Supporting Information

Tris((4-BMes$_2$)phenyl)methanide: a Carbanion with a Delocalised Triple Quinoidal Structure

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Table of Contents

1. Experimental details

Materials and methods: Unless otherwise noted, all chemicals were purchased from Adamas and used without further purification. Solvents were treated to remove water using a commercial solvent purification system (SPS) and deoxygenated using the freeze-pump-thaw method. THF used for recrystallisation was dried on the SPS and stored over NaK alloy in an argon-filled glove box from Innovative Technology Inc. Deionised water, purified with a Milli-Q system (18.2 MΩ cm), was used in all relevant experiments. All anhydrous and oxygen-free reactions were performed under an argon atmosphere in a glove box and monitored by TLC using silica gel. Column chromatography was carried out on silica gel (300-400 mesh).

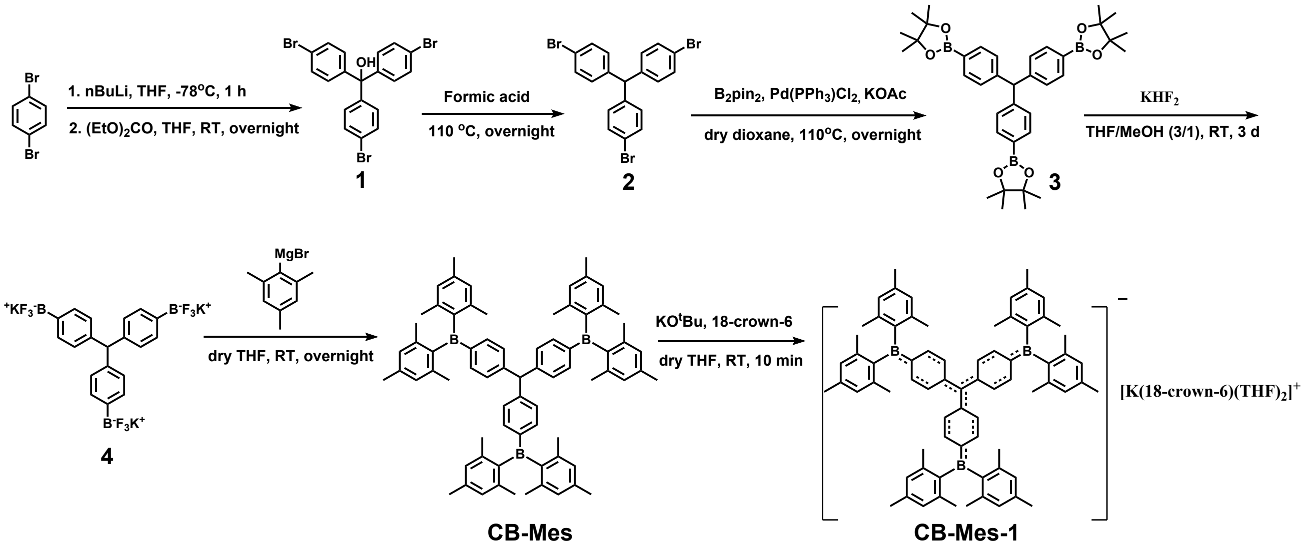
NMR spectra were recorded in DMSO-d_6, $CDCl_3$, or C_6D_6 on Bruker 500 MHz or 600 MHz (^{1}H) spectrometers. ^{1}H NMR spectra are referenced via the signal of the residual protonated solvent. ^{13}C NMR spectra are referenced via the ^{13}C resonance of the deuterated solvent. ^{11}B NMR spectra are referenced to external $BF_3{\cdot}OEt_2$. HRMS was performed using a Thermo Scientific Exactive Plus Orbitrap MS system with an Atmospheric Sample Analysis Probe (ASAP).

Crystal structure determinations: Crystals suitable for single-crystal X-ray diffraction were selected, coated in polybutyl oil, mounted on a polyimide microloop (MicroMounts fromMiTeGen) and transferred to a stream of cold nitrogen (Oxford Cryostream 800). Diffraction data were collected on a Rigaku Oxford Diffraction XtaLAB Synergy-R four-circle diffractometer with an HPA area detector (HyPix-Arc150) using multi-layer mirror monochromated Cu-Kα (1.54178 Å) radiation generated by a rotating-anode PhotonJet-R X-ray source. Data were collected at 100(2) K. The images were processed and corrected for Lorentz-polarization effects and absorption (empirical scaling). The crystal structures were solved using the intrinsic phasing method (SHELXT)[1] and Fourier expansion technique. All non-hydrogen atoms were refined in anisotropic approximation, with hydrogen atoms 'riding' in idealised positions, by full-matrix least squares against F^2 of all data, using SHELXL software[2] and the SHELXLE[3] graphical user interface. The unit cells of **CB-Mes-1** and **CB-Mes** contain THF solvent molecules which are strongly disordered. Diamond software was used for graphical representations.[4] Deposition numbers: CCDC 2504657 (for **CB-Mes**) and CCDC 2504659 (for **CB-Mes-1**) contain the supplementary crystallographic data for this paper. These data are provided free of charge by the joint Cambridge Crystallographic Data Centre and Fachinformationszentrum Karlsruhe Access Structures service. Crystallographic data and refinement parameters are listed in Table S1. Selected bond lengths, angles, and dihedral angles are listed in Table S2.

Photophysical measurements: All measurements were performed in standard quartz cuvettes (1 cm × 1 cm). All solutions for photophysical measurements had a concentration of ca. 1×10^{-5} M. UV−vis absorption spectra were recorded using a Perkin Elmer Lambda 465 UV-visible spectrophotometer. Steady-state fluorescence spectra were obtained using an Edinburgh Instrument FLS920 fluorescence spectrometer. Fluorescence quantum yields were measured using a calibrated integrating sphere (inner diameter: 150 mm) from Edinburgh Instruments combined with the FLS920 spectrophotometer described above. The longest wavelength absorption maximum of the compound in the respective solvent was chosen as the excitation wavelength. Fluorescence lifetimes were recorded using the time-correlated single-photon counting (TCSPC) method using the same FLS920 spectrometer described above. Solutions were excited with a picosecond pulsed diode laser at emission maximum of 316 nm. The full width at half maximum (FWHM) of the laser pulses were ca. 70–200 ps, while the instrument response function (IRF) had a FWHM of ca. 1.0 ns, measured from the scatter of a Ludox solution at the excitation wavelength. Decays were recorded to at least 10000 counts in the peak channel with a record length of at least 2048 channels. The quality of all decay fits was judged to be satisfactory based on the calculated values of the reduced χ^2 and Durbin−Watson parameters and visual inspection of the weighted and autocorrelated residuals.

Theoretical methods: All calculations (DFT and TD-DFT) were carried out with the Gaussian 16 program package.[5] The ground-state geometries were optimised using the ωB97XD functional in combination with the 6-31G+(d,p) basis set. The molecular structures obtained from single-crystal X-ray diffraction of **CB-Mes**, and **CB-Mes-1** were used as the starting geometries. For computational simplicity, the Mes (2,4,6-trimethylphenyl) groups were replaced with phenyl groups **(CB-Mes'** and **CB-Mes-1')**. This substitution retains the main electronic effects of the substituents while avoiding low-frequency imaginary vibrations associated with the rotational flexibility of the methyl groups. The optimised geometries were confirmed to be local minima by performing frequency calculations and obtaining only positive frequencies. Based on these optimised structures, the gas phase vertical transitions were calculated (singlets, 25 states) by TD-DFT using the B3LYP functional in combination with the 6-31G+(d,p) basis set. No symmetry constraints were used in any of the calculations. NBO calculations were performed based on the optimised structures at the ωB97XD/6-31G+(d,p) level.

2. Synthesis



Compounds **1**, **2**, and **3** were synthesised via literature procedures.[6]

Synthesis of potassium (methanetriyltris(benzene-4,1-diyl))tris(trifluoroborate) (**4**): KHF_2 (0.189 g, 2.43 mmol) was dissolved in 2.5 mL of water and added to a THF/MeOH (6 mL/6 mL) solution of compound **3** (101 mg, 0.160 mmol). The mixture was stirred at room temperature for 3 d to give a white suspension. The suspension was filtered, and the resulting white solid was washed with hot acetone and hexane to afford 80.0 mg (0.151 mmol, 94%) of **4** as a colourless powder. ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.18 (d, J = 4 Hz, 6H), 6.80 (d, J = 4 Hz, 6H), 5.21 (s, 1H) ppm.^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 147.2, 141.5, 130.9, 127.2, 56.4 ppm. The B-bonded C atom (147.2 ppm) of compound **4** gives rise to a very broad signal due to unresolved coupling and quadrupolar broadening. ^{19}F NMR (470 MHz, DMSO-d_6) δ 138.6 ppm. ^{11}B{^{1}H} NMR (160 MHz, DMSO-d_6) δ 3.4 ppm.

Synthesis of tris(4-(dimesitylboraneyl)phenyl)methane (**CB-Mes**): A solution (1 M) of the

Grignard reagent MesMgBr was prepared in THF, and 4.8 mL of the solution was slowly added to **4** (450 mg, 0.800 mmol) in dry THF (6 mL). The reaction mixture was stirred at room temperature for 3 d. After filtration through a pad of silica gel, all volatiles were removed from the filtrate *in vacuo*. The crude product was purified by column chromatography (silica gel; hexane/CH_2Cl_2 = 5/1) to give 108 mg (0.109 mmol, 14%) of **CB-Mes** as a colourless powder. mp. 270–271 °C; ^{1}H NMR (600 MHz, C_6D_6) δ 7.63 (d, J = 8 Hz, 6H), 7.11 (d, J = 8 Hz, 6H), 6.78 (s, 12H), 5.46 (s, 1H), 2.19 (s, 18H), 2.11 (s, 36H) ppm. ^{13}C{^{1}H} NMR (126 MHz, C_6D_6) δ 147.9, 144.9, 142.3, 141.0, 138.9, 137.0, 129.7, 128.9, 57.8, 23.8, 21.3 ppm. ^{11}B{^{1}H} NMR (193 MHz, C_6D_6) δ 73.3 (br) ppm. HRMS (APCI) m/z calcd for $C_{73}H_{78}B_3$ $[M]^+$ 987.6388, found: 987.6397.

Synthesis of tris(4-(dimesitylboraneyl)phenyl)methyl carbanion (**CB-Mes-1**): In an argon-filled glove box, **CB-Mes-1** (18 mg, 0.018 mmol), KO^{t}Bu (2.6 mg, 0.024 mmol), and 18-crown-6 (6.3 mg, 0.024 mmol) were dissolved in dry THF (2 mL) and the mixture was stirred for 10 min to form a dark green solution. Dry pentane was diffused into the above solution at –30 °C for 3 d. After filtration, the crystals were washed with hexane and dried under vacuum to afford **CB-Mes-1** as dark green crystals (10 mg, 39%). ^{1}H NMR (600 MHz, C_6D_6) δ 7.73 (d, J = 8.5 Hz, 6H), 7.53 (d, J = 8.5 Hz, 6H), 6.90 (s, 12H), 2.40 (s, 36H), 2.28 (s, 18H) ppm (the peaks at 3.58 (m, 8H) and 1.42 (m, 8H) ppm are the uncoordinated THF, the single peak at 2.95 (s, 40H) ppm includes one 18-crown-6 and two coordinated THF molecules). ^{13}C{^{1}H} NMR (126 MHz, C_6D_6) δ 150.9, 144.0, 141.0, 139.2, 136.8, 136.0, 128.6, 126.3,108.5, 24.2, 21.4 ppm. ^{11}B{^{1}H} NMR (193 MHz, C_6D_6) δ 66.1 (br) ppm.

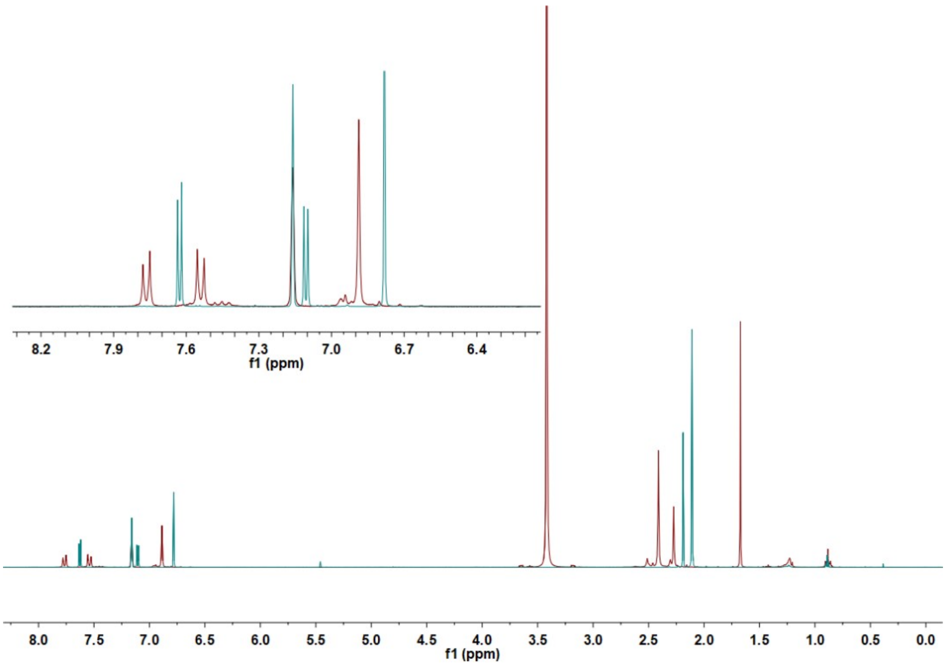


Figure S1. *In situ* ^{1}H NMR spectra of **CB-Mes-1** (brown line) and **CB-Mes** (green line).

3. Crystal structure determinations

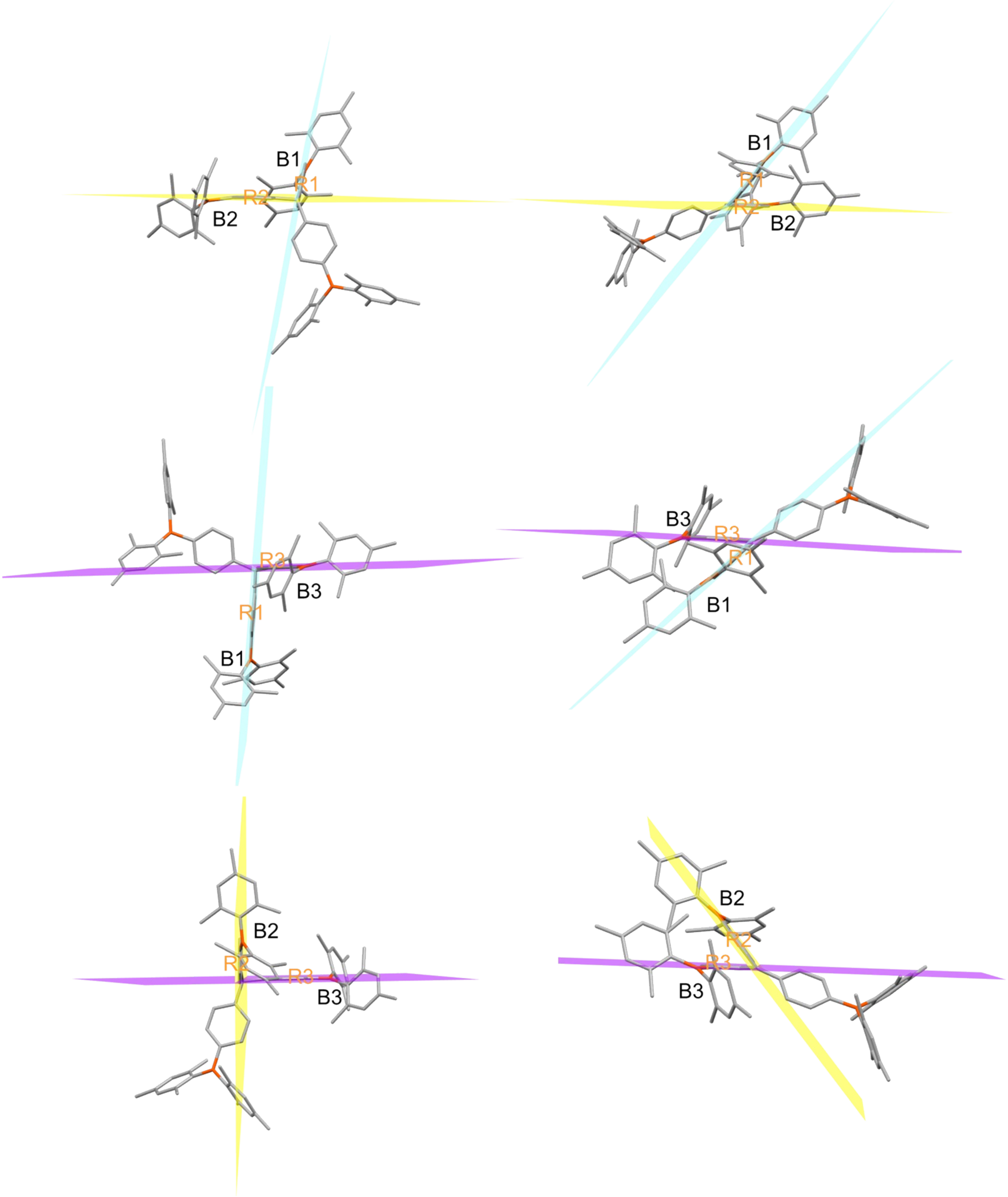


Figure S2. Side views of the molecular structures of **CB-Mes** (left) and **CB-Mes-1** (right). R1, R2, and R3 correspond to the three different central phenylene rings shown in Figure 2 and form bonds to the B1, B2, and B3 atoms, respectively.

Table S1. Crystallographic data and refinement parameters for **CB-Mes** and **CB-Mes-1**.

Compound	**CB-Mes**	**CB-Mes-1**
CCDC number	2504657	2504659
Empirical formula	$C_{73}H_{79}B_3 \cdot 3(C_4H_8O)$	$[C_{73}H_{78}B_3]^- \cdot [(C_{12}H_{24}KO_6)$ $2(C_4H_8O)]^+ \cdot 4.5(C_4H_8O)$
Formula weight [g·mol^{-1}]	1205.10	1759.86
T[K]	100(2)	100(2)
Crystal size (mm)	0.93x0.15x0.10 [a]	0.18x0.14x0.08
Crystal colour, habit	colourless block	green plate
Crystal system	monoclinic	triclinic
Space group	*Cc*	*P*
a [Å]	19.6219(2)	12.8289(2)
b [Å]	16.0897(2)	13.7960(3)
c [Å]	23.0540(3)	29.2020(5)
α [º]	90	85.135(2)
β [º]	91.9530(10)	87.8240(10)
γ [º]	90	82.0000(10)
V [Å^3]	7274.16(15)	5097.86(16)
Z	4	2
ρ_{calcd} [g/cm^3]	1.100	1.146
μ[mm^{-1}]	0.481	0.918
F(000)	2608	1908
θ [º]	3.553–74.501	3.039–68.249
Reflections collected	83191	57665
Unique reflections	13536	18462
Unique reflections with [I≥2σ(I)]	12158	11785
R_{int}	0.0361	0.0374
Parameters / restraints	916 / 205	1306 / 384
Goodness-of-fit on F^2	1.036	1.072
R_1 [I≥2σ(I)]	0.0758	0.0889
wR_2 [all data]	0.2243	0.3012
Largest diff. peak/hole [e Å^{-3}]	0.57 / -0.42	0.66 / -0.60

[a] The crystal of **CB-Mes** was a long needle with a dimension of 0.93 mm along the needle axis, which is much larger than the beam diameter (ca. 0.1 mm FWHM of a Gauss beam profile). The long needle was chosen in order to have appropriate thickness in the other dimensions and it was not cut in order to maintain its excellent diffraction quality. Absorption effects due to the anisotropic habit were corrected by considering the crystal faces on a Gaussian grid and a beam profile correction applying the CrysAlis$^{\mathrm{Pro}}$ program from Rigaku Oxford Diffraction.

Table S2. Bond lengths [Å], angles [°], dihedral angles [°], and torsion angles between phenyl rings R1, R2, and R3 [°] of $CHPh_3$ (CCDC number: 297234)[7] and $[CPh_3]^-[K(18\text{-}C\text{-}6)(THF)_2]^+$ (CCDC 1427375 with labeling from reference 6) from the literature (labelling of molecular structures shown in Figure S3).[a]

$CHPh_3$		**$CHPh_3$**		**$[CPh_3]^-[K(18\text{-}C\text{-}6)(THF)_2]^+$**	
C1–C2	1.530(4)	C20–C21	1.522(4)	C15–C6	1.467(4)
C1–C8	1.526(4)	C20–C27	1.528(4)	C15–C19	1.458(4)
C1–C14	1.517(4)	C20–C33	1.534(4)	C15–C22	1.438(3)
mean bond length **a**	1.524(2)		1.528(2)		1.454(2)
C2–C3	1.384(4)	C21–C22	1.388(4)	C6–C10	1.409(4)
C8–C9	1.387(4)	C27–C28	1.383(4)	C19–C9	1.401(3)
C14–C15	1.387(4)	C33–C34	1.388(4)	C22–C11	1.418(4)
C7–C2	1.402(4)	C26–C21	1.390(4)	C13–C6	1.414(3)
C13–C8	1.382(4)	C32–C27	1.393(4)	C12–C19	1.420(3)
C19–C14	1.385(4)	C38–C33	1.391(4)	C14–C22	1.433(4)
mean bond length **b**	1.389(2)		1.389(2)		1.416(1)
C3–C4	1.392(4)	C22–C23	1.394(4)	C10–C20	1.394(4)
C9–C10	1.386(5)	C28–C29	1.383(4)	C9–C16	1.395(5)
C15–C16	1.382(5)	C34–C35	1.379(4)	C11–C34	1.382(5)
C6–C7	1.384(4)	C25–C26	1.388(4)	C23–C13	1.387(5)
C12–C13	1.376(4)	C31–C32	1.375(5)	C21–C12	1.379(4)
C18–C19	1.394(5)	C37–C38	1.398(5)	C29–C14	1.375(5)
mean bond length **c**	1.386(2)		1.386(2)		1.385(2)
C4–C5	1.379(4)	C23–C24	1.376(4)	C20–C28	1.391(5)
C10–C11	1.389(6)	C29–C30	1.377(5)	C16–C26	1.372(4)
C16–C17	1.377(5)	C35–C36	1.373(5)	C34–C36	1.394(6)
C5–C6	1.376(4)	C24–C25	1.383(5)	C28–C23	1.374(6)
C11–C12	1.384(5)	C30–C31	1.387(6)	C26–C21	1.396(5)
C17–C18	1.377(6)	C36–C37	1.375(5)	C36–C29	1.378(5)
mean bond length **d**	1.380(2)		1.379(2)		1.384(2)
C19–C14–C1–C8	84.1(3)	C26–C21–C20–C33	66.9(3)	C13–C6–C15–C22	33.4(4)
C9–C8–C1–C2	80.9(3)	C38–C33–C20–C27	96.8(3)	C14–C22–C15–C19	18.2(4)
C7–C2–C1–C14	62.6(3)	C32–C27–C20–C21	77.1(3)	C12–C19–C15–C6	41.0(3)
C2–C1–C8	112.2(2)	C21–C20–C33	110.9(2)	C6–C15–C19	117.8(2)
C8–C1–C14	111.8(2)	C21–C20–C27	111.9(2)	C19–C15–C22	120.5(2)
C14–C1–C2	112.6(2)	C27–C20–C33	113.4(2)	C6–C15–C22	121.7(2)
sum of the angles	336.6		336.2		360.0
$\angle(R1_{C2},R2_{C8})$	85.6(1)	$\angle(R1_{C21},R2_{C27})$	86.0(1)	$\angle(R1_{C6},R2_{C19})$	62.8(1)
$\angle(R2_{C8},R3_{C14})$	81.9(1)	$\angle(R2_{C27},R3_{C33})$	70.2(1)	$\angle(R2_{C19},R3_{C22})$	51.9(1)
$\angle(R1_{C2},R3_{C14})$	80.8(1)	$\angle(R1_{C21},R3_{C33})$	85.9(1)	$\angle(R1_{C6},R3_{C22})$	43.8(1)

[a]Esd’s of the mean values were calculated from the esd’s of the individual values using the formula $\sqrt{\sum_{i=1}^{n}\sigma_i^2/n}$. For the nature of bonds **a**, **b**, **c**, **d**, and **e**, see the structure in Figure 2a.

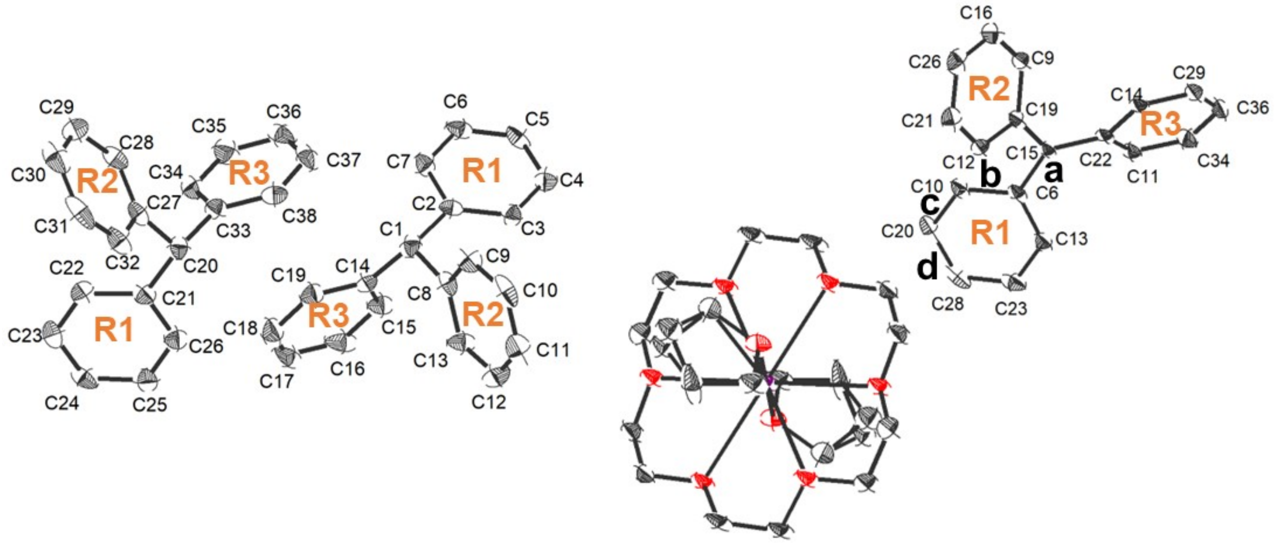
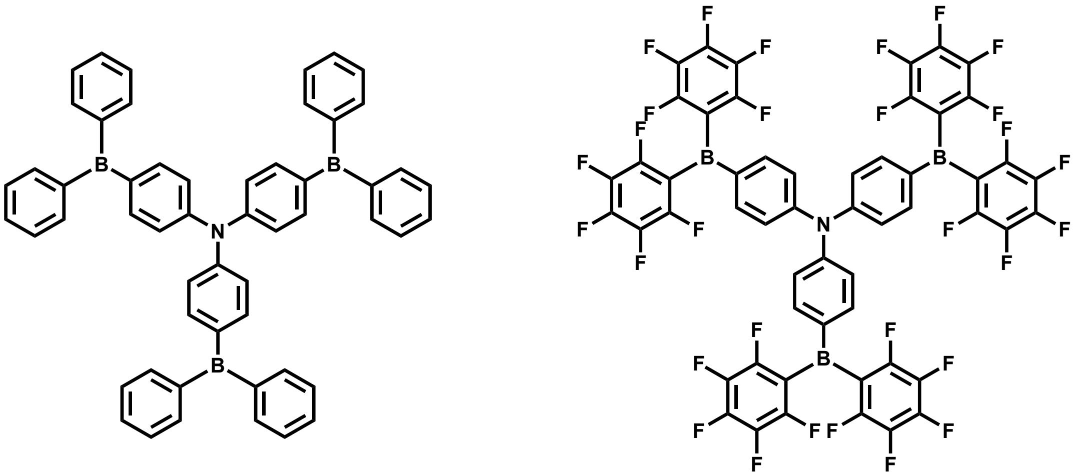


Figure S3. Crystal structures of $CHPh_3$ (left, CCDC number: 297234)[7] and $[CPh_3]^{-}[K(18\text{-}C\text{-}6)(THF)_2]^{+}$ (right, CCDC number: 1427375 with labeling from reference 6) from the literature.

We selected compounds **H** and **I** as representative N-containing analogues. For computational simplicity, the Mes (2,4,6-trimethylphenyl) groups in **G** (Figure 1) were replaced with phenyl groups (**H**, Figure S4). DFT and TD-DFT calculations on **H** and **I** were conducted at the same level as we used for the model compounds **CB-Mes’** and **CB-Mes-1’** in which the Mes groups were also replaced by phenyl groups. In addition, based on their optimised geometries, NBO calculations were performed. The bond lengths, Wiberg Index values, NPA charges on the boron atom, HOMO-LUMO energy levels, and oscillator strengths of these compounds are summarised in Table S3.


H

I

Figure S4. Chemical structures of compounds **H** and **I**.

Table S3. Calculated mean bond length, WBI value, NPA charge on boron, HOMO-LUMO energy level, absorption wavelength, and oscillator strength [Å] of **CB-Mes**, **CB-Mes-1**, compound **H**, and compound **I**.[a]

	CB-Mes	**CB-Mes-1**	**H**	**I**
a / Å	1.531	1.449	1.414	1.412
b / Å	1.402	1.420	1.400	1.401
c / Å	1.393	1.386	1.388	1.384
d / Å	1.411	1.413	1.407	1.408
e / Å	1.567	1.535	1.564	1.539
WBI(a)[b]	0.986	1.867	1.013	1.016
WBI(e)[b]	0.908	1.021	0.918	0.974
NPA charge on boron[b] / e^-	0.881	0.802	0.874	0.881
$\mathbf{E_{HOMO}}$ / eV	-8.414	-2.894	-7.186	-8.210
$\mathbf{E_{LUMO}}$ / eV	-0.253	-1.841	-0.344	-1.592
$\mathbf{E_{HOMO\text{-}LUMO}}$ / eV	8.161	1.053	6.842	6.618
λ_{abs} / nm	312	745	428	453
f	0.480	0.765	0.554	0.684

[a] For model compounds **CB-Mes'**, **CB-Mes-1'**, and **H**, the Mes groups were replaced by phenyl groups. For the nature of bonds **a**, **b**, **c**, **d**, and **e**, see the structure in Figure 2a and Table 1. [b] Average value.

4. Cyclic and differential pulse voltammograms

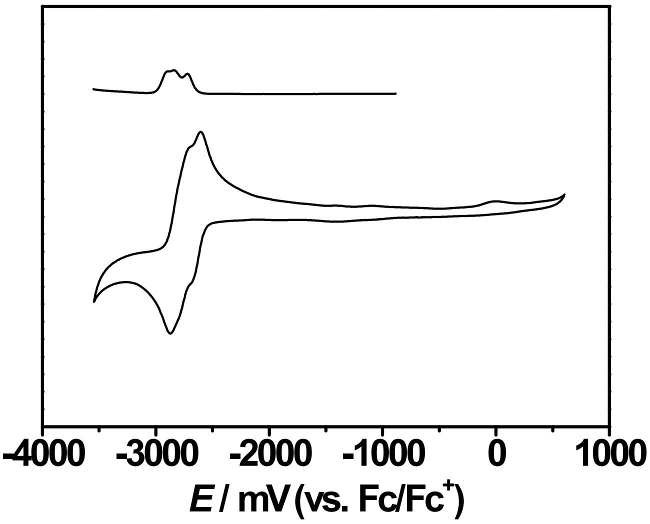


Figure S5. Cyclic (bottom) and differential pulse (top) voltammograms of **CB-Mes** (1 mM) in THF/0.1 M nBu_4NPF_6, vs. $Fc^{+/0}$, $v = 250$ mV/s, CV plotting convention: IUPAC.

5. Absorption and emission spectra

Table S4. Photophysical properties of **CB-Mes** in different solvents.

solvents	λ_{abs} /nm	λ_{fl} /nm	Stokes shift /cm^{-1}	τ /ns	Φ[a]	k_r[b] /10^7 s^{-1}	k_{nr} /10^7 s^{-1}	τ_0[c] /ns
Hexane	316	361	3945	1.4	0.20	14	57	7
Toluene	317	375	4879	1.5	0.25	17	50	6
DCM	316	388	5872	1.9	0.25	13	39	8
THF	316	386	5739	1.9	0.23	12	41	8
MeCN	316	399	6583	2.9	0.27	9.3	25	11

[a]fluorescence quantum yields (Φ) in solution were determined using absolute method; [b]Radiative (k_r) and nonradiative (k_{nr}) decay rate calculated by $k_r = \Phi/\tau$ and $k_{nr} = (1 - \Phi)/\tau$; [c]the pure radiative lifetime $\tau_0 = \tau/\Phi$.

6. Theoretical calculations

Table S5. Lowest energy singlet electronic transitions of **CB-Mes'** (TD-DFT B3LYP/6-31+G(d)).

State	***E* (eV)**	***λ* (nm)**	***f***	**Major contributions**
S_1^a	3.97	312	0.4787	H→L (0.84)
S_2^a	3.97	312	0.4787	H→L+1 (0.84)
S_3	4.14	299	0.0259	H→L+2 (0.93)
S_4	4.20	295	0.1672	H−2→L+1 (0.27) H−1→L (0.27)
S_5	4.23	293	0.0029	H−2→L (0.20) H−1→L+1 (0.19) H−1→L+2 (0.18)

^{a}These two states are degenerate due to C_3 symmetry.

Table S6. Lowest energy singlet electronic transitions of **CB-Mes-1'** (TD-DFT B3LYP/6-31+G(d)).

State	***E* (eV)**	***λ* (nm)**	***f***	**Major contributions**
S_1^a	1.66	745	0.7649	H→L (1.00)
S_2^a	1.66	745	0.7673	H→L+1 (1.00)
S_3	2.23	556	0.0000	H→L+2 (0.99)
S_4	2.60	476	0.0004	H→L+4 (0.95)
S_5^a	2.64	470	0.0001	H→L+5 (1.00)
S_6^a	2.64	470	0.0001	H→L+6 (1.00)
S_7	2.74	452	0.0029	H→L+7 (0.91)
S_8	2.79	445	0.0251	H→L+8 (1.00)

$^a S_1$ and S_2, and S_5 and S_6 are degenerate due to C_3 symmetry.

Cartesian coordinates and associated data for all optimised structures

CB-Mes’ (DFT wb97xd/6-31+g(d,p), S_0)

Total energy: − 2195.788786 hartree

Dipole moment: 0.020222 D

Imaginary frequencies: 0

Symbol	***X* / Å**	***Y* / Å**	***Z* / Å**
B	5.48448	1.5343	0.00153
C	1.41847	0.34012	-1.21415
B	-4.07228	3.9812	0.0285
C	2.02717	-0.23608	-0.09842
H	1.49971	-0.99344	0.47351
C	-0.005	-0.001	-1.63903
H	-0.00861	-0.00144	-2.73667
B	-1.41067	-5.51623	0.02999
C	3.30471	0.1568	0.29108
H	3.74724	-0.30013	1.17218
C	4.03955	1.11001	-0.43329
C	3.41798	1.66332	-1.56825
H	3.94984	2.40251	-2.16124
C	2.1308	1.29892	-1.94114
H	1.66632	1.7648	-2.8071
C	5.86621	1.56789	1.52319
C	4.92237	1.91621	2.50665
C	5.26048	1.96066	3.85625
H	4.51693	2.24846	4.59343
C	6.55192	1.62648	4.26021
C	7.50394	1.2637	3.30895
H	8.51008	0.99866	3.61957
C	7.16577	1.25064	1.95867
C	6.54804	1.92651	-1.0833
C	6.56455	1.31032	-2.34797
C	7.51508	1.64543	-3.30812
H	7.51552	1.14294	-4.27074
C	8.46002	2.63304	-3.03517
C	8.45844	3.27053	-1.79566
H	9.19024	4.04327	-1.58017
C	7.52312	2.90859	-0.83035
C	-1.01052	1.05991	-1.20668
C	-0.8048	1.8822	-0.09817
H	0.12208	1.8103	0.4628
C	-1.78195	2.79154	0.29767
H	-1.59896	3.40929	1.17281
C	-2.98418	2.94307	-0.41304
C	-3.16405	2.12036	-1.54075

H	-4.07785	2.20449	-2.12278
C	-2.20644	1.18891	-1.91981
H	-2.38594	0.54778	-2.77968
C	-4.27185	4.30845	1.55017
C	-4.0843	3.3271	2.54064
C	-4.27444	3.60991	3.89031
H	-4.13901	2.82963	4.63322
C	-4.63024	4.89789	4.2868
C	-4.80888	5.89388	3.32827
H	-5.08215	6.89965	3.63296
C	-4.64588	5.59525	1.97846
C	-0.41943	-1.4026	-1.20706
C	-1.20743	-1.6374	-0.07946
H	-1.58913	-0.79955	0.49618
C	-1.50351	-2.93865	0.31689
H	-2.10771	-3.09022	1.20733
C	-1.05906	-4.05409	-0.41239
C	-0.28531	-3.79667	-1.55931
H	0.07738	-4.62904	-2.15639
C	0.04124	-2.50125	-1.93895
H	0.66463	-2.33515	-2.81439
C	-1.54423	-5.86224	1.55462
C	-0.75362	-5.21634	2.52262
C	-0.85843	-5.52951	3.87488
H	-0.2248	-5.02717	4.59962
C	-1.78406	-6.48206	4.29746
C	-2.59063	-7.12789	3.36199
H	-3.31589	-7.8677	3.6872
C	-2.45883	-6.83004	2.00859
C	-1.62722	-6.63235	-1.0513
C	-1.26414	-7.96942	-0.80704
C	-1.44186	-8.95885	-1.76998
H	-1.13812	-9.98033	-1.56171
C	-2.01865	-8.63814	-2.99766
C	-2.40162	-7.32424	-3.26169
H	-2.85548	-7.07069	-4.21499
C	-2.19323	-6.33521	-2.30457
C	-6.30096	5.0362	-0.78039
C	-4.96381	4.69169	-1.04962
C	-4.45898	5.00886	-2.32385
C	-5.24335	5.65107	-3.27787
H	-4.82405	5.89909	-4.24832
C	-6.5698	5.96681	-2.98863
C	-7.10087	5.65156	-1.73916

H	-8.13484	5.89217	-1.51086
H	-7.18773	6.45745	-3.73487
H	-4.76822	5.12475	5.33986
H	9.19567	2.9051	-3.7863
H	6.81584	1.649	5.31341
H	-1.8765	-6.72059	5.35291
H	-2.1694	-9.41007	-3.74652
H	3.90906	2.168	2.20535
H	7.92035	0.97753	1.22583
H	-0.03609	-4.46377	2.20671
H	-3.08536	-7.34895	1.28804
H	-2.48625	-5.31255	-2.52668
H	-0.82375	-8.23471	0.15033
H	-6.7235	4.80632	0.19407
H	-3.42944	4.75827	-2.56541
H	-4.79966	6.37782	1.24029
H	-3.79614	2.32179	2.24517
H	5.82627	0.54644	-2.57702
H	7.53984	3.4048	0.13633

CB-Mes-1’ (DFT wb97xd/6-31+g(d,p), S_0)

Total energy: −2195.231408 hartree

Dipole moment: 0.022530 D

Imaginary frequencies: 0

Symbol	***X* / Å**	***Y* / Å**	***Z* / Å**
B	-0.38456	5.85488	0.00069
C	0.00114	-0.00604	0.00718
C	1.30033	-0.64437	0.01181
C	2.44174	-0.04532	-0.59112
H	2.32562	0.90777	-1.09752
C	3.67736	-0.65597	-0.58109
H	4.50932	-0.15677	-1.07394
C	3.89892	-1.9203	0.01903
C	2.7605	-2.51623	0.61631
H	2.87203	-3.47875	1.1117
C	1.52172	-1.91192	0.61973
H	0.69412	-2.40158	1.12328
C	6.56907	-1.78534	-0.43673
C	6.99592	-0.62486	0.24413
C	8.13863	0.06224	-0.18374
H	8.45368	0.95127	0.35865
C	8.86325	-0.3693	-1.28413
C	8.44556	-1.50592	-1.9705
H	9.00124	-1.84569	-2.84143

C	7.31868	-2.21671	-1.55836
C	5.42105	-4.11794	0.47761
C	6.22173	-4.44963	1.59786
C	6.34673	-5.77642	2.00875
H	6.95621	-6.0101	2.87861
C	5.7004	-6.80034	1.3222
C	4.91494	-6.48861	0.2231
H	4.40241	-7.28024	-0.31954
C	4.76111	-5.1636	-0.20322
C	-1.20371	-0.80914	0.00105
C	-1.25849	-2.0915	-0.61299
H	-0.37489	-2.46647	-1.1198
C	-2.40799	-2.85227	-0.61194
H	-2.39375	-3.81862	-1.11216
C	-3.61352	-2.41252	-0.01125
C	-3.55808	-1.13323	0.59528
H	-4.44764	-0.74913	1.09068
C	-2.41241	-0.36689	0.60784
H	-2.42064	0.59105	1.11835
C	-4.83759	-4.78633	-0.48338
C	-4.04785	-5.74137	0.19236
C	-4.02824	-7.07262	-0.24163
H	-3.41763	-7.79423	0.29713
C	-4.76612	-7.47719	-1.34348
C	-5.53974	-6.54192	-2.02487
H	-6.11345	-6.84774	-2.89668
C	-5.58826	-5.21251	-1.60624
C	-6.27896	-2.62766	0.44202
C	-6.96938	-3.16033	1.55807
C	-8.17962	-2.60395	1.97117
H	-8.689	-3.01886	2.83784
C	-8.73902	-1.52609	1.29092
C	-8.07361	-0.99691	0.19575
H	-8.49976	-0.15246	-0.34197
C	-6.85051	-1.52739	-0.23268
C	-0.09467	1.44087	0.00706
C	-1.16613	2.12855	-0.6262
H	-1.92015	1.55038	-1.15117
C	-1.25544	3.50464	-0.61753
H	-2.09031	3.97707	-1.13207
C	-0.28496	4.32694	0.00403
C	0.78454	3.6404	0.62777
H	1.55024	4.21954	1.14089
C	0.87669	2.26449	0.63944

H	1.69998	1.79169	1.16582
C	-1.75931	6.56919	-0.37604
C	-2.93666	6.30462	0.35986
C	-4.1282	6.96319	0.03767
H	-5.02179	6.75823	0.62303
C	-4.18522	7.86547	-1.01546
C	-3.03554	8.12443	-1.7538
H	-3.07289	8.82698	-2.58309
C	-1.82787	7.49773	-1.44127
C	0.88605	6.74315	0.37294
C	0.83378	7.6788	1.43284
C	1.94999	8.45865	1.74074
H	1.89601	9.16479	2.56605
C	3.12338	8.3469	1.0027
C	3.18364	7.43895	-0.04535
H	4.09611	7.34842	-0.63048
C	2.08758	6.62947	-0.36265
B	-4.88838	-3.26118	-0.01727
B	5.27298	-2.59624	0.0206
H	-5.11837	8.36544	-1.26001
H	3.98385	8.96507	1.24358
H	9.74428	0.17616	-1.61092
H	5.80657	-7.8315	1.64775
H	-4.73741	-8.5115	-1.67503
H	-9.68406	-1.10148	1.61824
H	-2.96571	5.6125	1.17535
H	-0.96766	7.72823	-2.0344
H	-0.04917	7.79938	2.02509
H	2.20611	5.94277	-1.17462
H	6.49913	-0.24049	1.11036
H	7.02545	-3.07854	-2.12064
H	6.72639	-3.69183	2.15995
H	4.15121	-5.00381	-1.06773
H	-3.46392	-5.50857	1.05822
H	-6.18723	-4.5235	-2.16426
H	-6.40495	-1.07534	-1.09409
H	-6.56883	-3.98127	2.11532

CB-Mes (TD-DFT B3LYP/6-31+G(d,p), S_1)

Total energy: − 2196.390444 hartree

Dipole moment: 0.050133 D

Symbol	***X*** **/ Å**	***Y*** **/ Å**	***Z*** **/ Å**
B	1.93423	-5.35329	0.01639
C	0.44184	-1.39007	-1.20845

B	3.67364	4.35138	0.02395
C	-0.08887	-2.03763	-0.09203
H	-0.88402	-1.56669	0.47796
C	-0.00343	0.0034	-1.63637
H	-0.003	0.00494	-2.73401
B	-5.60983	1.00352	0.02141
C	0.39756	-3.2816	0.30058
H	-0.02579	-3.75506	1.18237
C	1.40356	-3.94494	-0.42151
C	1.91045	-3.28625	-1.55721
H	2.68792	-3.76281	-2.14819
C	1.45184	-2.03044	-1.93304
H	1.88286	-1.53416	-2.79938
C	1.99517	-5.72911	1.53865
C	2.2698	-4.76011	2.52094
C	2.3387	-5.09178	3.8711
H	2.5685	-4.32741	4.60731
C	2.10357	-6.40436	4.27677
C	1.8151	-7.38257	3.32669
H	1.62731	-8.40556	3.63863
C	1.77734	-7.04842	1.97588
C	2.40579	-6.38618	-1.06646
C	1.7915	-6.45256	-2.3304
C	2.19715	-7.37712	-3.28872
H	1.69515	-7.41824	-4.2507
C	3.25424	-8.24329	-3.01476
C	3.89107	-8.19003	-1.77607
H	4.71771	-8.86012	-1.55991
C	3.4597	-7.28279	-0.81243
C	0.98029	1.08482	-1.2049
C	1.80684	0.94549	-0.08921
H	1.79616	0.01977	0.47814
C	2.64241	1.98684	0.30539
H	3.26486	1.854	1.18623
C	2.71493	3.19123	-0.41404
C	1.88975	3.30484	-1.54844
H	1.91423	4.21788	-2.13714
C	1.03003	2.28172	-1.92614
H	0.3842	2.40973	-2.79166
C	3.97192	4.58939	1.54589
C	2.99707	4.34291	2.52983
C	3.25324	4.56562	3.8798
H	2.47772	4.38254	4.61746
C	4.50926	5.01529	4.28349

C	5.49904	5.25441	3.33169
H	6.48018	5.60094	3.64211
C	5.22522	5.05734	1.98117
C	-1.43244	0.31377	-1.20674
C	-1.72663	1.09287	-0.08698
H	-0.92034	1.54271	0.48444
C	-3.04677	1.29365	0.30683
H	-3.24413	1.89371	1.19111
C	-4.1251	0.75863	-0.41735
C	-3.80933	-0.0054	-1.55628
H	-4.61151	-0.43661	-2.14906
C	-2.49285	-0.23645	-1.93331
H	-2.27959	-0.85444	-2.80235
C	-5.96599	1.1303	1.54429
C	-5.26458	0.40188	2.5224
C	-5.58649	0.50027	3.87309
H	-5.03978	-0.08545	4.606
C	-6.60537	1.35819	4.28365
C	-7.30785	2.10301	3.33784
H	-8.09965	2.77559	3.65366
C	-6.99936	1.97646	1.98633
C	-6.73931	1.11988	-1.06147
C	-8.04418	0.65774	-0.81055
C	-9.04475	0.74531	-1.77436
H	-10.03956	0.36616	-1.56063
C	-8.77011	1.32876	-3.01004
C	-7.48996	1.80901	-3.28083
H	-7.27275	2.26843	-4.24045
C	-6.48736	1.69066	-2.32243
C	4.59214	6.6336	-0.80465
C	4.33479	5.27413	-1.05926
C	4.69435	4.77433	-2.32426
C	5.29468	5.58537	-3.28317
H	5.5772	5.1704	-4.24603
C	5.52401	6.9325	-3.00862
C	5.16477	7.45841	-1.76879
H	5.33794	8.50824	-1.55213
H	5.98164	7.57073	-3.75872
H	4.71608	5.17921	5.33695
H	3.58076	-8.95795	-3.76446
H	2.14527	-6.6643	5.33038
H	-6.85149	1.44591	5.33776
H	-9.55157	1.40911	-3.75988
H	2.44426	-3.73102	2.21841

H	1.56297	-7.82265	1.24405
H	-4.46077	-0.26215	2.21591
H	-7.5623	2.55376	1.25776
H	-5.49049	2.05892	-2.54974
H	-8.27417	0.21123	0.15313
H	4.32749	7.05286	0.16241
H	4.51062	3.72824	-2.55445
H	6.00155	5.25854	1.24779
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H	0.97346	-5.77495	-2.56008
H	3.95697	-7.25921	0.15355

CB-Mes-1 (TD-DFT B3LYP/6-31+G(d,p), S$_1$)

Total energy: −2195.937378 hartree

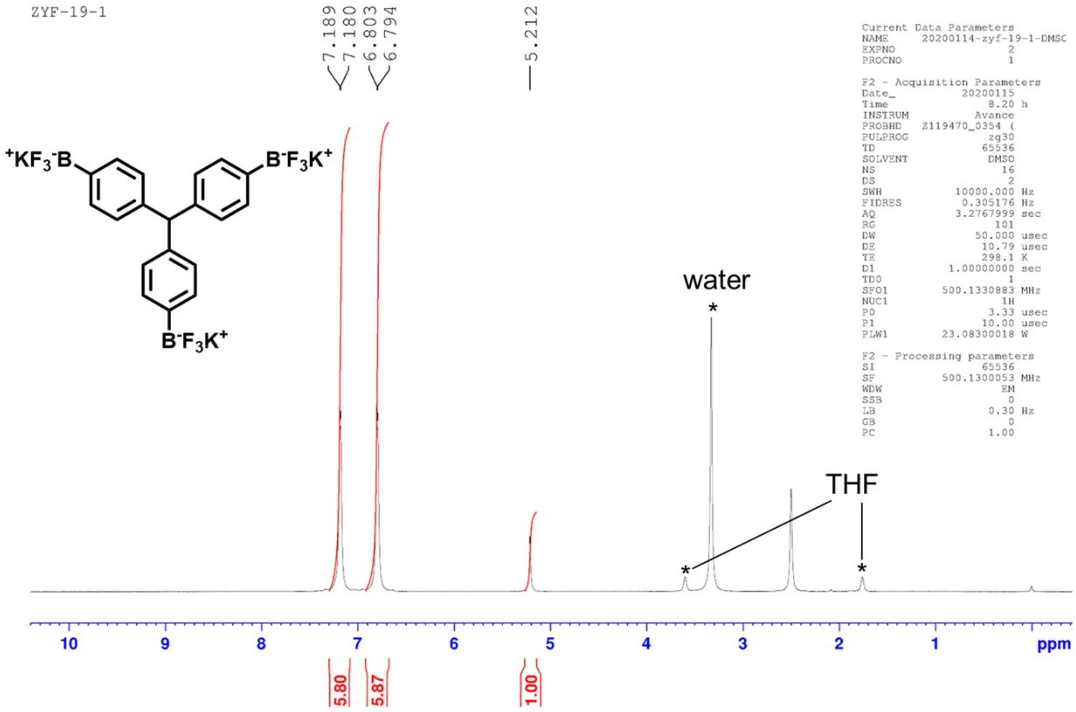
Dipole moment: 0.018760 D

Symbol	***X*** **/ Å**	***Y*** **/ Å**	***Z*** **/ Å**
B	-2.93591	-5.10072	-0.00103
C	-0.00029	0.00049	0.00129
C	1.44865	0.00213	0.00083
C	2.21023	-1.03123	0.61223
H	1.68682	-1.83126	1.12651
C	3.5897	-1.02998	0.60057
H	4.10916	-1.83823	1.11046
C	4.35051	0.00555	0.00078
C	3.58721	1.03902	-0.59938
H	4.10454	1.84827	-1.1098
C	2.20774	1.03702	-0.61102
H	1.68255	1.83553	-1.12581
C	6.70995	-1.32641	0.20922
C	6.29251	-2.54548	-0.35312
C	7.02673	-3.71784	-0.18565
H	6.68201	-4.64231	-0.6405
C	8.19665	-3.70561	0.57154
C	8.63284	-2.51188	1.14475
H	9.54418	-2.49319	1.73629
C	7.90461	-1.34061	0.95081
C	6.70677	1.3437	-0.20568
C	7.9023	1.36078	-0.94577
C	8.62778	2.53387	-1.13906
H	9.53991	2.51741	-1.72945
C	8.18778	3.72661	-0.56668
C	7.01689	3.73601	0.18905
H	6.66926	4.65971	0.64326
C	6.28549	2.56181	0.35589

C	-0.72659	1.25417	0.00142
C	-0.21227	2.43107	0.61134
H	0.74259	2.37859	1.12503
C	-0.90338	3.62494	0.59906
H	-0.4628	4.47969	1.10738
C	-2.18118	3.76516	0.00044
C	-2.69511	2.58655	-0.59753
H	-3.65535	2.62908	-1.10662
C	-2.00326	1.3931	-0.60881
H	-2.43261	0.5382	-1.12188
C	-2.20616	6.47473	0.20279
C	-0.94166	6.71958	-0.36093
C	-0.29215	7.94146	-0.1977
H	0.68082	8.10269	-0.65346
C	-0.88633	8.95163	0.55645
C	-2.13814	8.73567	1.13107
H	-2.60886	9.51795	1.72038
C	-2.78965	7.51936	0.9415
C	-4.51838	5.13631	-0.20466
C	-5.13271	6.16097	-0.94632
C	-6.51181	6.20205	-1.13666
H	-6.95501	6.99855	-1.72825
C	-7.32334	5.22608	-0.5598
C	-6.74421	4.20939	0.19728
H	-7.36923	3.44752	0.65476
C	-5.36127	4.16369	0.36121
C	-0.72312	-1.25551	0.001
C	-1.9973	-1.39961	0.61498
H	-2.42737	-0.54733	1.13176
C	-2.68572	-2.59508	0.60276
H	-3.64415	-2.64175	1.11488
C	-2.17038	-3.77051	-0.00016
C	-0.89493	-3.62511	-0.60249
H	-0.45354	-4.47683	-1.11506
C	-0.20726	-2.42919	-0.61353
H	0.74587	-2.37253	-1.13003
C	-4.50341	-5.14853	0.20811
C	-5.35093	-4.17626	-0.35138
C	-6.73318	-4.22629	-0.18272
H	-7.36186	-3.46454	-0.63534
C	-7.30685	-5.24717	0.57284
C	-6.49064	-6.22299	1.14332
H	-6.92959	-7.02274	1.73368
C	-5.11234	-6.17751	0.94823

C	-2.18936	-6.4797	-0.21116
C	-2.77261	-7.52284	-0.95216
C	-2.11901	-8.73703	-1.1479
H	-2.58955	-9.51812	-1.73891
C	-0.86531	-8.95249	-0.57723
C	-0.27132	-7.9439	0.17915
H	0.70314	-8.10472	0.63184
C	-0.92295	-6.72397	0.34844
B	-2.95008	5.09328	-0.00035
B	5.88513	0.0076	0.00148
H	-8.38351	-5.28356	0.71465
H	-0.35554	-9.90144	-0.71957
H	8.76635	-4.62006	0.71242
H	8.7553	4.6425	-0.70704
H	-0.37819	9.90216	0.69395
H	-8.40059	5.25911	-0.69787
H	-4.91516	-3.37041	-0.93566
H	-4.48948	-6.95509	1.38379
H	-3.75779	-7.375	-1.38788
H	-0.44552	-5.94233	0.93308
H	5.37754	-2.5699	-0.93873
H	8.2661	-0.4132	1.38845
H	8.2667	0.43413	-1.38263
H	5.36979	2.58406	0.94042
H	-0.464	5.93688	-0.94396
H	-3.77336	7.37097	1.38034
H	-4.92113	3.36091	0.94647
H	-4.51347	6.93864	-1.38688

7. NMR spectra



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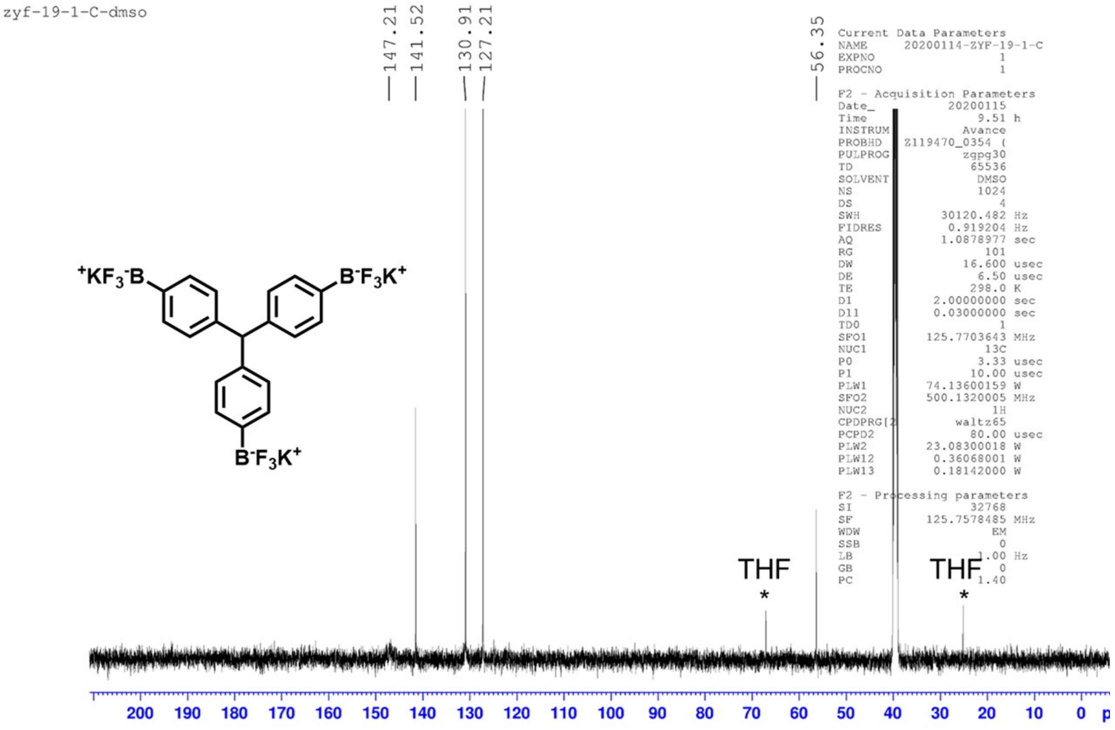
RG                     101
DW                  50.000 usec
DE                   10.79 usec
TE                   298.1 K
D1              1.00000000 sec
TD0                      1
SFO1           500.1330883 MHz
NUC1                    1H
P0                    3.33 usec
P1                   10.00 usec
PLW1           23.08300018 W

F2 - Processing parameters
SI                   65536
SF             500.1300053 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

Figure S6. ^{1}H NMR spectrum (500 MHz, DMSO-d_6) of compound **4**.



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Current Data Parameters
NAME      20200114-ZYF-19-1-C
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20200115
Time                  9.51 h
INSTRUM             Avance
PROBHD    Z119470_0354 (
PULPROG             zgpg30
TD                   65536
SOLVENT               DMSO
NS                    1024
DS                       4
SWH              30120.482 Hz
FIDRES            0.919204 Hz
AQ               1.0878977 sec
RG                     101
DW                  16.600 usec
DE                    6.50 usec
TE                   298.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1
SFO1           125.7703643 MHz
NUC1                   13C
P0                    3.33 usec
P1                   10.00 usec
PLW1           74.13600159 W
SFO2           500.1320005 MHz
NUC2                    1H
CPDPRG[2           waltz65
PCPD2                80.00 usec
PLW2           23.08300018 W
PLW12           0.36068001 W
PLW13           0.18142000 W

F2 - Processing parameters
SI                   32768
SF             125.7578485 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

Figure S7. ^{13}C{^{1}H} NMR spectrum (126 MHz, DMSO-d_6) of compound **4**.

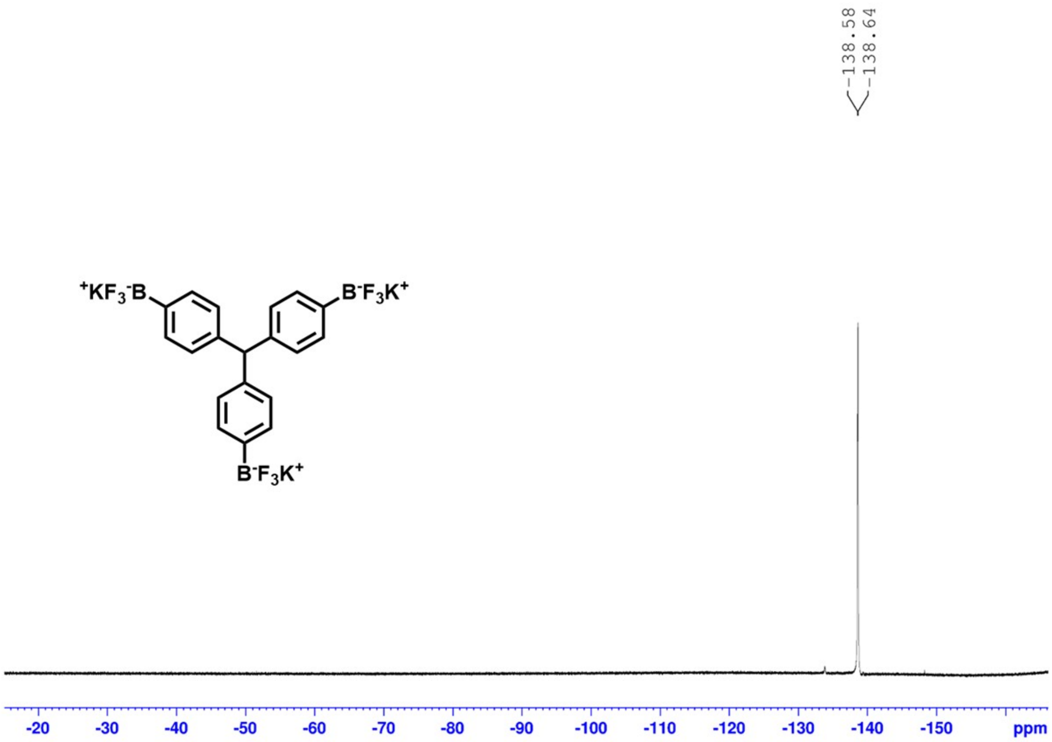


Figure S8. ^{19}F NMR spectrum (470 MHz, DMSO-d_6) of compound **4**.

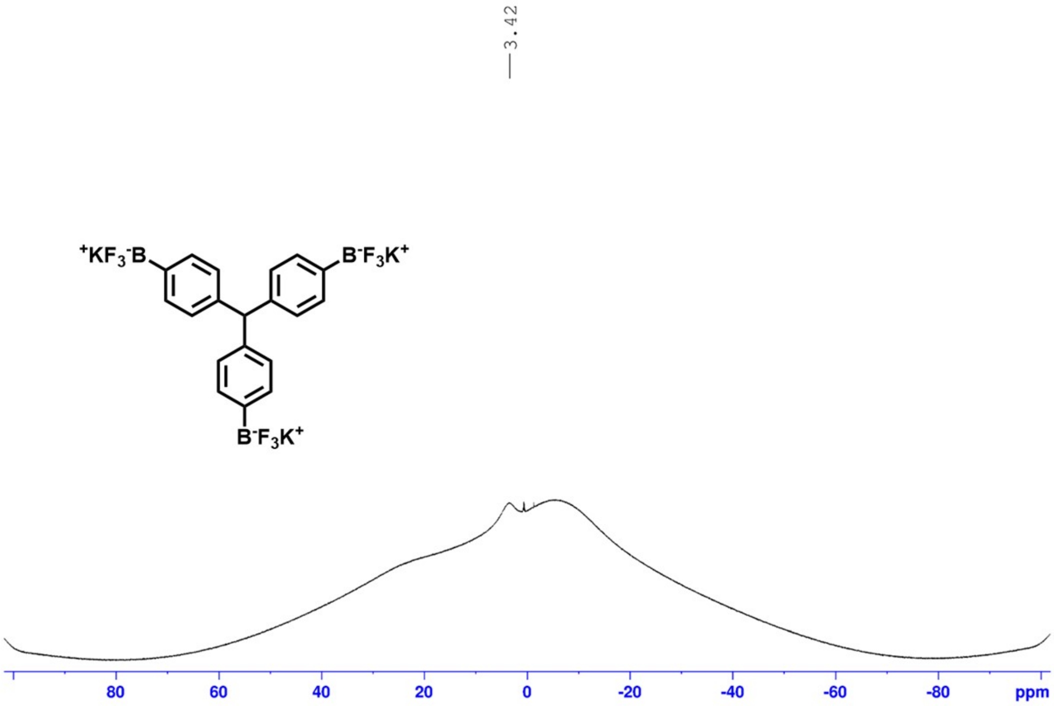


Figure S9. ^{11}B{^{1}H} NMR spectrum (160 MHz, DMSO-d_6) of compound **4**.

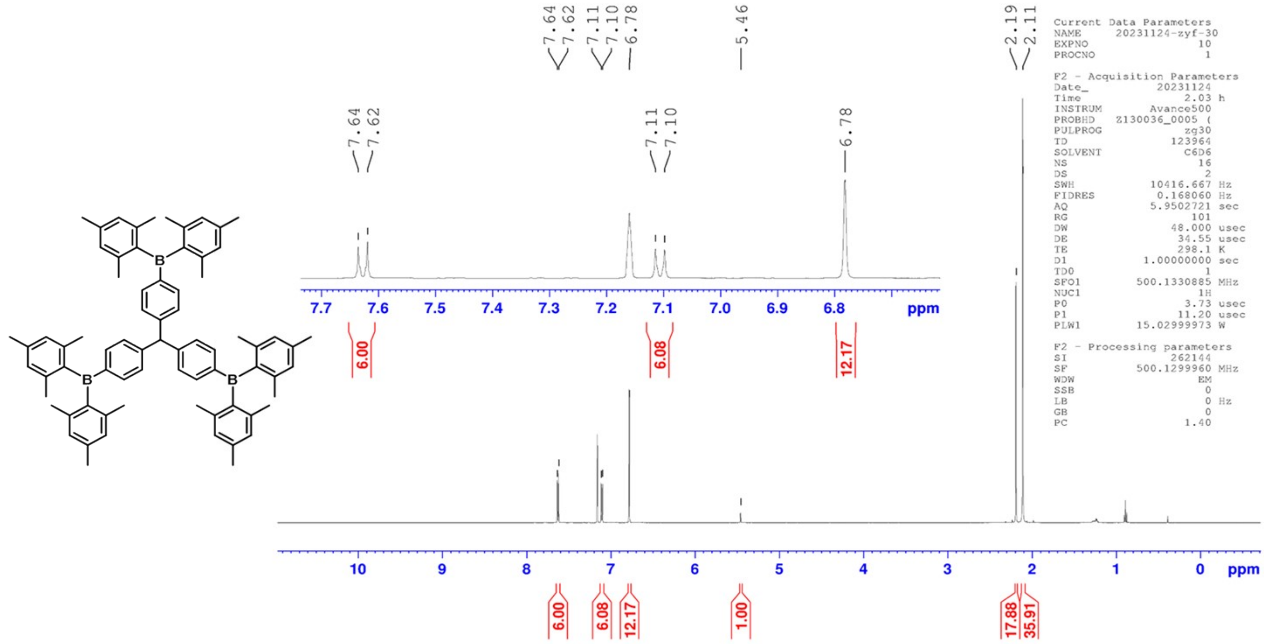


Figure S10. ^{1}H NMR spectrum (500 MHz, C_6D_6) of **CB-Mes**.

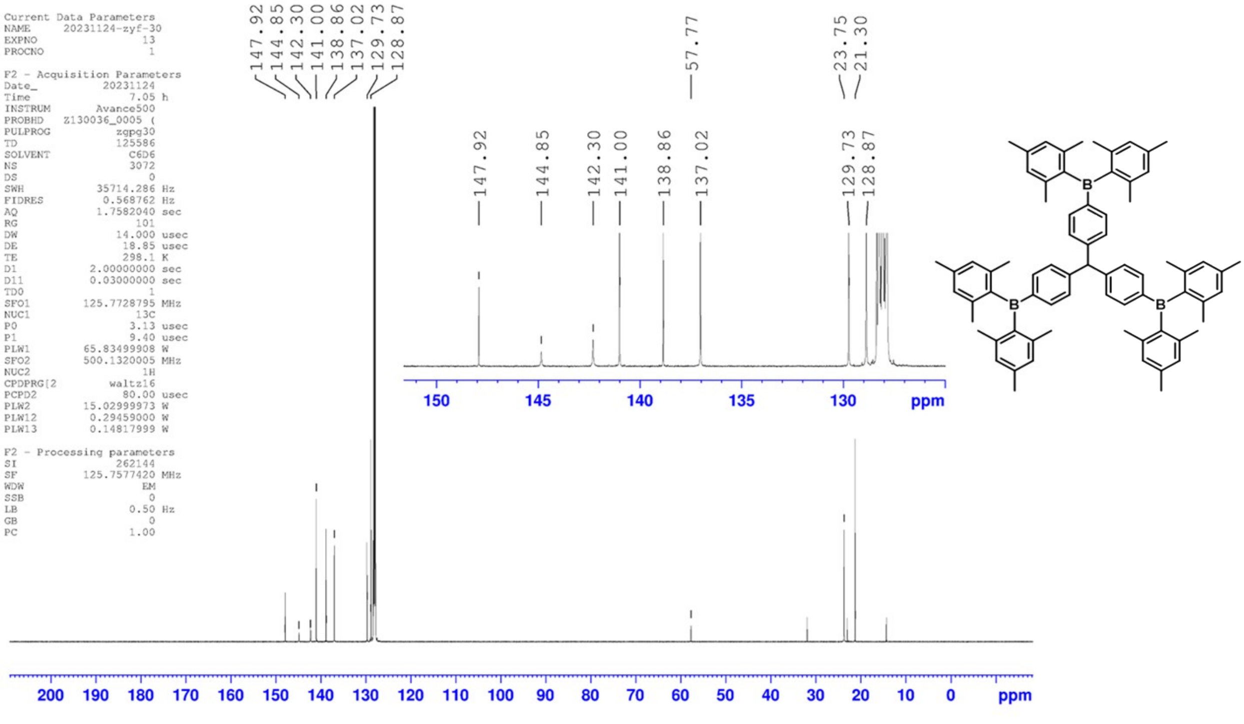
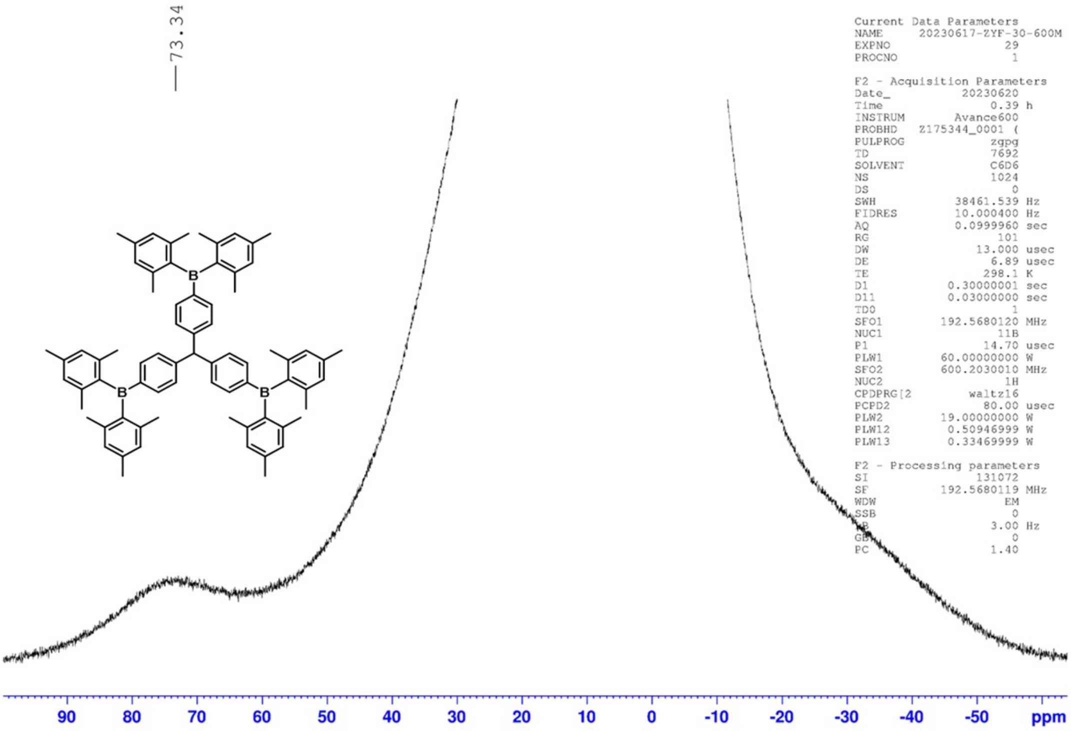


Figure S11. $^{13}C\{^1H\}$ NMR spectrum (150 MHz, C_6D_6) of **CB-Mes**.



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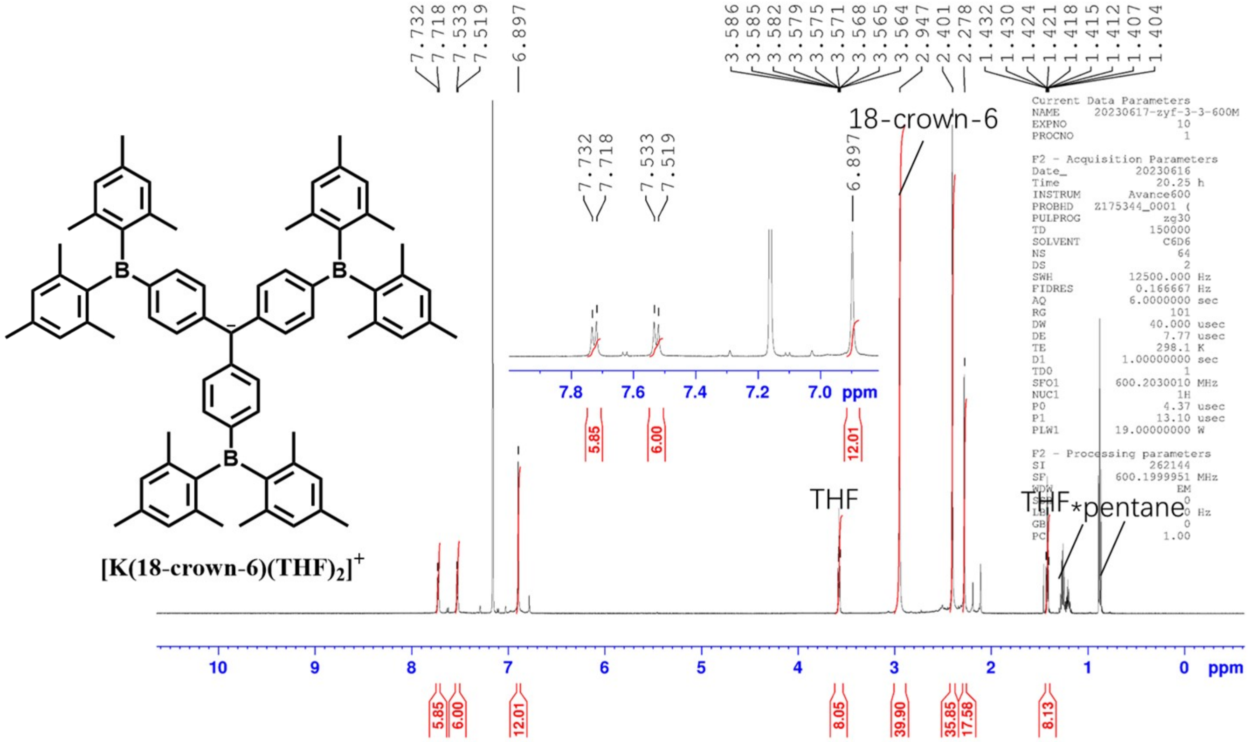
Current Data Parameters
NAME       20230617-ZYF-30-600M
EXPNO                    29
PROCNO                    1

F2 - Acquisition Parameters
Date_              20230620
Time                   0.39 h
INSTRUM           Avance600
PROBHD    Z175344_0001 (
PULPROG                zgpg
TD                     7692
SOLVENT                C6D6
NS                     1024
DS                        0
SWH               38461.539 Hz
FIDRES            10.000400 Hz
AQ                0.0999960 sec
RG                      101
DW                   13.000 usec
DE                     6.89 usec
TE                    298.1 K
D1               0.30000001 sec
D11              0.03000000 sec
TD0                       1
SFO1            192.5680120 MHz
NUC1                    11B
P1                    14.70 usec
PLW1            60.00000000 W
SFO2            600.2030010 MHz
NUC2                     1H
CPDPRG[2            waltz16
PCPD2                 80.00 usec
PLW2            19.00000000 W
PLW12            0.50946999 W
PLW13            0.33469999 W

F2 - Processing parameters
SI                   131072
SF              192.5680119 MHz
WDW                      EM
SSB                       0
LB                     3.00 Hz
GB                        0
PC                     1.40
```

Figure S12. $^{11}B\{^1H\}$ NMR spectrum (193 MHz, C_6D_6) of **CB-Mes**.



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Current Data Parameters
NAME       20230617-zyf-3-3-600M
EXPNO                    10
PROCNO                    1

F2 - Acquisition Parameters
Date_              20230616
Time                  20.25 h
INSTRUM           Avance600
PROBHD    Z175344_0001 (
PULPROG                zg30
TD                   150000
SOLVENT                C6D6
NS                       64
DS                        2
SWH               12500.000 Hz
FIDRES             0.166667 Hz
AQ                6.0000000 sec
RG                      101
DW                   40.000 usec
DE                     7.77 usec
TE                    298.1 K
D1               1.00000000 sec
TD0                       1
SFO1            600.2030010 MHz
NUC1                     1H
P0                     4.37 usec
P1                    13.10 usec
PLW1            19.00000000 W

F2 - Processing parameters
SI                   262144
SF              600.1999951 MHz
WDW                      EM
SSB                       0
LB                        0 Hz
GB                        0
PC                     1.00
```

Figure S13. ^1H NMR spectrum (500 MHz, C_6D_6) of **CB-Mes-1**.

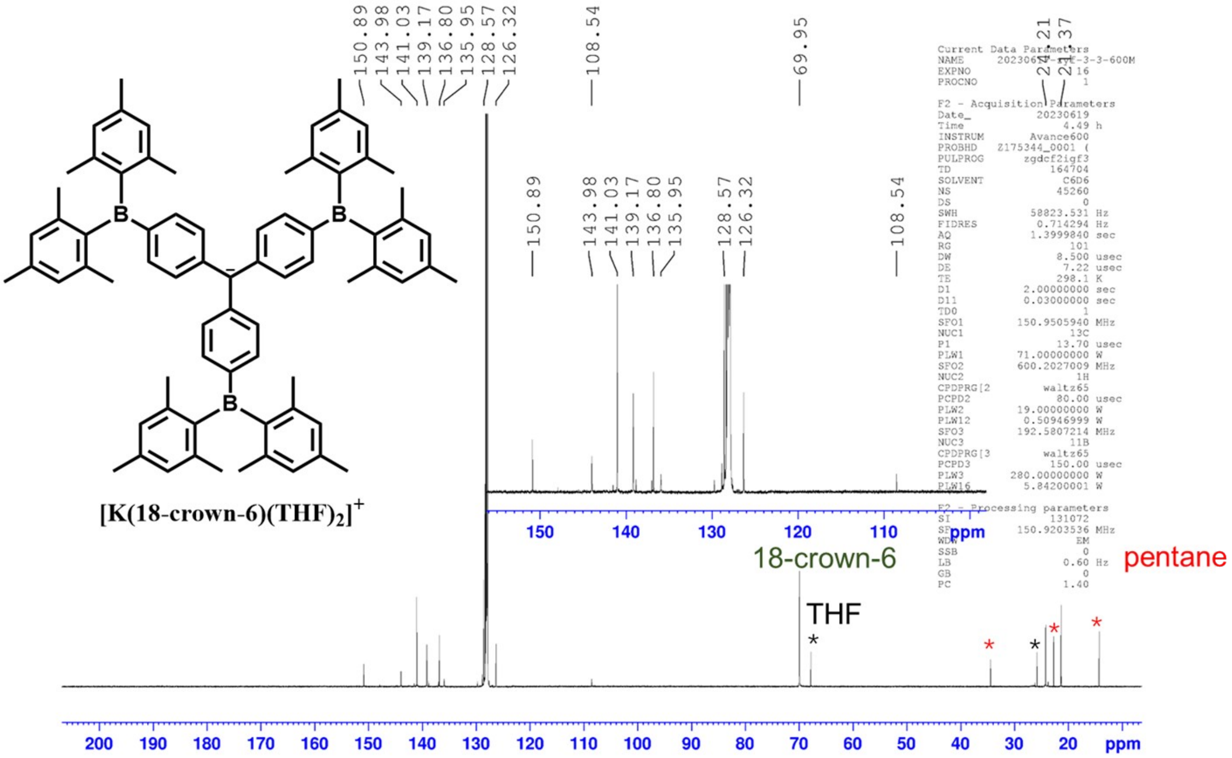

Figure S14. $^{13}C\{^1H\}$ NMR spectrum (150 MHz, C_6D_6) of **CB-Mes-1**.

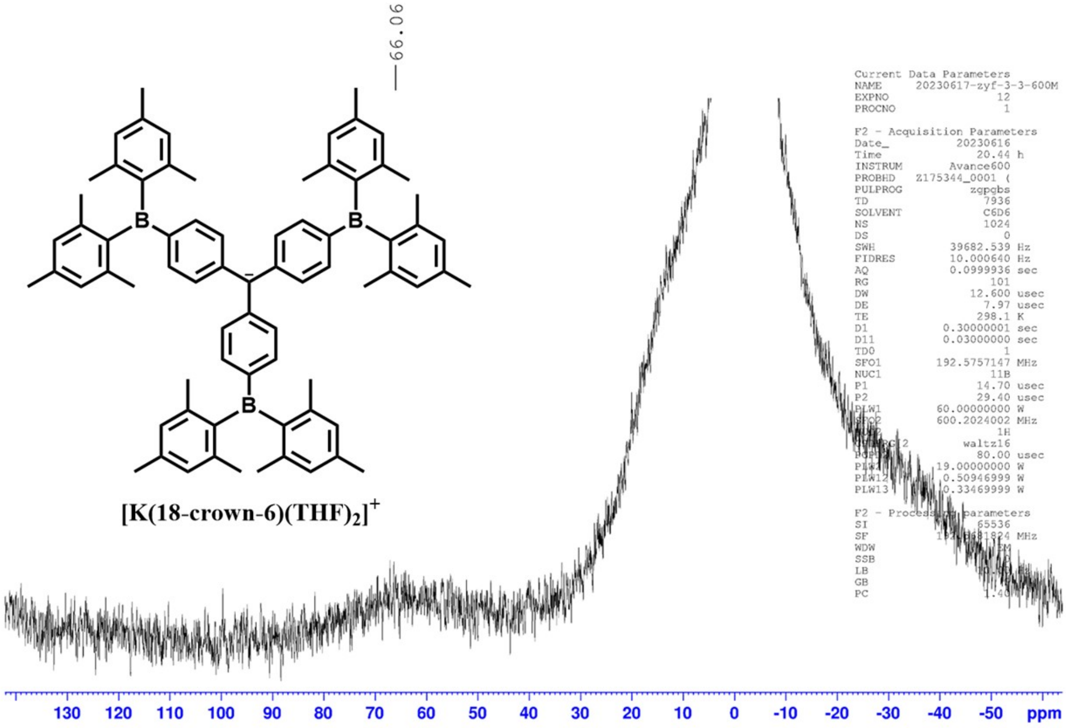

Figure S15. $^{11}B\{^1H\}$ NMR spectrum (193 MHz, C_6D_6) of **CB-Mes-1**.

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