Electronic Supplementary Information

BODIPY–*ortho*-Carborane–Tetraphenylethylene Triad: Synthesis, Characterization, and Properties

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General Information

All NMR spectra were recorded on Agilent VNMRS 500 MHz at 25 ^{o}C and chemical shifts were referenced internally using the residual solvent resonances. Mass spectra were measured on a MALDI (matrix assisted laser desorption ionization) BRUKER Microflex LT using DHB (2,5-Dihydroxybenzoic acid) as the matrix. All reagents and solvents were of reagent grade quality obtained from commercial suppliers.

A Varian Cary-Eclipse Luminescence Spectrometer was used for recording spectra and making fluorescence measurements.

Electrochemical measurements were carried out using a Gamry 600 Potentiostat/Galvanostat. The cell comprised inlets for a glassy carbon working electrode, a platinum wire counter electrode and a saturated calomel electrode (SCE) reference electrode. Typically, a 0.1 M solution of TBAP in CH_2Cl_2 containing the sample was purged with nitrogen for 20 min, and then the voltammograms were recorded at room temperature.

Single crystals of the compounds were mounted on a MicroMount (MiTeGen). Crystallographic data of the compounds were recorded on a Bruker D8 VENTURE single crystal X-ray diffractometer equipped with PHOTON 100 CMOS detector, using graphite monochromatized MoKα radiation (λ=0.71073 Å). All of the data were corrected for absorption effects using the multiscan method implemented in SADABS. The structures were solved by direct methods and refined on F^2 by fullmatrix least-squares using SHELXL 2014[1]. All the hydrogen atoms were added to their geometrically ideal positions. All non-hydrogen atoms were refined with anisotropic displacement parameters. The crystal and instrumental parameters used in the unit-cell determination and data collection are summarized in **Table S1.**

1D and 2D NMR spectra of 3 and 4

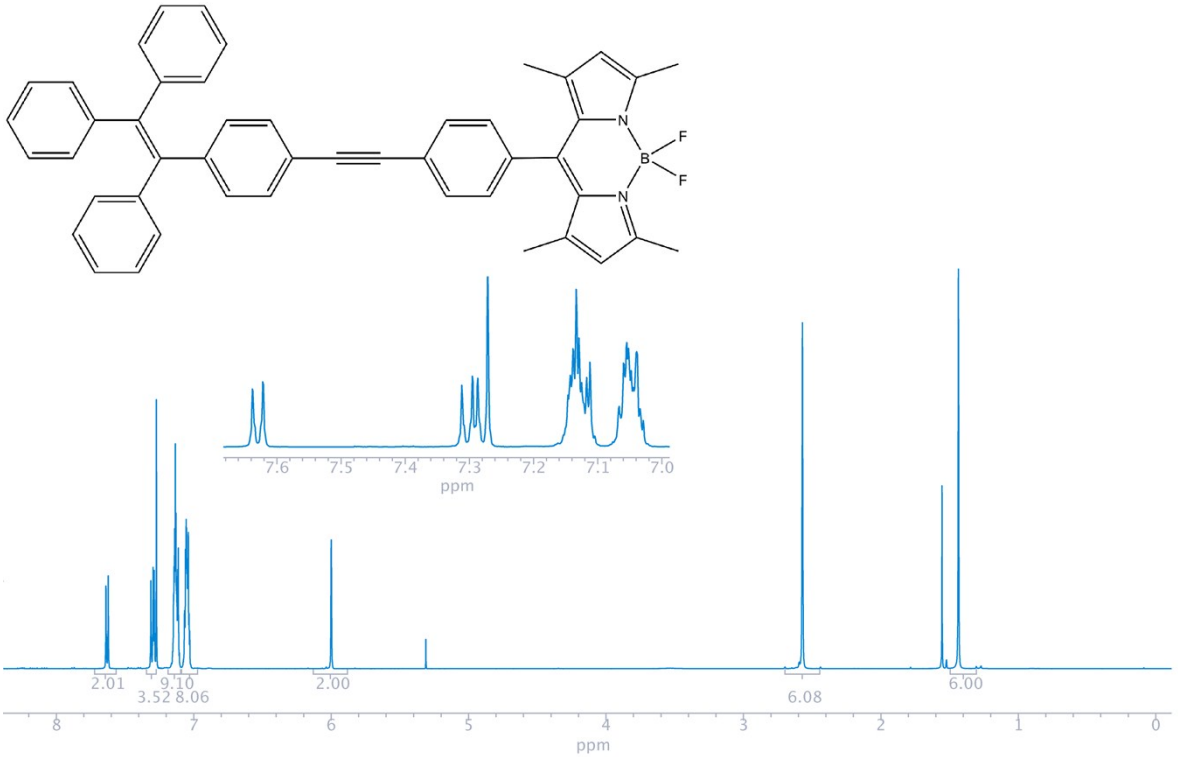

Fig. S1 ^{1}H NMR spectrum of 3 in $CDCl_3$.

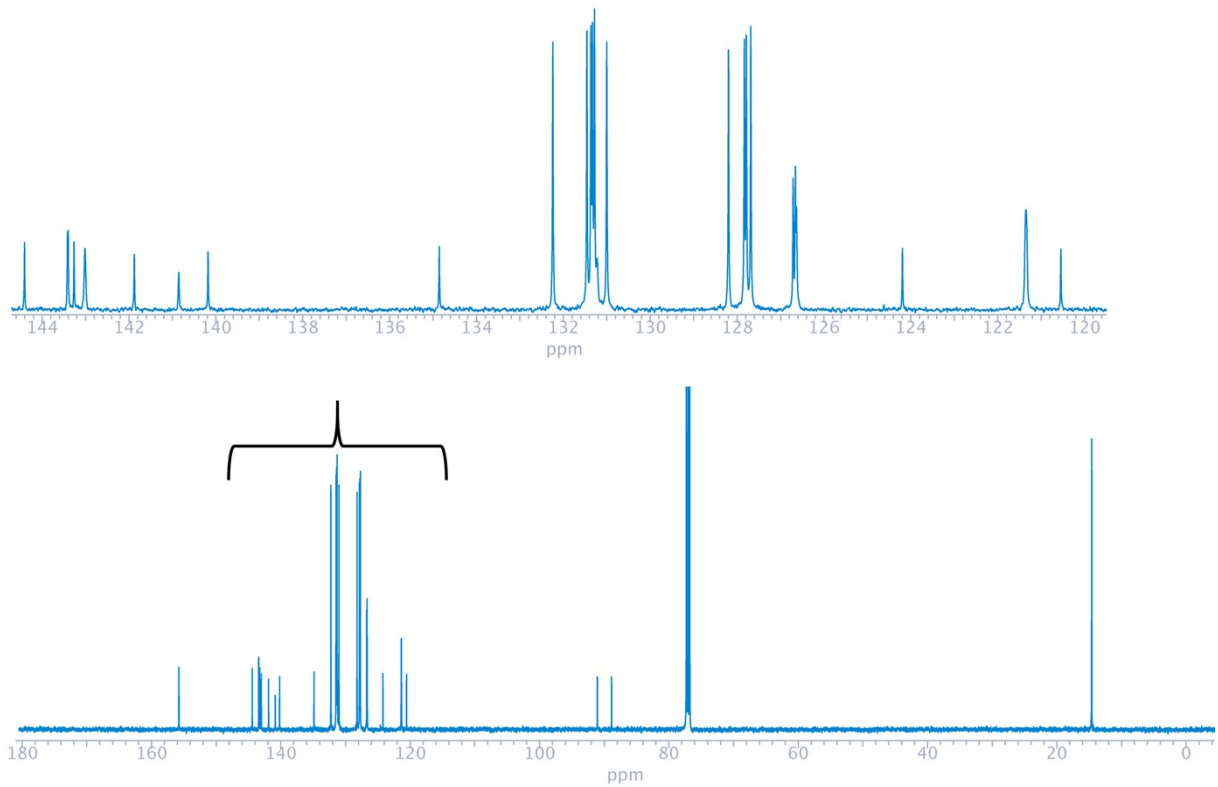

Fig. S2 ^{13}C NMR spectrum of **3** in $CDCl_3$.

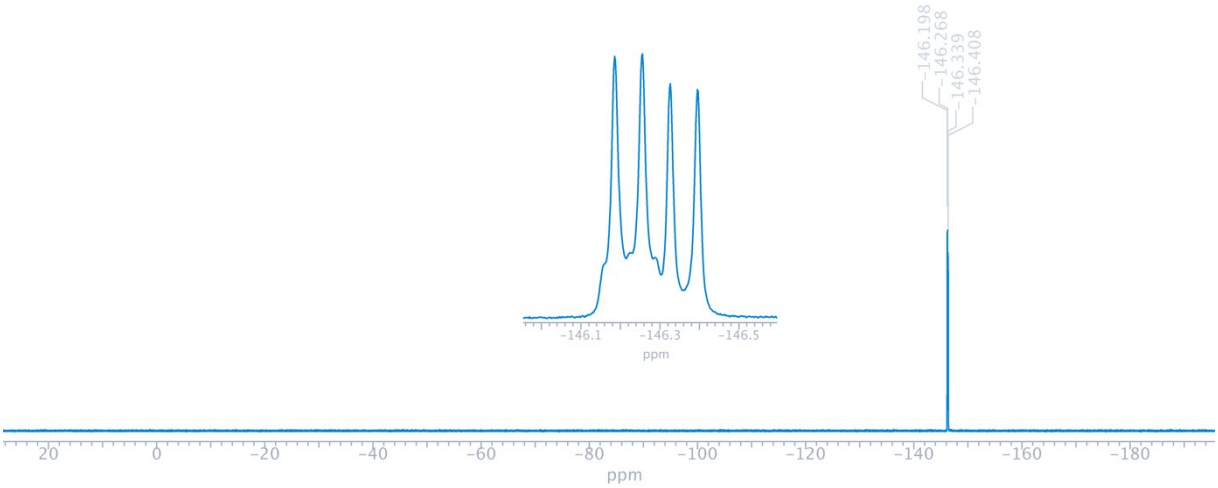

Fig. S3 ^{19}F NMR spectrum of **3** in $CDCl_3$.

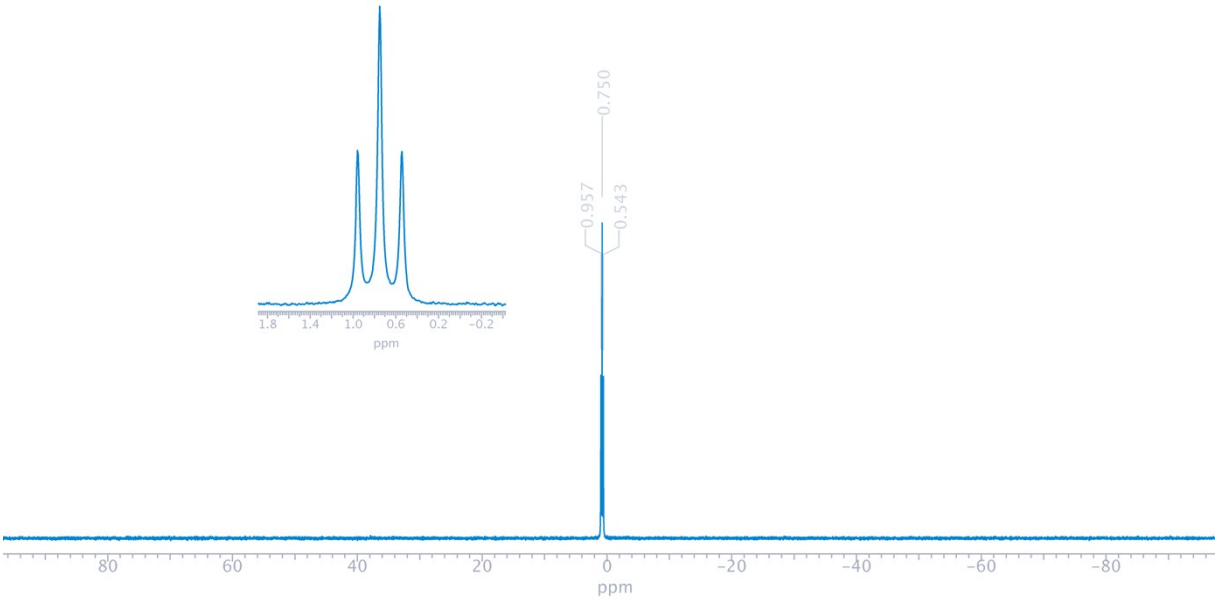

Fig. S4 ^{11}B NMR spectrum of **3** in $CDCl_3$.

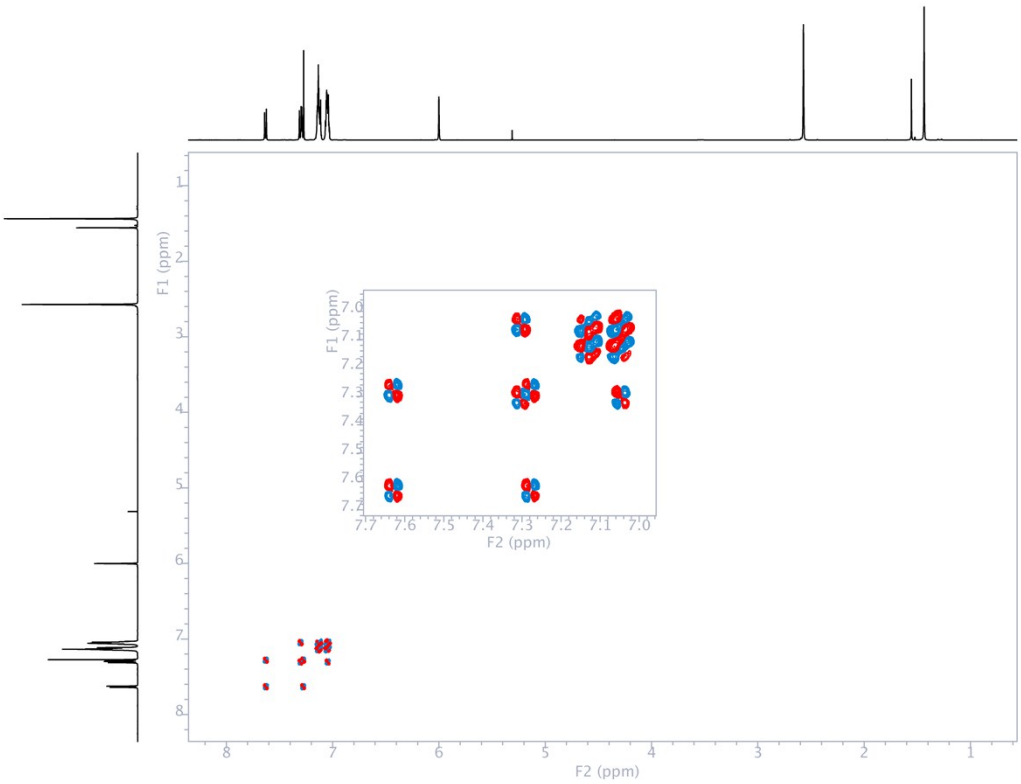

Fig. S5 COSY NMR spectrum of **3** in $CDCl_3$ (inset shows magnified aromatic region between 7-7.7 ppm).

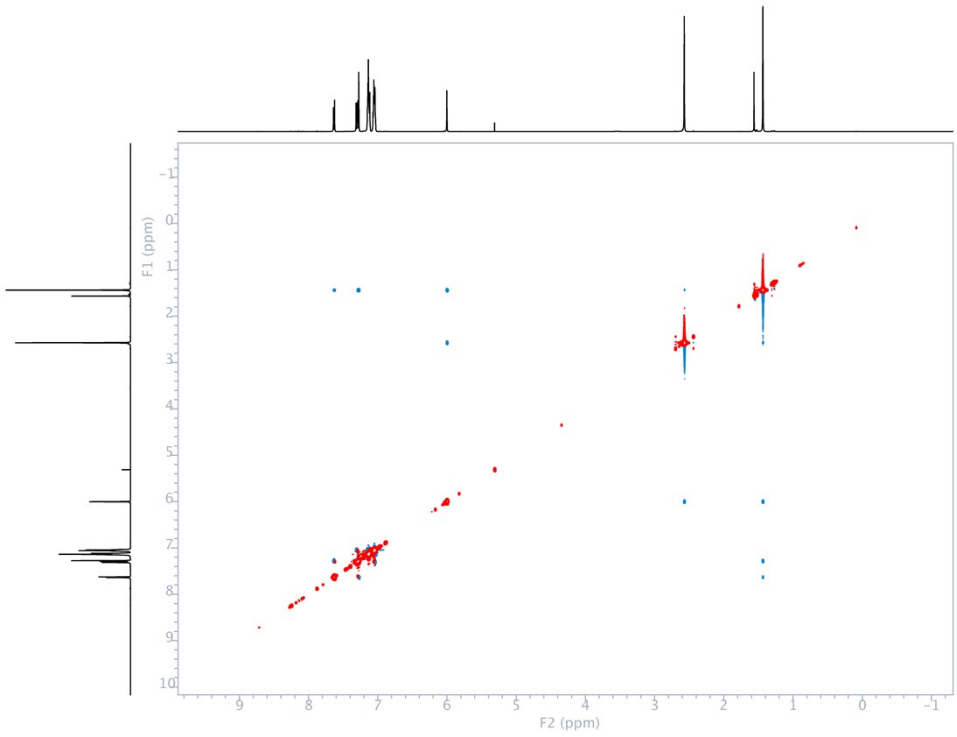

Fig. S6 NOESY NMR spectrum of **3** in $CDCl_3$.

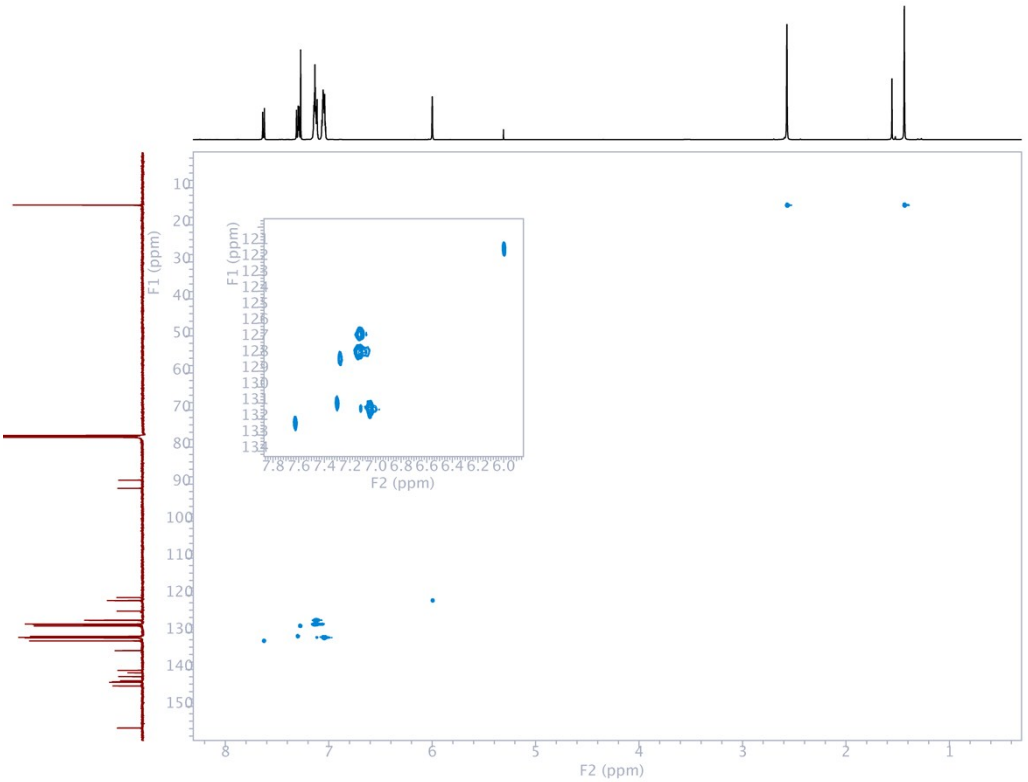

Fig. S7 ^{13}C HSQC spectrum of **3** in $CDCl_3$.

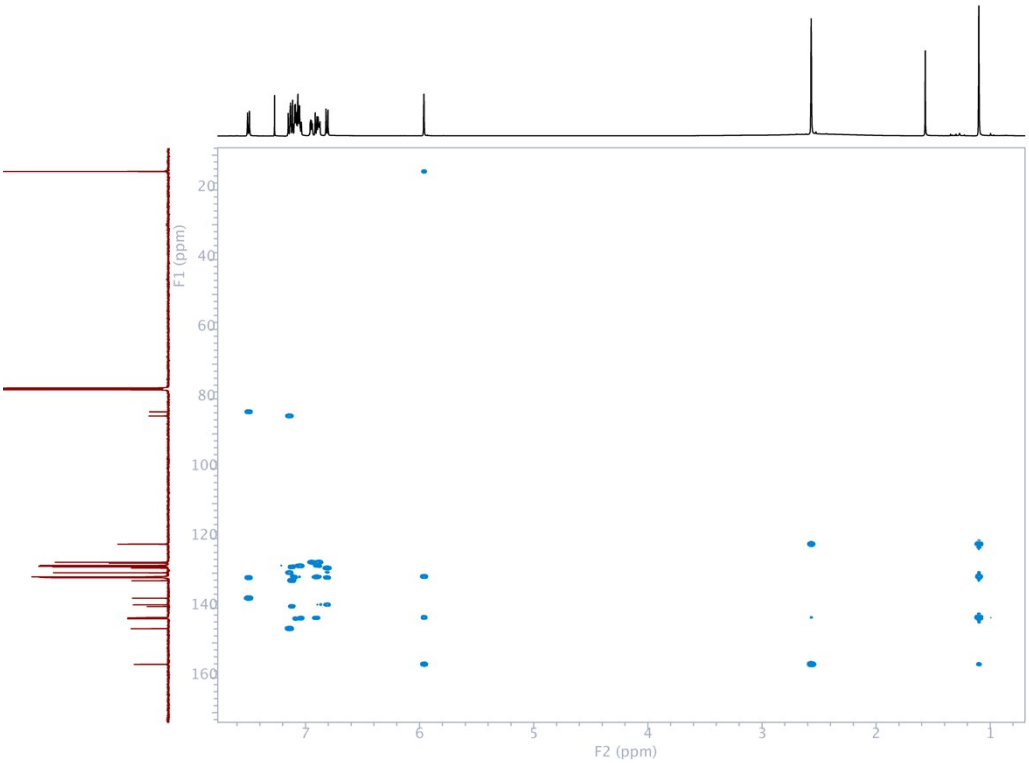

Fig. S8 HMBC spectrum of **3** in $CDCl_3$.

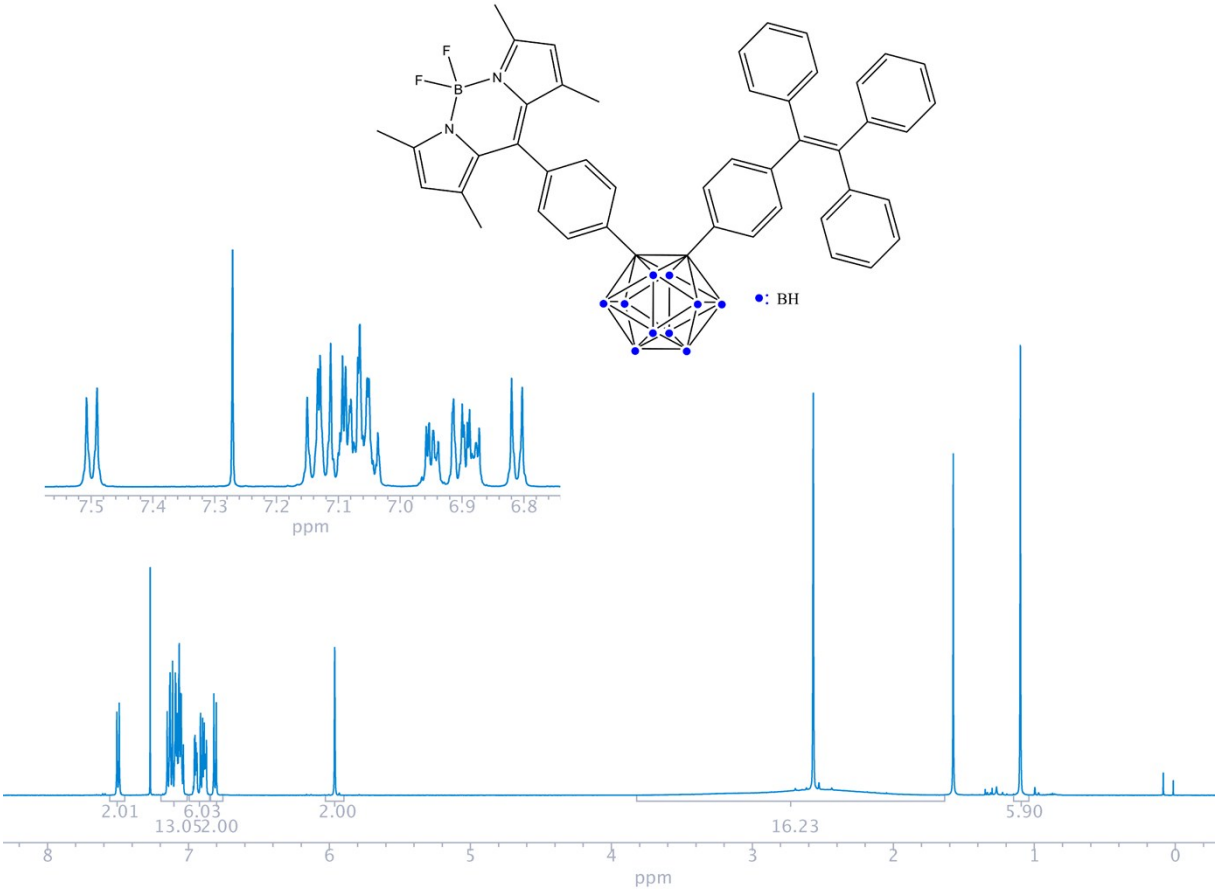

Fig. S9 ^{1}H NMR spectrum of **4** in $CDCl_3$.

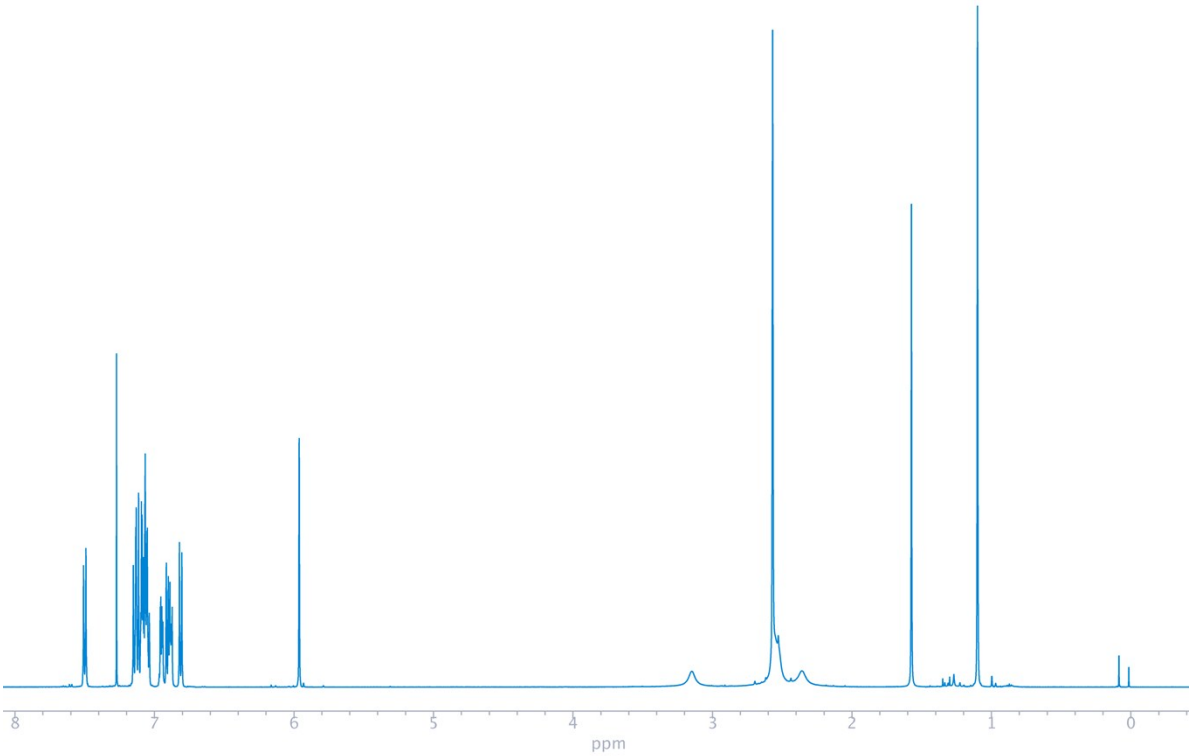

Fig. S10 $^{1}H\{^{11}B\}$ NMR spectrum of **4** in $CDCl_3$.

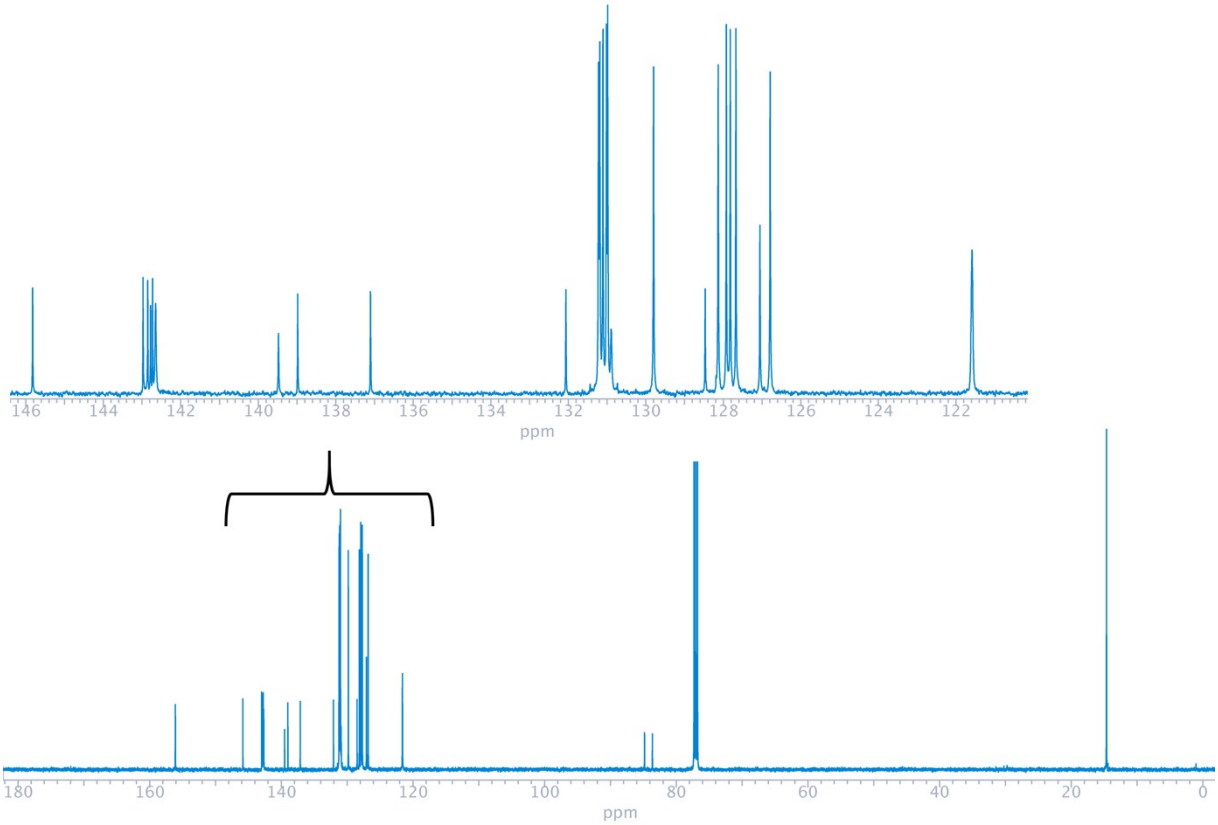

Fig. S11 ^{13}C NMR spectrum of **4** in $CDCl_3$.

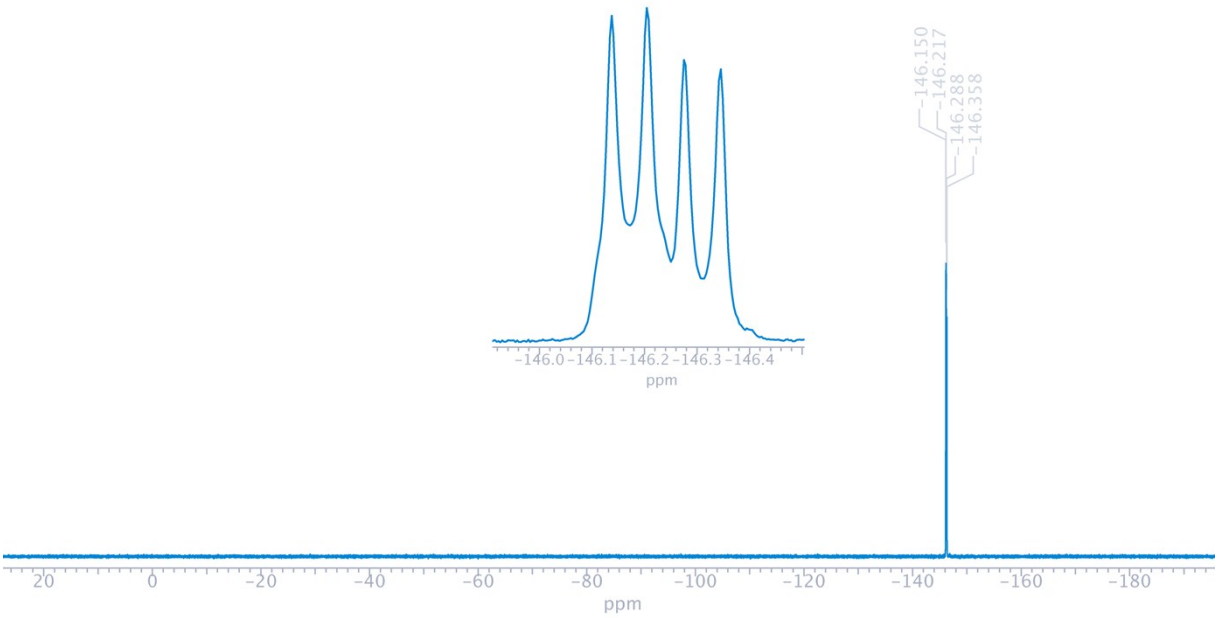

Fig. S12 ^{19}F NMR spectrum of **4** in $CDCl_3$.

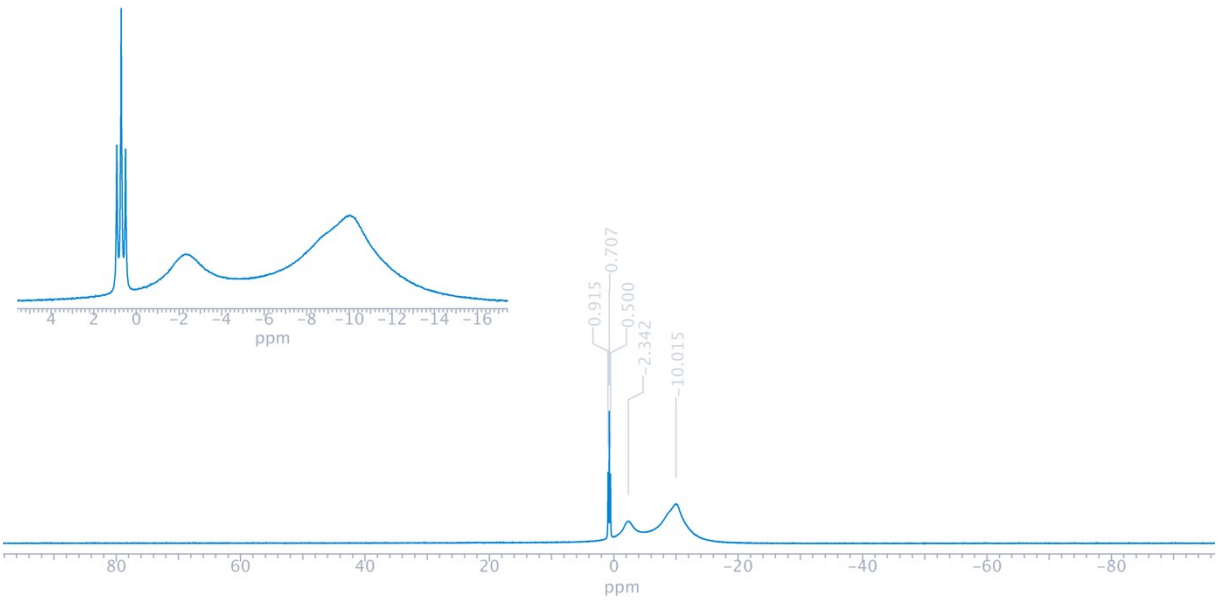

Fig. S13 ^{11}B NMR spectrum of **4** in $CDCl_3$.

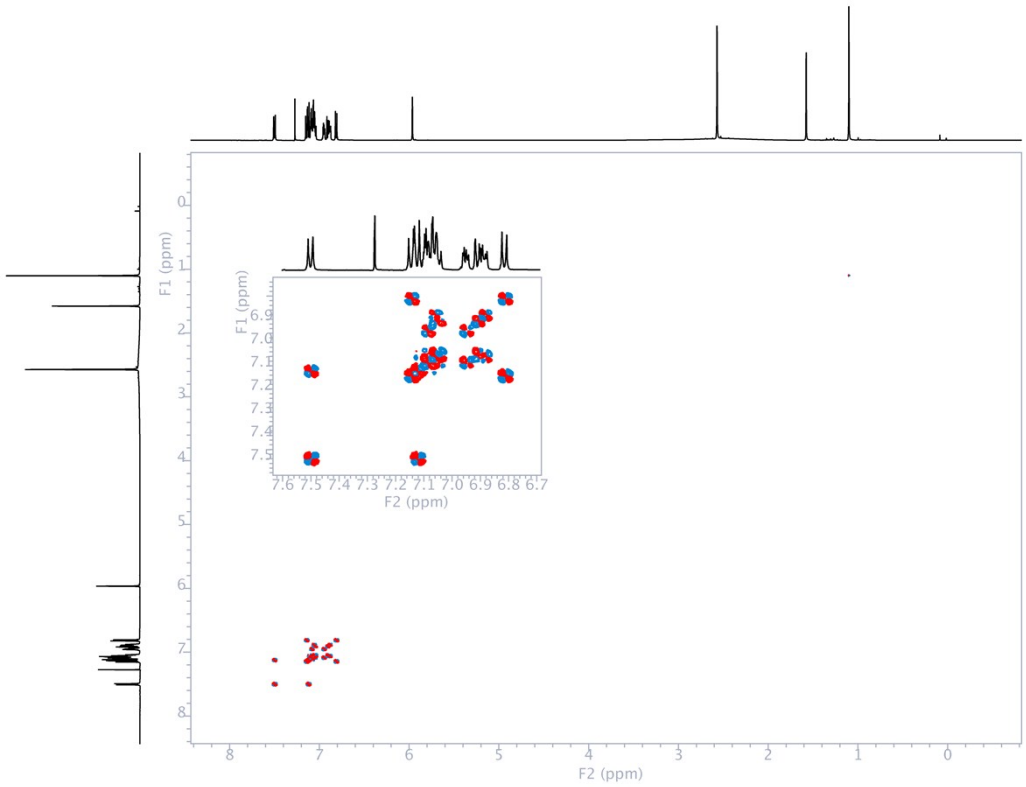

Fig. S14 COSY spectrum of **4** in $CDCl_3$ (inset shows magnified aromatic region between 6.7-7.6 ppm).

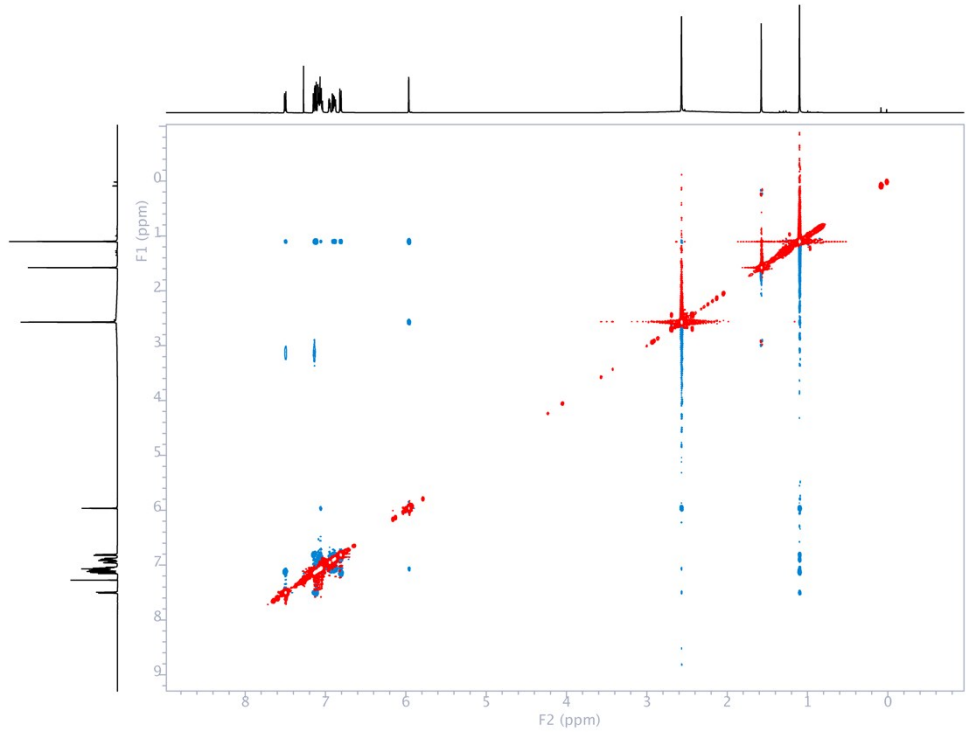

Fig. S15 NOESY spectrum of **4** in $CDCl_3$.

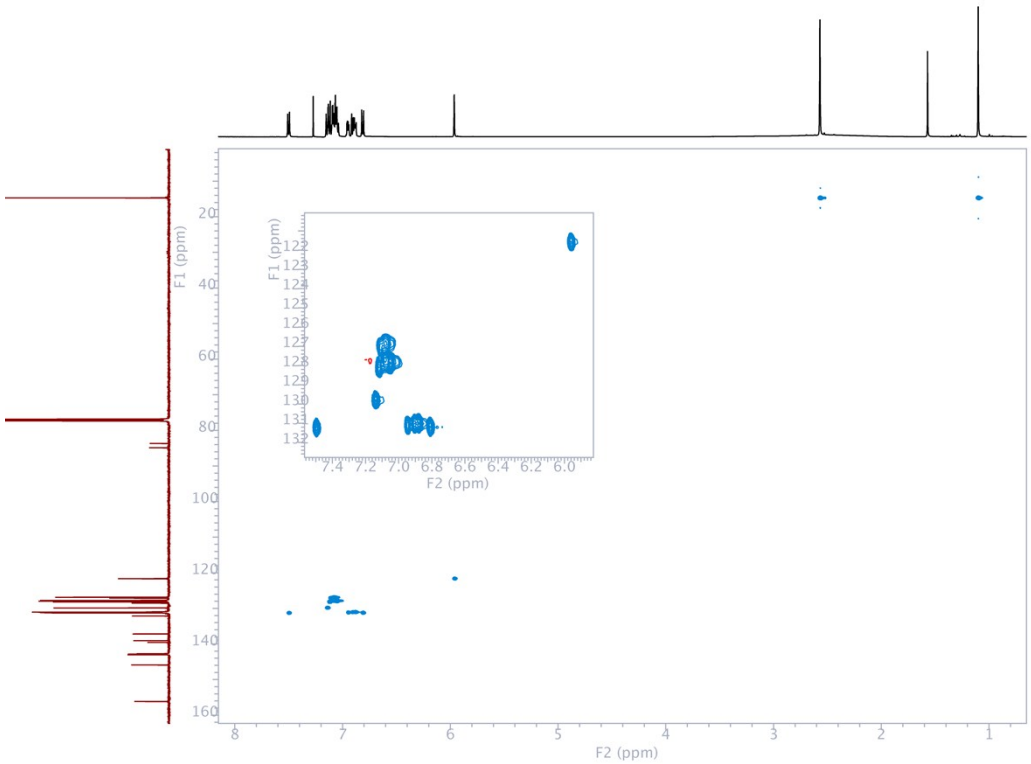

Fig. S16 HSQC spectrum of **4** in $CDCl_3$.

Fig. S17 HMBC spectrum of **4** in $CDCl_3$.

MALDI-TOF MS spectra of 3 and 4

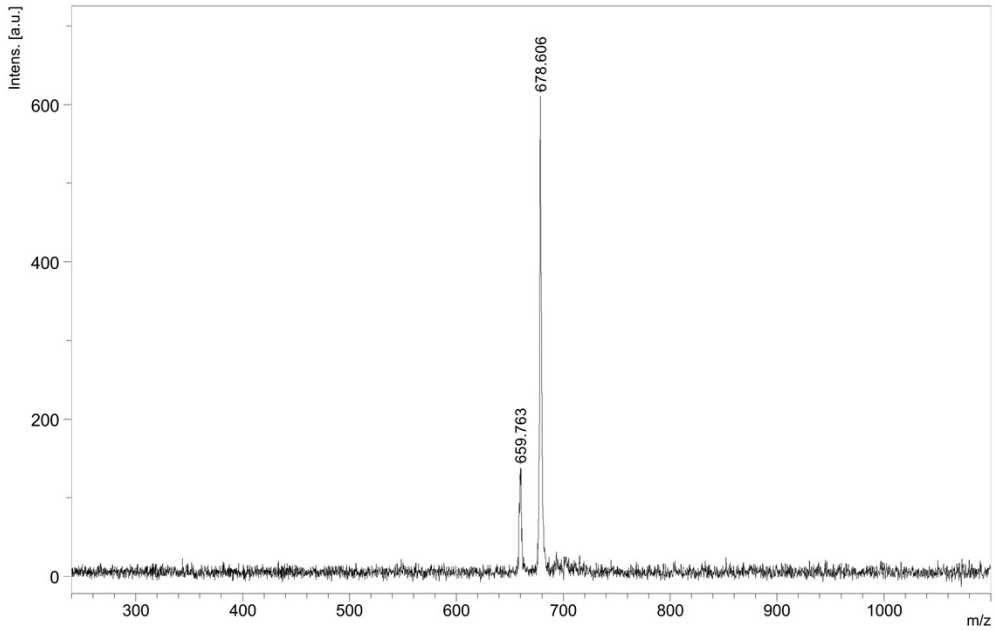

Fig. S18 Maldi-TOF MS spectrum of **3**.

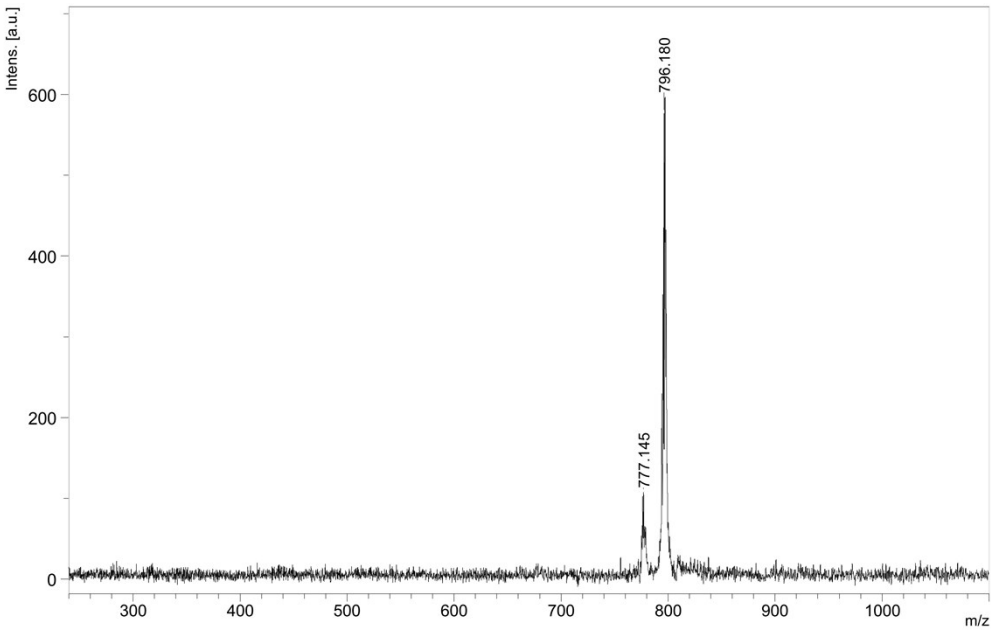

Fig. S19 Maldi-TOF MS spectrum of **4**.

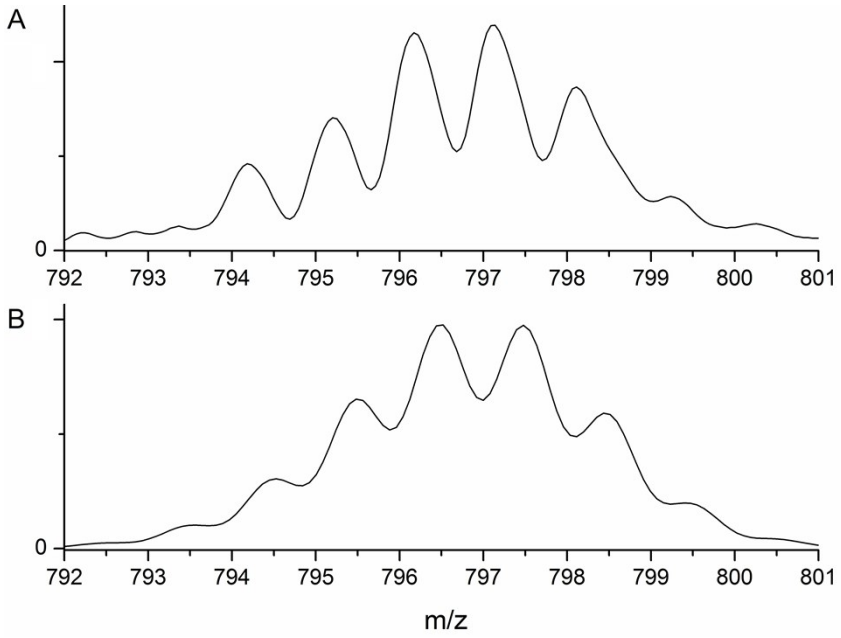

Fig. S20 MS isotop pattern of **4** A) measured B) calculated

X-ray structure of 3 and 4

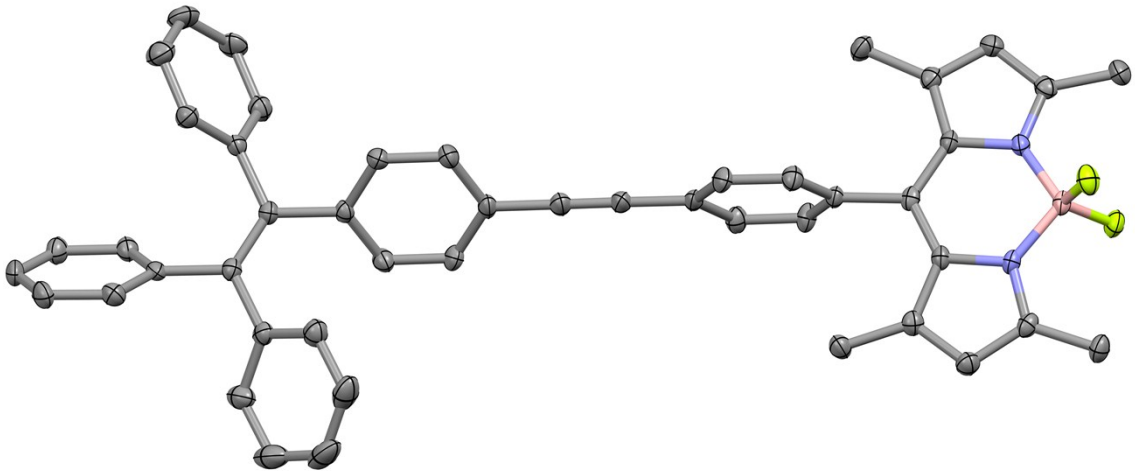

Fig. S21 X-Ray structure of **3**.

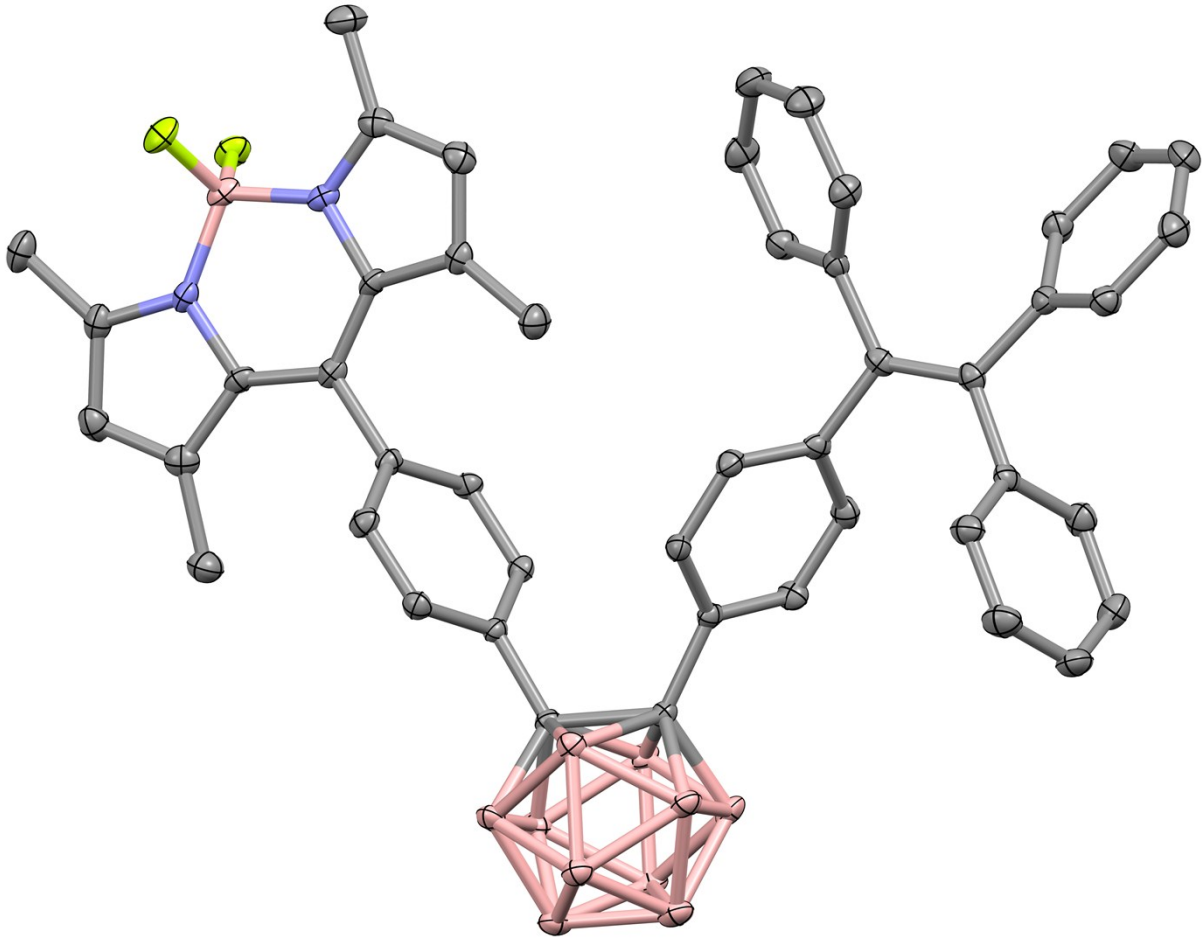

Fig. S22 X-Ray structure of **4**.

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Table S1. Crystal data and structure refinement details for compounds **3** and **4**

	3	**4**
CCDC No	1817439	1817440
Empirical formula	$C_{47}H_{37}BF_2N_2$	$C_{47}H_{47}B_{11}F_2N_2$, 2(CH_4O)
Formula weight (g/mol)	678.59	860.66
T(K)	100	100
λ(Å)	0.71073	0.71073
Crystal system, space group	Triclinic, P-1	Triclinic, P-1
Unit cell dimensions: (Å, °)		
a	8.4917(9)	13.4097(11)
b	10.9196(11)	13.5319(11)
c	20.148(2)	14.5334(12)
α	80.996(3)	63.934(2)
β	83.209(3)	80.524(2)
γ	76.283(3)	89.720(2)
V(Å3)	1786.2(3)	2329.9(3)
Z	2	2
Absorbtion coefficient (mm^{-1})	0.08	0.075
Dcalc (g/cm^3)	1.262	1.227
F(000)	712	904
Crystal size (mm)	0.03x0.2x0.4	0.12 x 0.13 x 0.22
θ Range for data collection (°)	1.94–28.55°	2.0-27.398
Index ranges	$-11 \leqslant h \leqslant 11$ $-14 \leqslant k \leqslant 14$ $-27 \leqslant l \leqslant 26$	$-17 \leqslant h \leqslant 17$ $-17 \leqslant k \leqslant 17$ $-18 \leqslant l \leqslant 18$
Reflections collected	70562	105125
Independent reflections	9033	10517
Max. and min. transmission	0.746 and 0.726	0.746, 0.724
Final *R* indices [$I \geqslant 2\sigma(I)$]	$R1 = 0.0596$, $wR2 = 0.1294$	$R1 = 0.0610$, $wR2 = 0.1195$
R indices (all data)	$R1 = 0.0977$, $wR2 = 0.1453$	$R1 = 0.1114$ $wR2 = 0.1366$
Goodness-of-fit on F^2	1.034	1.061
Largest difference in peak and hole (e $Å^{-3}$)	0.603/−0.265	0.282/-0.386

References

1. G. Sheldrick, *Acta Crystallographica Section C* **2015**, *71*, 3-8.