (º): B1–N1 1.521(2), B1–N2 1.508(2), B1–F1 1.430(2), B1–F2 1.427(2), F1–K2 2.6820(18), F2–K2 2.5746(18), N1–C1 1.388(2), N2–C9 1.399(2), C1–C2 1.371(3), C2–C3 1.430(3), C3–C4 1.407(3), C4–C5 1.431(3), C5–C6 1.380(3), C6–C7 1.464(3), C7–C8 1.472(2), C8–C9 1.349(3), N1–B1–N2 108.58(14), N1–B1–F1 111.19(15), N1–B1–F2 110.00(15), F1–B1–F2 104.09(13), F1–K2–F 50.70(4) , B1–F1–K2 54.49(8), B1–F2–K2 50.06(8).

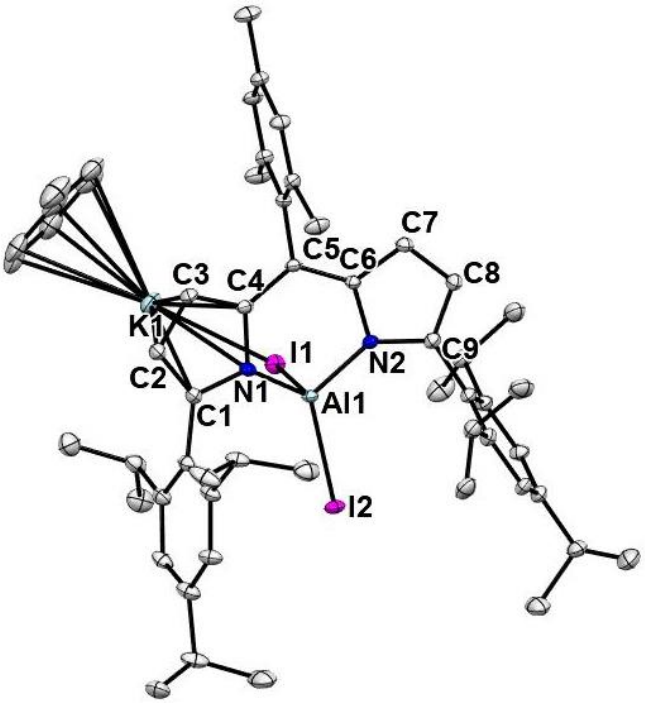


Fig. S16 Molecular structure of **5**. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are set at the 30% probability level. Selected bond distances (Å) and angles (o): Al1–N1 1.864(3), Al1–N2 1.845(3), Al1–I1 2.6139(12), Al1–I2 2.4935(11), I1–K1 3.4313(11), N1–C1 1.391(5), N2–C9 1.388(5), C1–C2 1.384(6), C2–C3 1.414(6), C3–C4 1.401(6), C4–C5 1.425(5), C5–C6 1.414(5), C6–C7 1.402(5) , C7–C8 1.406(6), C8–C9 1.385(6), N1–Al1–N2 99.56(14) , N1–Al1–I1 104.36(11) , N1–Al1–I2 119.70(11), I1–Al1–I2 106.96(4), Al1–I1–K1 84.78(3), K1–N1–Al1 105.87(14).

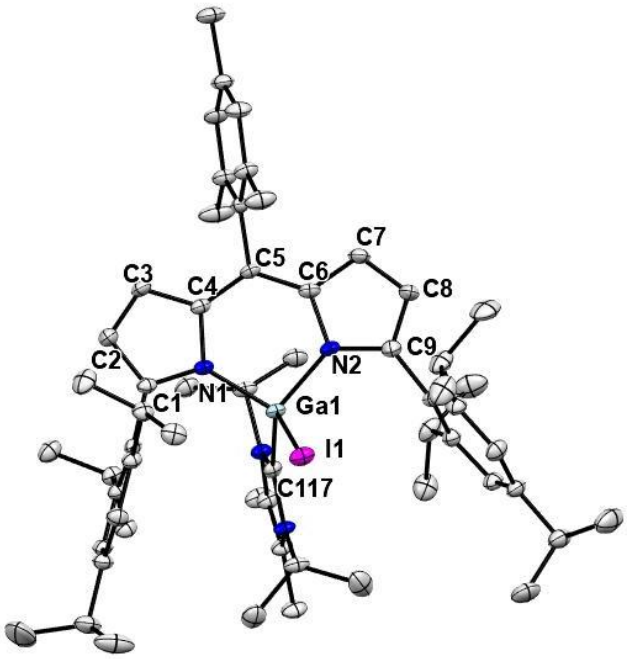


Fig. S17 Molecular structure of **6**. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are set at the 30% probability level. Selected bond distances (Å) and angles (o): Ga1–N1 1.899(3), Ga1–N2 1.906(3), Ga1–I1 2.5541(4), Ga1–C117 2.037(3), N1–C1 1.393(4), N2–C9 1.398(4), C1–C2 1.394(5), C2–C3 1.387(5), C3–C4 1.409(5), C4–C5 1.415(5), C5–C6 1.416(5), C6–C7 1.409(5), C7–C8 1.393(5), C8–C9 1.378(5), N1–Ga1–N2 100.43(11), N1–Ga1–I1 110.05(8), N1–Ga1–C117 110.88(12).

3. UV-vis absorption spectra and photoluminescence spectra of 1-3

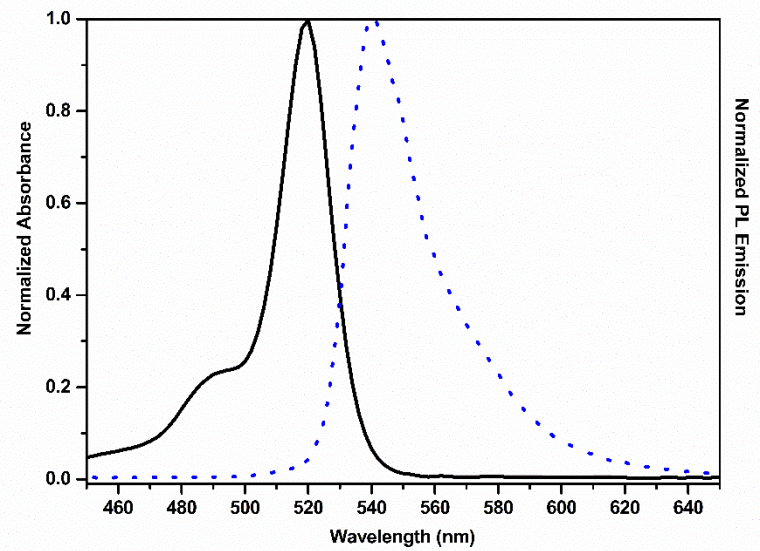


Fig. S18 UV-vis absorption spectra and photoluminescence spectra of **1** in hexane.

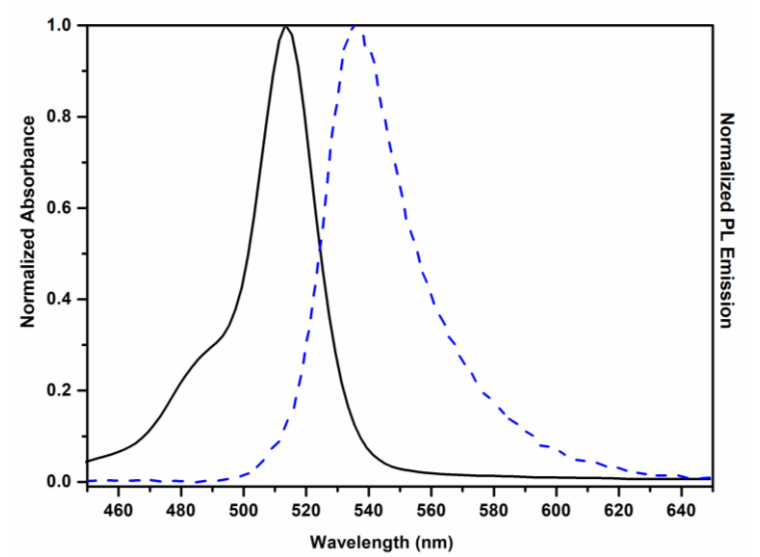


Fig. S19 UV-vis absorption spectra and photoluminescence spectra of **2** in hexane.

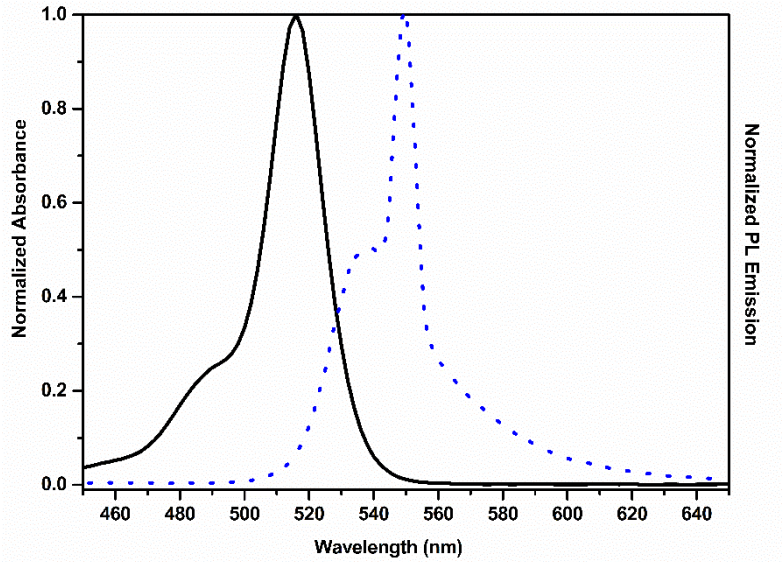


Fig. S20 UV-vis absorption spectra and photoluminescence spectra of **3** in hexane.

4. Theoretical calculations

All of the calculations were performed with Gaussian 16.[S2] The geometry optimization, frequency calculations, and spin density distributions were performed with the (U)B3LYP functional in conjunction with a basis set of Def2-SVP for C, H, N, B, F, and Al atoms and Def2-TZVP for I and Ga atoms, respectively, in the gas phase.[S3] To further figure out the absorption properties of **1**-**6**, time-dependent DFT (TD-DFT) calculations were carried out with the hybrid (U)B3LYP functional in conjunction with a basis set of Def2-SVP for C, H, N, B, F, and Al atoms and Def2-TZVP for I and Ga atoms, respectively. The calculated UV-vis absorption spectra agree well with the experimental data, and the calculated Kohn-Sham orbitals related to the observed transitions are shown in Tables S2. To gain further insight into the electronic structures, Multiwfn[S4] and VMD[S5] were also used.

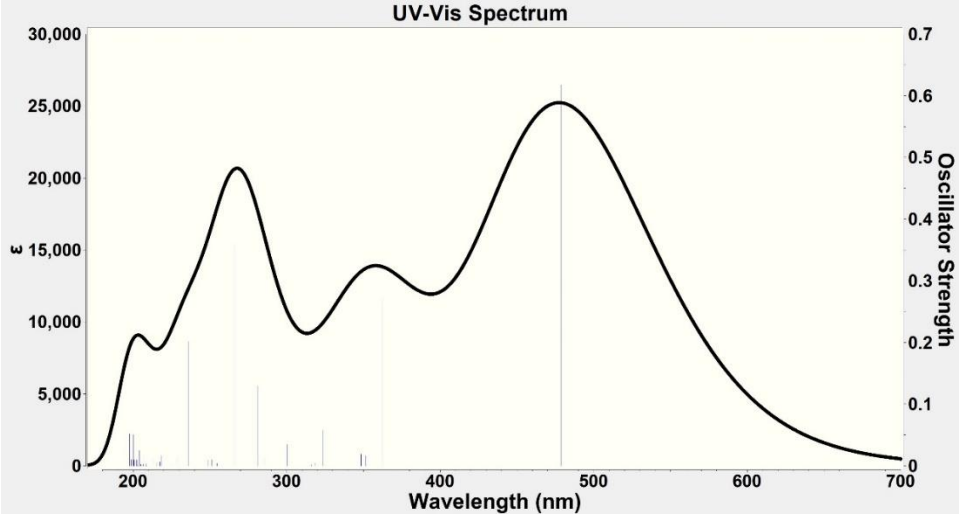


Fig. S21 Calculated UV-vis spectrum of **1′** at the time-dependent DFT (TDDFT)//B3LYP/Def2-SVP level.

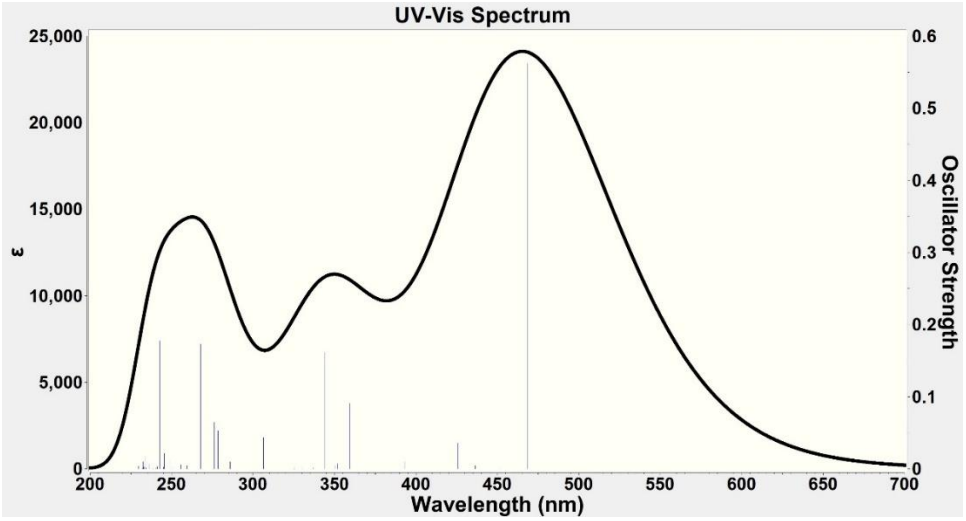


Fig. S22 Calculated UV-vis spectrum of **2′** at the time-dependent DFT (TDDFT)/ /B3LYP/C H N Al for Def2-SVP; I for Def2-TZVP level.

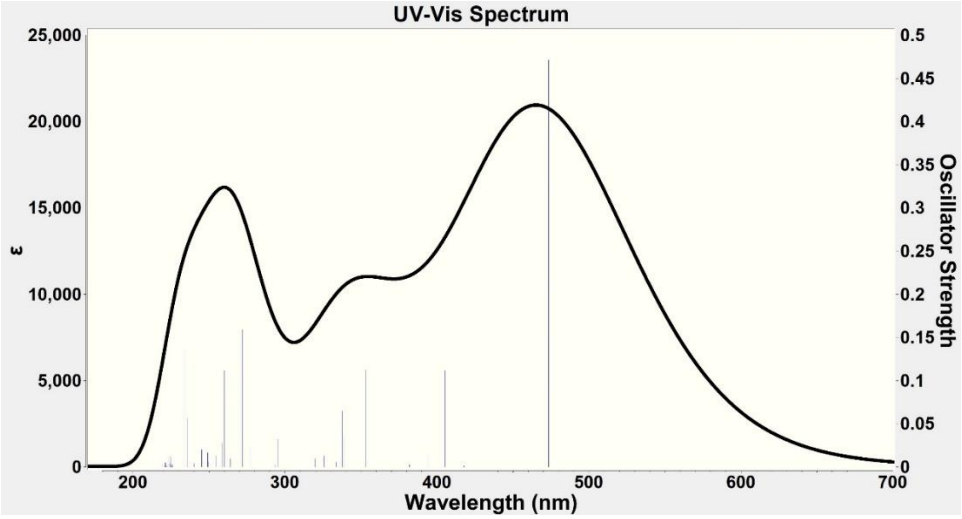


Fig. S23 Calculated UV-vis spectrum of **3′** at the time-dependent DFT (TDDFT)/ /B3LYP/Def2-SVP C H N for Def2-SVP; Ga I for Def2-TZVP level.

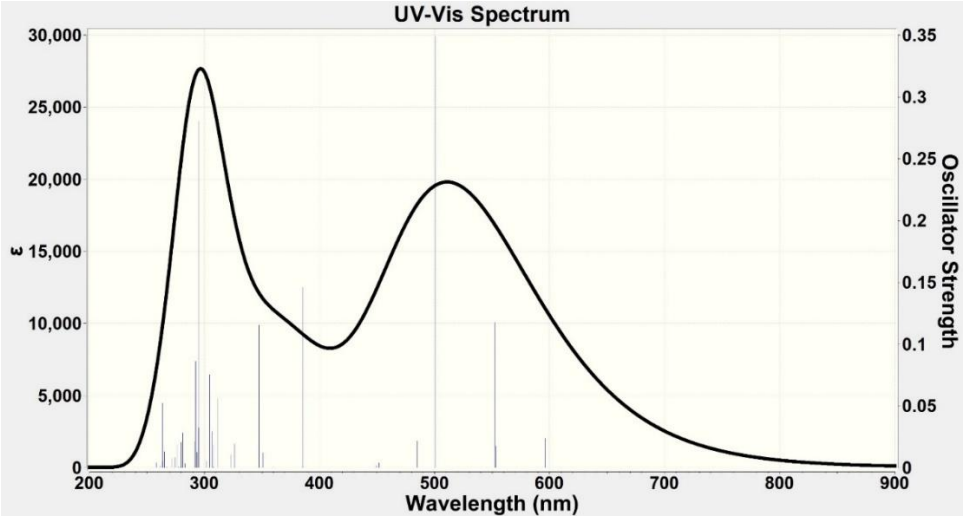


Fig. S24 Calculated UV-vis spectrum of **4′** at the time-dependent DFT (TDDFT)//UB3LYP/Def2-SVP level.

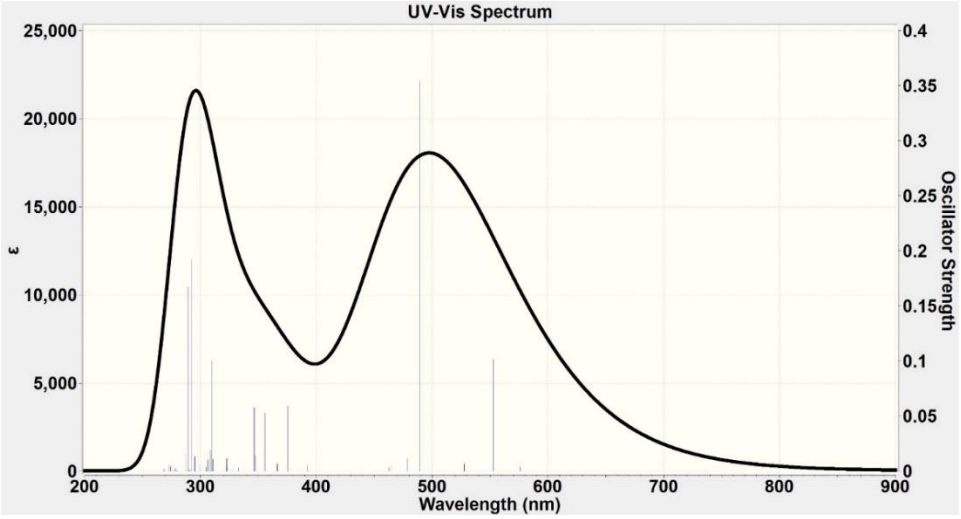


Fig. S25 Calculated UV-vis spectrum of **5′** at the time-dependent DFT level of (TDDFT)//UB3LYP/ Def2-SVP for C, H, N, and Al and Def2-TZVP for I.

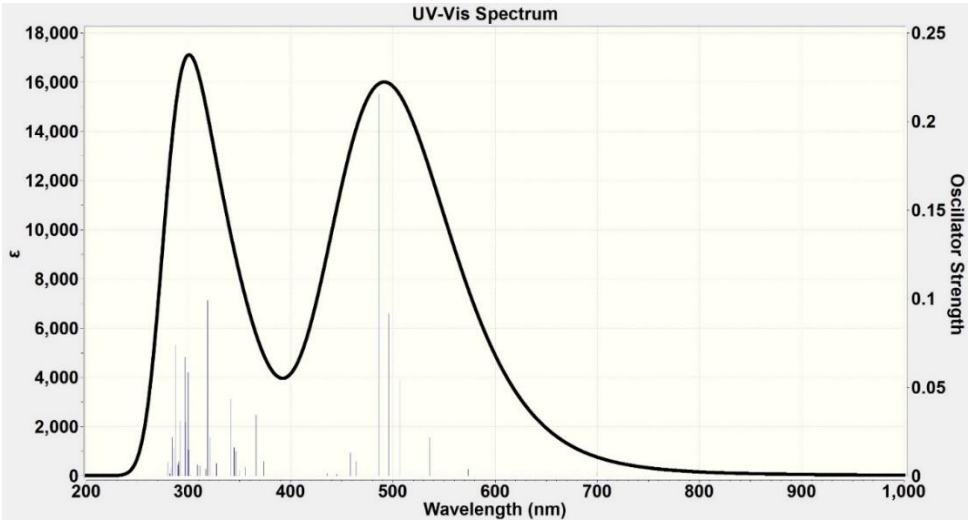
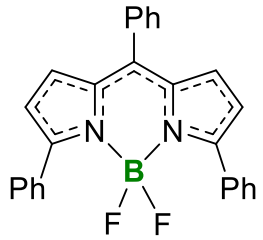


Fig. S26 Calculated UV-vis spectrum of **6′** at the time-dependent DFT level of (TDDFT)//UB3LYP/ Def2-SVP for C, H, and N, and Def2-TZVP for Ga and I.

Table S2. Calculated absorption properties of **1′-6′** including wavelength (nm), oscillator strength (f) and the related transition nature

	Energy/ ev	**Wavelength/ nm**	**Oscillator strength/ f**	**Transition nature and contributions**
1′	2.5695	482.52	0.6173	HOMO→LUMO (0.70645)
2′	2.6463	468.51	0.5621	HOMO→LUMO (0.69782)
3′	2.5978	477.26	0.4711	HOMO→LUMO (0.67875)
4′	2.4781	500.32	0.3489	SOMO (α)→LUMO+2 (α) (0.67081) SOMO-1(β)→SOMO (β) (0.57404) HOMO (α)→LUMO (α) (-0.42990)
5′	2.5348	489.13	0.3541	SOMO (α)→LUMO+1 (α) (0.60179) SOMO-1 (β)→SOMO (β) (0.66425) SOMO (α)→LUMO+2 (α) (-0.39385)
6′	2.3130	536.03	0.0215	HOMO(α)→LUMO+2(α) (0.97504)
	2.5514	485.94	0.2155	SOMO-1 (β)→SOMO (β) (0.65041) SOMO (α)→LUMO +1 (α) (0.38759) SOMO (α)→LUMO+4 (α) (-0.60522)

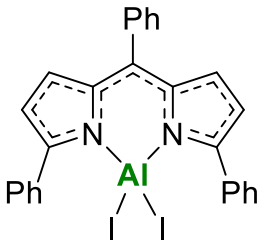
Coordinates for the optimized structure



1'

F	1.63525400	0.17650600	-1.13814500
F	1.63525100	-0.17650500	1.13815000
N	-0.06752700	1.26706400	0.13861200
N	-0.06752600	-1.26706400	-0.13861300
C	1.66811800	3.12848000	0.16473500
C	1.66812200	-3.12847800	-0.16473500
C	2.76848600	2.54213900	0.82082100
C	0.30134900	2.57640400	0.19377300
C	3.12456000	-4.95518200	0.55149800
H	3.25793500	-5.89256600	1.09753400
C	1.86973500	-4.34876300	0.51709200
C	2.76849000	-2.54213600	-0.82082200
C	4.02059200	-3.15778100	-0.78894300
H	4.85946500	-2.68844800	-1.30921500
C	1.86973000	4.34876600	-0.51709100
C	-1.45993500	1.21214000	0.13233000
C	-1.96577100	2.53600500	0.23535300
H	-3.01695300	2.80687000	0.29110100
C	4.02058800	3.15778500	0.78894200
H	4.85946100	2.68845300	1.30921400
C	-1.45993400	-1.21214200	-0.13233100
C	4.20759100	-4.36205600	-0.10469300
C	0.30135200	-2.57640400	-0.19377400
C	4.20758600	4.36206000	0.10469300
C	-0.87216000	3.38134100	0.25788300
H	-0.87778300	4.46464500	0.35093000
C	3.12455400	4.95518600	-0.55149700
H	3.25792700	5.89257100	-1.09753300
C	-4.36388100	0.69276100	-0.99285500
C	-1.96576800	-2.53600800	-0.23535600
H	-3.01694900	-2.80687400	-0.29110500
C	-3.64723200	-0.00000200	0.00000000
C	-4.36388100	-0.69276500	0.99285600
C	-5.76073000	0.68778900	-0.99396200
H	-6.30241000	1.22181700	-1.77873000
C	-0.87215500	-3.38134300	-0.25788600
H	-0.87777700	-4.46464600	-0.35093400
B	0.85710000	0.00000000	0.00000100
C	-2.15804700	-0.00000200	0.00000100
C	-5.76073000	-0.68779300	0.99396300
H	-6.30241000	-1.22182200	1.77873100
C	-6.46319700	-0.00000300	0.00000000

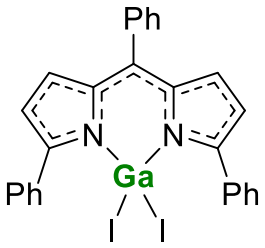
H	-7.55605800	-0.00000300	0.00000000
H	-3.81859100	1.22105300	-1.77784500
H	-3.81859100	-1.22105700	1.77784600
H	1.03612200	4.81169700	-1.04919800
H	5.19213100	4.83634800	0.08166400
H	2.63848200	1.60693200	1.36065300
H	1.03612800	-4.81169500	1.04919900
H	5.19213700	-4.83634200	-0.08166300
H	2.63848400	-1.60693000	-1.36065400



2'

I	-1.82962500	-0.56303200	2.08158900
I	-1.82962400	0.56303000	-2.08158600
Al	-0.47483700	0.00000000	0.00000100
N	0.78169500	-1.45048100	-0.19376500
N	0.78169900	1.45047900	0.19376700
C	-1.64824700	3.16959400	1.30761400
C	-0.73494400	3.47611400	0.28352800
C	2.79457800	-2.52365900	0.06368500
H	3.86179900	-2.68684100	0.18733800
C	0.56763200	2.79777500	0.15809700
C	2.16652000	1.25267300	0.05976900
C	7.12052500	-0.00001000	-0.00000100
C	5.02153600	-0.51429200	-1.09600200
C	2.16651600	-1.25267900	-0.05976800
C	-1.04740300	4.52029300	-0.61088300
C	2.79458500	2.52365100	-0.06368500
H	3.86180700	2.68682900	-0.18733900
C	2.81069000	-0.00000400	0.00000000
C	-0.73495600	-3.47610700	-0.28352900
C	1.79794200	-3.48055000	0.01317800
H	1.90922400	-4.56167900	0.05655100
C	-3.15837700	4.89116500	0.51503600
C	4.30581200	-0.00000600	0.00000000
C	5.02153800	0.51427800	1.09600100
C	-2.85087900	3.87060400	1.41831700
H	-3.54816600	3.61688700	2.22039600
C	6.41839900	-0.50732400	-1.09758100
H	6.96020000	-0.89902400	-1.96209600
C	6.41840100	0.50730600	1.09758000
H	6.96020300	0.89900400	1.96209400
C	1.79795300	3.48054400	-0.01318100
H	1.90923800	4.56167300	-0.05655700
C	-2.25059900	5.21576100	-0.49914200

H	-2.48486800	6.01074700	-1.21152400
C	0.56762400	-2.79777500	-0.15809700
C	-1.64825700	-3.16957900	-1.30761400
C	-2.25062200	-5.21574700	0.49913700
H	-2.48489500	-6.01073300	1.21151700
C	-2.85089300	-3.87058200	-1.41831900
H	-3.54817900	-3.61685800	-2.22039700
C	-1.04742100	-4.52028600	0.61088000
C	-3.15839800	-4.89114400	-0.51504100
H	8.21339300	-0.00001100	-0.00000100
H	4.47537700	0.90689500	1.95654700
H	4.47537400	-0.90690700	-1.95654700
H	-0.35018100	-4.76468100	1.41534400
H	-4.10219100	-5.43548300	-0.60150500
H	-1.41098800	-2.39199000	-2.03375800
H	-0.35016100	4.76468200	-1.41534800
H	-1.41098200	2.39200600	2.03375900
H	-4.10216800	5.43551000	0.60149900



3'

I	-2.41637800	0.01917100	-1.49640800
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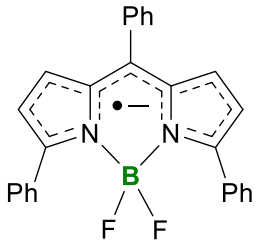
N	0.77894800	1.47404700	-0.17387200
C	0.53832000	-2.82522300	-0.28877000
C	2.15803100	1.23718800	-0.23155700
C	0.57883200	2.80009900	-0.39567900
C	-0.71974000	3.49702500	-0.42303600
C	-1.71025800	3.30130100	0.55605100
C	2.14128500	-1.28185900	-0.17006100
C	-2.17025800	-5.19551200	-1.40751400
H	-2.30830500	-5.95156500	-2.18454600
C	-0.95670700	4.44373400	-1.44084000
C	-0.77005600	-3.50386200	-0.34742800
C	1.82908700	3.44190700	-0.60574300
H	1.95928800	4.50560900	-0.79201700
C	4.99958700	0.41023900	0.92285200
C	-3.13751400	4.94159300	-0.51487600
C	2.77988500	-2.55228100	-0.27290700
H	3.85386800	-2.71707700	-0.27795400
C	-3.19974600	-4.92395400	-0.50009500
C	2.81170800	2.47787000	-0.48725000
H	3.88549300	2.61111400	-0.58921600

C	-2.15633000	5.15305400	-1.48942700
H	-2.32860700	5.87106000	-2.29517200
C	-3.01208200	-3.95268900	0.48651800
H	-3.80548100	-3.74060300	1.20721200
C	2.78267900	-0.02643700	-0.18247700
C	-1.80951800	-3.24765000	0.56430000
C	1.78382500	-3.50424100	-0.37351200
H	1.89980200	-4.58223100	-0.46072300
C	-2.90728700	4.01807500	0.50806900
H	-3.66260500	3.85322700	1.28022200
C	6.39695700	0.41405800	0.91429600
H	6.94204400	0.74780900	1.80079800
C	-0.96506400	-4.49846300	-1.32799700
C	4.28180900	-0.02663500	-0.20329600
C	7.09462100	-0.00658300	-0.22188800
C	4.99066900	-0.44920500	-1.34038300
C	6.38803300	-0.43481000	-1.34976700
H	6.92623200	-0.75812100	-2.24436900
H	8.18743200	0.00083100	-0.22906000
H	4.45595100	0.73963900	1.81136600
H	4.44073500	-0.77910800	-2.22479200
H	-4.07759600	5.49775400	-0.55222900
H	-0.20109400	4.60201500	-2.21359400
H	-1.53607300	2.60705100	1.37869500
H	-1.67054700	-2.51676100	1.36132700
H	-0.17011200	-4.70535400	-2.04805700
H	-4.14412800	-5.47067700	-0.56096700
I	-1.02614700	0.01649800	2.68686700

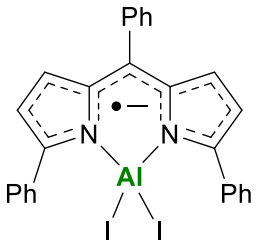


4'

F	1.62598900	0.16415600	-1.13872000
F	1.62599100	-0.16415400	1.13872100
N	-0.08579600	1.26471900	0.12271400
N	-0.08579400	-1.26472000	-0.12271000
C	1.68003000	3.13549600	0.14965500
C	1.68003600	-3.13549300	-0.14965400
C	2.81609700	2.49804800	0.69665000
C	0.31219500	2.59305400	0.18926700
C	3.12897800	-5.02500600	0.45206000

H	3.23920600	-6.01012700	0.91629500
C	1.87638800	-4.41279300	0.43057300
C	2.81610000	-2.49804400	-0.69665500
C	4.06927800	-3.11193200	-0.66580000
H	4.92629000	-2.58806600	-1.10023100
C	1.87637800	4.41279800	-0.43057000
C	-1.47264900	1.22568000	0.11907300
C	-1.95833300	2.54889900	0.24367000
H	-3.00334900	2.83687600	0.32076500
C	4.06927400	3.11193800	0.66579200
H	4.92628800	2.58807200	1.10021900
C	-1.47264700	-1.22568400	-0.11907000
C	4.24128000	-4.37830600	-0.09747500
C	0.31220100	-2.59305400	-0.18926300
C	4.24127100	4.37831400	0.09747100
C	-0.84381300	3.39080000	0.27123200
H	-0.84770700	4.47380900	0.38050800
C	3.12896600	5.02501300	-0.45205900
H	3.23919000	6.01013500	-0.91629200
C	-4.40914700	0.83857200	-0.86590200
C	-1.95832800	-2.54890400	-0.24366600
H	-3.00334300	-2.83688300	-0.32076000
C	-3.67125900	-0.00000300	-0.00000100
C	-4.40914800	-0.83857900	0.86590000
C	-5.80526900	0.83937700	-0.86501100
H	-6.34395600	1.49534200	-1.55582600
C	-0.84380600	-3.39080300	-0.27122700
H	-0.84769700	-4.47381200	-0.38050100
B	0.81417300	0.00000000	0.00000100
C	-2.19202600	-0.00000300	0.00000100
C	-5.80527100	-0.83938400	0.86500500
H	-6.34395900	-1.49535000	1.55581900
C	-6.51596500	-0.00000400	-0.00000400
H	-7.60970100	-0.00000400	-0.00000500
H	-3.86745000	1.48205500	-1.56180700

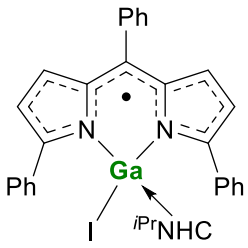
H	-3.86745300	-1.48206100	1.56180600
H	1.02768400	4.91882700	-0.89548900
H	5.22748100	4.85121800	0.07594500
H	2.70543000	1.51716600	1.15322200
H	1.02769700	-4.91882300	0.89549600
H	5.22749000	-4.85120800	-0.07595200
H	2.70542900	-1.51716500	-1.15323100



5'

I	-1.86085600	-0.55490900	2.06367000
I	-1.86085700	0.55490800	-2.06366800
Al	-0.39640000	0.00000000	0.00000100
N	0.79719200	-1.46424800	-0.17423600
N	0.79719300	1.46424700	0.17423600
C	-1.66048000	3.17037900	1.24629400
C	-0.72995900	3.51737100	0.24703900
C	2.78435400	-2.53028100	0.19747600
H	3.84476500	-2.69825500	0.36544400
C	0.56122800	2.83405100	0.07972800
C	2.17728900	1.26921600	0.00630700
C	7.16339600	-0.00000200	-0.00000100
C	5.05792100	-0.67250700	-1.00028200
C	2.17728800	-1.26921700	-0.00630700
C	-1.03485500	4.62841400	-0.57200300
C	2.78435600	2.53028000	-0.19747700
H	3.84476600	2.69825300	-0.36544500
C	2.83624000	-0.00000100	0.00000000
C	-0.72996200	-3.51737000	-0.24704000
C	1.77186400	-3.49423600	0.15741500
H	1.88718900	-4.57363500	0.24267000

C	-3.13400500	4.98323800	0.58766000
C	4.32437300	-0.00000100	0.00000000
C	5.05792100	0.67250400	1.00028200
C	-2.84779500	3.88746200	1.40695300
H	-3.55141400	3.58560100	2.18792100
C	6.45453100	-0.67275200	-1.00117700
H	6.99394400	-1.19661200	-1.79608400
C	6.45453200	0.67274900	1.00117600
H	6.99394500	1.19660800	1.79608200
C	1.77186600	3.49423500	-0.15741700
H	1.88719200	4.57363400	-0.24267300
C	-2.21459800	5.35158600	-0.40171800
H	-2.42723100	6.20031200	-1.05880100
C	0.56122600	-2.83405100	-0.07972800
C	-1.66048300	-3.17037400	-1.24629300
C	-2.21460200	-5.35158400	0.40171400
H	-2.42723600	-6.20031200	1.05879500
C	-2.84779900	-3.88745500	-1.40695300
H	-3.55141800	-3.58559000	-2.18791900
C	-1.03485800	-4.62841400	0.57199900
C	-3.13401000	-4.98323200	-0.58766300
H	8.25713800	-0.00000200	-0.00000100
H	4.51303100	1.19233600	1.79129200
H	4.51303000	-1.19233800	-1.79129200
H	-0.33999600	-4.90298800	1.36879900
H	-4.06528600	-5.54254100	-0.71438600
H	-1.44686100	-2.33816700	-1.91679200
H	-0.33999200	4.90298500	-1.36880300
H	-1.44685900	2.33817400	1.91679500
H	-4.06528000	5.54254900	0.71438300



6'

I	-0.76078900	0.11685600	-3.05559500
Ga	-0.03434400	0.04870300	-0.55459500
N	1.07592700	-1.49718000	-0.22913300
N	1.21965800	1.47594800	-0.20686800
N	-2.85431500	-0.03897400	0.86614000
N	-1.17044900	-0.02769200	2.23922900
C	-1.50044200	0.02386100	0.92161100
C	0.75177200	-2.82460900	0.02998300
C	2.59289300	1.19690200	-0.11617300
C	-3.38439800	-0.13432400	2.15074100
C	1.06051700	2.85327000	-0.08241600
C	-0.20068800	3.61537400	-0.10981200
C	0.22999100	0.06173300	2.74202500
H	0.84330200	0.06125400	1.83710000
C	-3.63020700	0.03812900	-0.40097300
H	-2.86090300	0.00660900	-1.18221600
C	-0.41685400	4.60569700	0.87663100
C	2.45113700	-1.34493100	-0.01788800
C	-2.31939200	-0.12796500	3.01864200
C	-2.50207600	-4.05400100	-1.51138500
H	-3.05619100	-3.94719700	-2.44803500
C	-1.15951900	3.49909800	-1.13639100
C	-0.56361100	-3.46201200	-0.14696300
C	-4.54215300	-1.17212500	-0.61296100
H	-4.01354500	-2.11448700	-0.41494700
H	-4.86187600	-1.18549400	-1.66618700
H	-5.45220400	-1.13320200	0.00244800
C	2.31996300	3.44239000	0.07101100
H	2.49837300	4.51245600	0.16266800

C	-2.35201500	-0.25649400	4.50845800
H	-2.05117300	-1.26288900	4.84105300
H	-3.37257600	-0.08299100	4.87422300
H	-1.69653900	0.46924500	5.00767300
C	5.34648100	0.27604200	1.18224000
C	0.49427700	1.39416500	3.44864100
H	0.17502300	2.23944300	2.82255800
H	1.57635500	1.49576000	3.61993900
H	-0.00500100	1.46857400	4.42627400
C	-2.47737400	5.30776800	-0.18848900
C	2.97817000	-2.60126700	0.36409700
H	4.02184600	-2.80024800	0.59207400
C	-2.96185400	-4.92905500	-0.52145400
C	0.64443500	-1.16874400	3.55150100
H	0.18478300	-1.20344700	4.54951500
H	1.73559600	-1.14410100	3.68906000
H	0.40477000	-2.09461000	3.00884600
C	-4.36476100	1.37395900	-0.53598500
H	-5.21413700	1.46278100	0.15810300
H	-4.76592500	1.45632200	-1.55791200
H	-3.68598900	2.22143100	-0.37147600
C	3.28026000	2.42648900	0.02044900
H	4.35873600	2.54067900	0.07982600
C	-2.27798500	4.33660900	-1.17480800
H	-2.98913700	4.24182100	-2.00003900
C	-2.22291600	-5.07251500	0.65843600
H	-2.56682700	-5.75530400	1.44044500
C	3.17006700	-0.10865400	-0.06330700
C	-1.04296600	-4.35051300	0.84249100
C	1.91248400	-3.50807800	0.40973300
H	1.96222000	-4.57166200	0.63742900
C	-1.53665900	5.43735300	0.83891400
H	-1.67478100	6.19387100	1.61638100
C	6.73608000	0.16450300	1.28217200
H	7.24777900	0.54357700	2.17123700

C	-1.32232500	-3.32827600	-1.32815700
C	-4.83594400	-0.26895500	2.48499700
H	-5.46049900	0.45536200	1.94526200
H	-4.98675200	-0.09604100	3.55867600
H	-5.21867400	-1.27668900	2.25775000
C	4.65733000	-0.20685700	0.05383600
C	7.47003300	-0.43502900	0.25425300
C	5.41154300	-0.81222900	-0.96925800
C	6.80080200	-0.92395800	-0.87209400
H	7.36435700	-1.39236800	-1.68366600
H	8.55707400	-0.52186800	0.33104800
H	4.77979400	0.73915300	1.99347900
H	4.89370500	-1.19382300	-1.85243300
H	-3.35023200	5.96459900	-0.22618200
H	-1.00075100	2.78319700	-1.94327000
H	0.31472500	4.71749400	1.68048400
H	-0.47024300	-4.47253300	1.76517800
H	-0.95762600	-2.68726700	-2.13122700
H	-3.88068800	-5.50176400	-0.67181900

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