# Configuration-Controllable Synthesis of Z/E Isomers Based on *o*−Carborane−functionalized Tetraphenylethene

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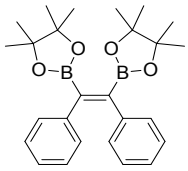
## CONTENTS

## I. General method

In this work, all the synthetic steps were carried out under an inert argon atmosphere using standard Schlenk and glovebox techniques. Commercial reagents were used without any further purification after purchasing. THF and toluene were distilled on sodium/benzophenone.(Z)-1,2-diphenyl-1,2-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethene (**Z-S1**),[S1] (E)-1,2-dibromo-1,2-diphenylethene (**E-S1**),[S2] were synthesized according to literature procedures. $B_{10}H_{12}(CH_3CN)_2$ was synthesized by a modified method according to literature reports.[S3] NMR spectra ($^1H$−, $^{13}C$−, and $^{11}B$−) were recorded on DRX−400 at ambient temperature. $CDCl_3$ was used as deuterated reagent unless specified. Mass spectra were measured with ESI−MS (LCQ Fleet, Thermo Fisher Scientific). UV−VIS absorption spectra were recorded with Shimadzu UV−3600 spectrophotometers. FL and PL spectra were recorded on a Hitachi F−7000 fluorescence spectrophotometer. Melting points were measured with X4 digital melting point displayer. Integrating Sphere (The FLS980 spectrometer) is used for measurements of fluorescence quantum yields and spectral reflectance. X−ray diffraction data were collected on a Bruker Smart CCD Apex DUO diffractometer with graphite monochromated Mo Kα radiation (λ = 0.71073 Å) using the ω−2θ scan mode.

## II. Synthesis and Spectral data

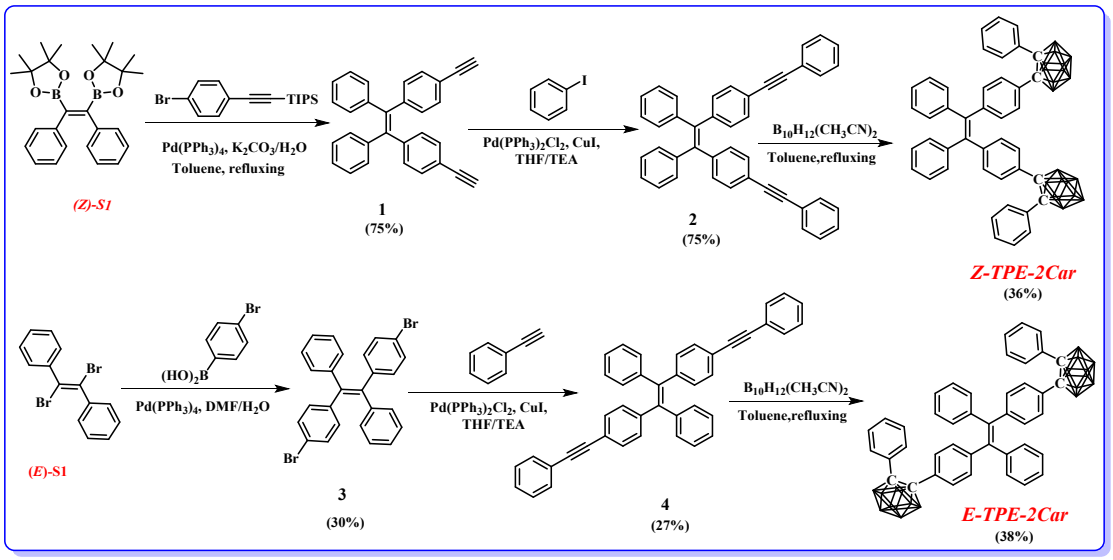


**(Z-S1). Preparation of (Z)-1,2-diphenyl-1,2-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethane**

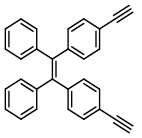
To a degassed solution of diphenylacetylene (1958 mg, 11 mmol) and bis(pinacolato)diboron (2.539 g, 10 mmol) in DMF (10 mL) was added $Pt(PPh_3)_4$ (248 mg, 2.0 mol%). The reaction mixture was heated to 80℃ for 24 hours. After this time, the reaction was diluted with $Et_2O$ (20 mL) and washed with saturated aqueous $NH_4Cl$(2 x 10 mL). The organic phase was dried over $MgSO_4$ and concentrated under reduced pressure. Recrystallisation from EtOH afforded the title compound as a white

solid (3.80 g, 8.8 mmol, 88%). $^1$H-NMR (400 MHz, Chloroform-*d*) δ 7.05 (p, *J* = 6.9 Hz, 6H, Ar-*H*), 6.94 (d, *J* = 7.0 Hz, 4H, Ar-*H*), 1.32 (s, 24H, C*H*$_3$).

**2. Synthesis of compounds *Z*-TPE-2Car and *E*-TPE-2Car.**



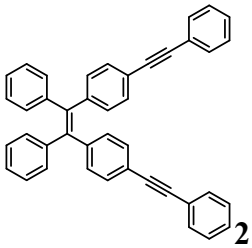

**Scheme S1.** Synthesis of compounds **Z-TPE-2Car and E-TPE-2Car**.



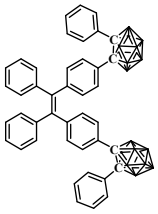
**1**:To a toluene degassed solution (100mL) of (Z)-1,2-diphenyl-1,2-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethane (1.30 g, 3 mmol, 1 equiv), ((4-bromophenyl)ethynyl)triisopropylsilane (3.04 g, 9 mmol, 3 equiv), $K_2CO_3$ (1.944 g, 18 mmol, 6 equiv), $Pd(PPh_3)_4$ (176 mg, 5 mol%), was added at room temperature. The resulting reaction mixture was refluxed for 24 h. Subsequently, the solvent was removed in vacuum, and then the reaction mixture was extracted by $CH_2Cl_2$ and washed with water and brine. The organic layer was dried over $Na_2SO_4$, concentrated in vacuum and purified with a silica column (eluent: PE) to afford the product as pale yellow solid.

The soild from above was dissolved in THF (40 mL). TBAF (9 mL, 9 mmol) was added. The solution was stirred at room temperature overnight. Subsequently, the solvent was removed in vacuum, and then the reaction mixture was extracted by $CH_2Cl_2$ and washed with water and brine. The organic layer was dried over $Na_2SO_4$, concentrated in vacuum and purified with a silica column (eluent: PE : DCM = 5 : 1 )

to afford the product as white solid （0.86 g， 75%）. $^{1}$H-NMR (400 MHz, Chloroform-*d*) $\delta_{H/ppm}$ 7.24 (s, 2H, Ar-*H*), 7.12 – 7.08 (m, 8H, Ar-*H*), 7.00 (d, *J* = 4.6 Hz, 8H, Ar-*H*), 3.05 (s, 2H, CC*H*). $^{13}$C-NMR (101 MHz, $CDCl_3$) δ 144.04, 142.93, 140.89, 131.62, 131.24, 127.93, 127.77, 126.79, 120.19, 83.63, 77.48, 77.32, 77.00, 76.68. HRMS (APCI-FTMS): *m/z* calcd for $C_{30}H_{20}$; [M+H] 381.4980; found 381.1631.

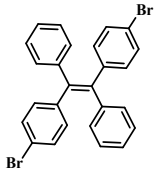


**2**: $Pd(PPh_3)_2Cl_2$ (53 mg, 0.075 mmol) was added to a degassed solution of **1** (0.60 g, 1.5 mmol), Iodobenzene (0.9643 mg, 4.50 mmol), $PPh_3$ （39 mg, 0.15 mmol）and CuI (29 mg, 0.15 mmol) in triethylamine (60 mL) and toluene (100 mL). The resulting mixture was stirred at room temperature overnight under a $N_2$ atmosphere. The reaction mixture was poured into a 10% $NH_4Cl$ solution and extracted with $CH_2Cl_2$. The organic layer was washed with water, dried over $Na_2SO_4$, and concentrated under reduced pressure. The residue was purified by recrystallization from $CH_2Cl_2$ /PE(5:1) to afford **2** (600 mg, 75%).$^{1}$H-NMR (400 MHz, Chloroform-*d*) δ 7.53 – 7.49 (m, 4H, Ar-*H*), 7.36 – 7.29 (m, 10H, Ar-*H*), 7.13 (dd, J = 4.0, 2.4 Hz, 6H, Ar-*H*), 7.06 – 7.02 (m, 8H, Ar-*H* ). $^{13}$C-NMR (101 MHz, Chloroform-d) δ 143.61, 143.09, 140.91, 131.54, 131.36, 131.07, 130.93, 128.29, 128.17, 127.91, 127.75, 126.74, 123.23, 121.34, 89.79, 89.44. HRMS (APCI-FTMS): *m/z* calcd for $C_{42}H_{28}$; [M+H] 533.6940; found 533.2267.

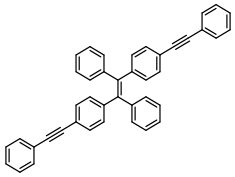


**Z-TPE-2Car:** To a toluene solution (80 mL) of (Z)-1,2-diphenyl-1,2-bis(4-(phenylethynyl)phenyl)ethene (**2**) (0.600 g, 1.13 mmol), $B_{10}H_{12}(CH_3CN)_2$ (0.670 g, 3.28mmol) was added at room temperature. The resulting reaction mixture was refluxed for three days. MeOH (40 mL) was then added to quench the reaction. Excessive solvent was removed under vacuum, and the resulting solid was filtered and dissolved in $CH_2Cl_2$. After removal of solvent, an orange red solid was afforded. The

crude product was purified by column chromatography using PE / $CH_2Cl_2$ (V / V = 7:1) as eluent and afford **Z-TPE-2Car** as a yellow solid (0.31 g, 36%).$^1$H-NMR (400 MHz, Chloroform-*d*) δ 7.38 (t, *J* = 8.3 Hz, 6H), 7.23 (t, *J* = 7.8 Hz, 4H), 7.04 (dd, *J* = 10.8, 8.1 Hz, 10H, Ar-*H*), 6.70 (d, *J* = 6.8 Hz, 4H, Ar-*H*), 6.57 (d, *J* = 8.4 Hz, 4H Ar-*H*). $^{13}$C-NMR (101 MHz, $CDCl_3$) δ 144.81, 142.58, 140.08, 131.03, 130.91, 130.62, 130.07, 128.90, 128.17, 127.73, 126.93, 85.17, 84.99, 77.32, 77.00, 76.68. $^{11}$B-NMR (128 MHz, Chloroform-d) δ -1.90 (12B), -8.52 (8B). HRMS (APCI-FTMS): *m/z* calcd for $C_{42}H_{48}B_{20}$; [M] 769.0460; found 768.5791. Melting Point: 236-238 ℃.

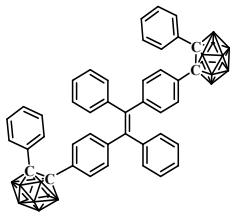



**3：** To a DMF solution (80mL) of (E)-1,2-dibromo-1,2-diphenylethene **(E-S1)** (2.0g, 5.92 mmol, 1 equiv), (4-bromophenyl)boronic acid (3.2 g, 15.9 mmol, 3 equiv), $K_3PO_4$ (1.26 g, 5.92 mmol, 1 equiv), $Pd(PPh_3)_4$ (156 mg, 3 mol%), was added at room temperature. The resulting reaction mixture was refluxed for 24 h. Subsequently, the solvent was removed in vacuum, and then the reaction mixture was extracted by $CH_2Cl_2$ and washed with water and brine. The organic layer was dried over $Na_2SO_4$, concentrated in vacuum and purified with a silica column (PE : DCM = 10:1) to afford the product as a white solid. $^1$H-NMR (400 MHz, Chloroform-d) δ 7.30 – 7.18 (m, 4H, Ar-*H*), 7.14 – 7.08 (m, 7H, Ar-*H*), 7.00 (dh, J = 9.7, 3.6 Hz, 5H, Ar-*H*), 6.91 – 6.87 (m, 2H, Ar-*H*). $^{13}$C-NMR (101 MHz, Chloroform-d) δ 143.39, 143.30, 143.20, 142.90, 142.68, 142.28, 141.59, 140.28, 139.64, 132.95, 132.87, 131.27, 131.20, 131.08, 130.83, 128.00, 127.86, 127.76, 127.66, 126.82, 126.68, 126.62, 126.57, 120.77, 120.42. HRMS (APCI-FTMS): *m/z* calcd for $C_{26}H_{18}Br_2$; [M+H] 491.2460; found 491.9734.



**4：** $Pd(PPh_3)_2Cl_2$ (55 mg, 0.078 mmol) was added to a degassed

solution of **3** (0.75 g, 1.53 mmol), ethynylbenzene (0.62g, 6.09 mmol), $PPh_3$ （105 mg, 0.38 mmol）and CuI (25 mg, 0.13 mmol) in triethylamine (50 mL) and toluene (50 mL). The resulting mixture was heated to 80℃ overnight under a $N_2$ atmosphere. The reaction mixture was poured into a 10% $NH_4Cl$ solution and extracted with $CH_2Cl_2$. The organic layer was washed with water, dried over $Na_2SO_4$, and concentrated under reduced pressure. The residue was purified by recrystallization from PE / $CH_2Cl_2$ (7:1) to afford **4** (220 mg, 27%) . $^1$H-NMR (400 MHz, Chloroform-d) δ 7.50 (dd, J = 6.4, 3.0 Hz, 4H, Ar-*H*), 7.36 – 7.28 (m, 9H, Ar-*H*), 7.19 – 7.09 (m, 7H, Ar-*H*), 7.03 (d, J = 8.4 Hz, 8H, Ar-*H*).$^{13}$C-NMR (101 MHz, Chloroform-*d*) δ 143.10, 140.93, 131.55, 131.36, 131.08, 130.94, 128.30, 128.18, 127.92, 127.75, 126.74, 121.35, 89.79, 89.45. HRMS (APCI-FTMS): *m/z* calcd for $C_{42}H_{28}$; [M+H] 533.6940; found 533.2264.



***E*-TPE-2Car:** To a toluene solution (50 mL) of (E)-1,2-diphenyl-1,2-bis(4-(phenylethynyl)phenyl)ethene (**4**) (0.220g, 0.41 mmol), $B_{10}H_{12}(CH_3CN)_2$ (0.40 g, 1.96mmol) was added at room temperature. The resulting reaction mixture was refluxed for three days. MeOH (20 mL) was then added to quench the reaction. Excessive solvent was removed under vacuum, and the resulting solid was filtered and dissolved in $CH_2Cl_2$. After removal of solvent, a yellow solid was afforded. The crude product was purified by column chromatography using PE / $CH_2Cl_2$ (V / V = 7:1) as eluent and afford ***E*-TPE-2Car** as a light yellow solid (0.12 g, 38%). $^1$H-NMR (400 MHz, Methylene Chloride-$d^2$) δ 7.41 (t, J = 7.9 Hz, 7H, Ar-H), 7.25 (t, J = 7.7 Hz, 4H, Ar-H), 7.06 (dd, J = 18.1, 7.9 Hz, 9H， Ar-H), 6.73 (d, J = 7.0 Hz, 4H, Ar-H), 6.59 (d, J = 8.3 Hz, 4H, Ar-H ). $^{13}$C-NMR (101 MHz, Methylene Chloride-d) δ 145.35, 131.37, 131.25, 131.04, 130.60, 130.52, 128.62, 128.08, 127.23, 85.81, 54.38, 54.11, 53.84, 53.57, 53.30. $^{11}$B-NMR (160 MHz, Chloroform-*d*) δ -2.57 (4B), -10.67 (16B). HRMS (APCI-FTMS): *m/z* calcd for $C_{42}H_{48}B_{20}$; [M+ H] 769.0460; found 769.5775. Melting

Point: 237-239℃.

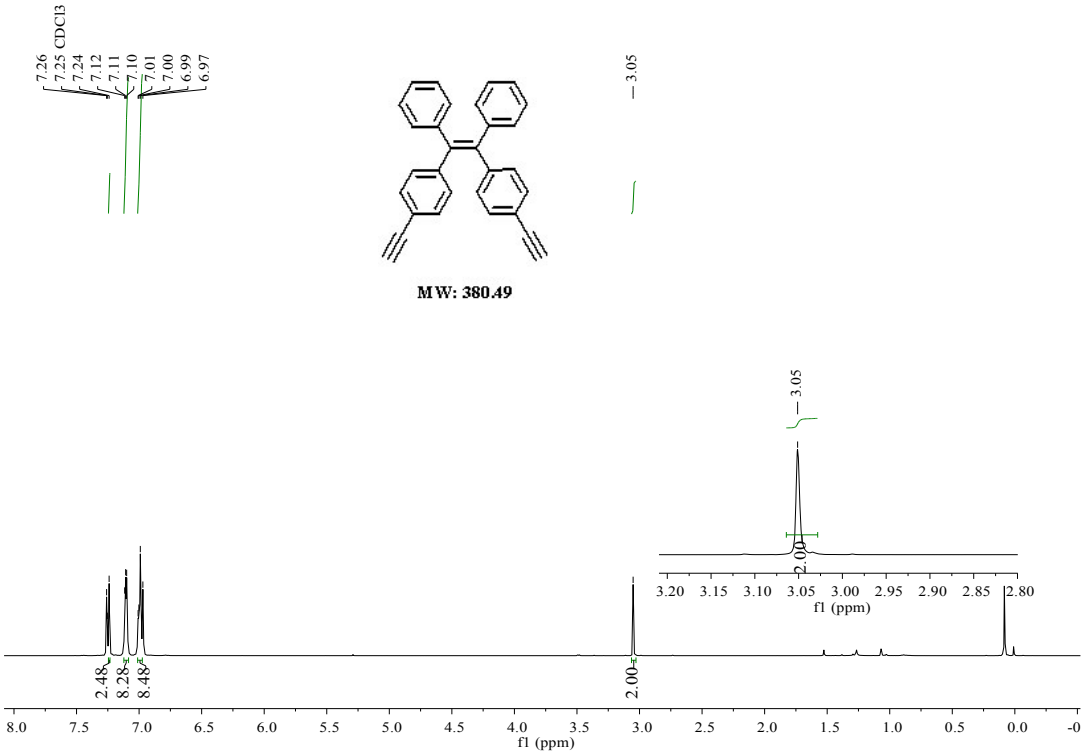



Figure.S1 The $^{1}$H-NMR (400 MHz, Chloroform-d) spectrum of compound **1**.

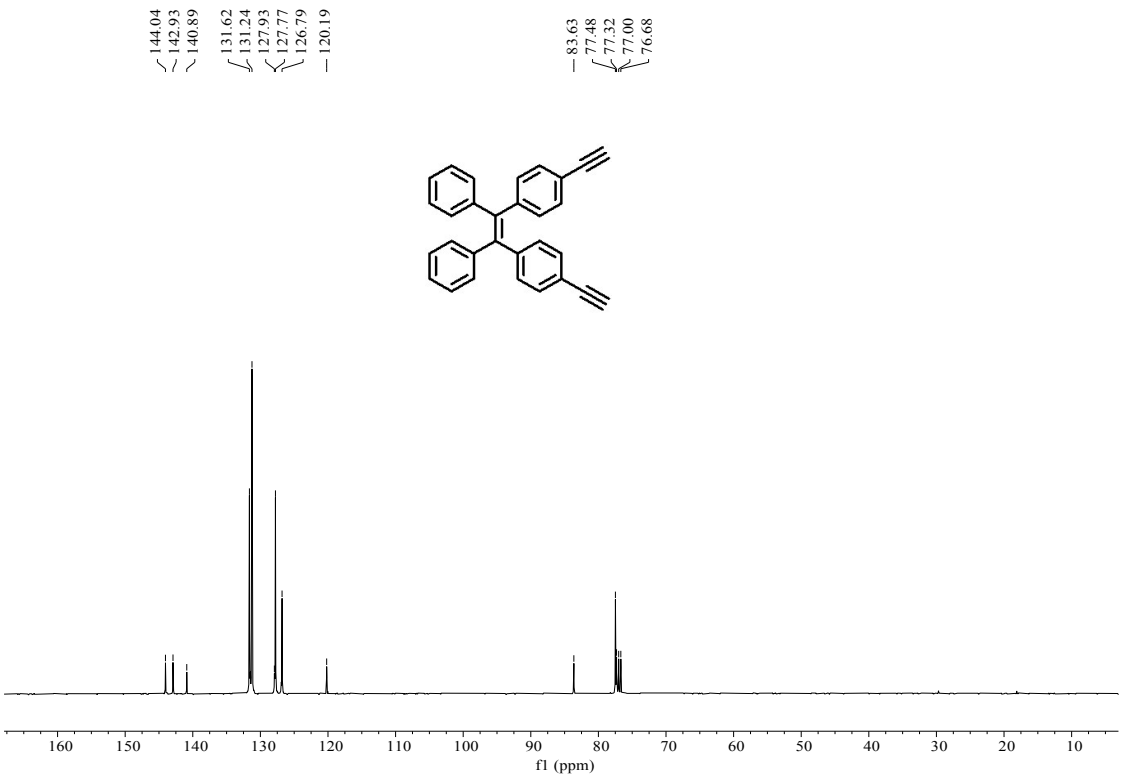


Figure S2. The $^{13}$C-NMR (101 MHz, Chloroform-*d*) spectrum of compound **1**.

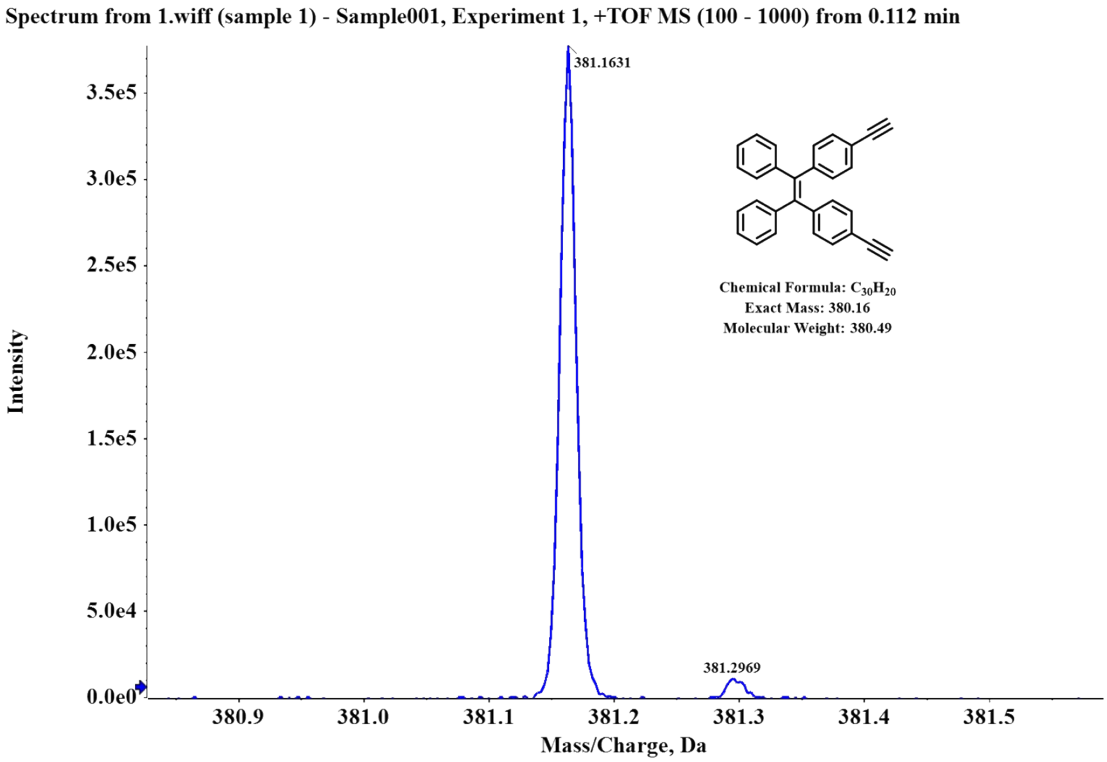



Figure.S3. The HRMS (APCI) spectrum of compound **1**.

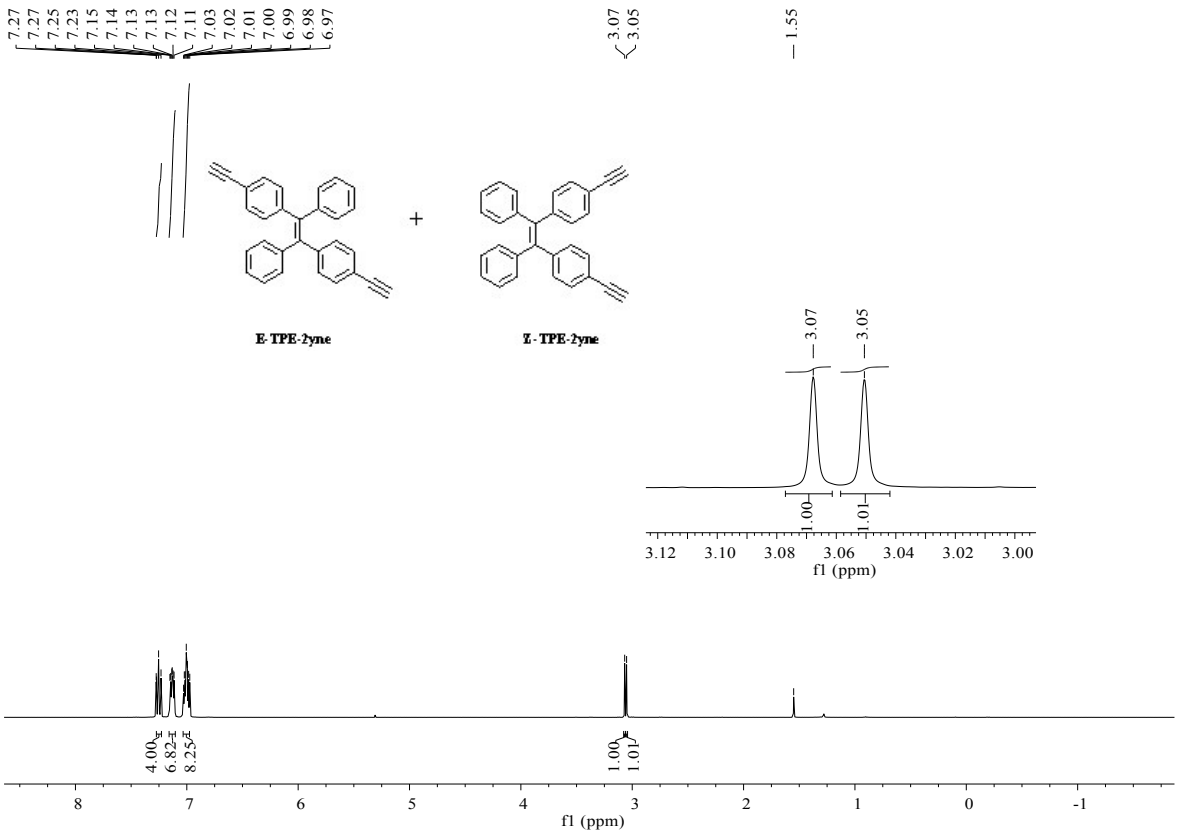



Figure.S4 The $^{1}$H-NMR (400 MHz, Chloroform-d) spectrum of isomers **1** (by McMurry method).

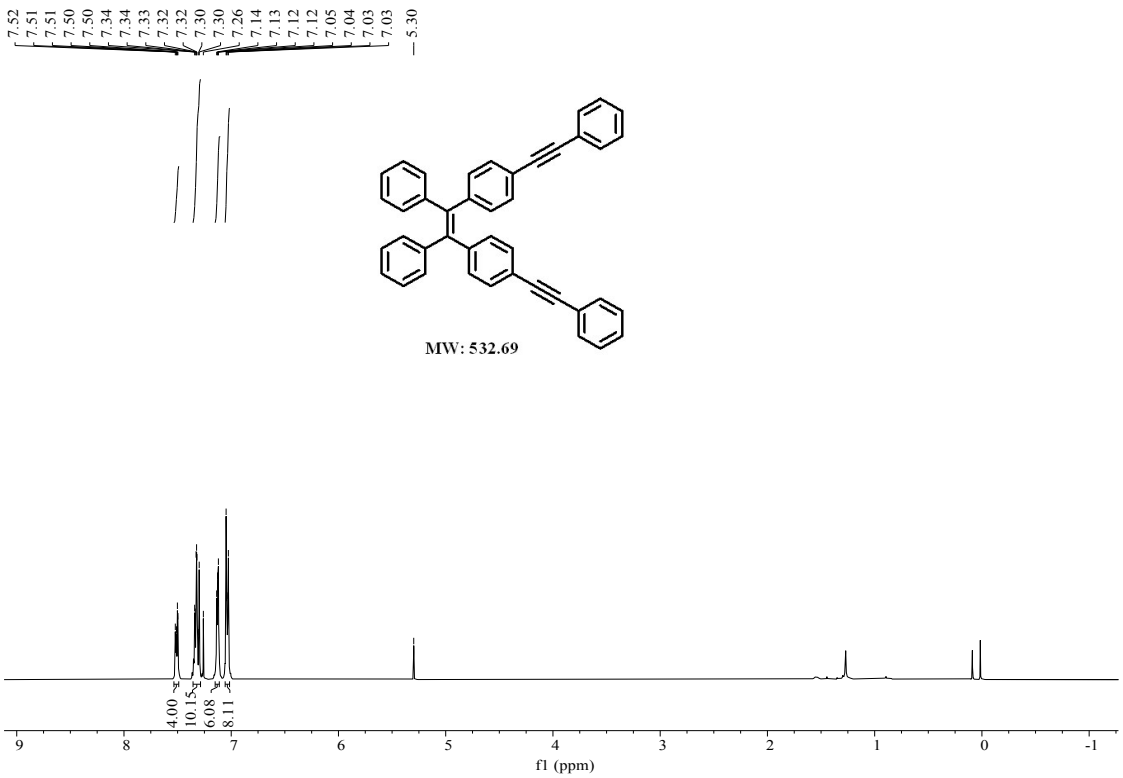



Figure S5. The $^{1}$H-NMR (400 MHz, Chloroform-d) spectrum of compound **2**.

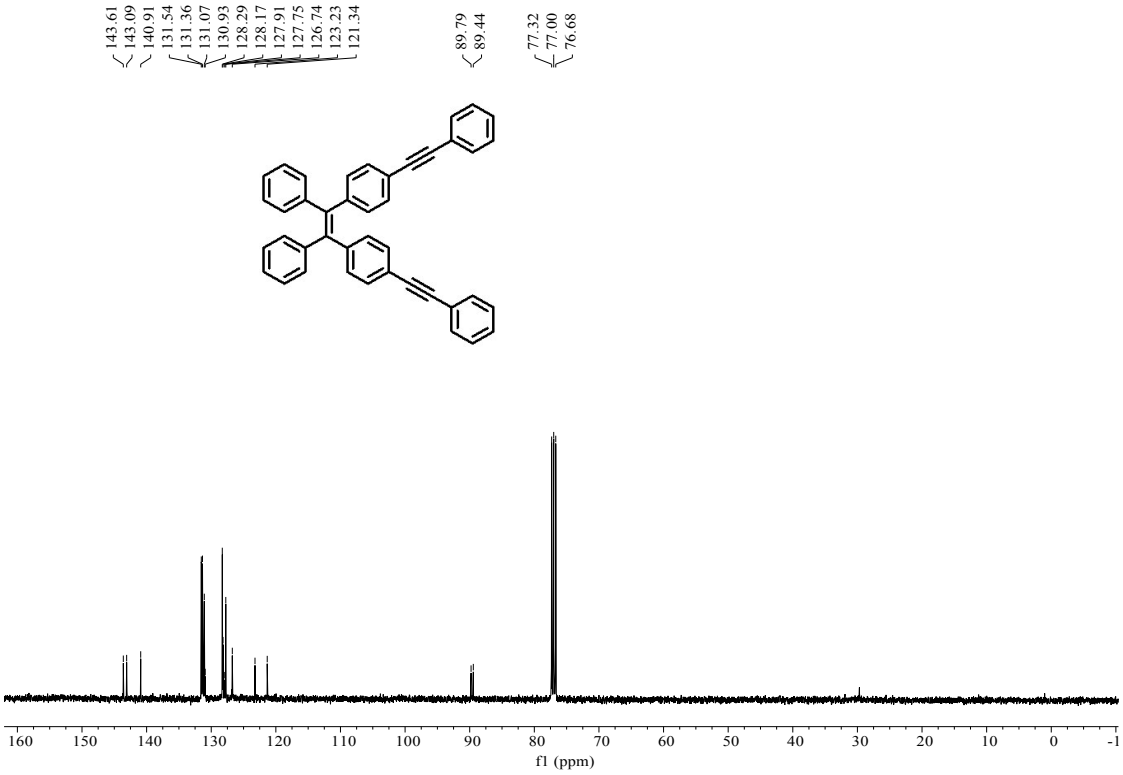


Figure S6. The $^{13}$C-NMR (101 MHz, Chloroform-*d*) spectrum of compound 2.

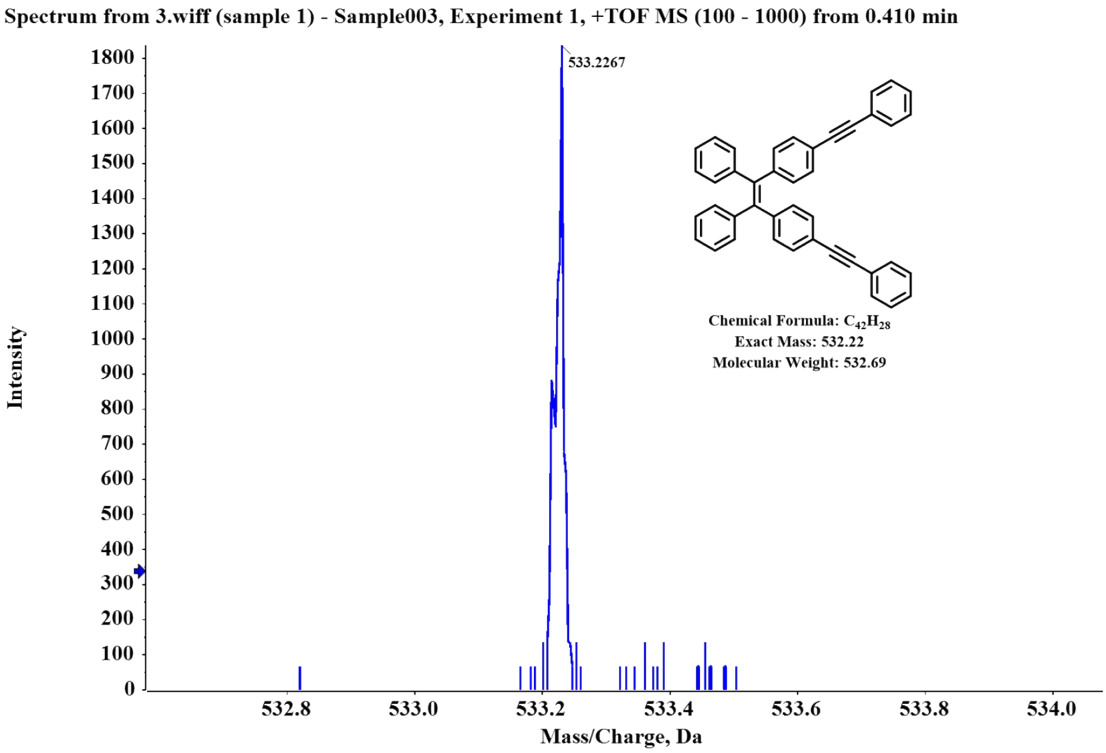



Figure.S7. The HRMS (APCI) spectrum of compound **2**.

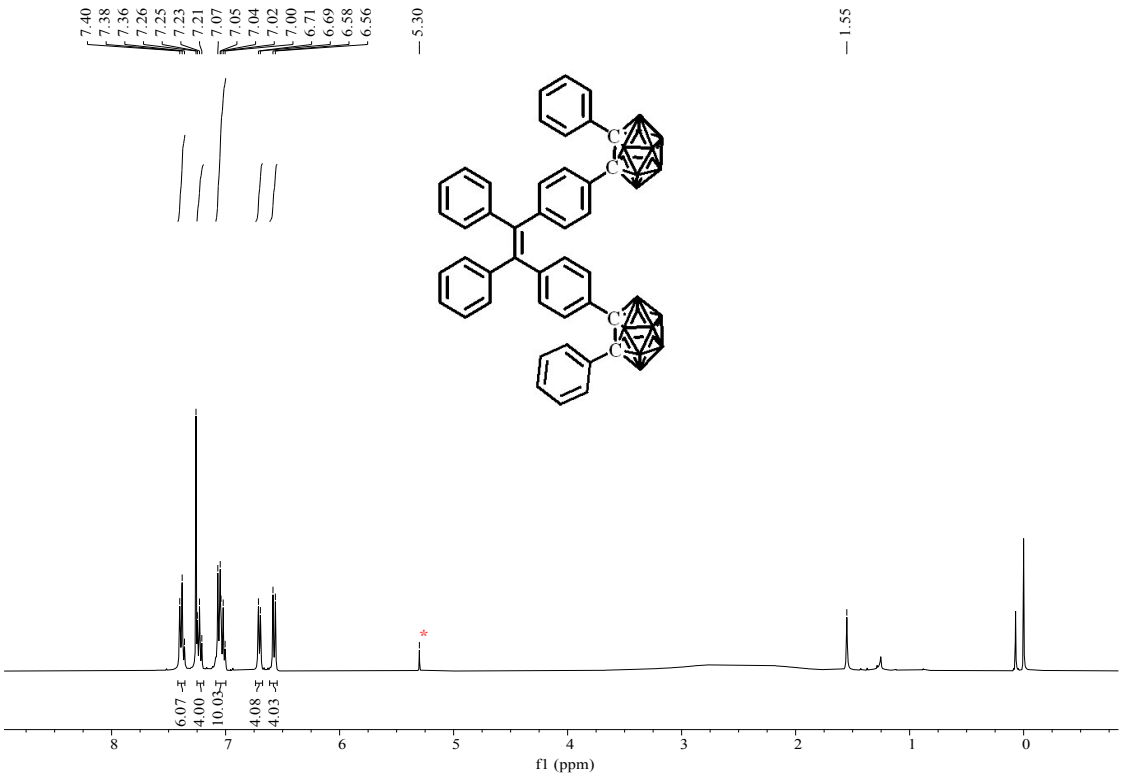



Figure S8. The $^{1}$H-NMR (400 MHz, Chloroform-d) spectrum of compound **Z-TPE-2Car**.

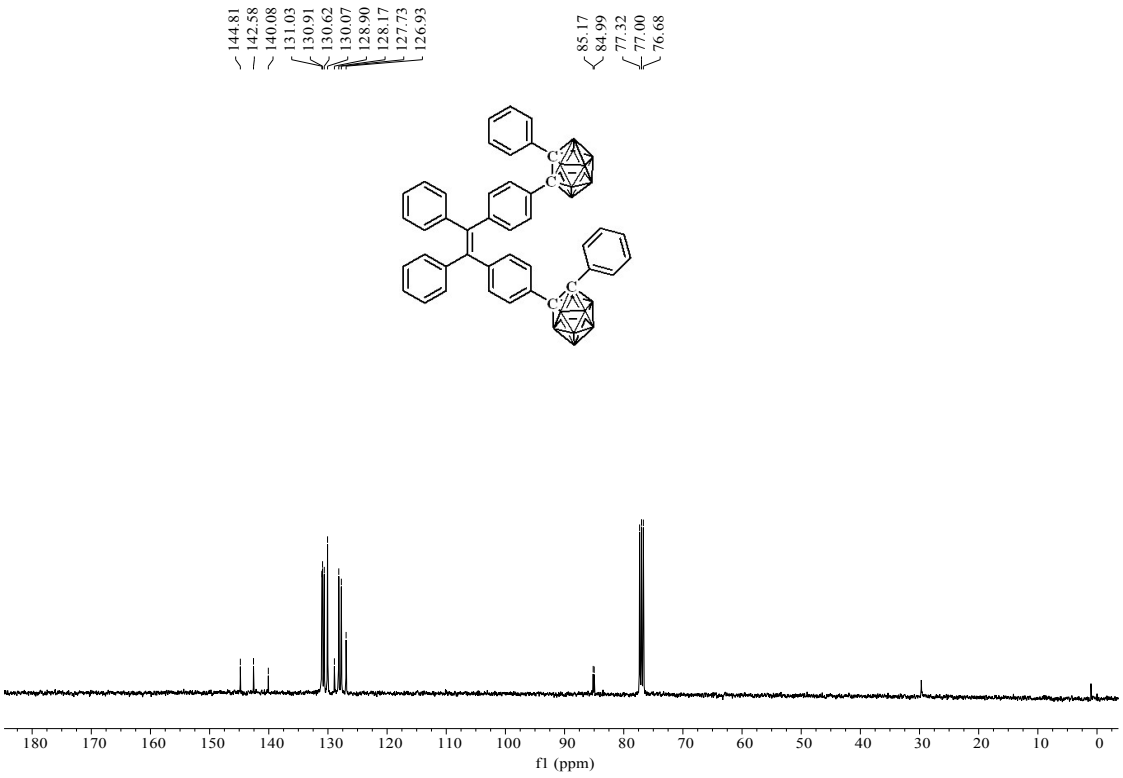


Figure S9. The $^{13}$C-NMR (101 MHz, Chloroform-*d*) spectrum of compound ***Z*-TPE-2Car**.

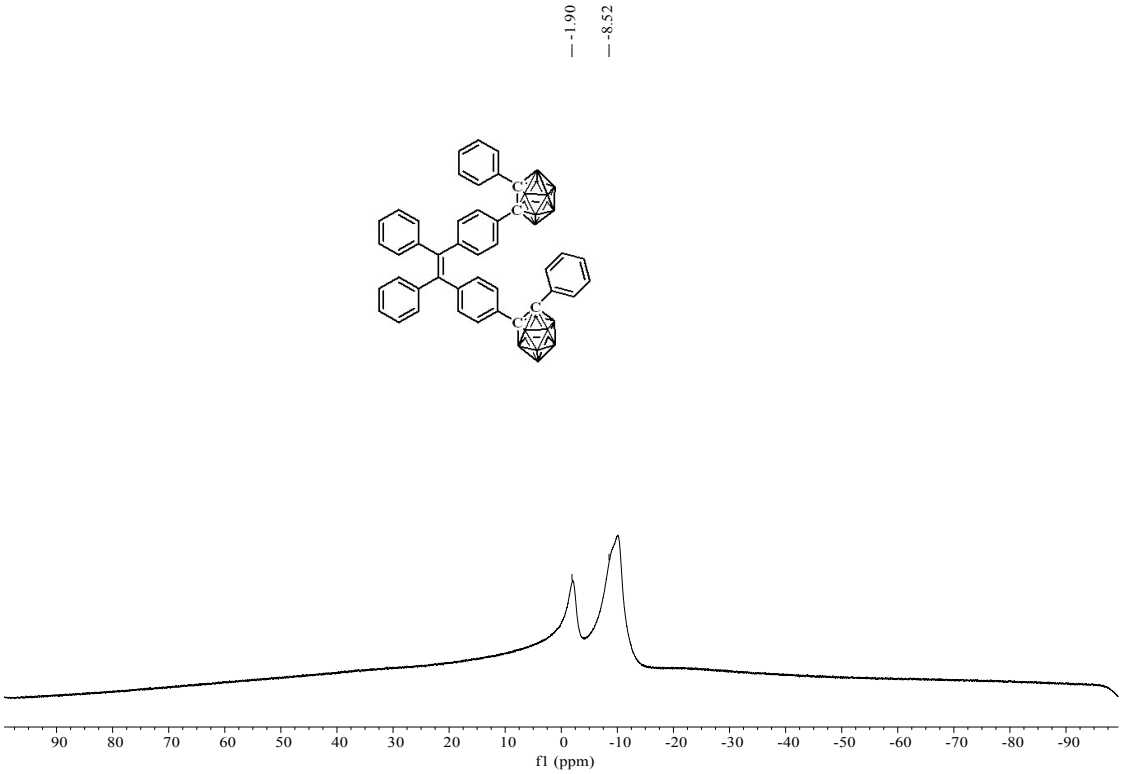



Figure.S10. The $^{11}$B−NMR (160 MHz, $CDCl_3$) spectrum of compound ***Z*-TPE-2Car**.

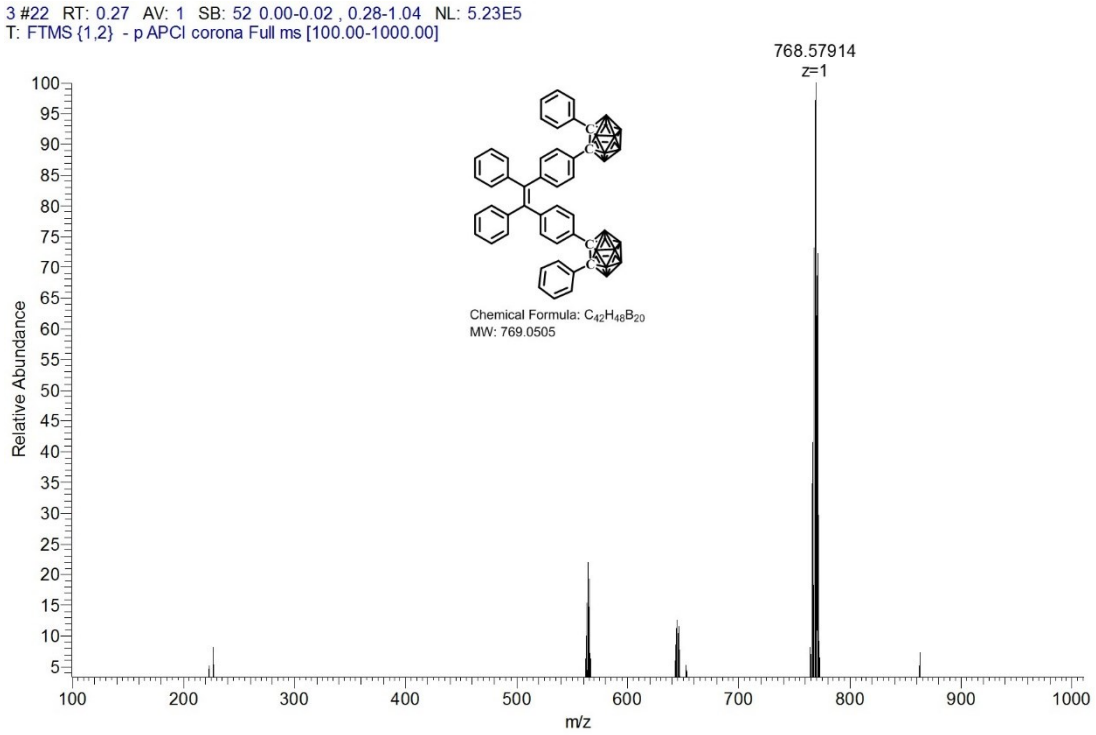



Figure.S11. The HRMS (APCI) spectrum of compound ***Z*-TPE-2Car**.

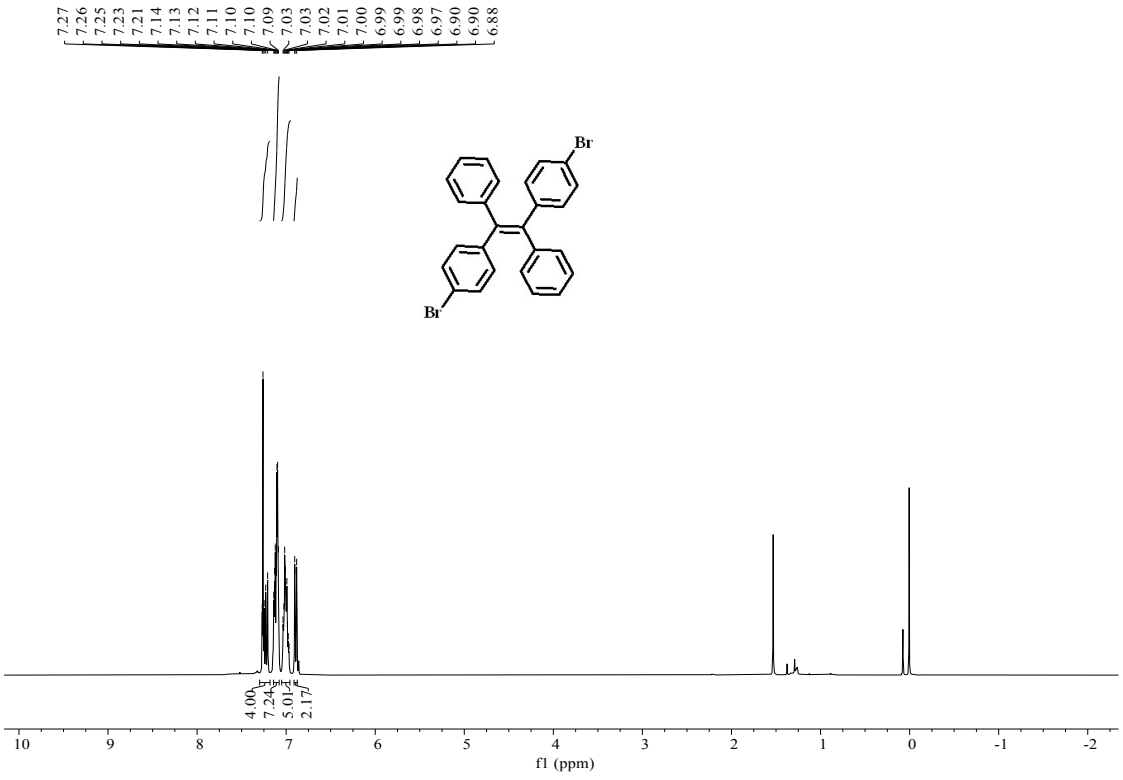



Figure S12. The $^{1}$H-NMR (400 MHz, Chloroform-d) spectrum of compound **3**.

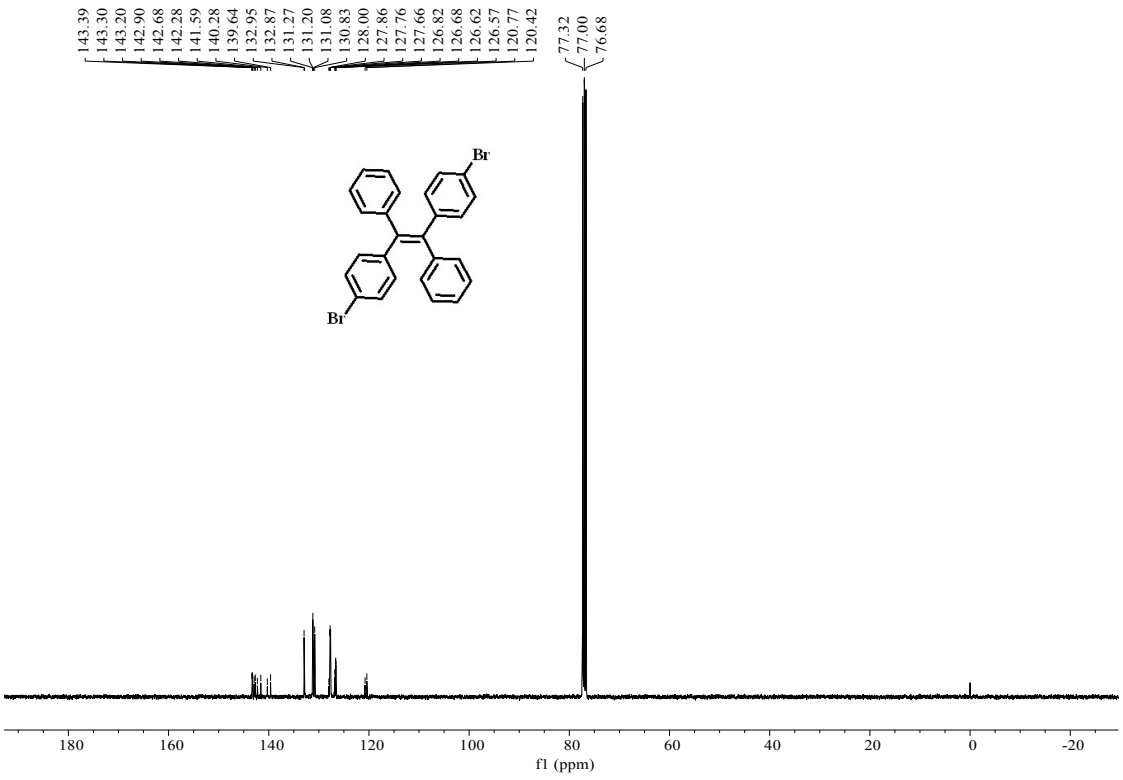


Figure S13. The $^{13}$C-NMR (101 MHz, Chloroform-*d*) spectrum of compound **3**.

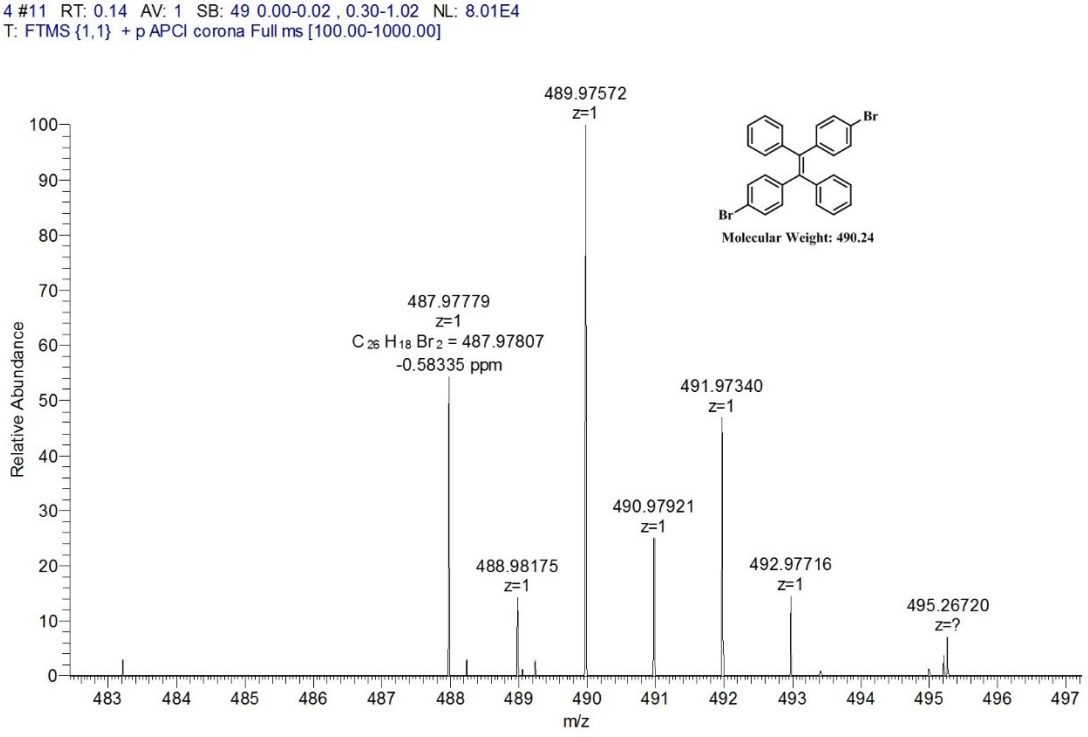



Figure S14. The HRMS (APCI) spectrum of compound **3**.

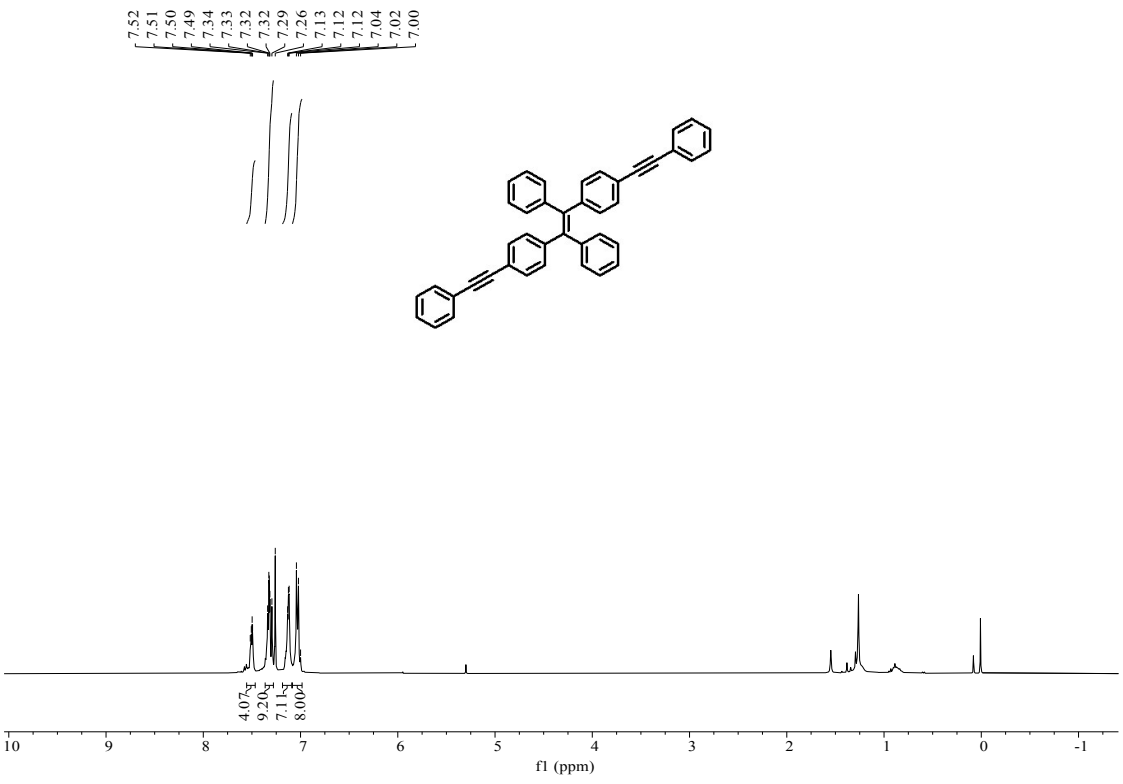



Figure S15. The $^{1}$H-NMR (400 MHz, Chloroform-d) spectrum of compound **4**.

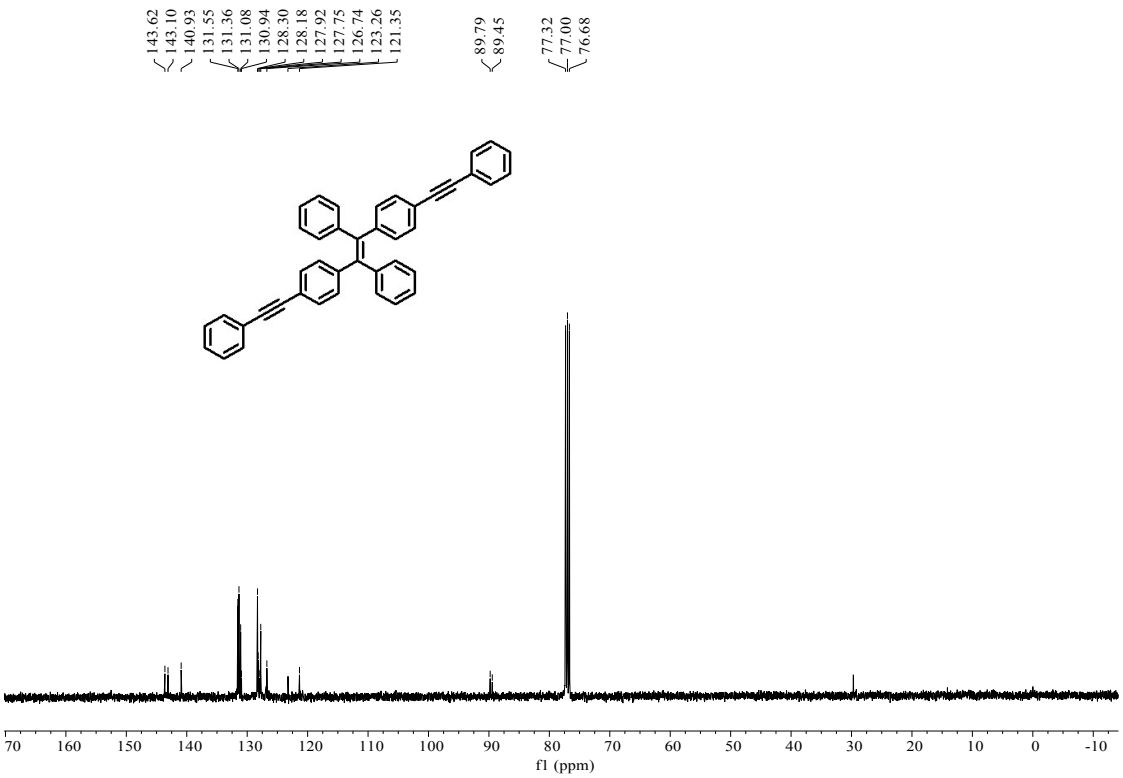



Figure S16. The $^{13}$C-NMR (101 MHz, Chloroform-*d*) spectrum of compound **4**.

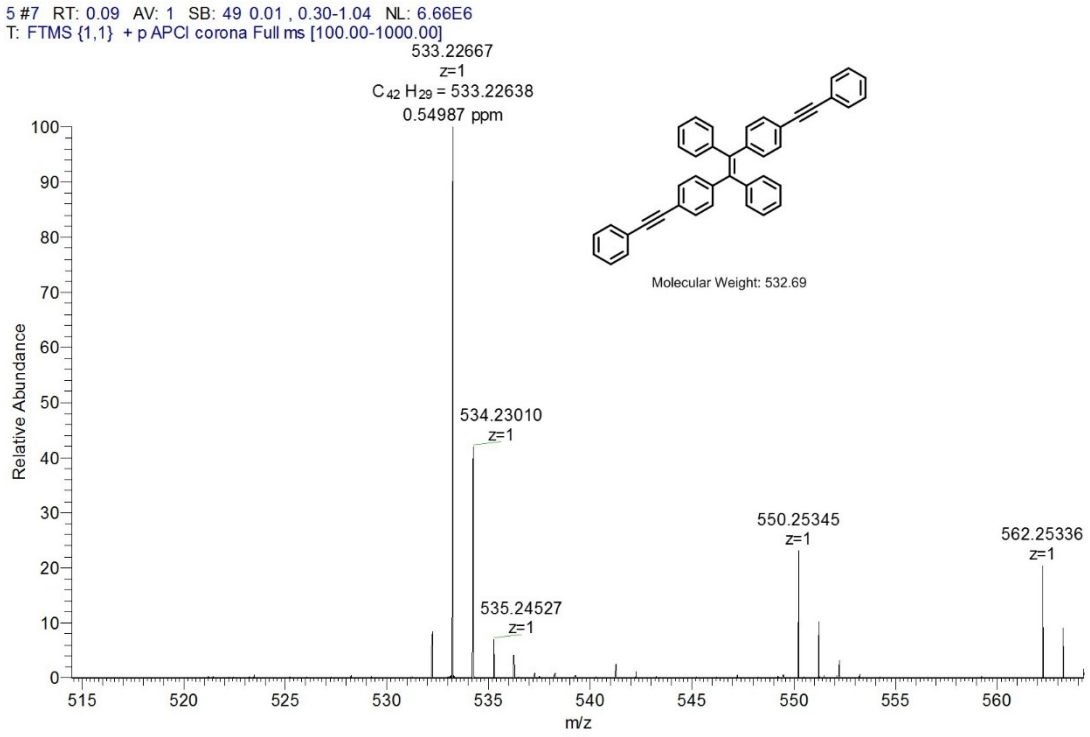



Figure S17. The HRMS (APCI) spectrum of compound **4**.

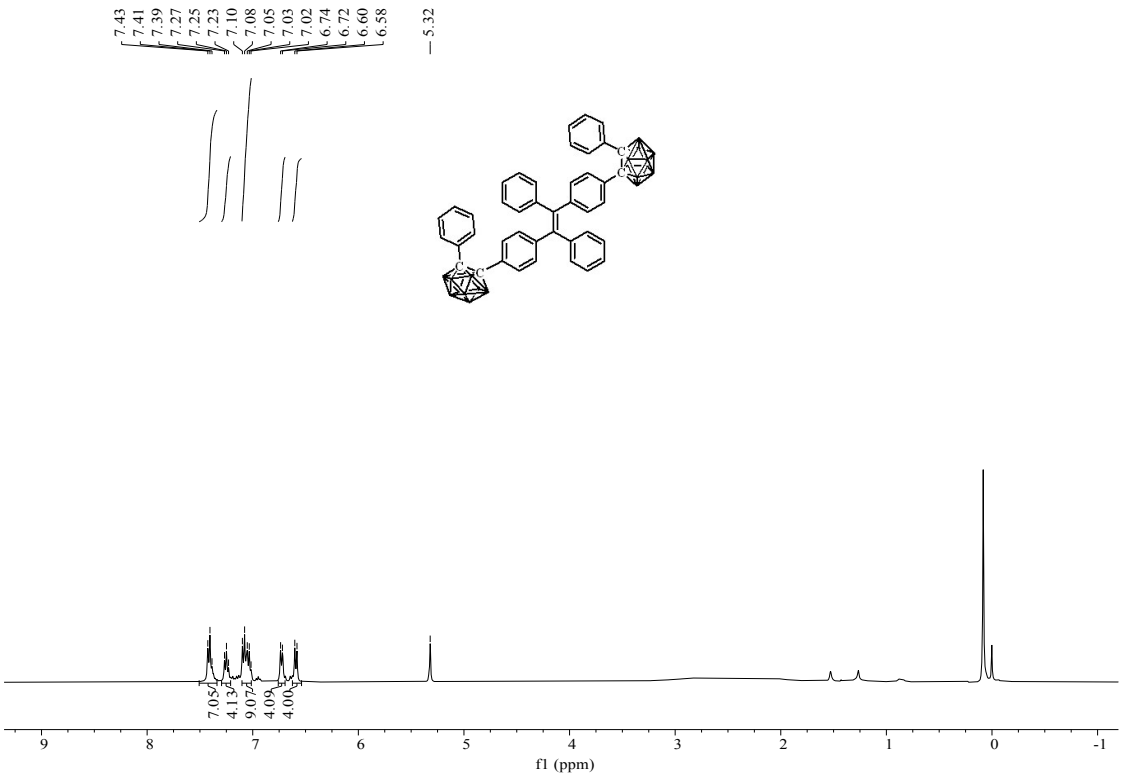



Figure S18. The $^{1}$H-NMR (400 MHz, Methylene Chloride-$d^2$) spectrum of compound ***E*-TPE-2Car**.

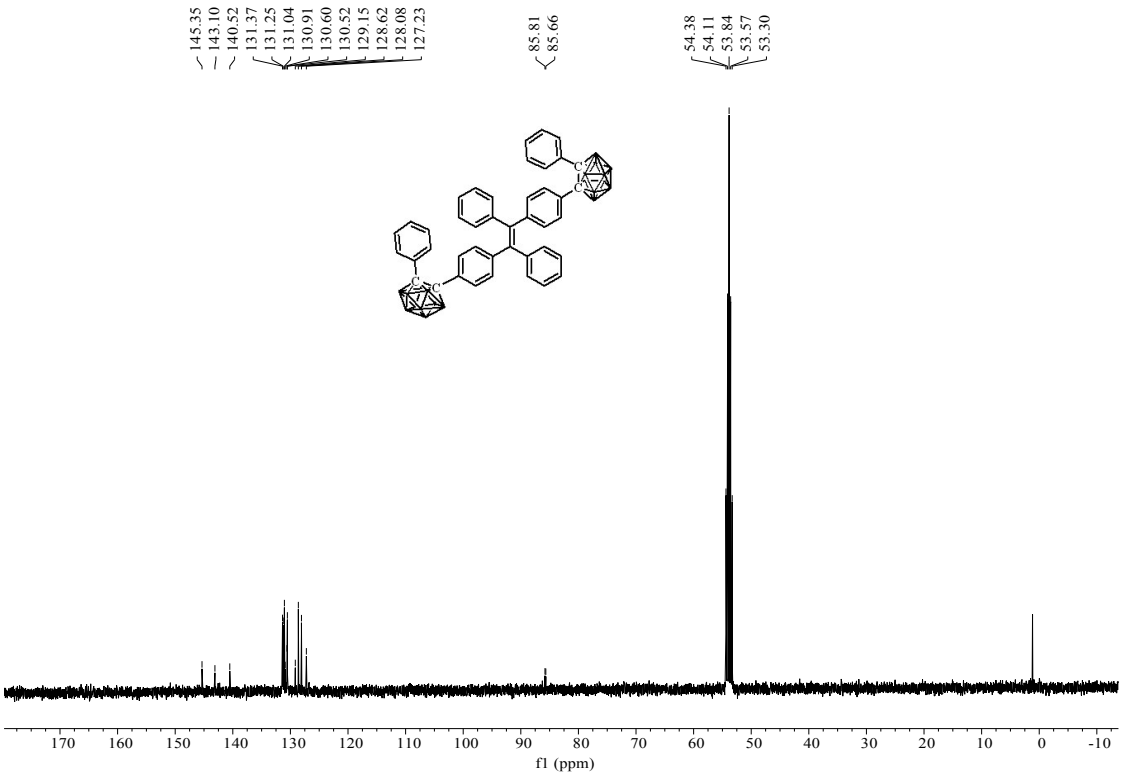



Figure S19. The $^{13}$C-NMR (101 MHz, Methylene Chloride-$d^2$) spectrum of compound ***E*-TPE-**

**2Car**.

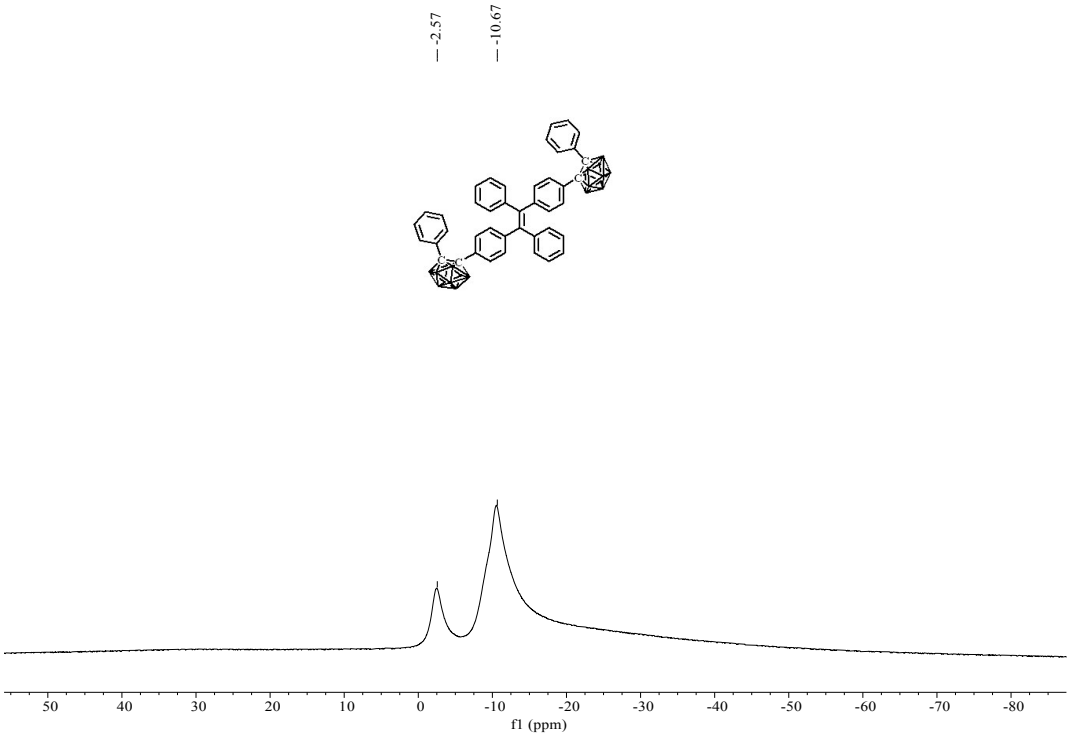



Figure S20. The $^{11}B-NMR$ (160 MHz, Methylene Chloride-$d^2$) spectrum of compound **E-TPE-2Car**.

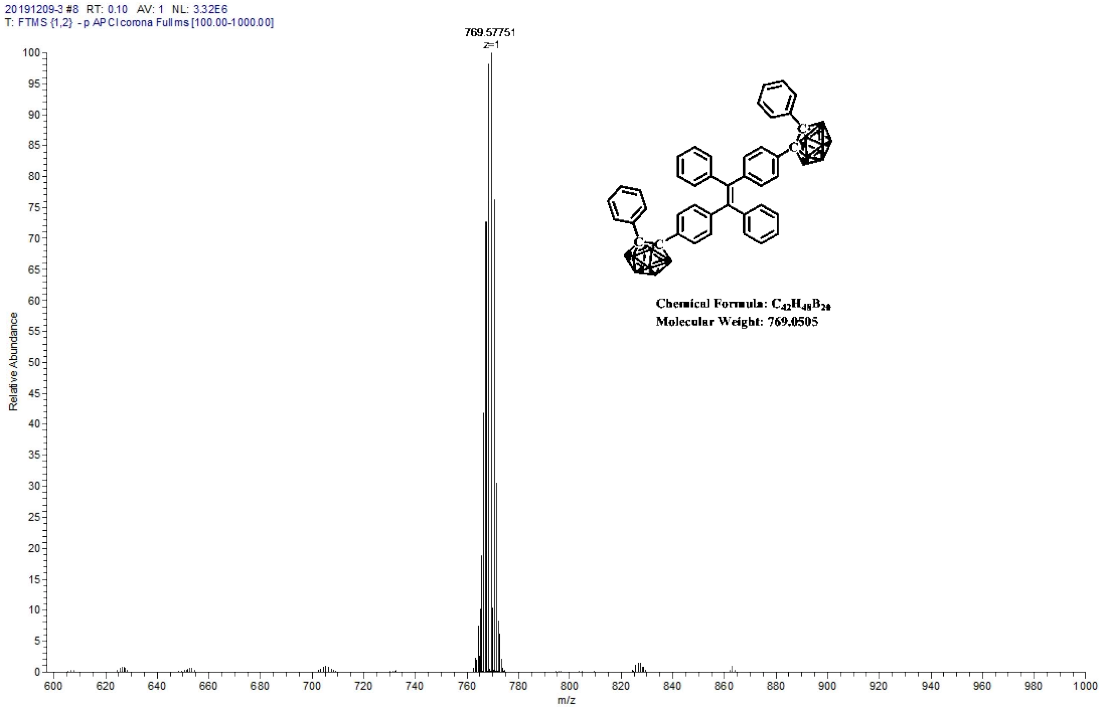



Figure S21. The HRMS (APCI) spectrum of compound **E-TPE-2Car**.

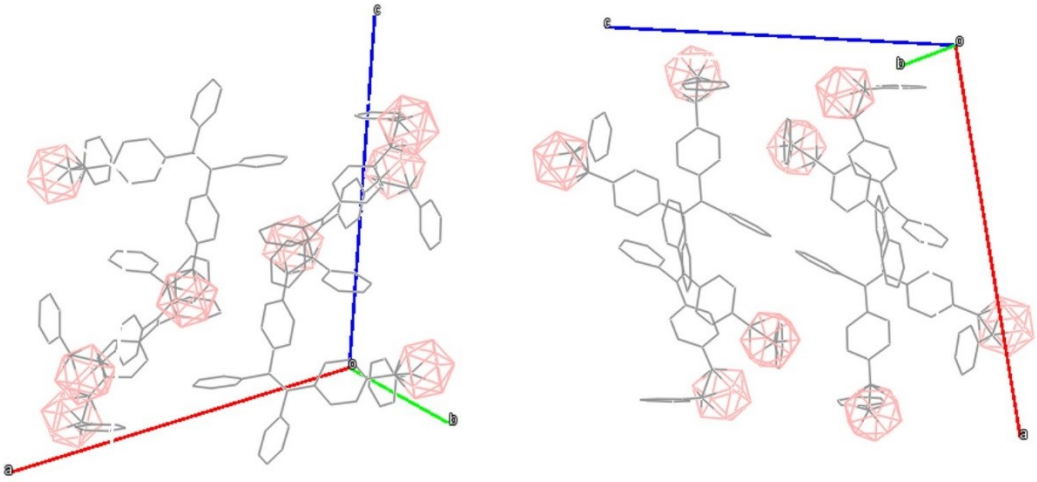


Figure S22. The crystal stacking diagram of ***Z*-TPE-2Car**.

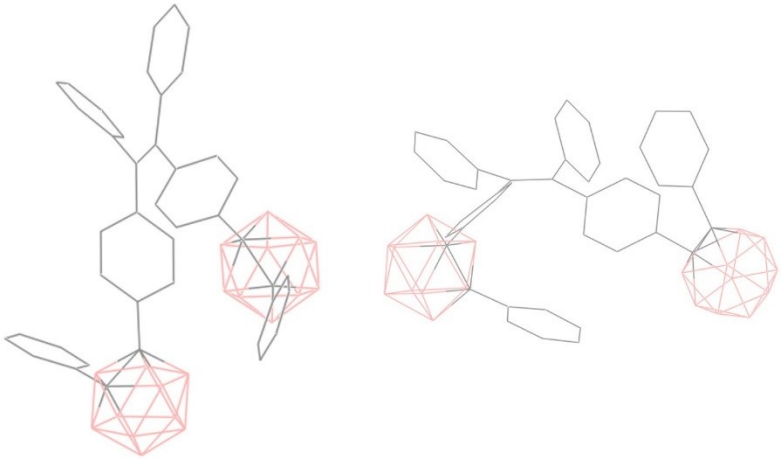


Figure S23. The orientation of the two carbon-terminal substituted benzene rings of carborane. (Facing the tetraphenylethylene structure on the two different sides).

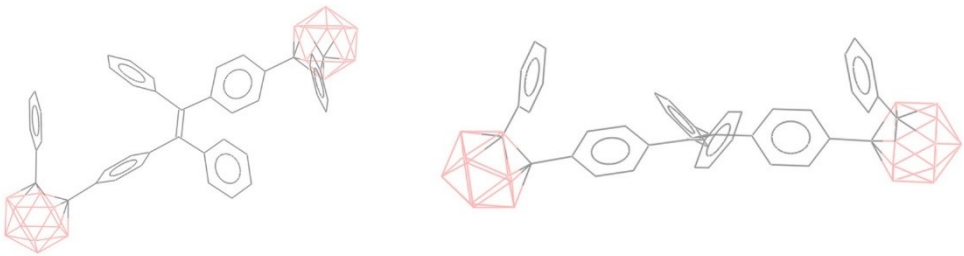


Figure S24. The orientation of the two carbon-terminal substituted benzene rings of carborane. (Facing the tetraphenylethylene structure on the same side).

**III. X−ray structure determination**: X−ray diffraction data were collected on a Bruker Smart CCD Apex DUO diffractometer with graphite monochromated Mo Kα radiation (λ = 0.71073 Å) using the ω−2θ scan mode. The data were corrected for Lorenz and polarization effects. The structure was solved by direct methods and refined on $F^2$ by full−matrix least−squares methods

using SHELXTL−2000. All calculations and molecular graphics were carried out on a computer using the SHELX−2000 program package, Mercury, and Diamond. Although the crystal structure of this compound has been reported and the CCDC number has been obtained, we obtained it from a pure compound, so the CCDC number has not been reapplied. CCDC **1569226** contains the supplementary crystallographic data for this paper.[S4] These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB21EZ, UK; fax: (+44) 1223−336−033; or deposit@ccdc.cam.ac.uk).

**IV. Quantum yields determination**: Absolute quantum yields of all compounds in THF/water or in solid state were measured by employing an integrating sphere.

The Principle of Absolute Quantum Yield Measurements

The absolute fluorescence quantum yield, $\eta$, is, by definition, the ratio of the number of photons emitted to the number of photons absorbed:

$$\eta = \frac{N^{em}}{N^{abs}} \quad (1)$$

There are two different methods for the measurement of the absolute fluorescence quantum yield: "Direct Excitation" measurements and "Direct & Indirect Excitation" measurements.

With "Direct Excitation" measurements one records the scatter and the emission of the sample being directly exited by the radiation from the excitation monochromator only, whereas with "Direct and Indirect Excitation" one also records the emission of the sample while it is in a position where it is only indirectly excited by excitation radiation bouncing within the sphere.

"Direct Excitation" Method

This method only requires two experimental setups, see figure 1.

Note that with the "Direct Excitation" method the emission measurement actually contains the information of both direct and indirect excitation, as photons that pass the sample in the direct excitation beam may still be absorbed after scattering in the sphere.


Figure 1. Two different measurement configurations required for Direct Excitation measurements:

(A) reference sample (solvent only) in sample position (1); (B) test sample in position 1 (position 2 remains empty for both measurements.)

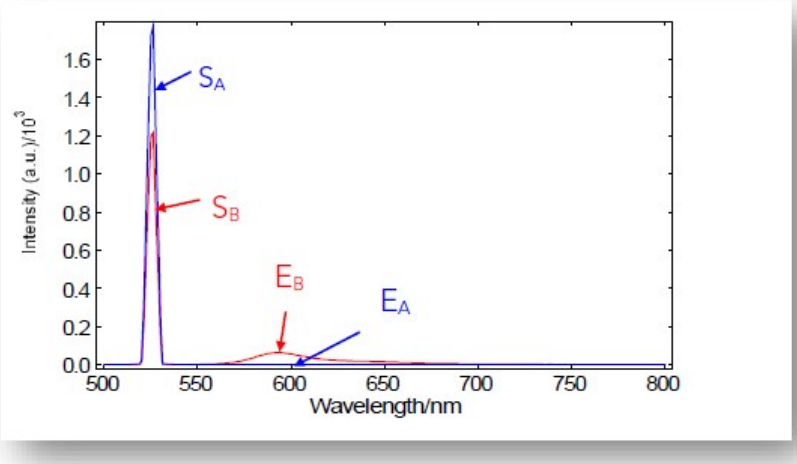



Figure 2. Spectral scans of the excitation scatter region or S-region (peaks on the left) and the emission region (E-region) of the sample and the solvent. The indices "A" and "B" refer to the experimental setup illustrated in Figure 1. Note that the quantities $S_A$, $S_B$, $E_A$, and $E_B$ refer to the integral of the scans.

The absolute fluorescence quantum yield, calculated with the "Direct Excitation" method is calculated as follows:

$$\eta_{DExc} = \frac{E_B - E_A}{S_A - S_B} \qquad (2)$$

$E_A(\lambda)$ and $S_A(\lambda)$, as well as $E_B(\lambda)$ and $S_B(\lambda)$ may be measured in four individual scans. However, it is often convenient to measure these spectra in two scans only. For the calculation of the integrals, the selection of the integral regions, and the final calculation of $\eta_{DExc}$ use the quantum yield wizard that is supplied with the F980 software.

If the sphere background, $E_A(\lambda)$, is sufficiently low the measurement of this region may be omitted to save measurement time. In this case the equation degrades to:

$$\eta_{DExc} = \frac{E_B}{S_A - S_B} \qquad (3)$$

**V. PL Spectra data**: UV−VIS absorption spectra were recorded with Shimadzu UV−3600 spectrophotometers. FL and PL spectra were recorded on a Hitachi F−7000 fluorescence spectrophotometer.

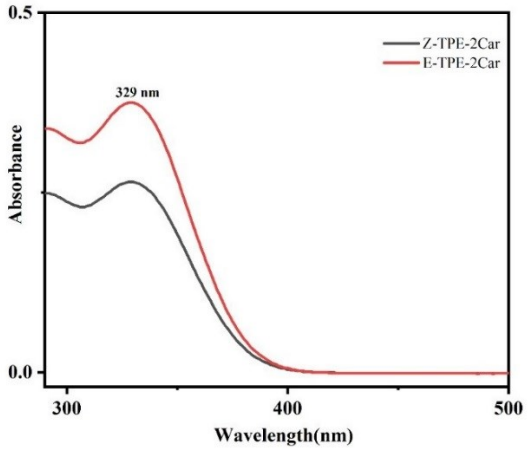



Figure S25. The absorption spectra of ***Z*-TPE-2Car** and ***E*-TPE-2Car** in THF ($1.0 \times 10^{-5}$ M) at room temperature.

**VI. Quantum chemical calculations**: Geometries of all complexes were optimized using density functional theory (DFT) method. The electronic transition energies including electron correlation effects were computed by TD−DFT method using B3LYP functional (TD−B3LYP). The 6−31G(d, p) basis set was used to treat all atoms. All calculations described here were performed by using Gaussian 09 program.[S5]

**VII. Cyclic voltammetry (CV):** Electrochemical determination: Cyclic Volta metric experiments were carried out with an IM6ex (Zahner) using three electrode cell assemblies. All measurements were carried out in a one-compartment cell under Argon, equipped with a glassy-carbon working electrode, a platinum wire counter electrode, and a Ag / $Ag^+$ reference electrode under a scan rate of 100 mV $s^{-1}$. The supporting electrolyte was a 0.10 mol $L^{-1}$ acetonitrile solution of tetrabutyl-ammonium hexafluorophosphate ($Bu_4NPF_6$). Each oxidation potential was calibrated with ferrocene as a reference.

Table S1. The electrochemical properties data sheet of the isomers.

| Compound | Eox (eV) | HOMO (eV) | $\lambda_{cross\text{-}point}$ (nm) | LUMO（eV） | Eg（eV） |
|---|---|---|---|---|---|
| ***Z*-TPE-2Car** | 0.90 | -5.70 | 425 | -2.78 | 2.92 |
| ***E*-TPE-2Car** | 0.90 | -5.70 | 422 | -2.76 | 2.94 |

## VIII. References

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