Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Cage Carbon-substitute Does Matter for Aggregation-Induced Emission Features of *o*-Carborane-Functionalized Anthracene Triads

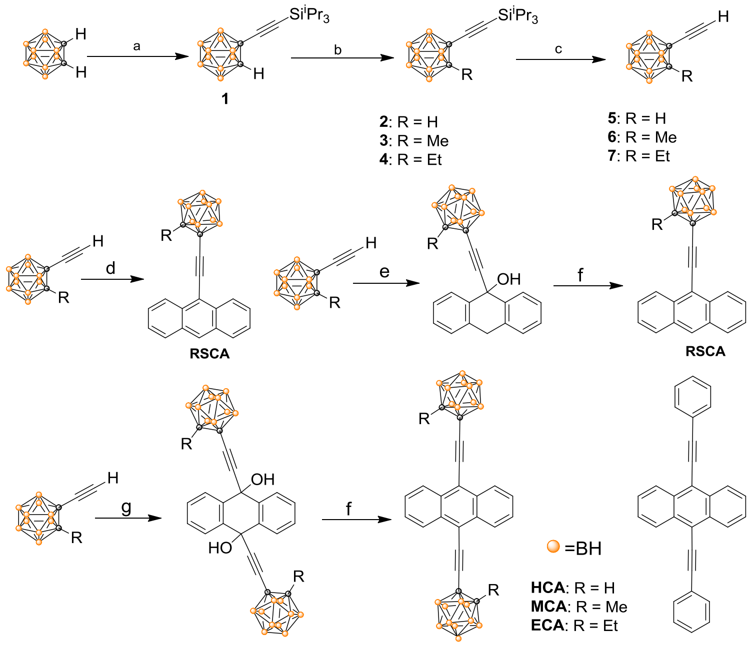
Xueyan Wu,[a] Jixi Guo,[a] * Yangjian Quan,[b] Wei Jia,[a] Dianzeng Jia,[a*] Yi Chen,[a] and Zuowei Xie[b]

[a]Key Laboratory of Energy Materials Chemistry, Ministry of Education; Key Laboratory of Advanced Functional Materials, Autonomous Region; Institute of Applied Chemistry, Xinjiang University, Urumqi, 830046, Xinjiang P. R. China. Email: jxguo1012@163.com; jdz@xju.edu.cn; Fax: +86-991-8588883; Tel: +86-991-8583083.

[b]Department of Chemistry and State Key Laboratory of Synthetic Chemistry, The Chinese University of Hong Kong, Shatin, N. T., Hong Kong, China.

Table of Contents

1. Synthesis



Scheme S1. (a) *n*-BuLi, Ether, THF, 0 °C, CuCl, r.t. 1-bromo-2-triisopropylsilylacetylene, Reflux, 83%; (b) *n*-BuLi, THF, 0 °C, RI, 0 °C, 90%; (c) KF, *n*-Bu_4NBr CH_2Cl_2, H_2O; (d) 9-Bromoanthracene, $Pd(PPh_3)_2Cl_2$, PPh_3, CuI, NEt_3, Ar, 90 °C, 8 h; (e) n-BuLi, Tol, 0 °C, Anthrone, 100 °C, H_2O; (f) $SnCl_2$, Tol, 50 °C; (g) *n*-BuLi, Tol, 0 °C, 9,10-Anthracenedione, 100 °C , H_2O.

Synthesis of 1-triisopropylsilylethynyl-*o*-carborane (1).

This compound was synthesized using the modified procedures reported in literature.[1] To a mixed ether/THF solution (150 mL in 1/1) of *o*-carborane (5.77 g, 40 mmol) was slowly added *n*-BuLi (30 mL, 48 mmol, 1.6 M in hexane) at 0 °C, and the mixture was stirred at room temperature for 3 h. After addition of anhydrous CuCl (7.13 g, 72 mmol), the mixture was vigorously stirred for 2 h at room temperature and then heated to reflux for 30 min. To the above solution was slowly added 1-bromo-2-triisopropylsilylacetylene (12.54 g, 48 mmol) with vigorous stirring at room temperature. The reaction mixture was stirred at room temperature for 1 h and then heated to reflux for 2 h. The reaction was then quenched with aqueous HCl (20 mL, 3 N) with stirring. The organic layer was separated, washed with water and then dried over Na_2SO_4. Removal of solvents under reduced pressure yielded a crude oil. The crude product was purified by column chromatography on silica gel using hexane as eluent to give **1** as colorless oil (10.78 g, 83%). ^1H NMR (400 MHz, CD_2Cl_2): δ 3.97 (s, 1H) (cage H), 1.06 (br m, 21H). $^{13}C\{^1H\}$ NMR (100 MHz, CD_2Cl_2): δ 100.27, 83.56 ($C{\equiv}C$), 63.85, 61.77 (cage C), 18.66, 11.42 (iPr). $^{11}B\{^1H\}$ NMR (128 MHz, CD_2Cl_2): δ -5.01 (1B), -6.76 (1B), -11.81 (2B), -12.75 (4B), -15.72 (2B). HRMS: m/z calcd for C13H32B10Si $[M]^+$: 324.3279. Found: 324.3278.

Synthesis of 1-triisopropylsilylethynyl-2-alkyl-*o*-carborane (2 and 3).

A representative procedure. To a diethyl ether solution (30 mL) of 1-triisopropylsilylethynyl-*o*-carborane (3.25 g, 10 mmol) was slowly added *n*-BuLi (7.5 ml, 12 mmol, 1.6 M in hexane) at 0 °C, and the resulting mixture was stirred at room temperature for 2 h. The above solution was cooled to 0 °C, to which was slowly added alkyl iodide (15 mmol) with vigorous stirring, and the reaction mixture was stirred at room temperature for 12 h. After hydrolysis with water and extraction with diethyl ether (3 × 30 mL), the ether solutions were combined and concentrated to dryness in vacuo. The residue was purified by column chromatography on silica gel using n-hexane as eluent to give the products **2** and **3**.

1-Triisopropylsilylethynyl-2-methyl-*o*-carborane (**2**): Yield 94%. Colorless oil. ^{1}H NMR (400 MHz, CD_2Cl_2): δ 2.17 (s, 3H), 1.08 (br m, 21H). ^{13}C{^{1}H} NMR (100 MHz, CD_2Cl_2): δ 98.93, 87.30 (C≡C), 77.12, 67.04 (cage C), 24.27, 18.67, 11.44. ^{11}B NMR (128 MHz,CD_2Cl_2): δ -3.37 (1B), -6.73 (1B), -8.30 (2B), -10.11 (6B). HRMS: m/z calcd for $C_{14}H_{34}B_{10}Si$[M]$^+$: 338.3436. Found: 338.3433.

1-Triisopropylsilylethynyl-2-ethyl-*o*-carborane (**3**): Yield 98%. Colorless oil. ^{1}H NMR (400 MHz, CD_2Cl_2): δ 2.47 (q, J = 7.6 Hz, 2H), 1.18 (t, J = 7.6 Hz, 3H), 1.06 (br m, 21H). ^{13}C{^{1}H} NMR (100 MHz, CD_2Cl_2): δ 98.66, 87.33 (C≡C), 82.92, 67.83 (cage C), 30.06,18.61, 14.14, 11.39. ^{11}B{^{1}H} NMR (128 MHz, CD_2Cl_2): δ -3.74 (1B), -5.99 (1B), -9.27 (2B), -10.38 (4B), -11.88 (2B). HRMS: m/z calcd for $C_{15}H_{36}B_{10}Si$ [M]$^+$: 352.3593. Found: 352.3595.

Synthesis of 1-ethynyl-2-alkyl-*o*-carboranes (4-6). A representative procedure.

All compounds were synthesized using the modified procedures reported in literature 3 1-Triisopropylsilylethynyl-2-alkyl-*o*-carborane (5.0 mmol), KF (2.91 g, 50 mmol), Bu_4NBr (0.16 g, 0.5 mmol), water (10 mL) and CH_2Cl_2 (25 mL) were mixed and stirred vigorously at room temperature overnight until all of the starting materials had disappeared. The lower layer was separated and the aqueous layer was extracted with CH_2Cl_2 (3 × 30 mL). The combined CH_2Cl_2 solutions were dried over Na_2SO_4. After removal of the solvent in vacuum, the residue was purified by column chromatography on silica gel using n-hexane as eluent to give the desired products **4-6**.

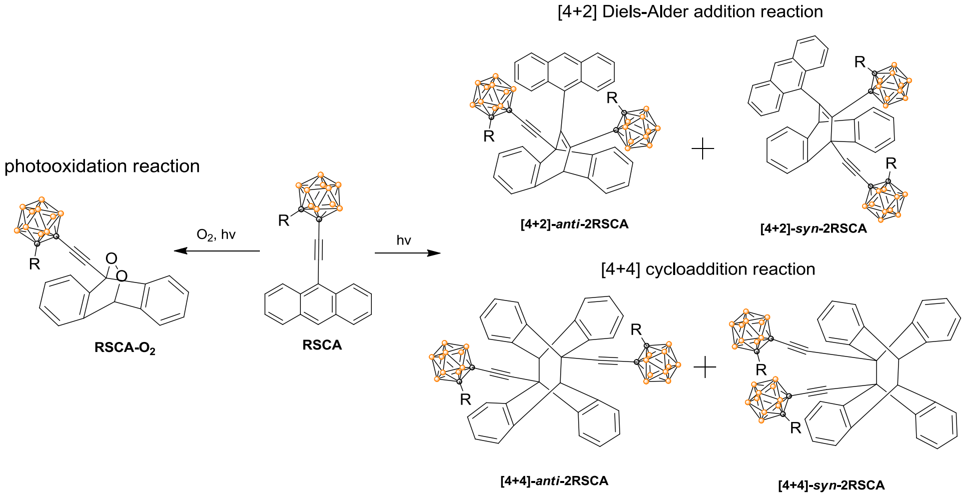
1-Ethynyl-*o*-carborane (**4**): Yield 90%. White solid. Mp: 84.1-86.3°C. ^{1}H NMR (400 MHz, CD_2Cl_2): δ 3.99 (s, 1H), 2.34 (s, 1H). ^{13}C{^{1}H} NMR (100 MHz, CD_2Cl_2): δ 77.49, 68.16(C≡C), 63.38, 60.20 (cage C). ^{11}B{^{1}H} NMR (128 MHz, CD_2Cl_2): δ -2.64 (1B), -4.04 (1B), -9.49 (2B), -10.98 (4B), -13.41 (2B). HRMS: m/z calcd for $C_5H_{14}B_{10}$ [M]$^+$: 168.1939. Found: 168.1938.

1-Ethynyl-2-methyl-*o*-carborane (**5**): Yield 91%. White solid. M.p: 118.7-119.8°C. ^{1}H NMR (400 MHz, CD_2Cl_2): δ 2.57 (s, 1H), 2.19 (s, 3H). ^{13}C{^{1}H}NMR (100 MHz, CD_2Cl_2): δ 77.21, 71.92 (C≡C), 76.37, 65.55 (cage C), 24.28. ^{11}B{^{1}H} NMR (128 MHz, CD_2Cl_2): δ -2.57 (1B), -6.23 (1B), -8.10 (2B), -9.67 (6B). HRMS: m/z calcd for $C_5H_{14}B_{10}$ [M]$^+$: 182.2093. Found: 182.2091.

1-Ethynyl-2-ethyl-*o*-carborane (**6**): Yield 95%. Colorless oil. ^{1}H NMR (400 MHz, CD_2Cl_2): δ 2.56 (s, 1H), 2.47 (q, J = 7.6 Hz, 2H), 1.20 (t, J = 7.6 Hz, 3H). ^{13}C{^{1}H}NMR (100 MHz, CD_2Cl_2): δ 82.98, 71.91 (C≡C), 76.14, 65.38 (cage C), 30.10, 14.24. ^{11}B{^{1}H}NMR (128 MHz, CD_2Cl_2): δ -3.52 (1B), -6.10 (1B), -9.56 (2B), -10.40 (4B), -12.09 (2B). HRMS: m/z calcd for $C_6H_{16}B_{10}$ [M]$^+$: 196.2253. Found: 196.2252

Synthesis of pentacenediols (7-9). A representative procedure.

To a toluene solution (30 mL) of 1-ethynyl-2-alkyl-*o*-carborane **4-6** (3.0 mmol) was added nBuLi (1.88 mL, 3.0 mmol, 1.6 M in hexane) dropwise at 0 °C, and the resulting mixture was stirred for 12 h at room temperature. Compound 9,10-Dioxoanthracene (0.21 g, 1.0 mmol) was added to the above solution and the reaction mixture was heated at 100 °C for 12 h. The reaction was then quenched with water (5 mL) and extracted with CH_2Cl_2 (3 × 30 mL). The organic solutions were combined, washed with brine, and dried over anhydrous Na_2SO_4. After removal of the solvent, the residue was purified by column chromatography on silica gel using n-hexane/CH_2Cl_2 (1/1 in v/v) as eluent to give the desired products **7-9** and the product were used without further purification.



Scheme S2. The possible pathways of destroy the chemical structure of the mono-*o*-carboranyl complexes.

2. UV–Vis absorption and fluorescence emission spectra

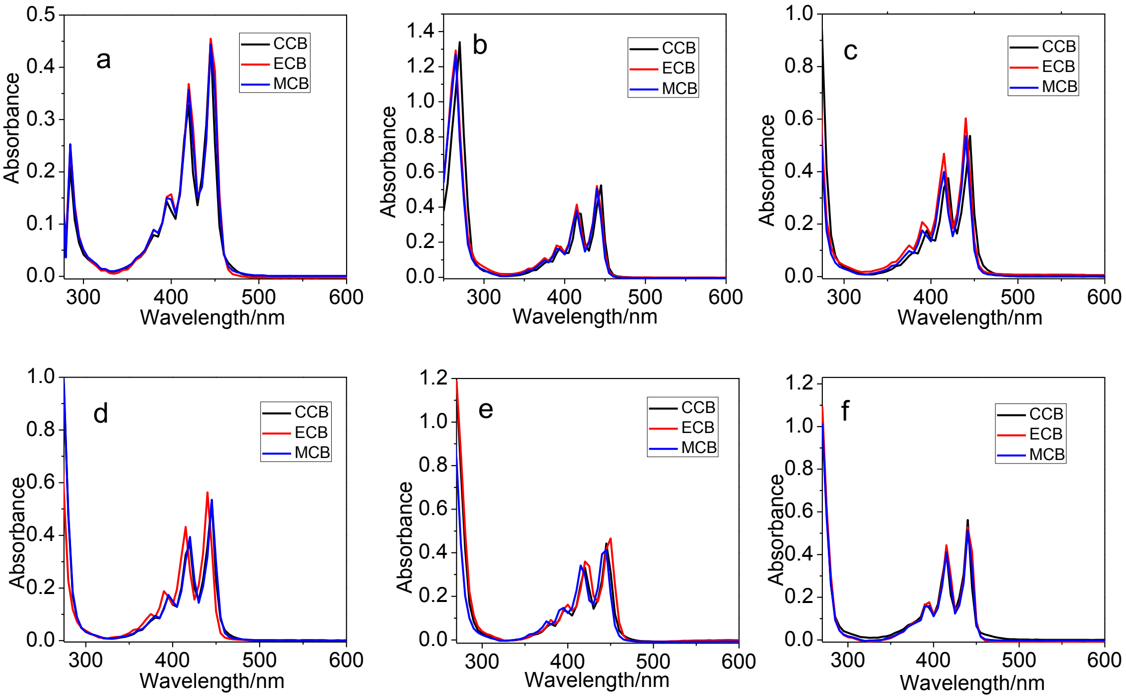


Fig.S1 UV-Vis absorption of **HCA**, **ECA** and **MCA** in (a) Toluene, (b) THF, (c) DCM, (d) Chloroform, (e) DMF, (f) n-hexane. *c* = 1.0 × 10^{-5} M, 20 °C.

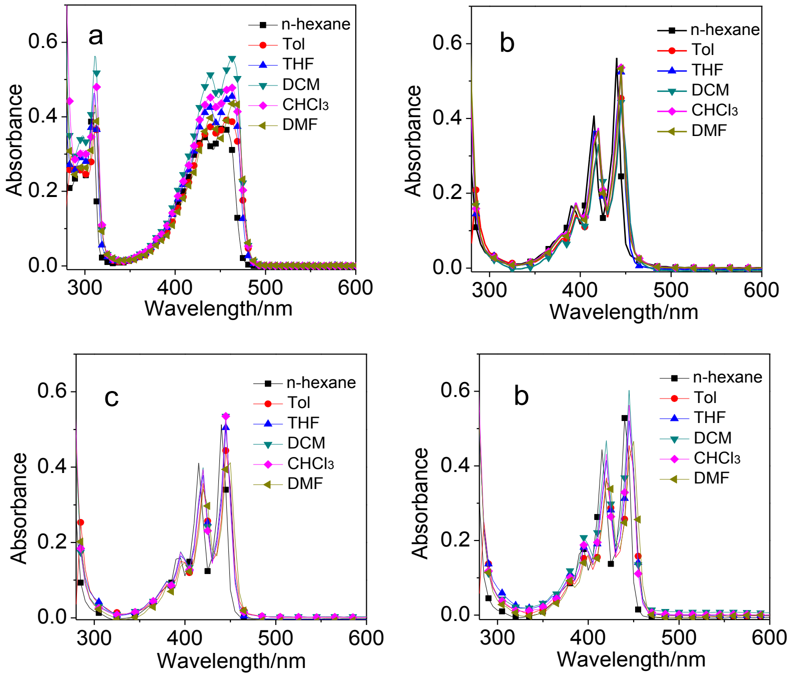


Fig.S2 UV-Vis absorption of (a) **BPEA,**(b) **HCA**, (c) **MCA** and (d) **ECA** in different solvents. $c = 1.0 \times 10^{-5}$ M, 20 °C.

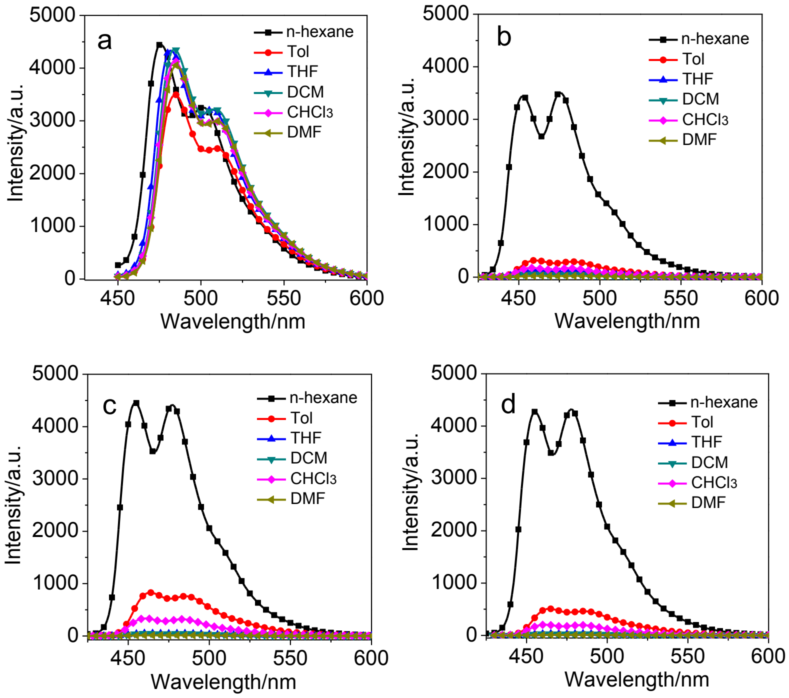


Fig.S3 Fluorescence spectra of (a) **BPEA,** (b) **HCA**, (c) **MCA** and (d) **ECA** in different solvents. (λ_{ex} = 420 nm). $c = 1.0 \times 10^{-5}$ M, 20 °C.

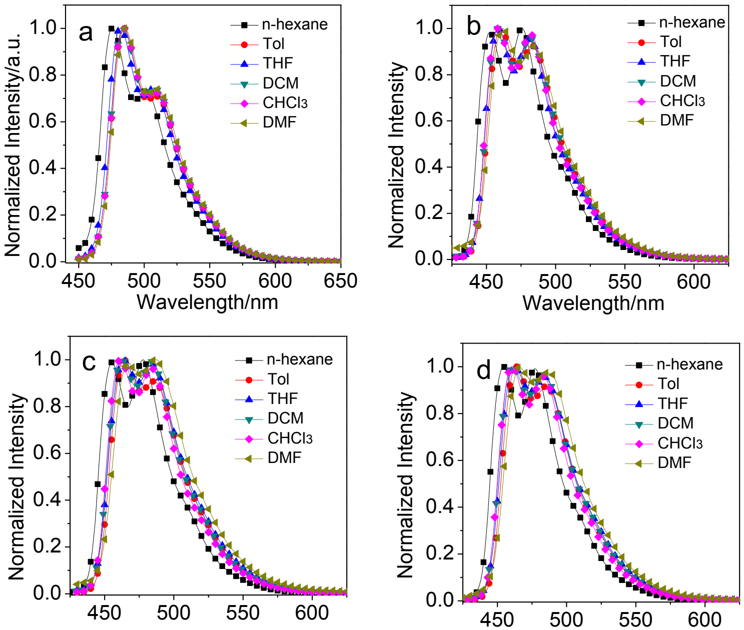


Fig.S4 Normalized fluorescence spectra of (a) **BPEA**, (b) **HCA**, (c) **MCA** and (d) **ECA** in different solvents. The compounds were excited at the $\lambda_{\max,\mathrm{abs}}$. $c = 1.0 \times 10^{-5}$ M, 20 °C.

3. AIE attributes of the triads

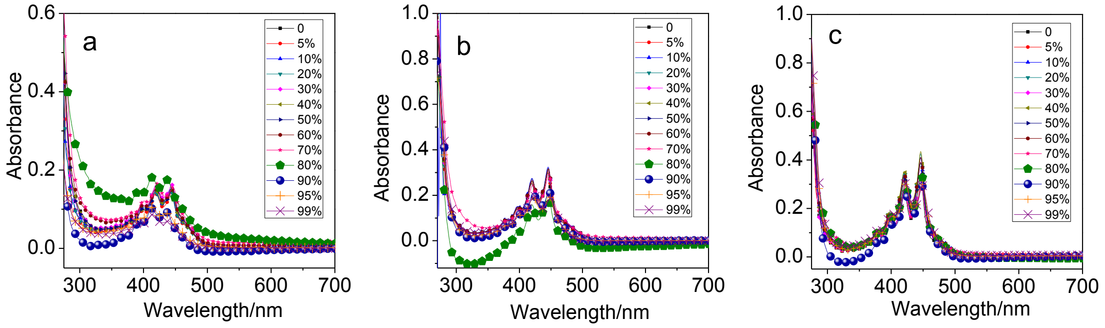


Fig.S5 UV-vis spectra of (a) **HCA**, (b) **MCA** and (c) **ECA** in THF/water mixtures with different water fractions (f_w).

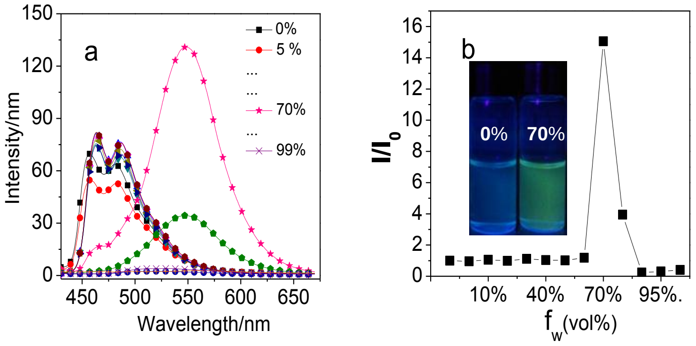


Fig.S6 (a) Fluorescence spectra of **HCA** in THF/water mixtures with different water volume fractions，(b) PL intensity enhancement ratio I/I₀ versus water fraction curves, where I₀ is the PL intensity in pure THF solution. Inset: photographs taken under UV illumination for **HCA** in the different water fractions. (λ_{ex} = 420 nm), *c* = 1.0 × 10^{-5} M, 20 °C.

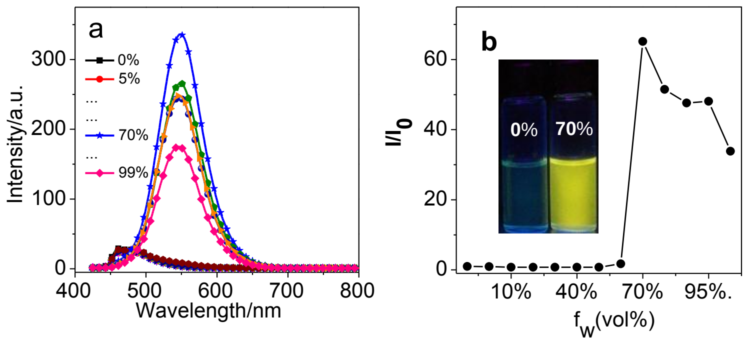


Fig.S7 (a) Fluorescence spectra of **ECA** in THF/water mixtures with different water volume fractions，(b) PL intensity enhancement ratio I/I₀ versus water fraction curves, where I₀ is the PL intensity in pure THF solution. Inset: photographs taken under UV illumination for **ECA** in the different water fractions. (λ_{ex} = 420 nm), *c* = 1.0 × 10^{-5} M, 20 °C.

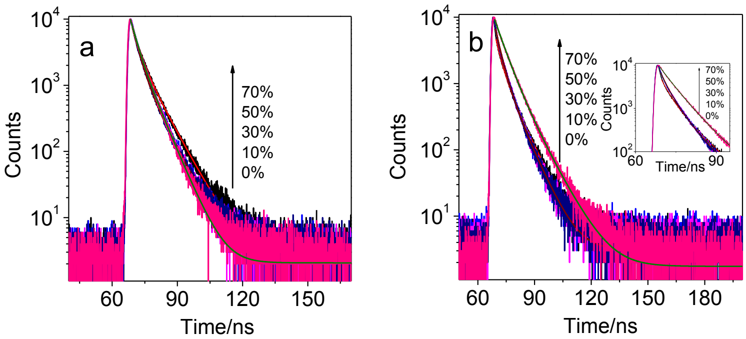


Fig.S8 Decay profiles of fluorescence lifetime measurement of (a) **HCA** (E_m= 555 nm), (b) **MCA** (E_m= 550 nm) in THF with various water volume fractions (c = 1.0 × 10^{-5} M). 20 °C.

Table S1. Photoluminescence lifetime of **HCA**, **MCA** and **ECA** in different water fractions.

f_w	τ_f^a(ns)		
	HCA	**MCA**	**ECA**
0%	0.63(40.7%), 7.61(50.3%)	0.48(75.1%), 8.41(24.9%)	0.43(78.7%), 6.05(21.3%)
10%	2.91(51.0%), 6.62(41.0%)	0.70(44.6%), 6.53(55.4%)	0.62(45.0%), 5.27(55.0%)
30%	2.89(50.9%), 6.48(49.1%)	2.68(35.3%), 6.01(64.7%)	0.52(10.8%), 4.74(89.2%)
50%	2.92(53.4%), 7.16(46.6%)	2.79(21.8%), 6.83(78.2%)	0.50 (8.3%), 4.61(91.7%)
70%	2.80(63.4%), 6.68(36.6%)	4.72(63.3%), 8.05(36.7%)	3.86(60.1%), 7.75(39.9%)

[a] Fluorescence lifetime.

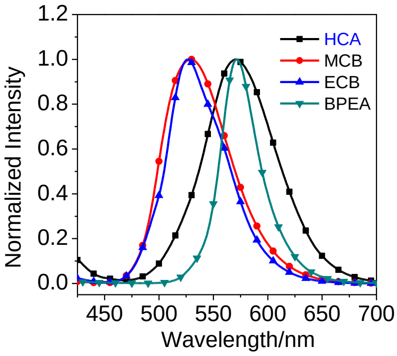


Fig.S9 Normalized fluorescence spectra of **BPEA**, **HCA**, **MCA** and **ECA** in the solid state. (λ_{ex} = 420 nm), 20 °C.

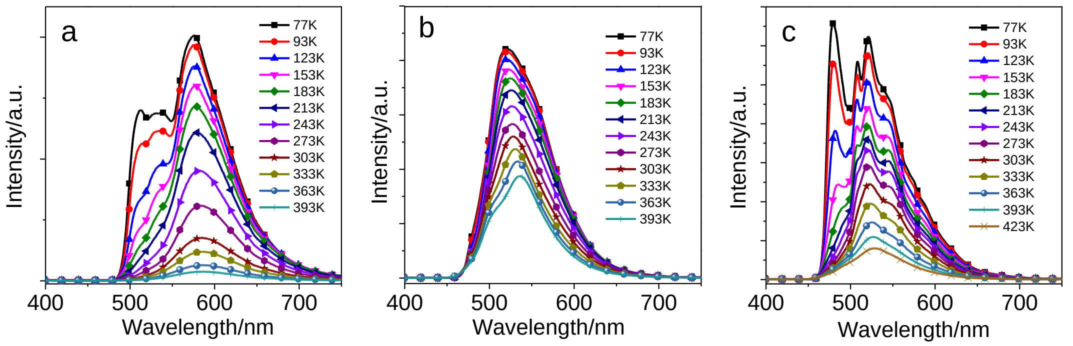


Fig.S10 PL spectra of (a) **HCA**, (b) **MCA** and (c) **ECA** in the solid state during heating from 77 to 393 K.

4.Time-resolved Florescence Measurements

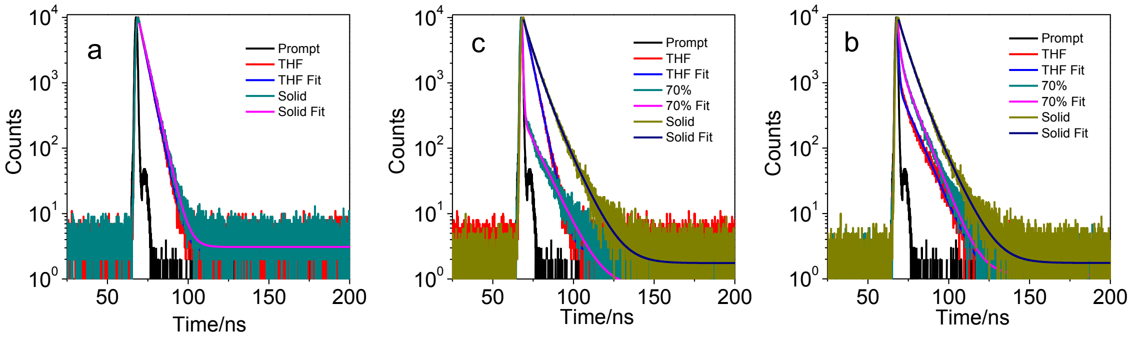


Fig.S11 Decay profiles of fluorescence lifetime measurement of (a) **BPEA**, (b) **HCA** and (c) **ECA** in various state. 20 °C.

Table S2. Photoluminescence lifetime of **BPEA**, **HCA**, **MCA** and **ECA** in different conditions.

Compound	*τ[a](ns)*		
	Sol[b]	*Agg*[c]	Solid [d]
BPEA	3.92(100%)	–[e]	4.73(100%)
HCA	0.63(40.7%), 7.61(50.3%)	2.80(63.4%), 5.68(36.6%)	4.19(77.1%), 7.81(22.9%)
MCA	0.48(65.1%), 8.41(34.9%)	4.64(61.6%), 8.55(38.4%)	4.38(87.9%), 18.4(12.1%)
ECA	0.43(78.7%), 6.05(21.3%)	4.72(63.3%), 8.05(36.7%)	4.39(81.0%), 14.5(19.0%)

[a] Fluorescence lifetime. [b] In pure THF. [c] f_W=70%. [d] In the solid state. [e] Not applicable or not observed.

Table S3. Emission properties of compounds in different states

Compound	*State*	k_r ^{d}(10^{7}s^{-1})	k_{nr} ^{d}(10^{7}s^{-1})
BPEA	*Sol*^{a}	21.70	3.81
	Agg^b	–^{e}	–^{e}
	Solid ^{c}	5.34	15.80
HCA	*Sol*^{a}	0.77	23.72
	Agg^b	1.04	20.58
	Solid ^{c}	1.40	18.59
MCA	*Sol*^{a}	0.28	30.49
	Agg^b	1.40	1.49
	Solid ^{c}	7.06	9.41
ECA	*Sol*^{a}	0.50	60.82
	Agg^b	1.61	15.23
	Solid ^{c}	5.01	10.10

[a] In pure THF. [b] f_W=70%. [c] In the solid state. [d] Fluorescence emission rate constant (k_r) and non-radiative decay rate constant (k_{nr}) were calculated as follows: $k_r=\Phi_f/\tau_f$, $k_{nr}=(1-\Phi_f)/\tau_f$. [e] Not detected.

5. Crystal Packing from X-ray Crystallography

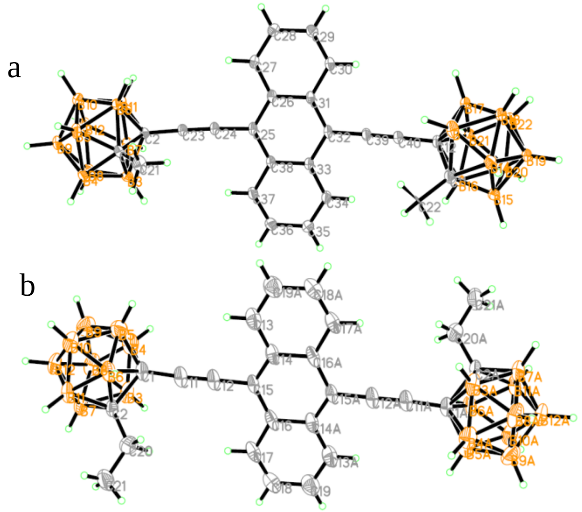


Fig.S12 ORTEP plots showing the crystal structures of (a) **MCA** and (b) **ECA** with ellipsoids at 30% probability and atom numbering scheme.

Table S4. Crystal data and structure refinement for **MCA** and **ECA**.

Compounds	**MCA**	**ECA**
CCDC	1545548	1545547
Empirical formula	$C_{24}H_{34}B_{20}$	$C_{26}H_{38}B_{20}$
Formula weight	538.71	566.76
Temperature, K	173(2)	298(2)
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Triclinic
Space group	P2(1)/c	P-1
Unit cell dimensions	a = 13.1826(13) Å.	a = 6.8517(4) Å
	b =20.410(2) Å.	b = 7.8881(6) Å
	c = 13.5543(14) Å.	c = 16.0370(11) Å
	α = 90 °	α = 83.056(2) °
	β = 118.359(2) °	β = 86.331(2) °
	γ = 90 °	γ = 76.6190(10) °
Volume, Å^3	3209.1(6)	836.45(10)
Z	4	2
Calculated density, g/cm^3	1.115	1.125
Absorption coefficient, mm^{-1}	0.054	0.054
F(000)	1112	294
Crystal size, mm^3	0.50 × 0.40 × 0.30	0.40 × 0.30 × 0.20
Theta range, degree	1.98–25.25°	2.56–25.25°
Limiting indices	$-15 \leq h \leq 15$	$-8 \leq h \leq 8$
	$-24 \leq k \leq 24$	$-9 \leq k \leq 9$
	$-15 \leq l \leq 12$	$-19 \leq l \leq 19$
Reflections collected / unique	32464 / 5645 [R(int) = 0.0364]	22732 / 3015 [R(int) = 0.0377]
Data / restraints / parameters	5645 / 0 / 402	3015 / 2 / 273
Goodness-of-fit on F^2	1.090	1.054
Final R indices [I >2 σ (I)]	R_1 = 0.0687, wR_2 = 0.1999	R_1 = 0.0732, wR_2 = 0.1946
R indices (all data)	R_1 = 0.0875, wR_2 = 0.2242	R_1 = 0.0942, wR_2 = 0.2124
Largest diff. peak and hole	0.814 and -0.256 e·Å^{-3}	0.232 and -0.250 e·Å^{-3}

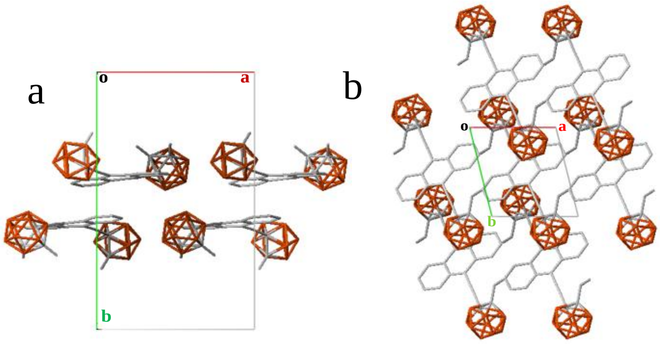


Fig.S13 Molecular packings of **MCA** (a) in the c-axis and **ECA** (b) in the c-axis in a single unit cell by the Mercury program. Carbon (gray) and boron (orange), hydrogen atoms are omitted for clarity.

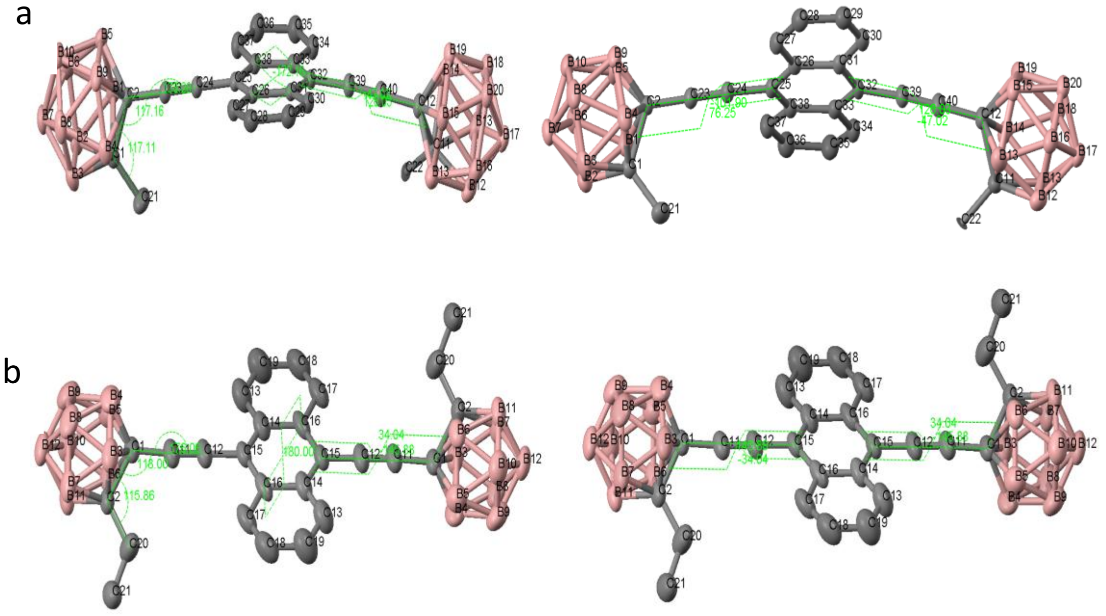


Fig.S14 Selected bond length and torsion angles for (a) **MCA** and (b)**ECA** by the Mercury program. Carbon (gray) and boron (orange), hydrogen atoms are omitted for clarity.

Table S5. Selected bond length [Å] and torsion angles [°] for **MCA** and **ECA**.

	Bond lengths [Å]		Bond angles[°]		Torsion angles[°]	
MCA	C(1)-C(2)	1.689(3)	C(21)-C(1)-C(2)	117.1(2)	C(11)-C(12)-C(32)-C(33)	-47.02
					C(1)-C(2)-C(25)-C(38)	76.25
	C(2)-C(23)	1.432(3)	C(23)-C(2)-C(1)	117.2(19)	C(11)-C(12)-C(32)-C(31)	-126.03
					C(1)-C(2)-C(25)-C(26)	-101.90
	C(23)-C(24)	1.196(3)	C(24)-C(23)-C(2)	178.2(3)	C(29)-C(26)-C(33)-C(36)	-172.16
ECA	C(1)-C(2)	1.687(3)	C(11)-C(1)-C(2)	118.0(2)	C(2)-C(1)-C(15)-C(16)	34.04
	C(1)-C(11)	1.430(3)	C(20)-C(2)-C(1)	115.87(19)	C(2)-C(1)-C(15)-C(14)	-145.88
	C(11)-C(12)	1.185(3)	C(12)-C(11)-C(1)	176.0(3)	C(18)-C(16)-C(16A)-C(18A)	180.00

6. Electrochemical studies of the compounds

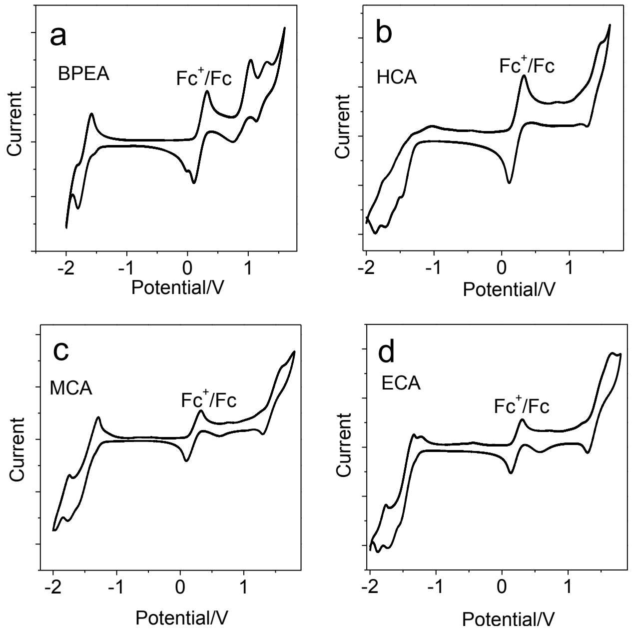


Fig. S15 Cyclic voltammogram of (a) **BPEA**, (b) **HCA**, (c) **MCA**, (d) **ECA**. For (a)–(d), c = 1.0 × 10^{-3} M. In deaerated CH_2Cl_2 solutions containing the compounds, 0.10 M Bu_4NPF_6 as supporting electrode, $Ag/AgNO_3$ as reference electrode, Scan rates: 100 mV/s. For all compounds Ferrocene (Fc) (c = 1.0 × 10^{-3} M) was used as internal reference. 20 °C.

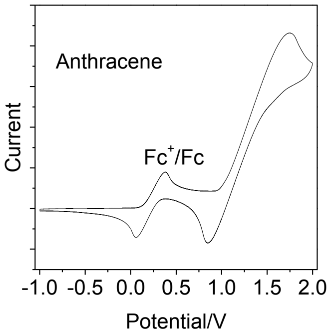


Fig. S16 Cyclic voltammogram of Anthracene, c = 1.0 × 10^{-3} M. In deaerated CH_2Cl_2 solutions containing the compounds, 0.10 M Bu_4NPF_6 as supporting electrode, $Ag/AgNO_3$ as reference electrode, Scan rates: 100 mV/s. Ferrocene (Fc) (c = 1.0 × 10^{-3} M) was used as internal reference. 20 °C.

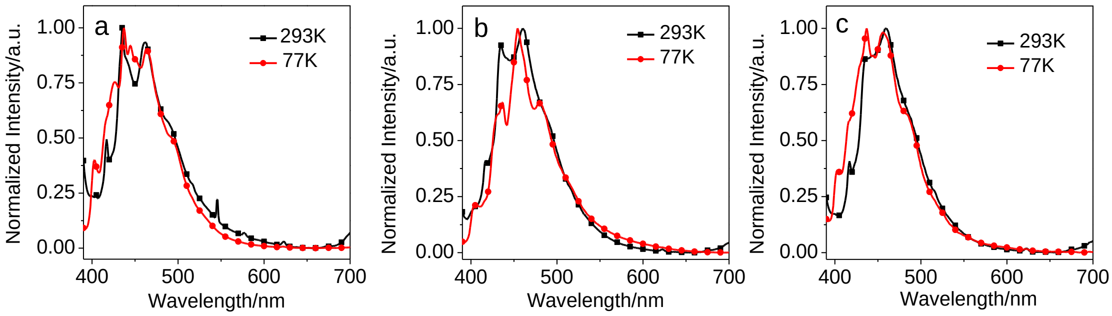


Fig. S17 Normalized PL spectra of (a) **HCA**, (b) **MCA**, (c) **ECA** in 2-MeTHF at r.t. (black line) and 77 K (red line).

7. NMR Spectra of all target compounds

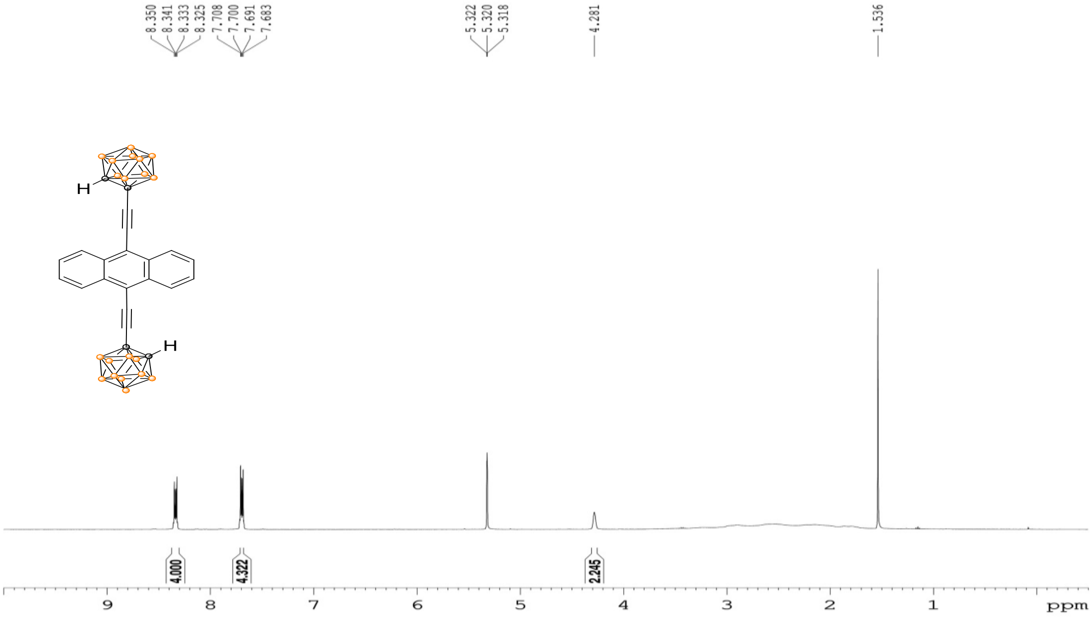


Fig. S18 ^{1}H NMR of **HCA** (400 MHz, CD_2Cl_2).

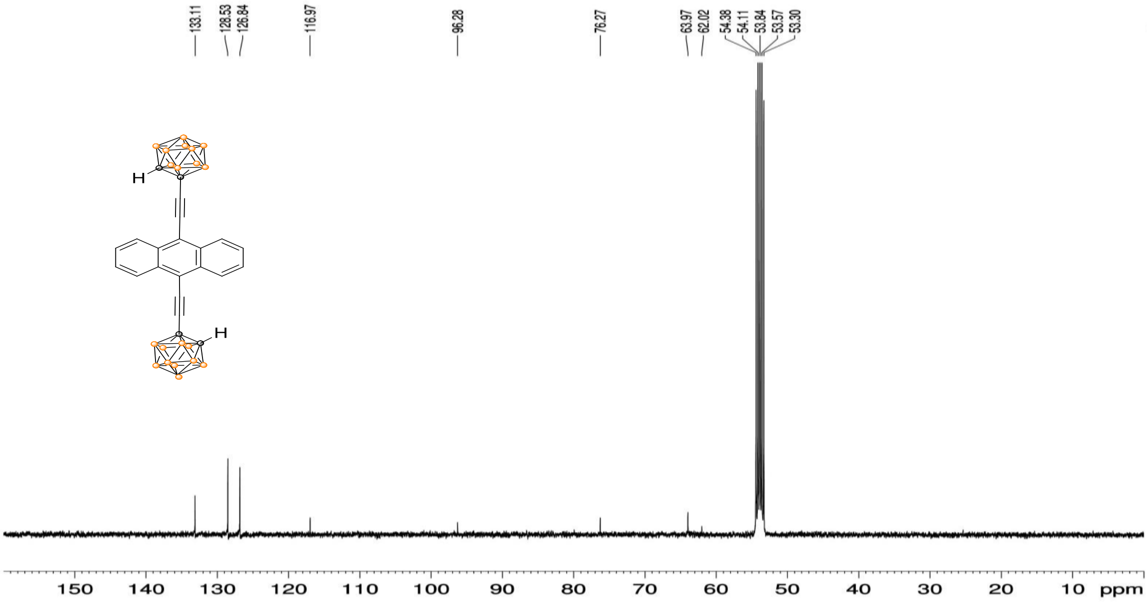


Fig. S19 $^{13}C\{^1H\}$ NMR of **HCA** (100 MHz, CD_2Cl_2).

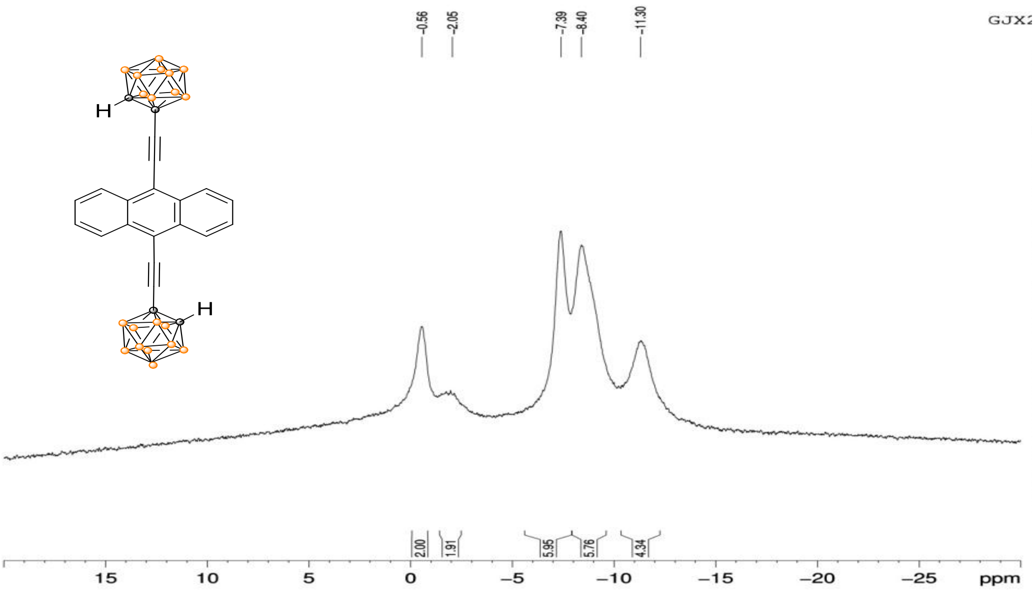
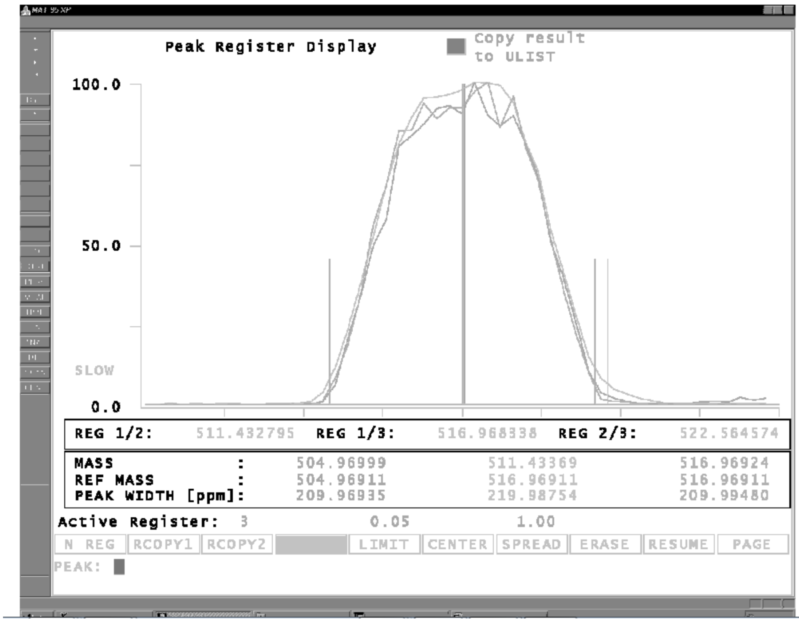


Fig. S20 $^{11}B\{^1H\}$ NMR of **HCA** (128 MHz, CD_2Cl_2).

Accurate Mass Measurement



```
REG 1/2:     511.432795   REG 1/3:     516.968338   REG 2/3:     522.564574

MASS              :     504.96999          511.43369          516.96924
REF MASS          :     504.96911          516.96911          516.96911
PEAK WIDTH [ppm]:       209.96935          219.98754          209.99480
Active Register:   3          0.05          1.00
PEAK:
```

Molecular formula
$C_{22}B_{20}H_{30}$
$[M]^+$ (theoretical)
= 511.4329

Fig. S21 HRMS of **HCA**.

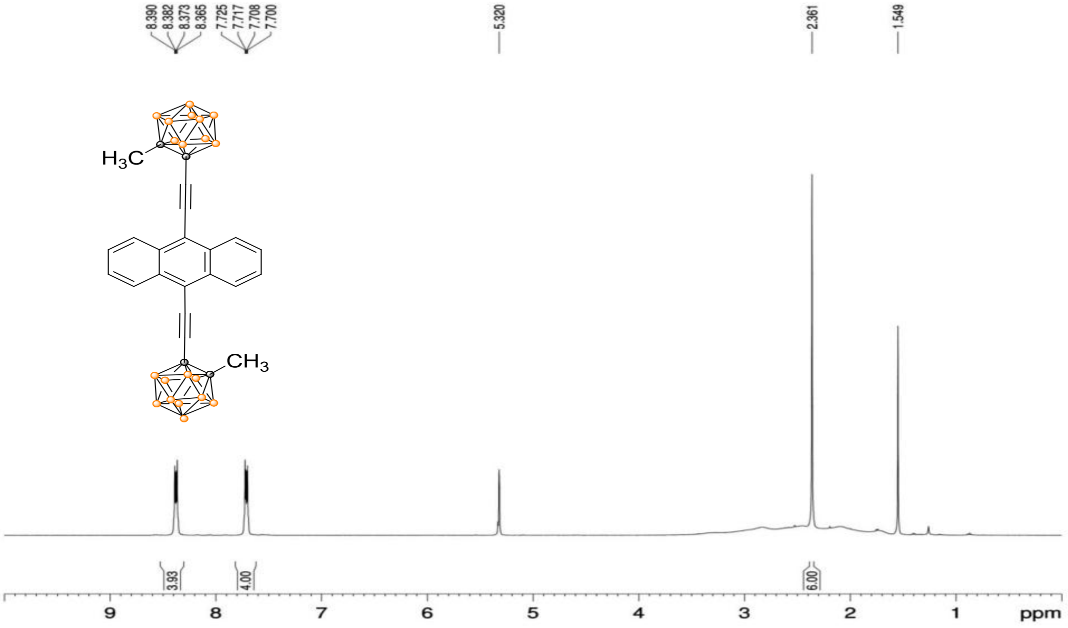


Fig. S22 ^{1}H NMR of **MCA** (400 MHz, CD_2Cl_2).

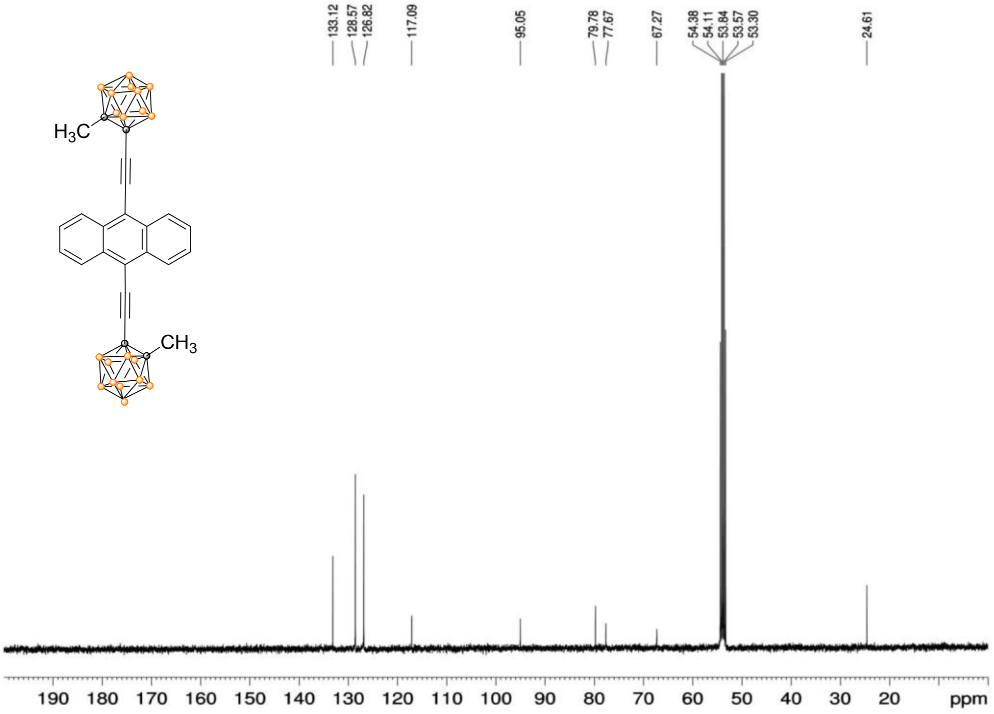


Fig. S23 $^{13}C\{^1H\}$ NMR of **MCA** (100 MHz, CD_2Cl_2).

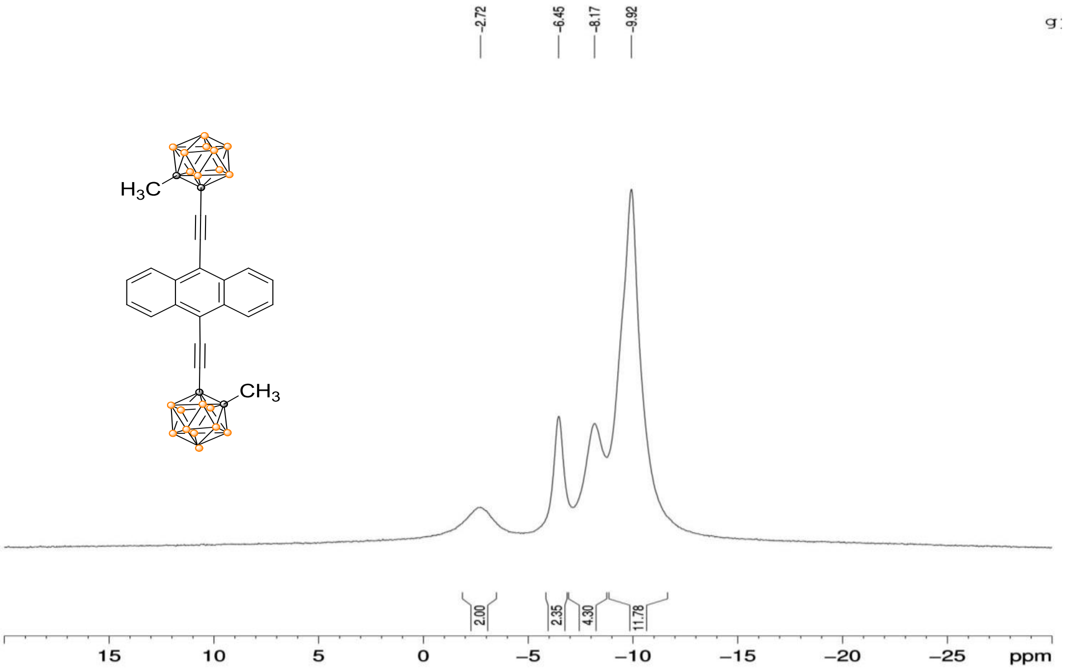
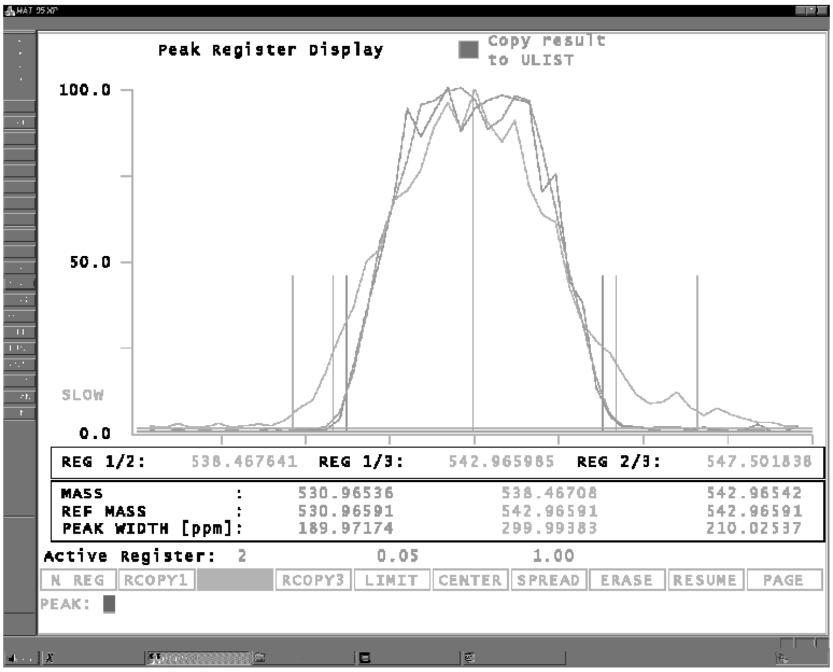


Fig. S24 $^{11}B\{^{1}H\}$ NMR of **MCA** (128 MHz, CD_2Cl_2).

Accurate Mass Measurement



```
REG 1/2:    538.467641  REG 1/3:     542.965985  REG 2/3:     547.501838

MASS             :    530.96536       538.46708       542.96542
REF MASS         :    530.96591       542.96591       542.96591
PEAK WIDTH [ppm]:     189.97174       299.99383       210.02537
Active Register:  2          0.05          1.00
```

Molecular formula
$C_{24}B_{20}H_{34}$
$[M]^+$ (theoretical)
= 538.4675

Fig. S25 HRMS of **MCA**.

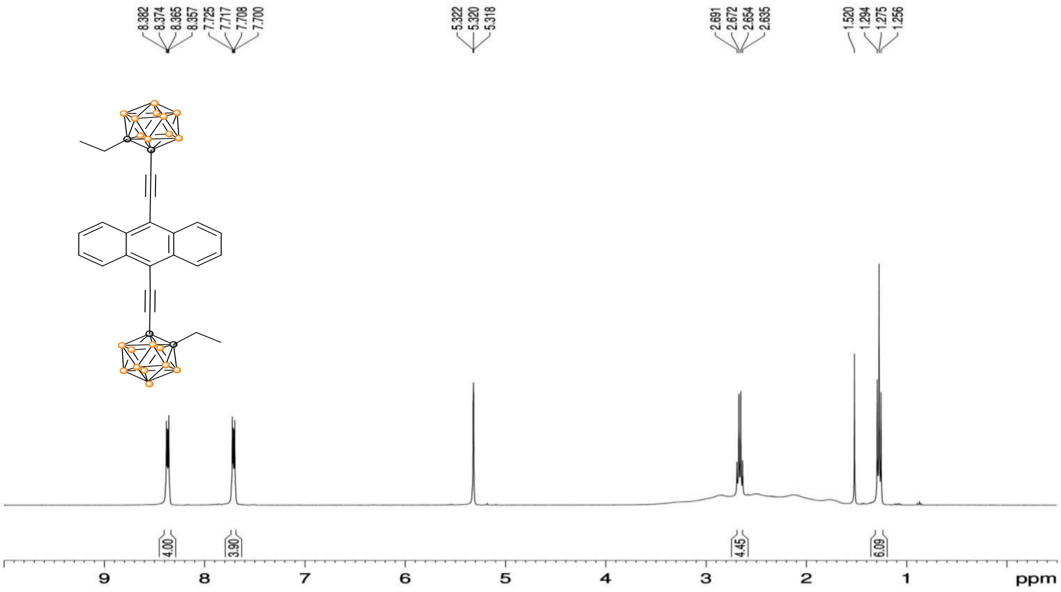


Fig. S26 ^{1}H NMR of **ECA** (400 MHz, CD_2Cl_2).

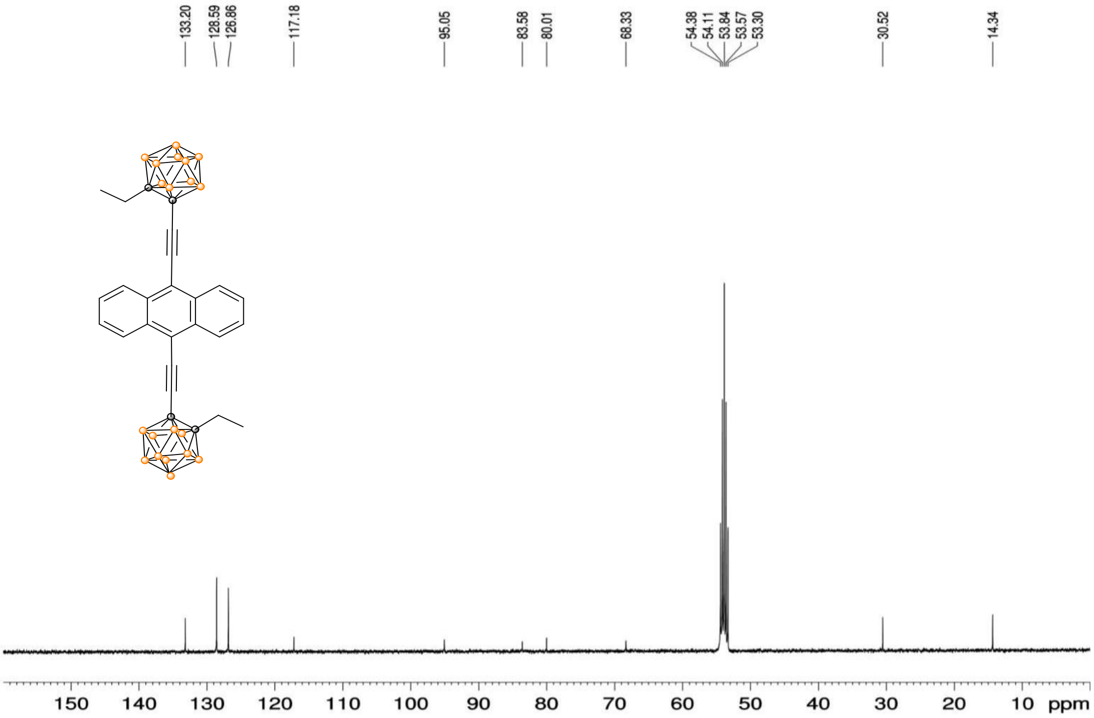


Fig. S27 $^{13}C\{^1H\}$ NMR of **ECA** (100 MHz, CD_2Cl_2).

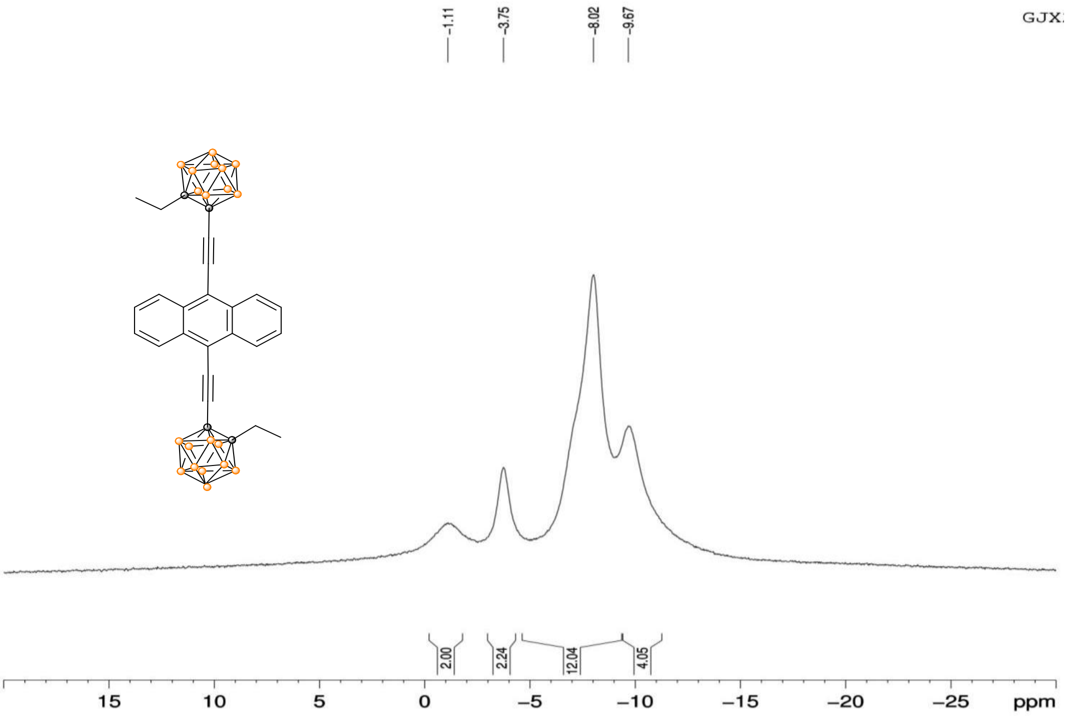
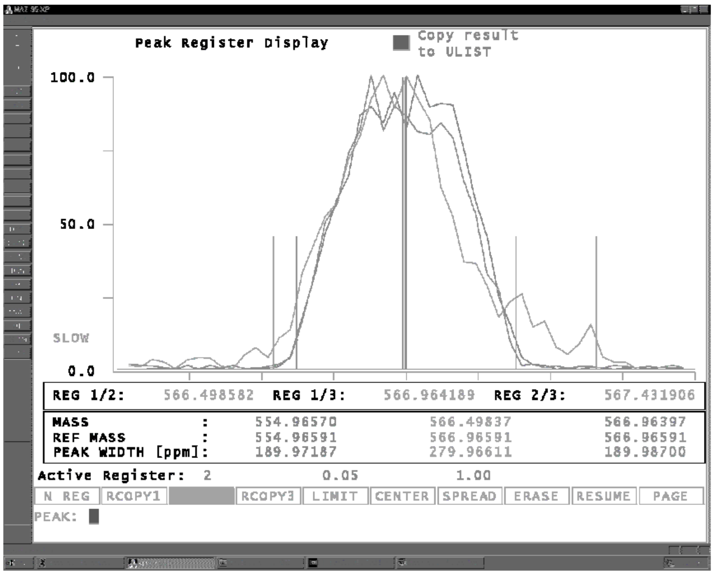


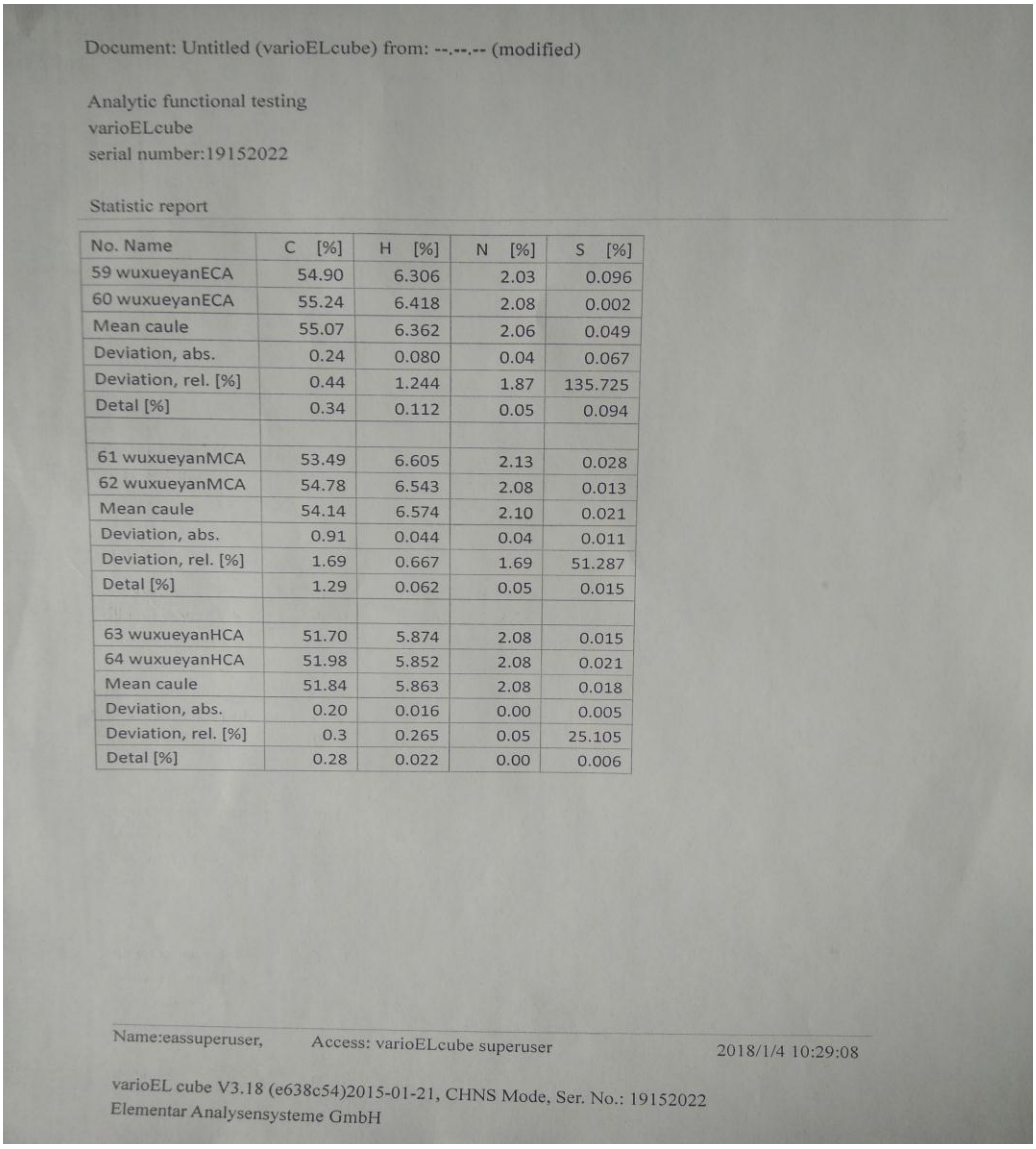
Fig. S28 $^{11}B\{^{1}H\}$ NMR of **ECA** (128 MHz, CD_2Cl_2).



```
REG 1/2:     566.498582  REG 1/3:     566.964189  REG 2/3:     567.431906

MASS               :   554.96570       566.49837       566.96397
REF MASS           :   554.96591       566.96591       566.96591
PEAK WIDTH [ppm]:      189.97187       279.96611       189.98700

Active Register:  2          0.05         1.00

PEAK:
```

Molecular formula
$C_{26}B_{20}H_{38}$
$[M]^+$ (theoretical)
= 566.4989

Fig. S29 HRMS of **ECA**.



Document: Untitled (varioELcube) from: --.--.-- (modified)

Analytic functional testing
varioELcube
serial number:19152022

Statistic report

No. Name	C [%]	H [%]	N [%]	S [%]
59 wuxueyanECA	54.90	6.306	2.03	0.096
60 wuxueyanECA	55.24	6.418	2.08	0.002
Mean caule	55.07	6.362	2.06	0.049
Deviation, abs.	0.24	0.080	0.04	0.067
Deviation, rel. [%]	0.44	1.244	1.87	135.725
Detal [%]	0.34	0.112	0.05	0.094
61 wuxueyanMCA	53.49	6.605	2.13	0.028
62 wuxueyanMCA	54.78	6.543	2.08	0.013
Mean caule	54.14	6.574	2.10	0.021
Deviation, abs.	0.91	0.044	0.04	0.011
Deviation, rel. [%]	1.69	0.667	1.69	51.287
Detal [%]	1.29	0.062	0.05	0.015
63 wuxueyanHCA	51.70	5.874	2.08	0.015
64 wuxueyanHCA	51.98	5.852	2.08	0.021
Mean caule	51.84	5.863	2.08	0.018
Deviation, abs.	0.20	0.016	0.00	0.005
Deviation, rel. [%]	0.3	0.265	0.05	25.105
Detal [%]	0.28	0.022	0.00	0.006

Name:eassuperuser, Access: varioELcube superuser 2018/1/4 10:29:08

varioEL cube V3.18 (e638c54)2015-01-21, CHNS Mode, Ser. No.: 19152022
Elementar Analysensysteme GmbH

Fig. S30 The elemental analysis of compounds of **HCA, MCA** and **ECA**.

Reference:

[1] (a) J. A. DuPont and M. F. Hawthorne, *J. Am. Chem. Soc.*, 1964, 86, 1642–1643; (b) J. Guo, D. Liu, J. Zhang, J. Zhang, Q. Miao and Z. Xie. Chem. Commun., 2015, 51, 12004–12007.