Electronic Supplementary Information

Conductance of *o*-Carborane-Based Wires with Different Substitution Patterns

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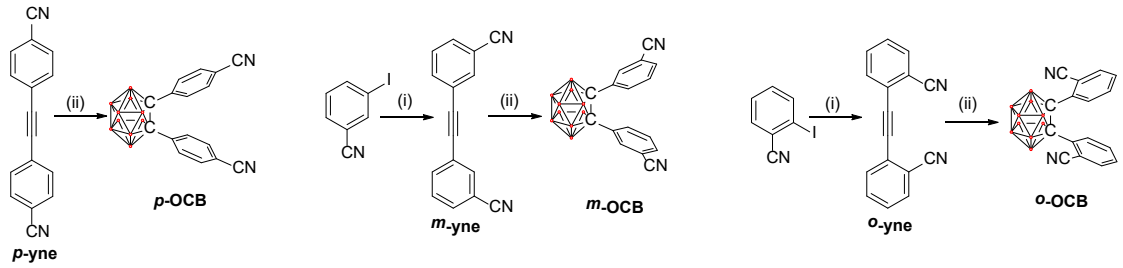
1. Synthesis of wires



(i) ***p*-yne**, ***m*-yne** and ***o*-yne** were prepared according to a previously published method.[1] MeCN was degassed with Ar for 20 min. A 250 mL three-neck round-bottom flask with a magnetic stir bar was added with CuI (57 mg, 0.30 mmol, 0.1 equiv), $Pd(OAc)_2$ (34 mg, 0.15 mmol, 0.05 equiv) and PPh_3 (79 mg, 0.30 mmol, 0.1 equiv). Then MeCN (30 mL), TEA (10 mL), aryl iodides (687 mg, 3 mmol, 1 equiv) and CaC_2 (749 mg, w % = 77 %, 9 mmol, 3 equiv) were added. The mixture was stirred at room temperature overnight under Ar atmosphere. The reaction mixture was then filtrated through diatomite and washed with CH_2Cl_2. The filtrate was dried under reduced pressure and subjected to silica gel flash chromatography.

(ii) A typical procedure for the preparation of *o*-carborane derivatives.[2, 3] The mixture of alkyne (269 mg, 1.18 mmol, 1 equiv) and $B_{10}H_{12}(MeCN)_2$ (240 mg, 1.20 mmol, 1.02 equiv) was dissolved in toluene and refluxed for 48 h under Ar atmosphere. The reaction mixture was cooled down to room temperature and was quenched by adding methanol. The solution was dried under reduced pressure. Then the product was dissolved with CH_2Cl_2 and filter out the insoluble matter. The filtrate was extracted, then dried under reduced pressure and subjected to silica gel flash chromatography.

***p*-yne**. Chromatography (Petroleum ether/CH_2Cl_2, 2:1 v/v). Yield 95%, colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.67 (d, J = 7.4 Hz, 4H), 7.63 (d, J = 7.2 Hz, 4H). ^{13}C NMR (126 MHz, $CDCl_3$): δ (ppm) 132.4, 132.3, 127.2, 118.4 (CN), 112.6, 91.7 (C≡C). HRMS (ESI+): $C_{16}H_9N_2$ $[M+H]^+$ require 229.0760, found 229.0760.

***m*-yne**. Chromatography (Petroleum ether/CH_2Cl_2, 2:1 v/v). Yield 87%, colorless solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.82 (t, J = 1.7 Hz, 2H), 7.75 (dt, J = 7.9, 1.4 Hz, 2H), 7.65 (dt, J = 7.8, 1.4 Hz, 2H), 7.50 (t, J = 7.8 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 135.9, 135.2, 132.2, 129.6, 124.1, 118.0 (CN), 113.3, 89.2 (C≡C). HRMS (ESI+): $C_{16}H_8N_2K$ $[M+K]^+$ require 267.0319, found 267.0320.

***o*-yne**. Chromatography (Petroleum ether/CH_2Cl_2, 2:1 v/v). Yield 82%, colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.77 (d, J = 7.9 Hz, 2H), 7.71 (d, J = 7.9 Hz, 2H), 7.62 (t, J = 7.7 Hz, 2H), 7.48 (t, J = 7.7 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$): δ (ppm) 133.2, 132.9, 132.7, 129.4, 126.1, 117.4 (CN), 115.5, 91.5 (C≡C). HRMS (ESI+): $C_{16}H_8N_2K$ $[M+K]^+$ require 267.0319, found 267.0321.

***p*-OCB**. Chromatography (Petroleum ether/CH_2Cl_2, 1:1 v/v). Yield 45%, colorless solid. ^{1}H NMR (400MHz, $CDCl_3$): δ (ppm) 7.55 (d, J = 7.2 Hz, 4H), 7.49 (d, J = 8.2 Hz, 4H), 4.03 – 1.59 (m, 10H, B-H). ^{13}C NMR (101MHz, $CDCl_3$): δ (ppm) 134.7, 132.4, 131.3, 117.3 (CN), 115.0, 83.2 (B-C). ^{11}B NMR (128MHz, $CDCl_3$): δ (ppm) –0.78, –1.96, –9.10, –10.23, –12.02. HRMS (ESI+): $C_{16}B_{10}H_{18}N_2Na$ $[M+Na]^+$ require 369.2365, found 369.2363.

***m*-OCB**. Chromatography (Petroleum ether/CH_2Cl_2, 1:1 v/v). Yield 14%, colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) δ 7.73-7.65 (m, 4H), 7.59 (d, J = 6.7 Hz, 2H), 7.36 (t, J = 7.9 Hz, 2H), 3.45-1.75 (m, 10H). ^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 134.7, 134.2, 134.0, 131.9, 129.9, 117.4(CN), 113.5, 82.9 (B-C). ^{11}B NMR (128 MHz, $CDCl_3$): δ (ppm) –0.76, –1.95, –9.19, –10.17, –12.34. HRMS (ESI+): $C_{16}B_{10}H_{18}N_2Na$ $[M+Na]^+$ require 369.2365, found 369.2365.

***o*-OCB**. Chromatography (Petroleum ether/CH_2Cl_2, 1:1 v/v). Yield 38%, colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.79 – 7.72 (m, 2H), 7.70 – 7.64 (m, 2H), 7.44 – 7.37 (m, 4H), 3.90 – 1.84 (m, 10H, B-H). ^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 137.6, 133.2, 133.0, 131.0, 130.7, 117.9(CN), 114.8, 84.9 (B-C). ^{11}B NMR (128 MHz, $CDCl_3$): δ (ppm) –0.11, –1.08, –8.22, –9.47, –11.78. HRMS (ESI+): $C_{16}B_{10}H_{18}N_2Na$ $[M+Na]^+$ require 369.2365, found 369.2363.

2. Theoretical calculations

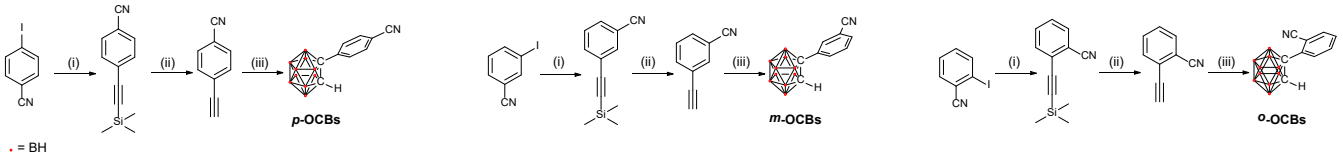
The optimized molecules: All the theoretical calculations were performed with Gaussian 09 software package.[4] Geometry optimizations and frequency calculations were performed on the 6-31+G (d, p) basis set. During the theoretical calculations, there is no imaginary frequency existed.

The single point energy: RB3LYP/6-31+G (d,p).

Table S1 Calculated energy levels of frontier molecular orbital of ***p*-OCB, *m*-OCB** and ***o*-OCB**.

Wires	HOMO (eV)	LUMO (eV)	Gap (eV)
***p*-OCB**	−8.00	−2.78	5.22
***m*-OCB**	−8.01	−2.45	5.56
***o*-OCB**	−7.91	−2.59	5.32

3. Synthesis of wires with one anchor



(i) A typical Sonogashira coupling for these: a 250 mL three-neck round-bottom flask with a magnetic stir bar was added with aryl iodide (687 mg, 3.00 mmol, 1 equiv), CuI (57 mg, 0.30 mmol, 0.1 equiv), $Pd(PPh_3)_2Cl_2$ (105 mg, 0.15 mmol, 0.05 equiv) and PPh_3 (40 mg, 0.15 mmol, 0.1 equiv). Then THF/TEA (3:1, v/v, 30 mL/10 mL) and TMSA (354 mg, 3.60 mmol, 1.2 equiv) were added. The mixture was stirred at 65°C for 24 h under Ar atmosphere. The reaction mixture was then filtrated through diatomite and washed with CH_2Cl_2. The filtrate was dried under reduced pressure and subjected to silica gel flash chromatography. (ii) The preliminary products (0.1 equiv) were reacted with K_2CO_3 (0.1 equiv) in MeOH at room temperature for 3~5 h. Then the reaction mixture was dried under reduced pressure and subjected to silica gel flash chromatography. (iii) A typical procedure for the preparation of these *o*-carborane derivatives.[5] The products of the previous step were reacted with $B_{10}H_{12}(MeCN)_2$ in toluene to obtain the target product. The mixture of alkyne (1 equiv) and $B_{10}H_{12}(MeCN)_2$ (1.02 equiv) was dissolved in toluene and refluxed for 48 h under Ar atmosphere. The reaction mixture was cooled down to room temperature and was quenched by adding methanol. The solution was dried under reduced pressure. Then the product was dissolved with CH_2Cl_2 and filter out the insoluble matter. The filtrate was extracted and then dried under reduced pressure and subjected to silica gel flash chromatography. Reactions involving air-sensitive materials were prepared under Ar by using standard Schlenk technology. Toluene is distilled from sodium/benzophenone. Other chemicals were purchased from commercial suppliers and were used directly upon receipt.

4-[(trimethylsilyl)ethynyl]benzonitrile. Chromatography (Petroleum ether/CH_2Cl_2, 1:1, v/v). Yield 95%, colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.55 (dd, J = 23.2, 8.2 Hz, 4H), 0.26 (s, 9H). **4-ethynylbenzonitrile**. Chromatography (Petroleum ether/CH_2Cl_2, 1:1, v/v). Yield 97%, colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.58 (dd, J = 21.1, 8.3 Hz, 4H), 3.30 (s, 1H).

3-[(trimethylsilyl)ethynyl]benzonitrile. Chromatography (Petroleum ether/CH_2Cl_2, 1:1, v/v). Yield 90%, pale yellow oily liquid. ^{1}H NMR (400 MHz, $CDCl_3$): 7.73 (s, 1H), 7.65 (d, J = 7.8 Hz, 1H), 7.57 (d, J = 7.8 Hz, 1H), 7.41 (t, J = 7.8 Hz, 1H), 0.25 (s, 9H). **3-ethynylbenzonitrile**. Chromatography (Petroleum ether/CH_2Cl_2, 1:1, v/v). Yield 87%, pale yellow oily liquid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.75 (s, 1H), 7.69 (d, J = 7.8 Hz, 1H), 7.62 (d, J = 7.8 Hz, 1H), 7.44 (t, J = 7.8 Hz, 1H), 3.19 (s, 1H).

2-[(trimethylsilyl)ethynyl]benzonitrile. Chromatography (Petroleum ether/CH_2Cl_2, 1:1, v/v). Yield 92%, pale yellow oily liquid. ^{1}H NMR (400 MHz, $CDCl_3$): 7.63 (d, J = 7.8 Hz, 1H), 7.58 – 7.49 (m, 2H), 7.39 (t, J = 7.6 Hz, 1H), 0.29 (s, 9H). **2-ethynylbenzonitrile**. Chromatography (Petroleum ether/CH_2Cl_2, 1:1, v/v). Yield 91%, pale violet powder. ^{1}H NMR (400 MHz, $CDCl_3$): 7.67 (d, J = 7.8 Hz, 1H), 7.62 (d, J = 7.8 Hz, 1H), 7.56 (t, J = 7.7 Hz, 1H), 7.45 (t, J = 7.7 Hz, 1H), 3.48 (s, 1H).

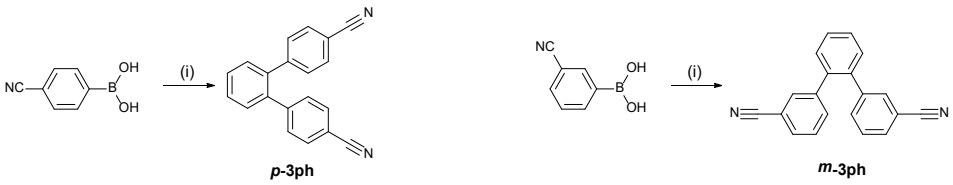
***p*-OCBs**. Chromatography (Petroleum ether/CH_2Cl_2, 2:1, v/v). Yield 50%, colorless solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ

(ppm) δ 7.68 – 7.64 (m, 2H), 7.63 – 7.59 (m, 2H), 3.98 (s, 1H), 3.35 – 1.69 (m, 10H). ^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 138.2, 132.7, 128.4, 117.5(CN), 114.3, 74.7 (B-C), 59.8 (B-C-H). ^{11}B NMR (128 MHz, $CDCl_3$): δ (ppm) –1.13, –2.33, –2.91, –4.05, –7.92, –9.10, –10.18, –10.61, –11.46, –11.95, –13.19. HRMS (ESI+): $C_{16}B_{10}H_{18}N_2K$ $[M+K]^+$ require 284.1839, found 284.1800.

***m*-OCBs**. Chromatography (Petroleum ether/CH_2Cl_2, 2:1, v/v). Yield 34%, colorless solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) δ 7.79 – 7.76 (m, 1H), 7.74 (ddd, *J* = 8.1, 2.2, 1.1 Hz, 1H), 7.70 (dt, *J* = 7.8, 1.3 Hz, 1H), 7.50 (t, *J* = 7.6 Hz, 1H), 3.96 (s, 1H), 3.05 – 1.76 (m, 10H). ^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 135.2, 133.5, 132.0, 131.3, 130.1, 117.6 (CN), 113.7, 74.5 (B-C), 60.1 (B-C-H). ^{11}B NMR (128 MHz, $CDCl_3$): δ (ppm) –1.03, –2.21, –3.02, –4.20, –7.96, –10.19, –10.73, –11.44, –11.92, –13.14. HRMS (ESI+): $C_{16}B_{10}H_{18}N_2K$ $[M+K]^+$ require 284.1839, found 284.1803.

***o*-OCBs**. Chromatography (Petroleum ether/CH_2Cl_2, 2:1, v/v). Yield 39%, colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) δ 7.88 (d, *J* = 8.3 Hz, 1H), 7.69 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.63 (td, *J* = 7.9, 1.6 Hz, 1H), 7.52 (td, *J* = 7.6, 1.2 Hz, 1H), 5.20 (s, 1H), 3.24 – 1.80 (m, 10H). ^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 136.3, 135.2, 133.6, 132.1, 130.0, 118.1 (CN), 108.9, 74.2 (B-C), 58.0 (B-C-H). ^{11}B NMR (128 MHz, $CDCl_3$): δ (ppm) –1.95, –3.12, –7.73, –9.04, –10.44, –11.97, –12.07, –13.43. HRMS (ESI+): $C_{16}B_{10}H_{18}N_2K$ $[M+K]^+$ require 284.1839, found 284.1796.

4. Synthesis of the triphenyl molecules.



A typical Suzuki coupling for these: (i) a 250 mL three-neck round-bottom flask with a magnetic stir bar was added with cyanophenylboronic acid (294 mg, 2 mmol, 2 equiv), 1,2-diiodobenzene (330 mg, 1 mmol, 1 equiv), $Pd(PPh_3)_4$ (23 mg, 0.02 mmol, 0.02 equiv), K_2CO_3 (1106 mg, 8 mmol, 8 equiv), then toluene/EtOH/H_2O (4:1:2, v/v, 20 mL/5 mL/10 mL) were added. The mixture was stirred at 85°C for 48 h under Ar atmosphere. The solution was dried under reduced pressure. Then the product was extracted with ethyl acetate and then dried under reduced pressure and subjected to silica gel flash chromatography. Reactions involving air-sensitive materials were prepared under Ar by using standard Schlenk technology.

***p*-3ph**. Chromatography (Petroleum ether/CH_2Cl_2, 3:1, v/v). Yield 58%, colorless solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) δ 7.57 – 7.48 (m, 6H), 7.43 (dd, *J* = 5.7, 3.3 Hz, 2H), 7.23 – 7.19 (m, 4H). ^{13}C NMR (126 MHz, $CDCl_3$): δ (ppm) 145.7, 138.8, 132.2, 130.8, 130.6, 129.05, 118.8 (CN), 111.06. HRMS (ESI+): $C_{20}H_{13}N_2$ $[M+H]^+$ require 281.1073, found 281.1073.

***m*-3ph**. Chromatography (Petroleum ether/CH_2Cl_2, 3:1, v/v). Yield 53%, colorless solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) δ 7.56 – 7.49 (m, 4H), 7.45 – 7.39 (m, 4H), 7.34 (t, *J* = 7.7 Hz, 2H), 7.30 (dt, *J* = 8.0, 1.6 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$): δ (ppm) 142.1, 138.3, 134.3, 133.2, 130.8, 130.7, 129.1, 128.9, 118.6 (CN), 112.6. HRMS (ESI+): $C_{20}H_{13}N_2$ $[M+H]^+$ require 281.1073, found 281.1070.

5. NMR

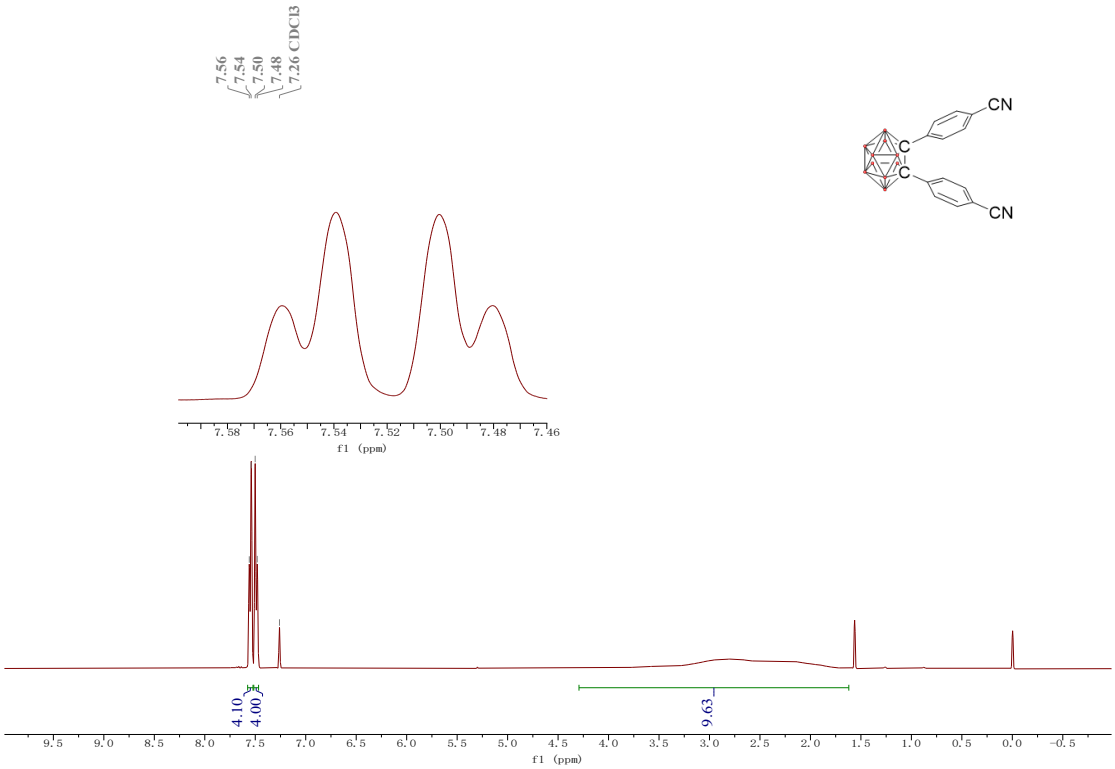


Fig. S1 ^{1}H NMR spectrum of ***p*-OCB** ($CDCl_3$)

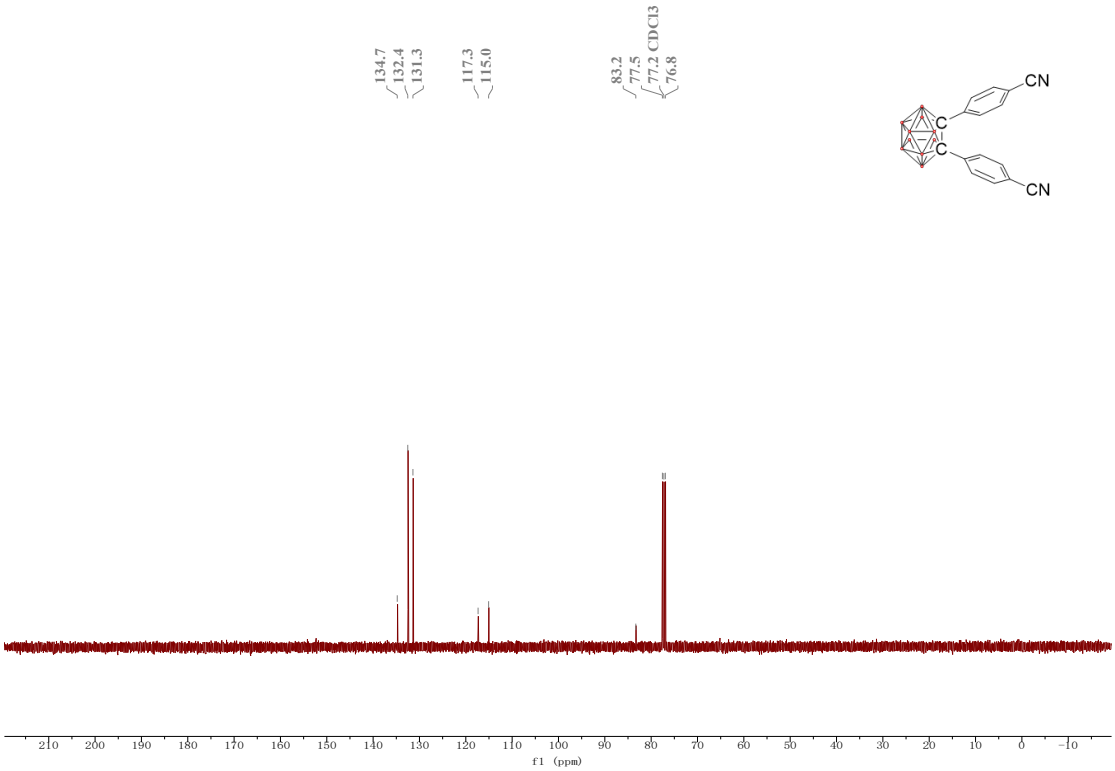


Fig. S2 ^{13}C NMR spectrum of ***p*-OCB** ($CDCl_3$)

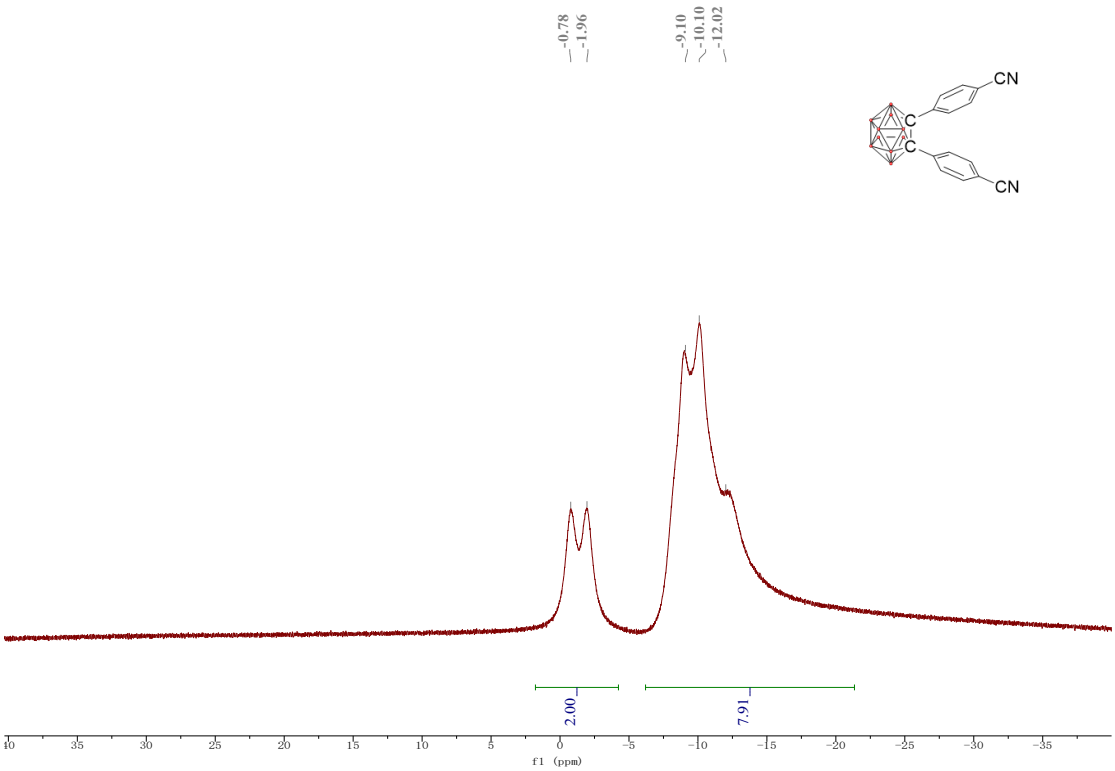


Fig. S3 ^{11}B NMR spectrum of ***p*-OCB** ($CDCl_3$)

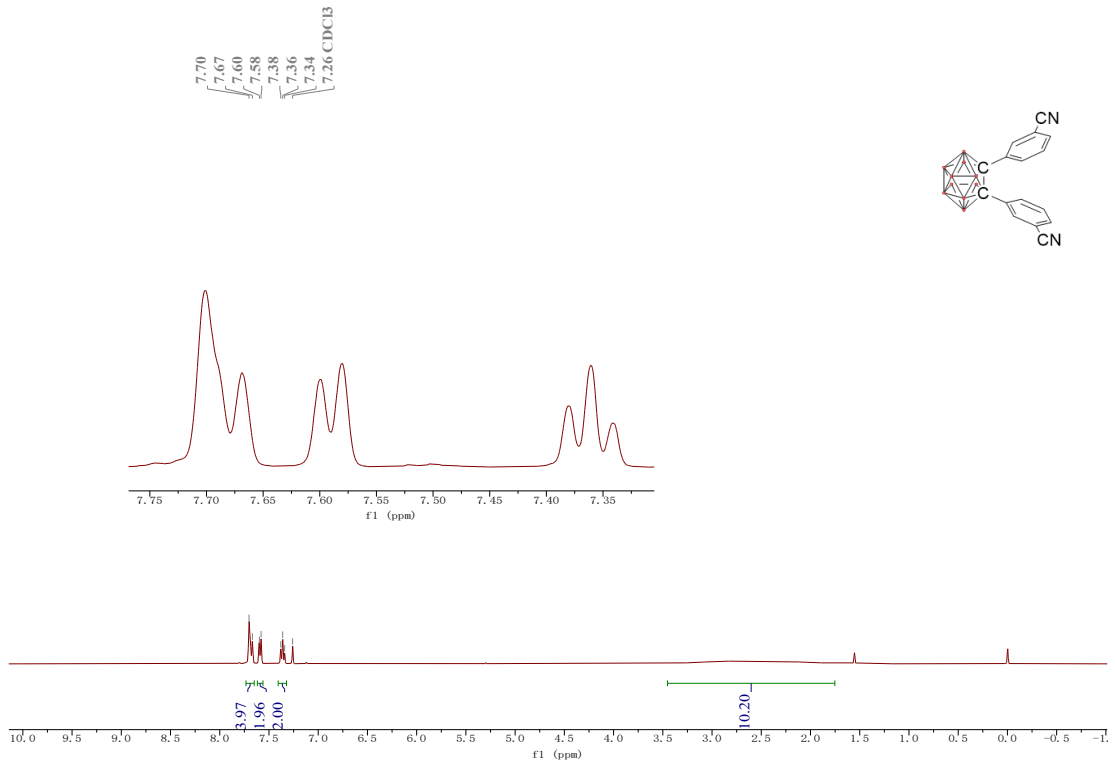


Fig. S4 ^{1}H NMR spectrum of ***m*-OCB** ($CDCl_3$)

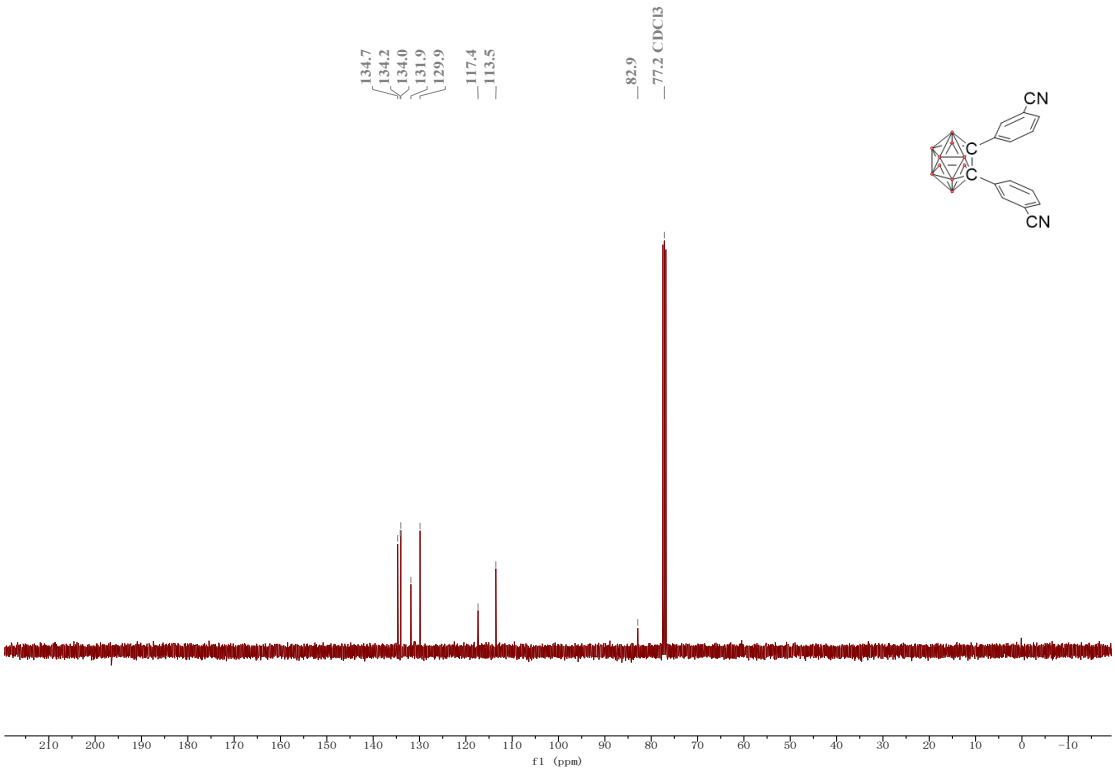


Fig. S5 ^{13}C NMR spectrum of ***m*-OCB** ($CDCl_3$)

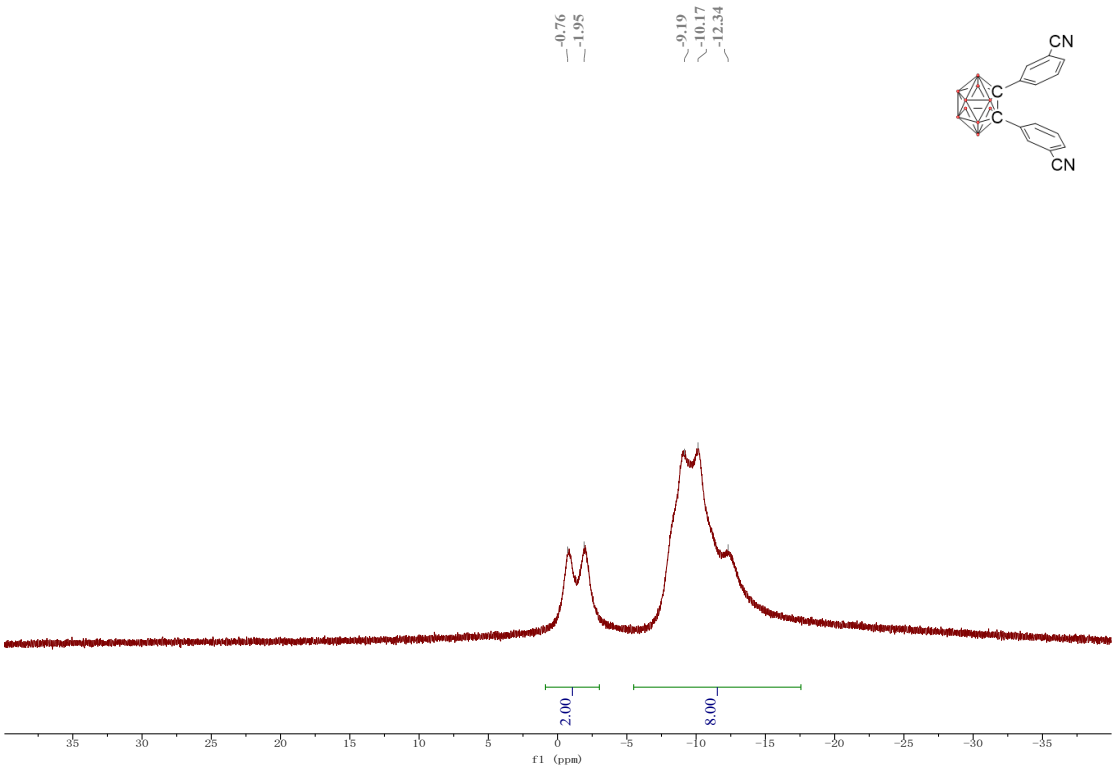


Fig. S6 ^{11}B NMR spectrum of ***m*-OCB** ($CDCl_3$)

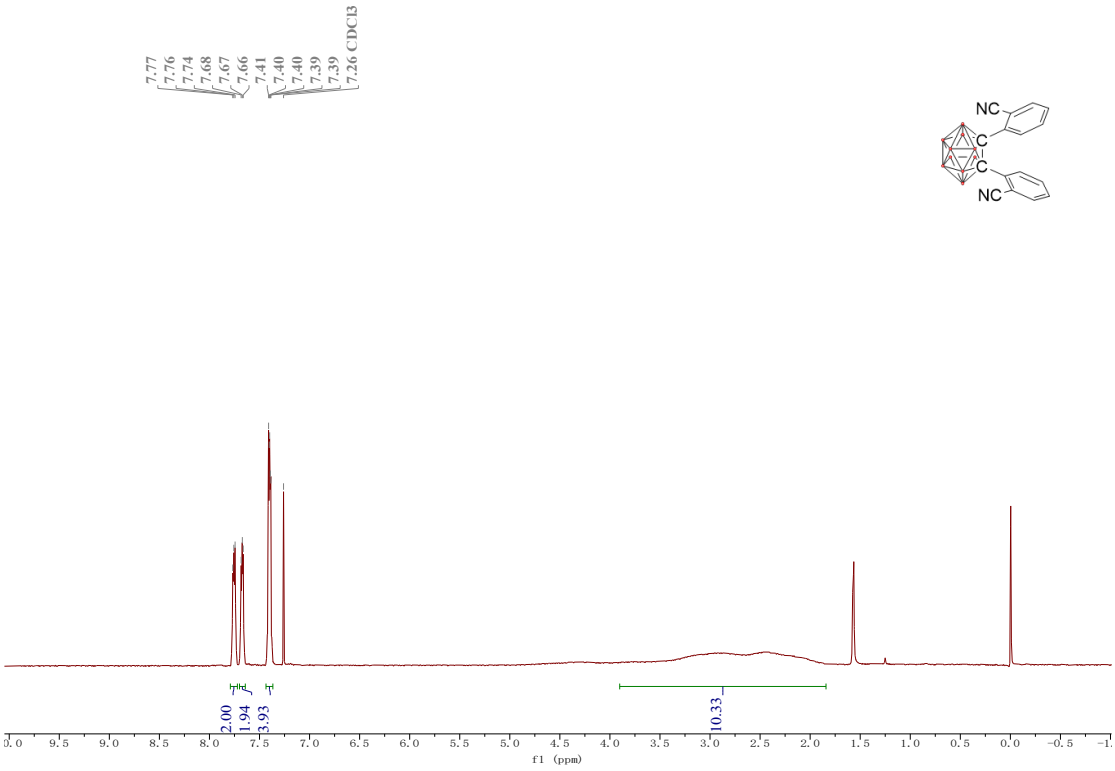


Fig. S7 ^{1}H NMR spectrum of ***o*-OCB** ($CDCl_3$)

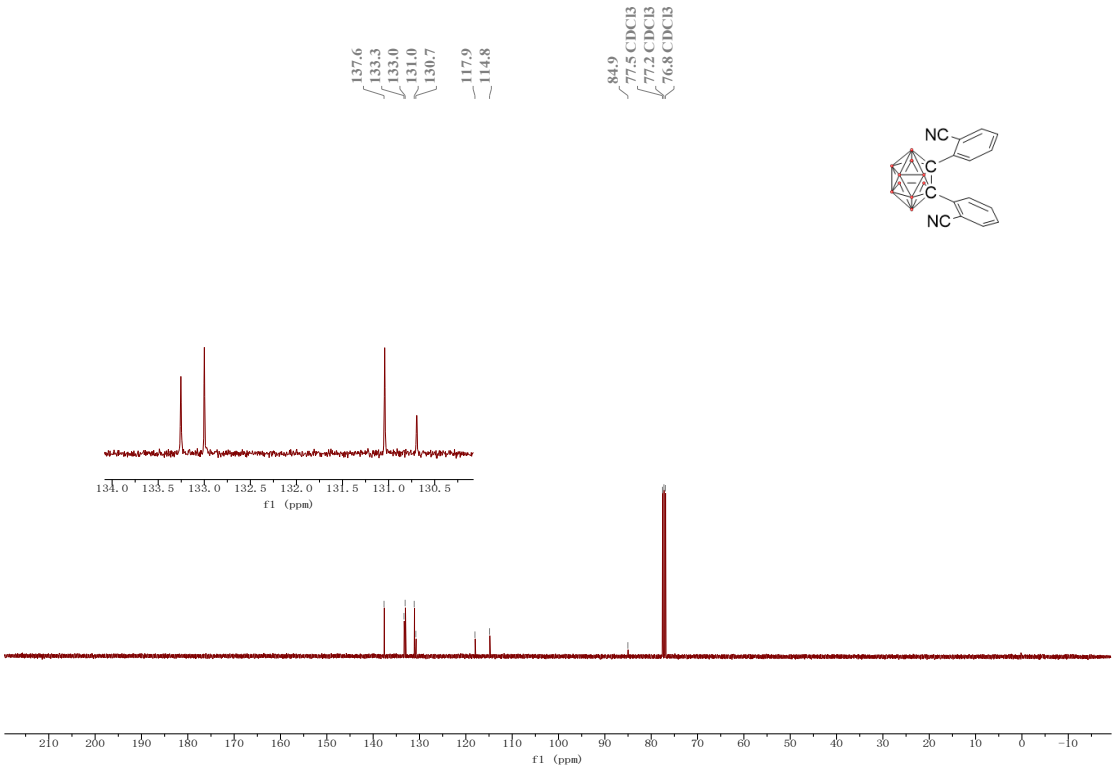


Fig. S8 ^{13}C NMR spectrum of ***o*-OCB** ($CDCl_3$)

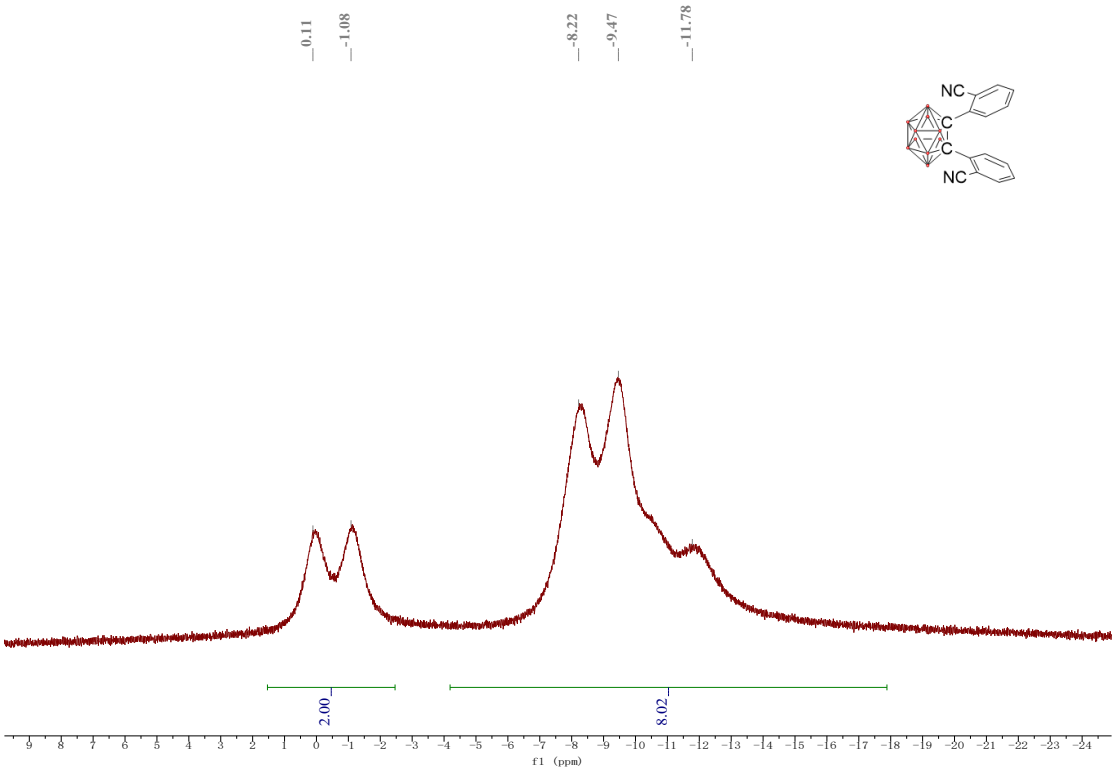


Fig. S9 ^{11}B NMR spectrum of ***o*-OCB** ($CDCl_3$)

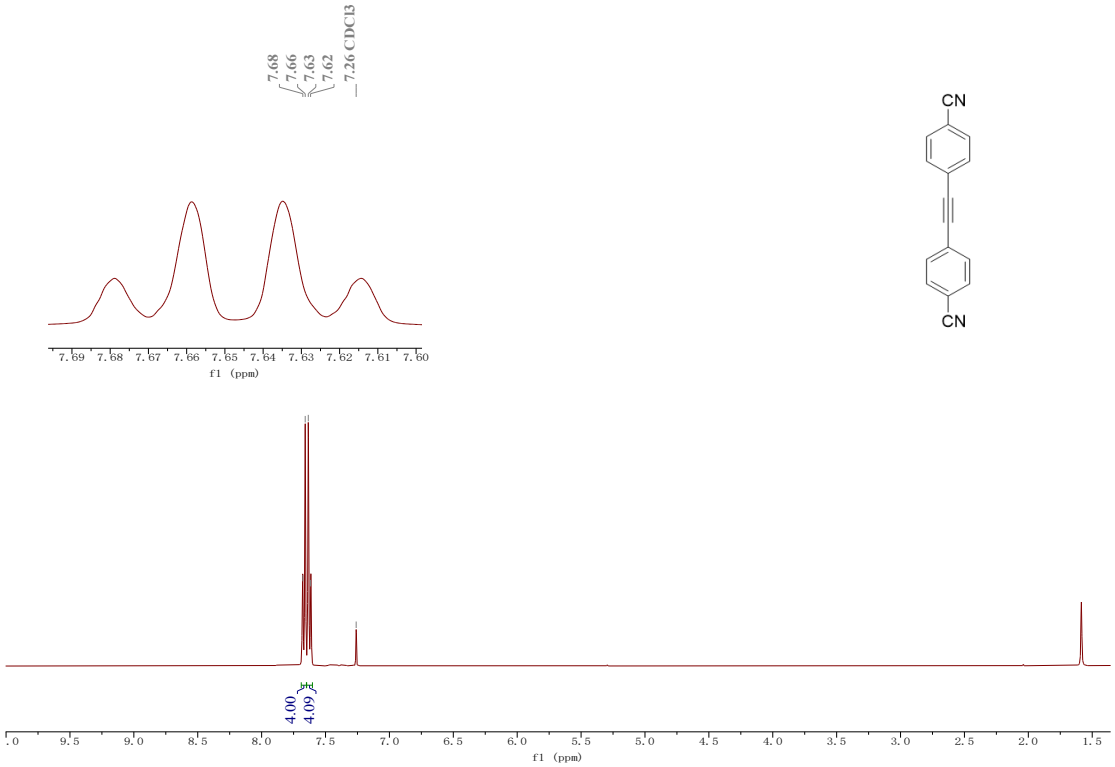


Fig. S10 ^{1}H NMR spectrum of ***p*-yne** ($CDCl_3$)

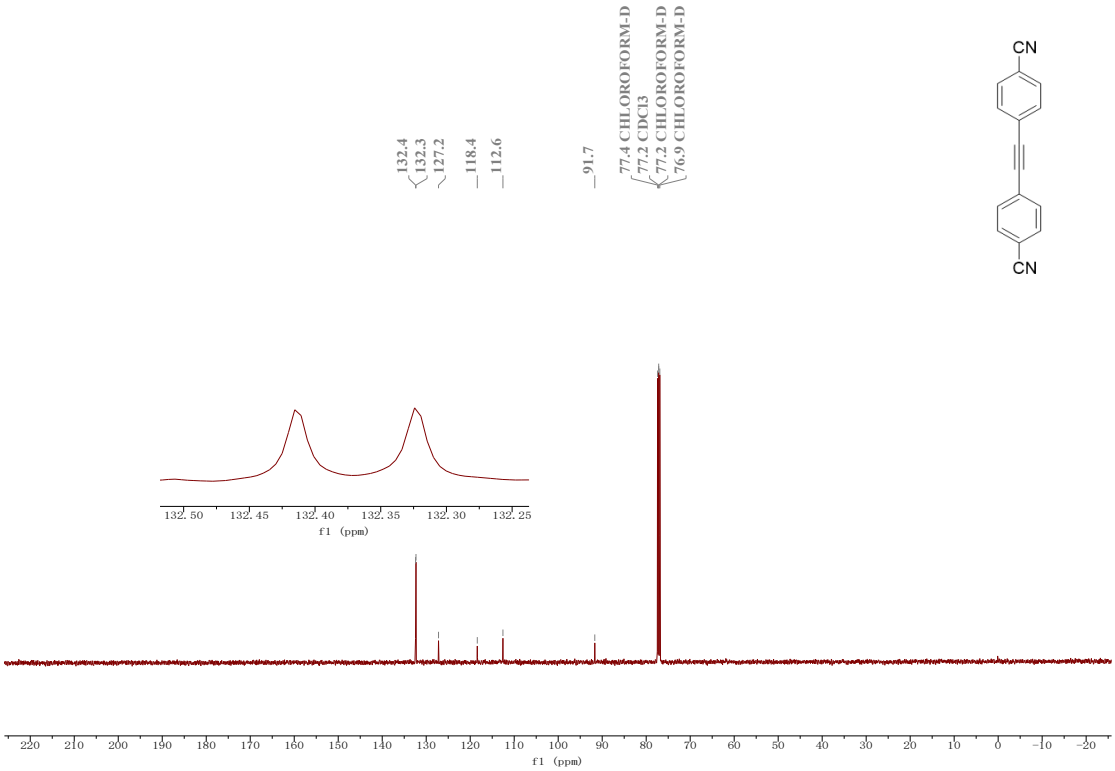


Fig. S11 ^{13}C NMR spectrum of ***p*-yne** ($CDCl_3$)

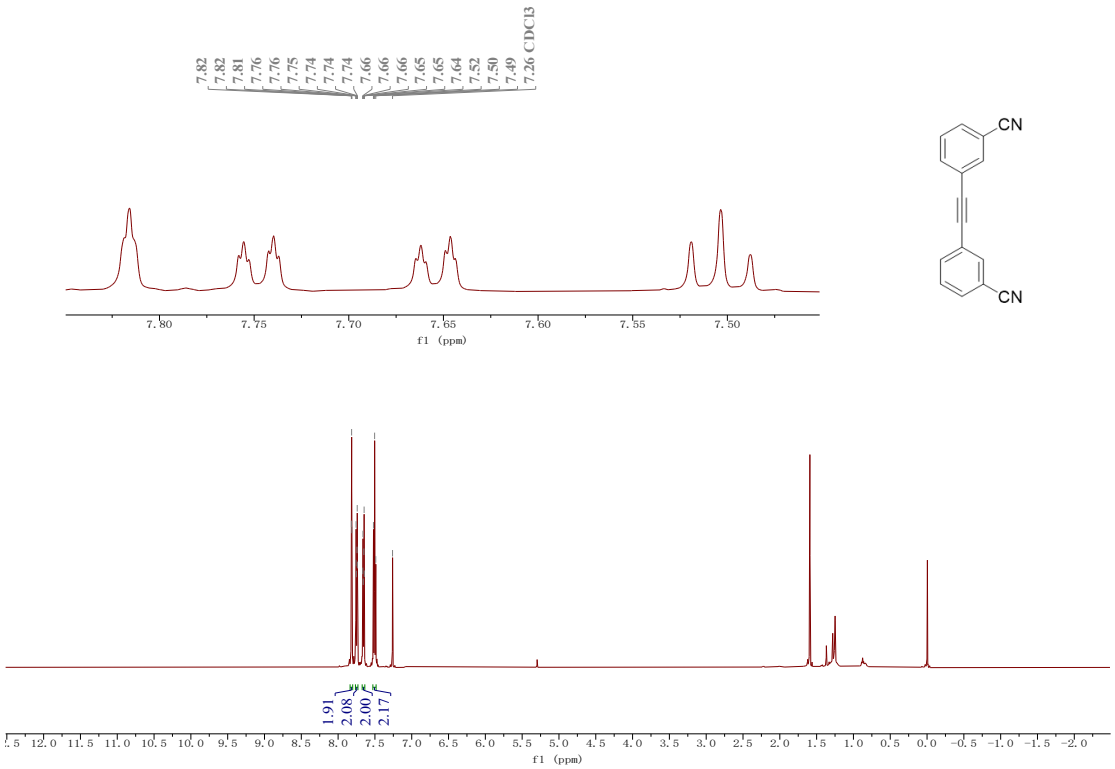


Fig. S12 ^{1}H NMR spectrum of ***m*-yne** ($CDCl_3$)

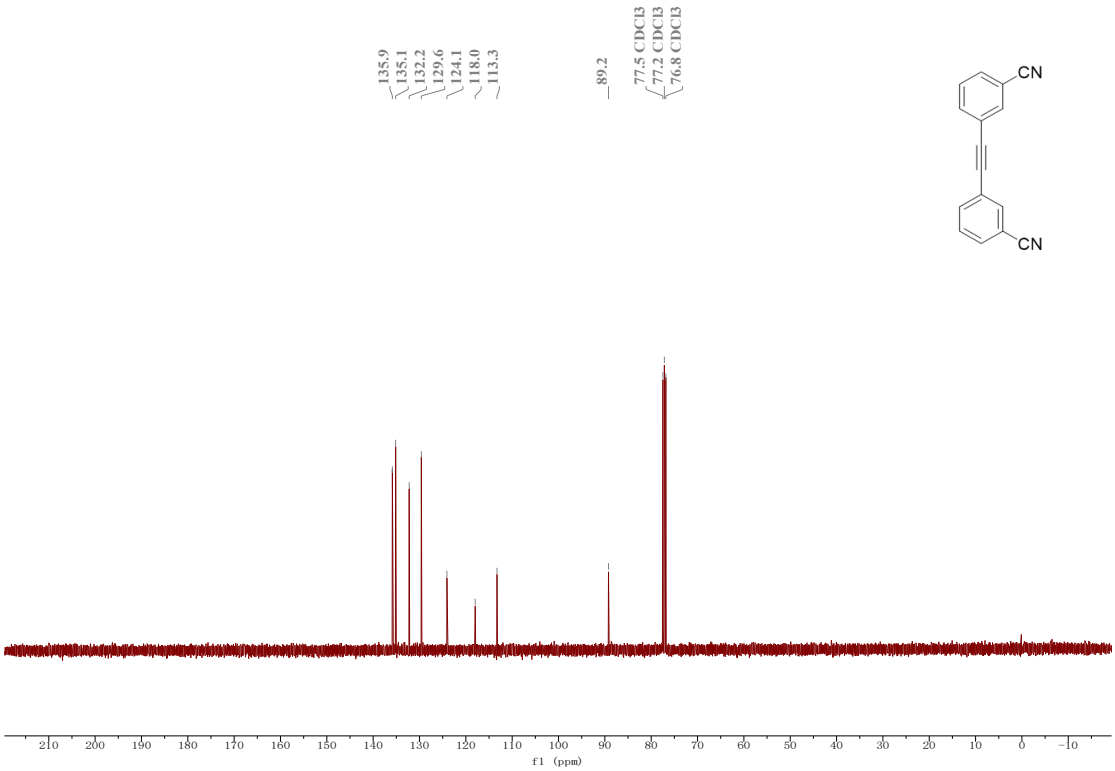


Fig. S13 ^{13}C NMR spectrum of ***m*-yne** ($CDCl_3$)

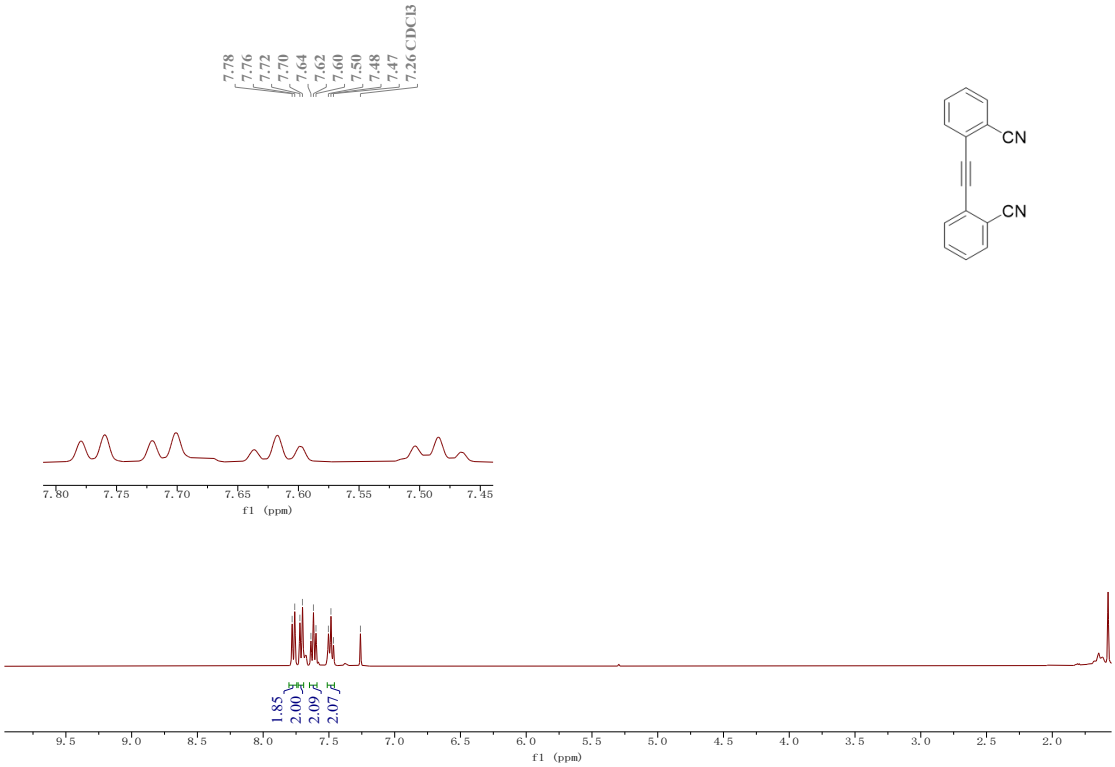


Fig. S14 ^{1}H NMR spectrum of ***o*-yne** ($CDCl_3$)

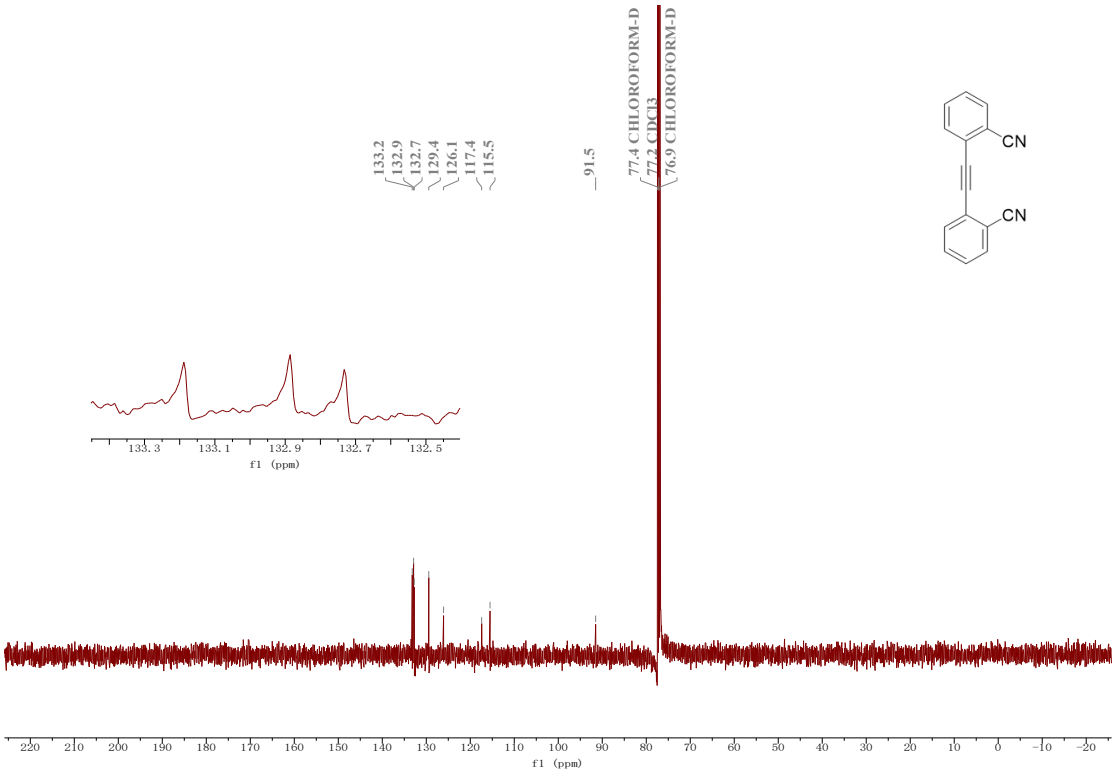


Fig. S15 ^{13}C NMR spectrum of ***o*-yne** ($CDCl_3$)

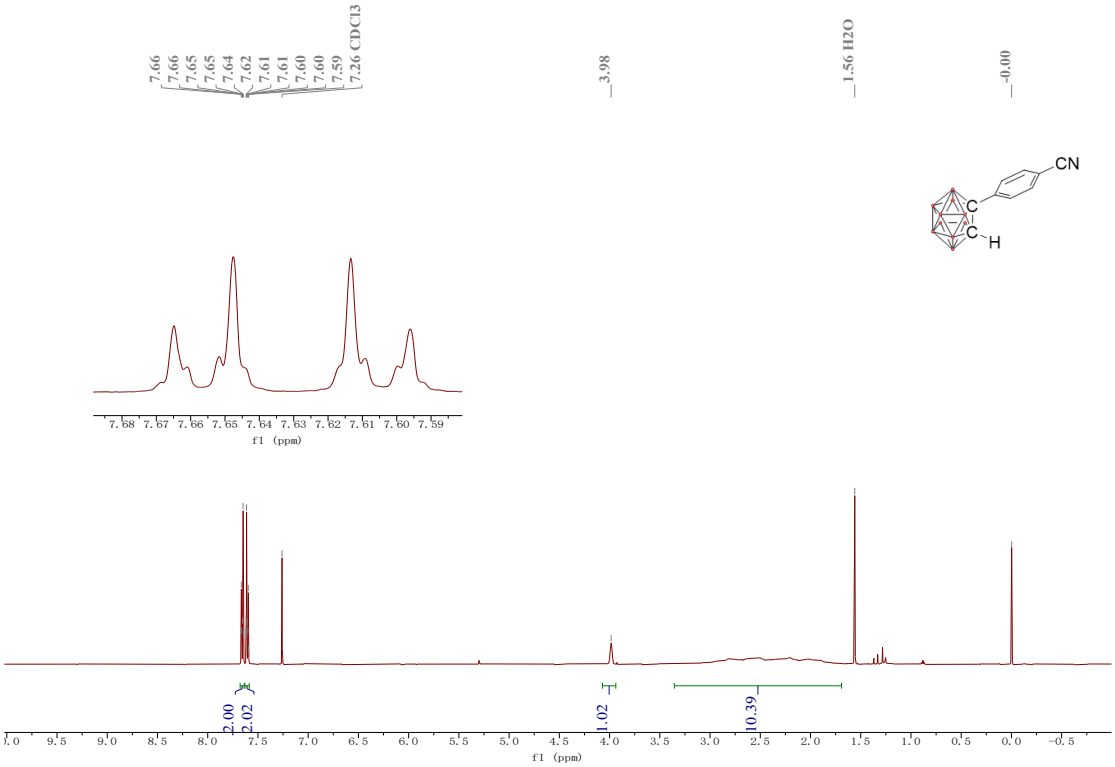


Fig. S16 ^{1}H NMR spectrum of ***p*-OCBs** ($CDCl_3$)

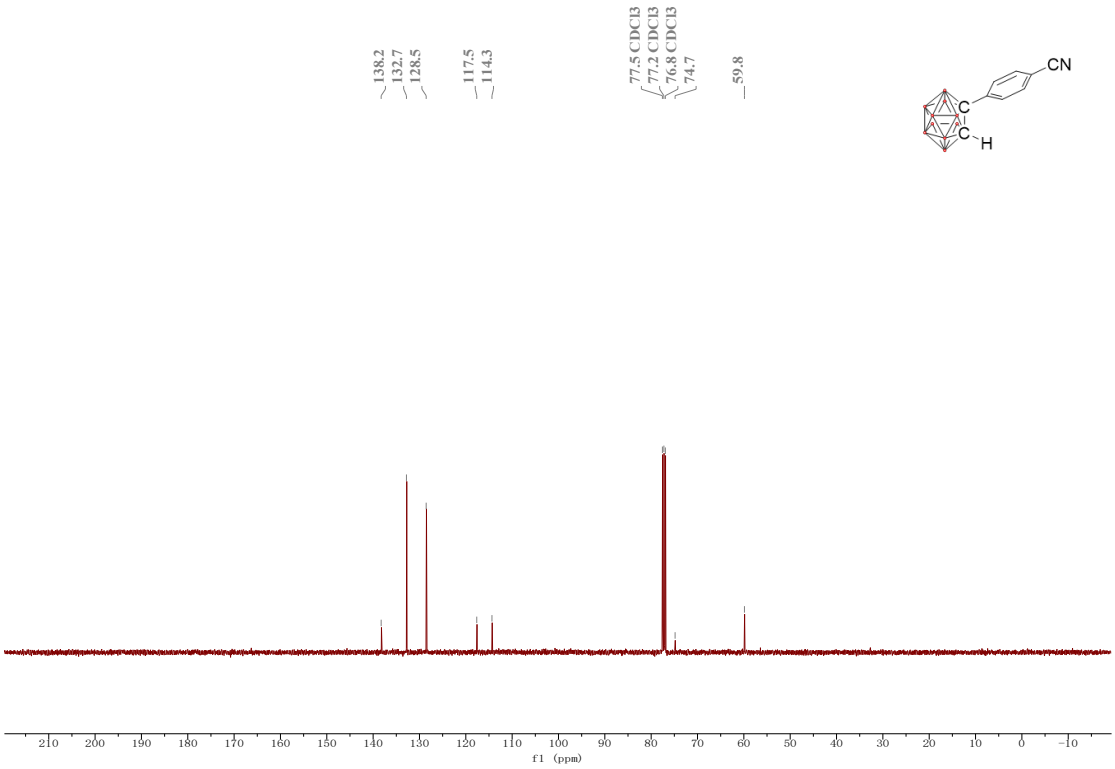


Fig. S17 ^{13}C NMR spectrum of ***p*-OCBs** ($CDCl_3$)

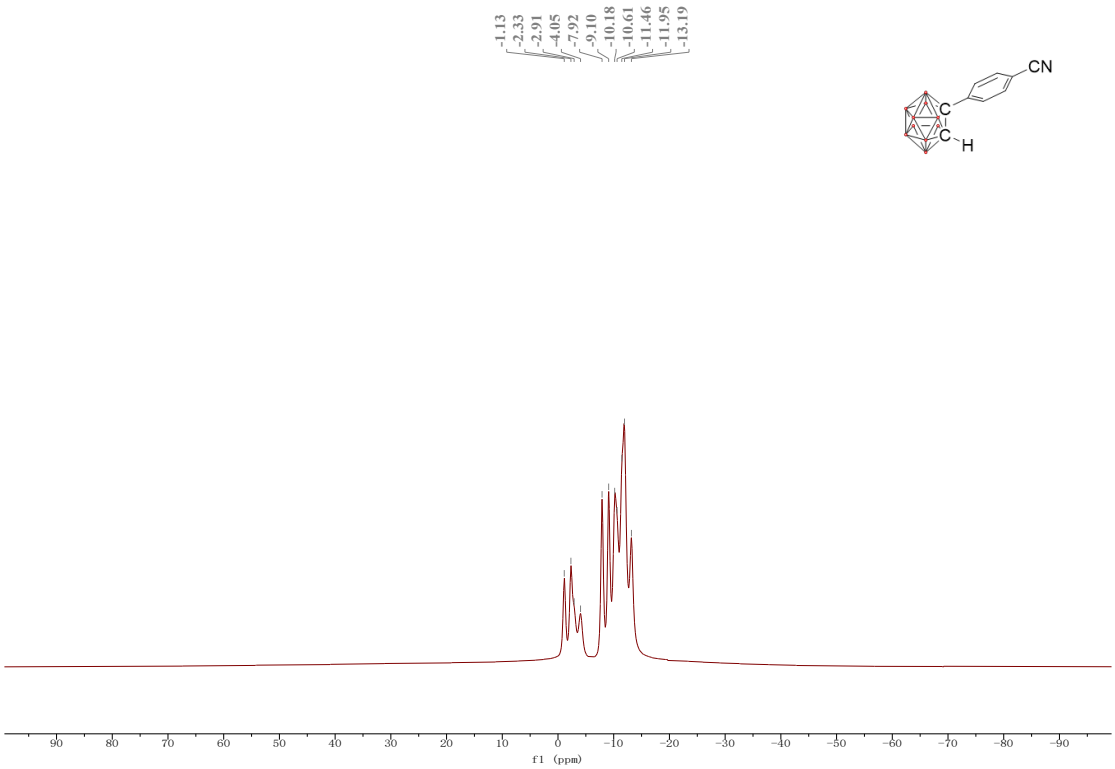


Fig. S18 ^{11}B NMR spectrum of ***p*-OCBs** ($CDCl_3$)

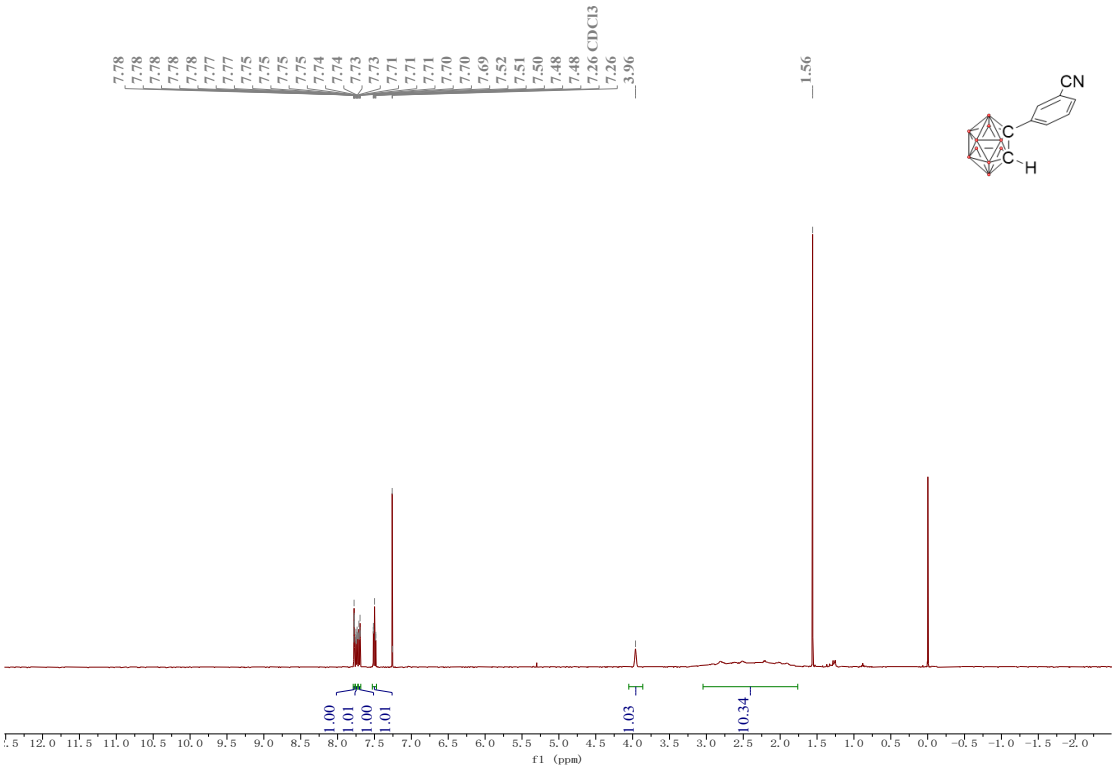


Fig. S19 ^{1}H NMR spectrum of ***m*-OCBs** ($CDCl_3$)

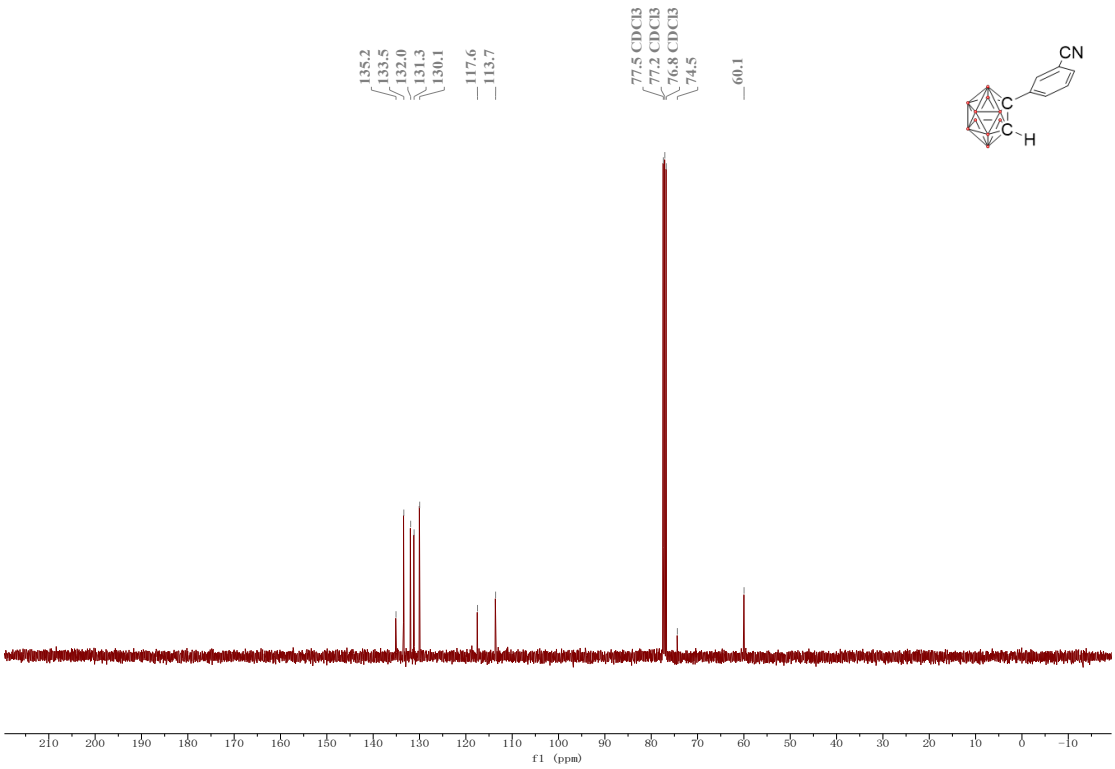


Fig. S20 ^{11}C NMR spectrum of ***m*-OCBs** ($CDCl_3$)

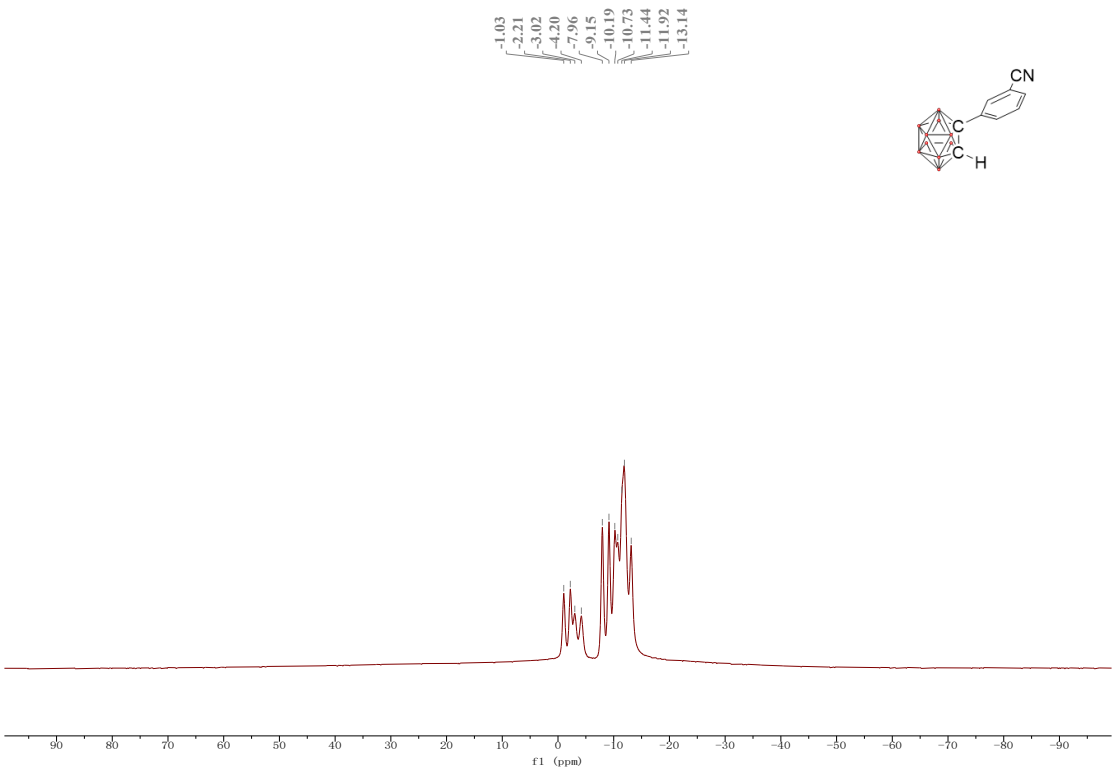


Fig. S21 ^{13}C NMR spectrum of ***m*-OCBs** ($CDCl_3$)

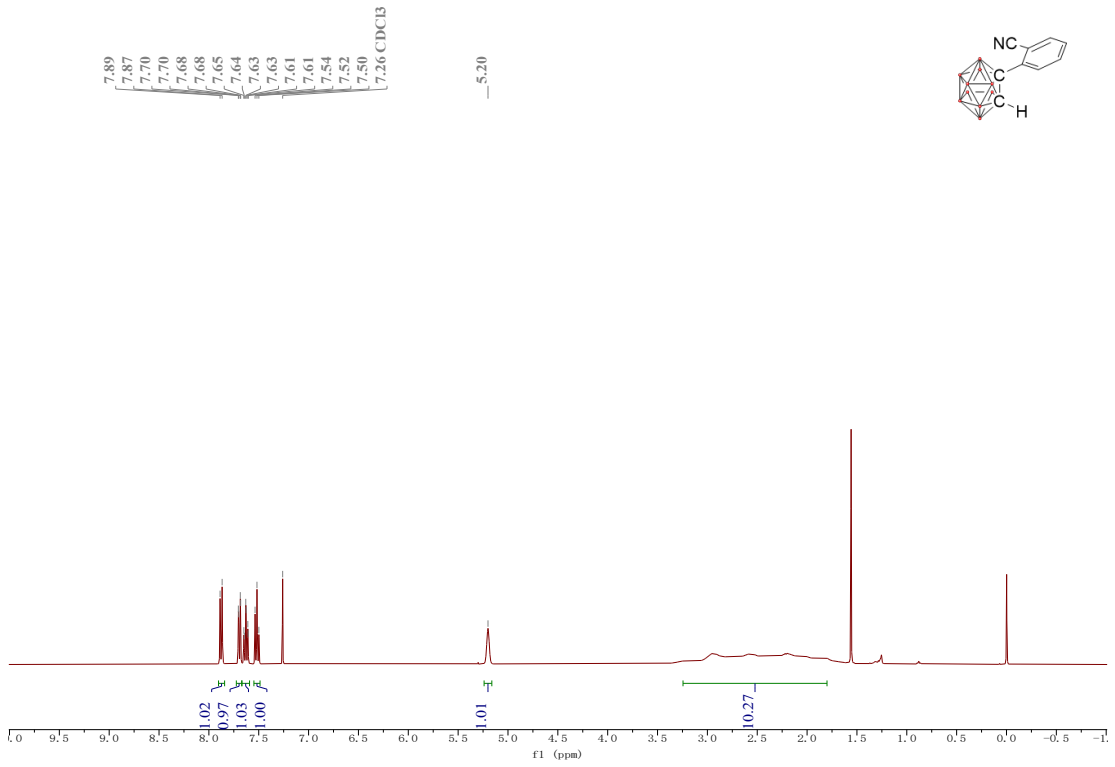


Fig. S22 ^{1}H NMR spectrum of ***o*-OCBs** ($CDCl_3$)

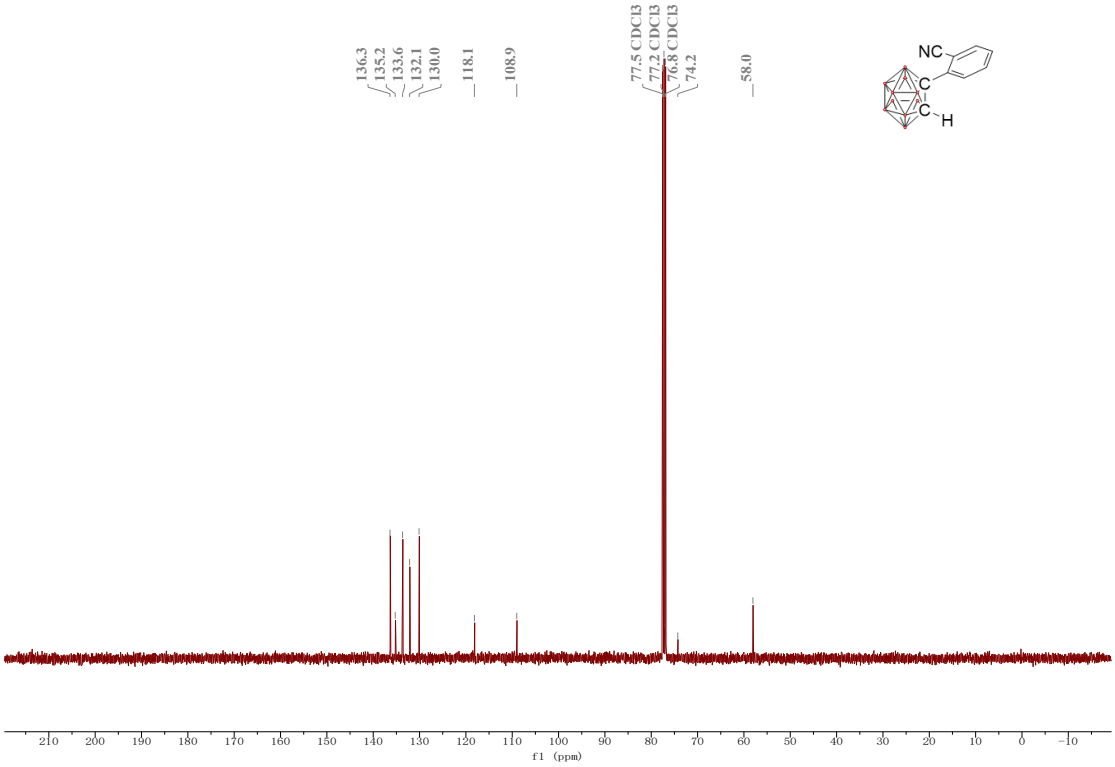


Fig. S23 ^{13}C NMR spectrum of ***o*-OCBs** ($CDCl_3$)

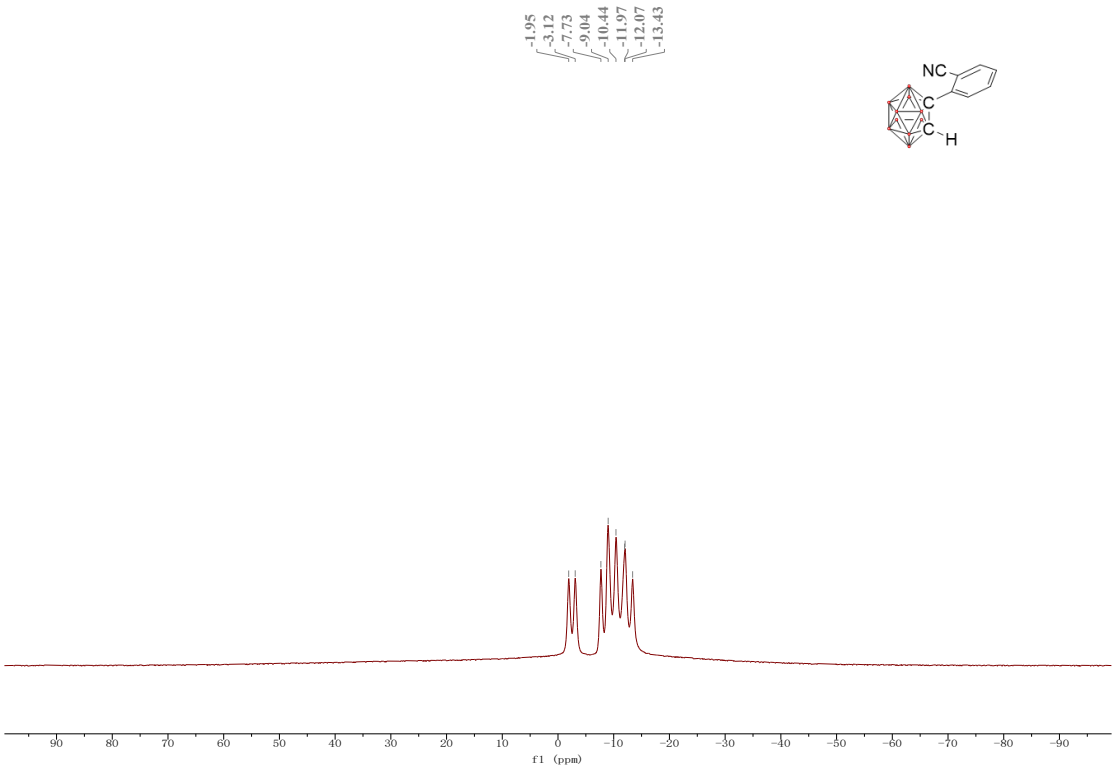


Fig. S24 ^{11}B NMR spectrum of ***o*-OCBs** ($CDCl_3$)

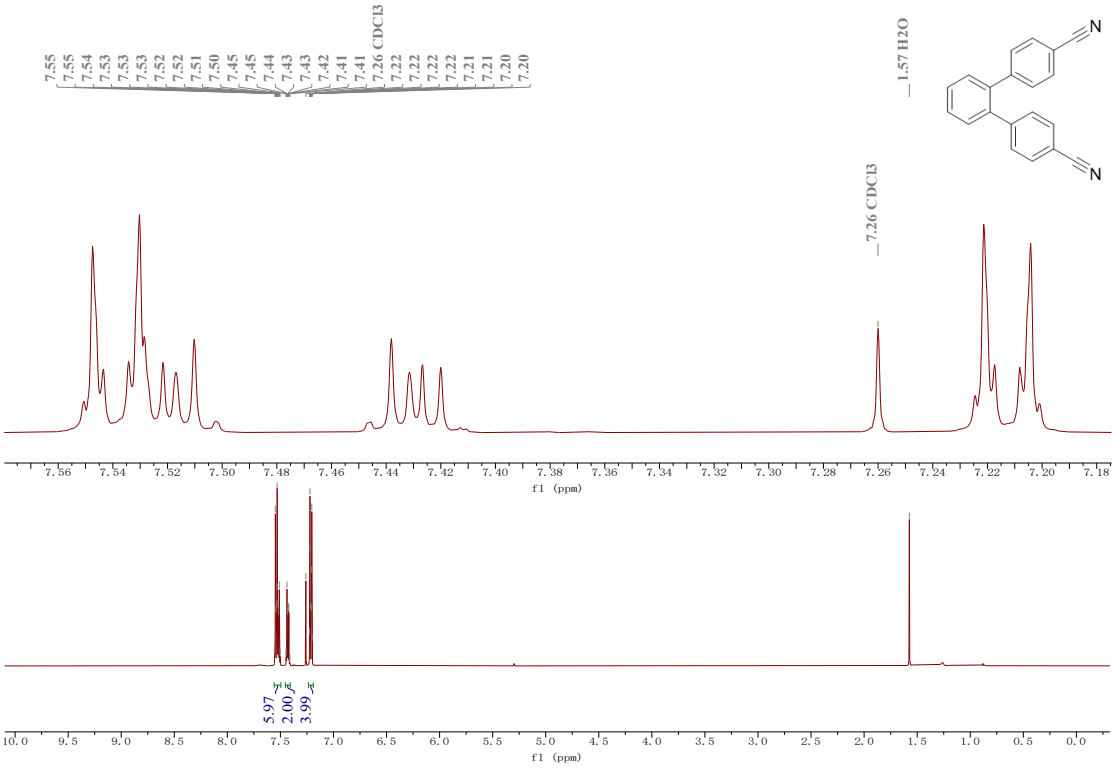


Fig. S25 ^{1}H NMR spectrum of ***p*-3ph** ($CDCl_3$)

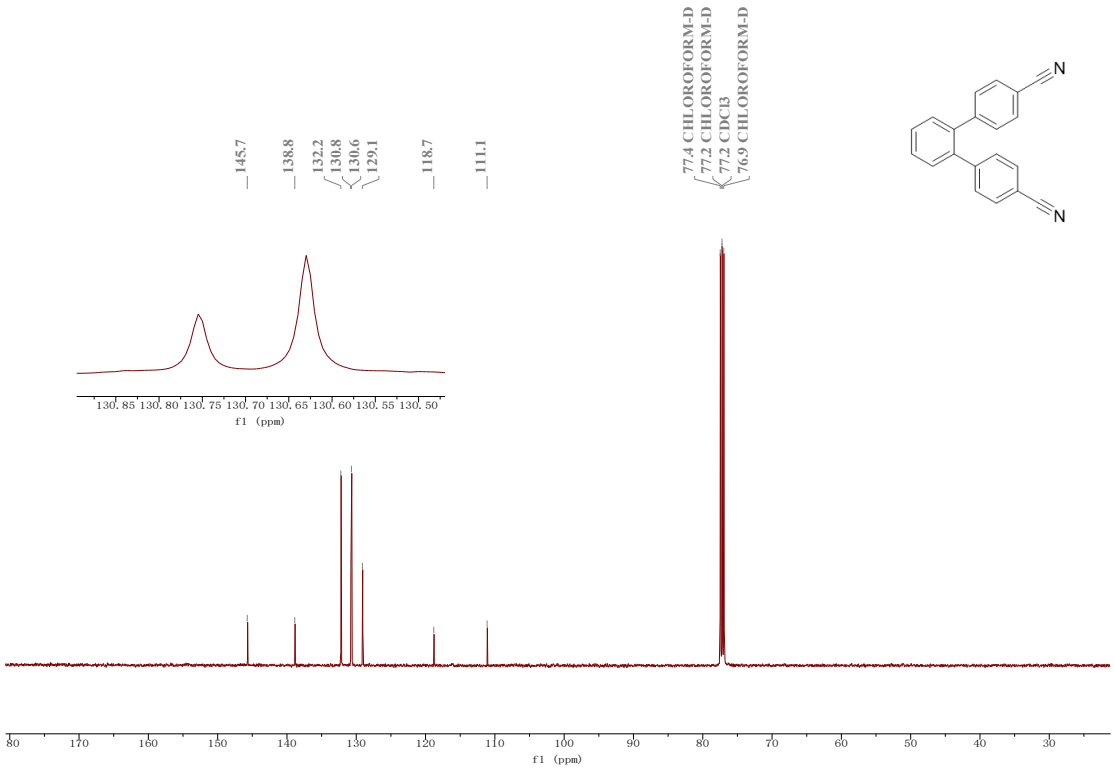


Fig. S26 ^{13}C NMR spectrum of ***p*-3ph** ($CDCl_3$)

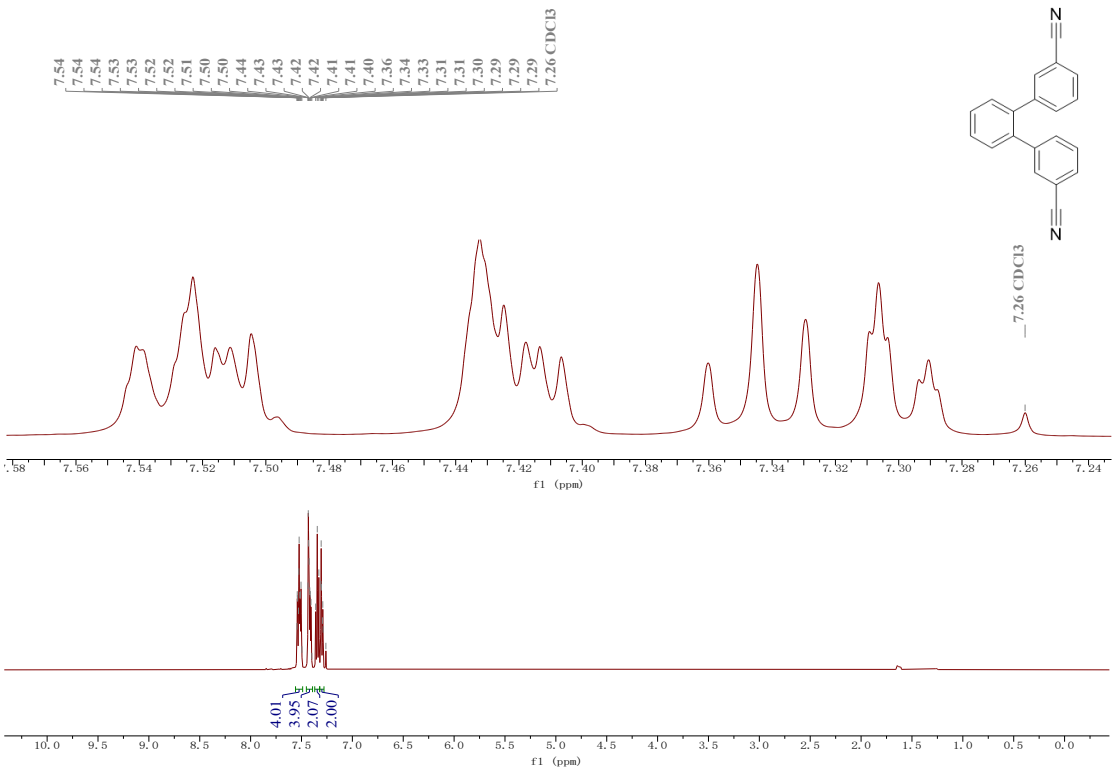


Fig. S27 ^{1}H NMR spectrum of ***m*-3ph** ($CDCl_3$)

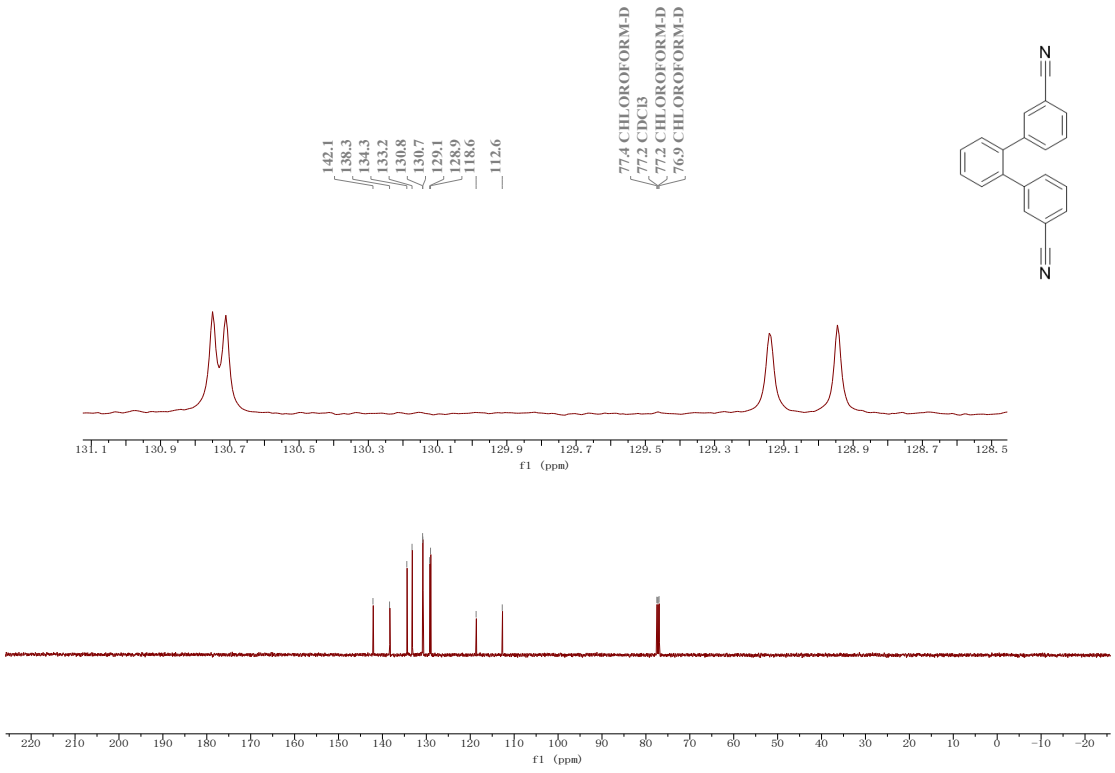


Fig. S28 ^{13}C NMR spectrum of ***m*-3ph** ($CDCl_3$)

6. MS

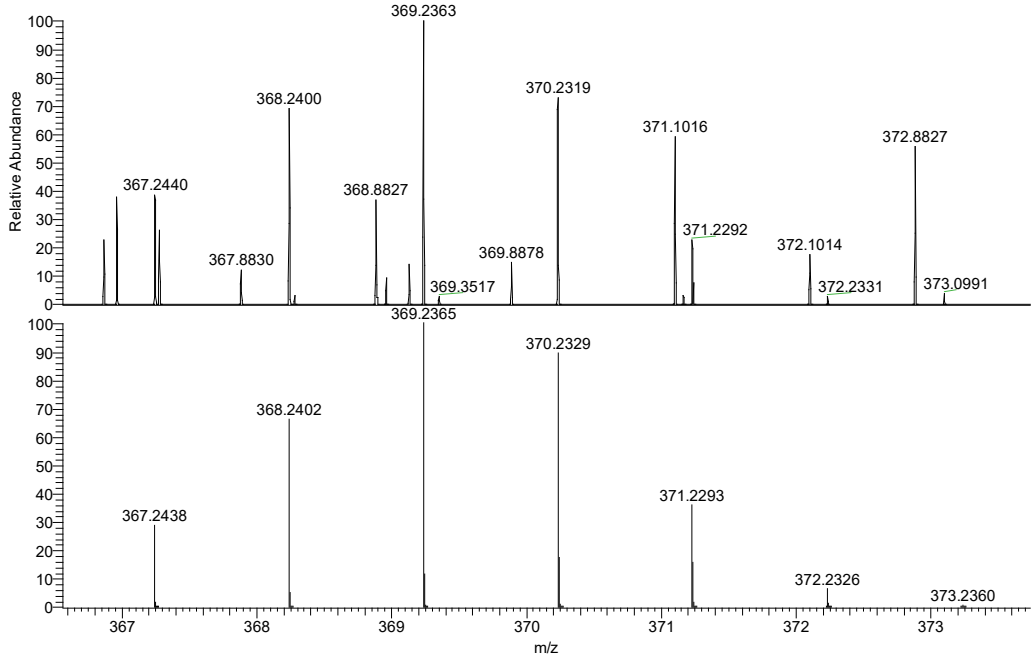


Fig. S29 MS of ***p*-OCB**

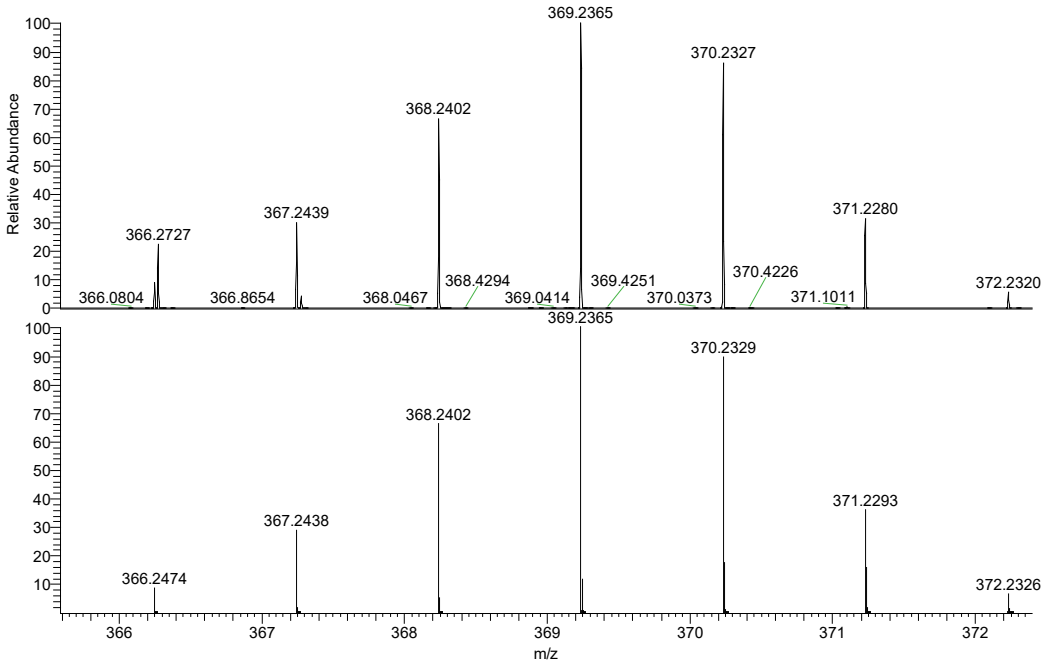


Fig. S30 MS of ***m*-OCB**

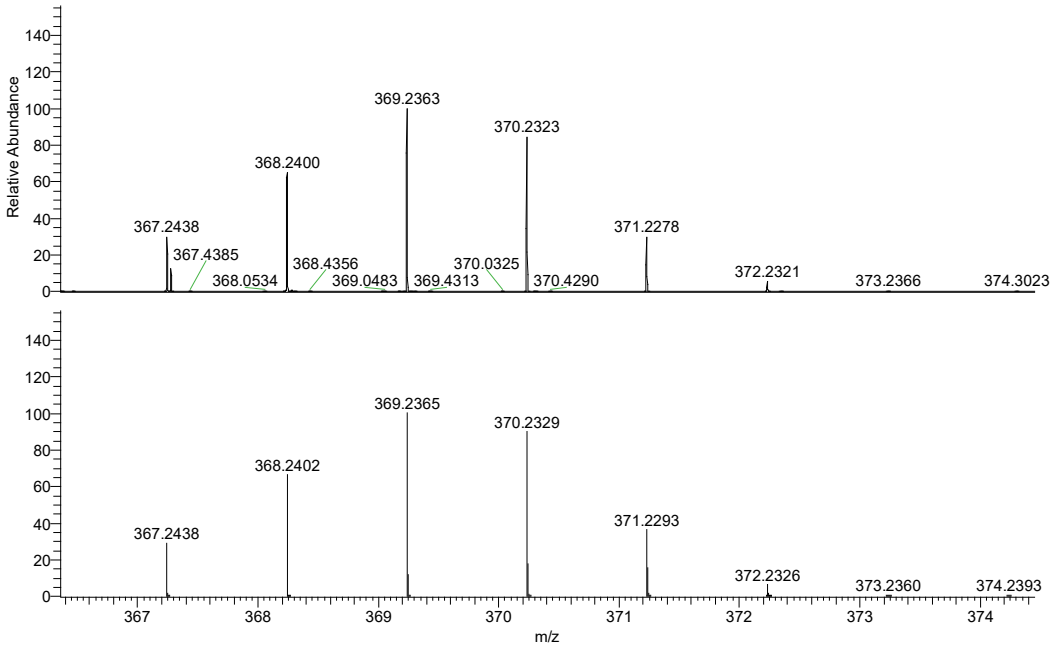


Fig. S31 MS of ***o*-OCB**

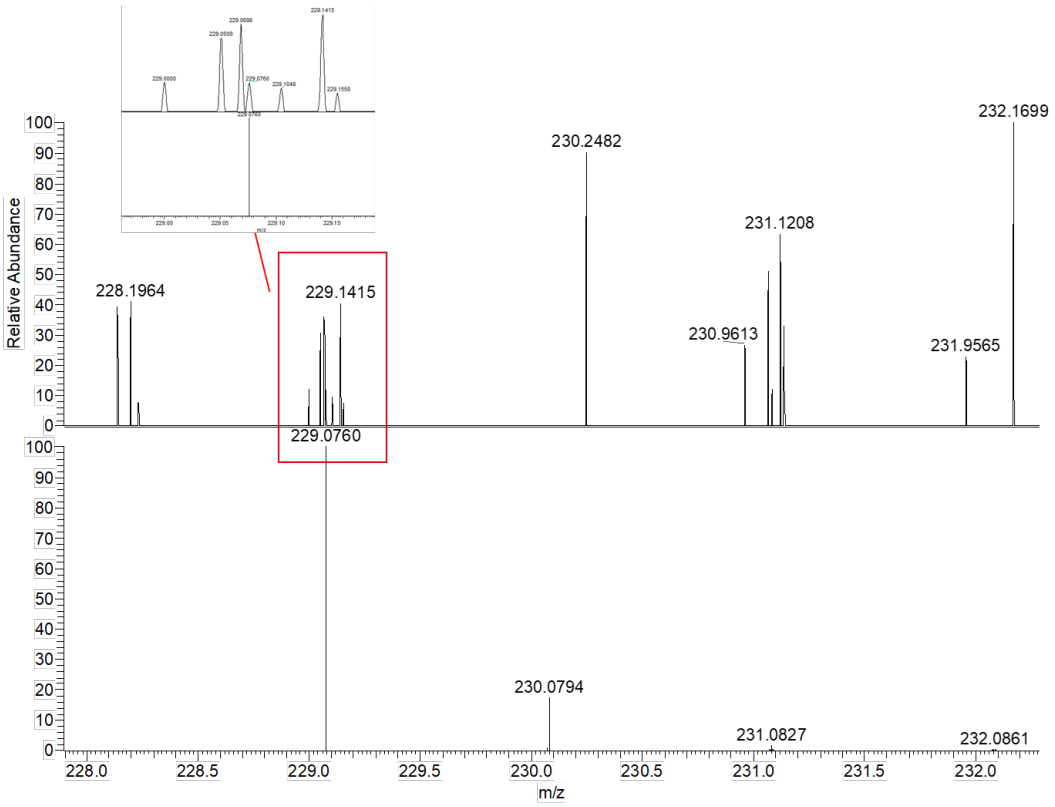


Fig. S32 MS of ***p*-yne**

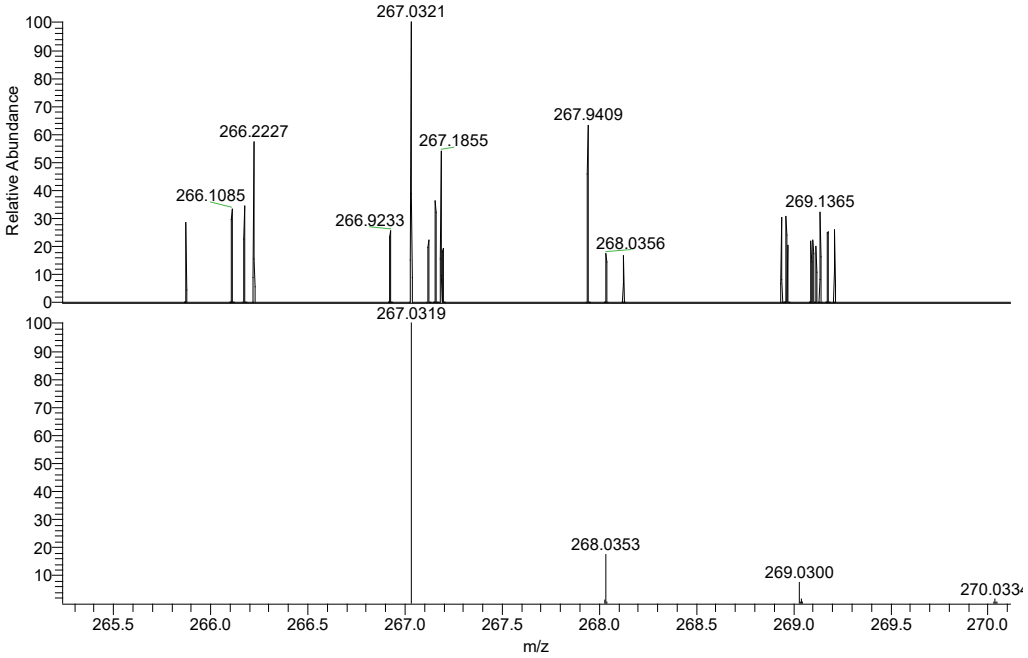


Fig. S33 MS of ***m*-yne**

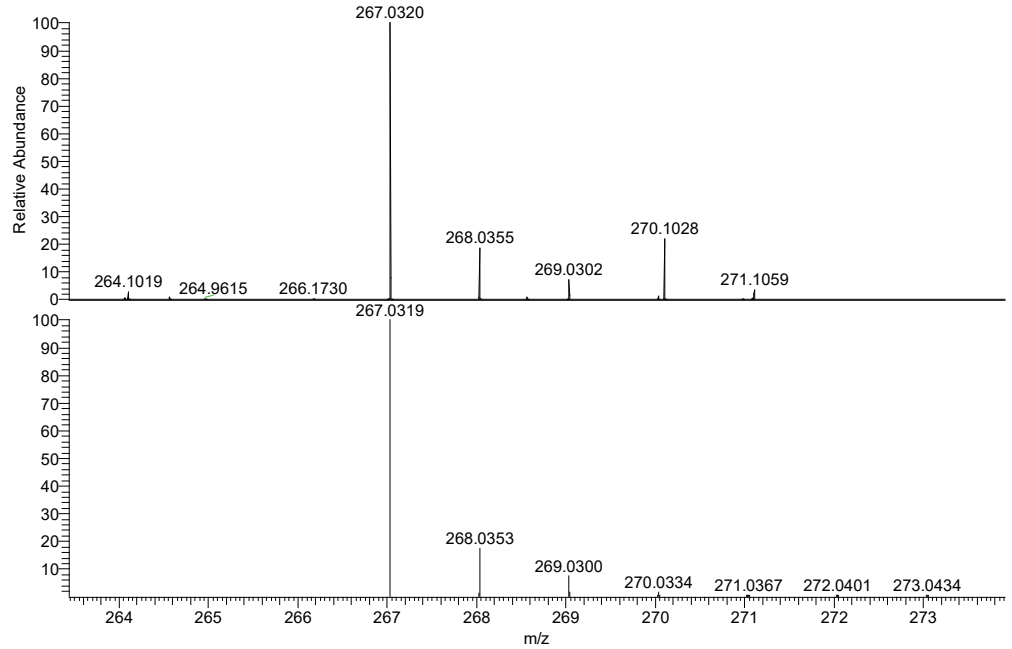


Fig. S34 MS of ***o*-yne**

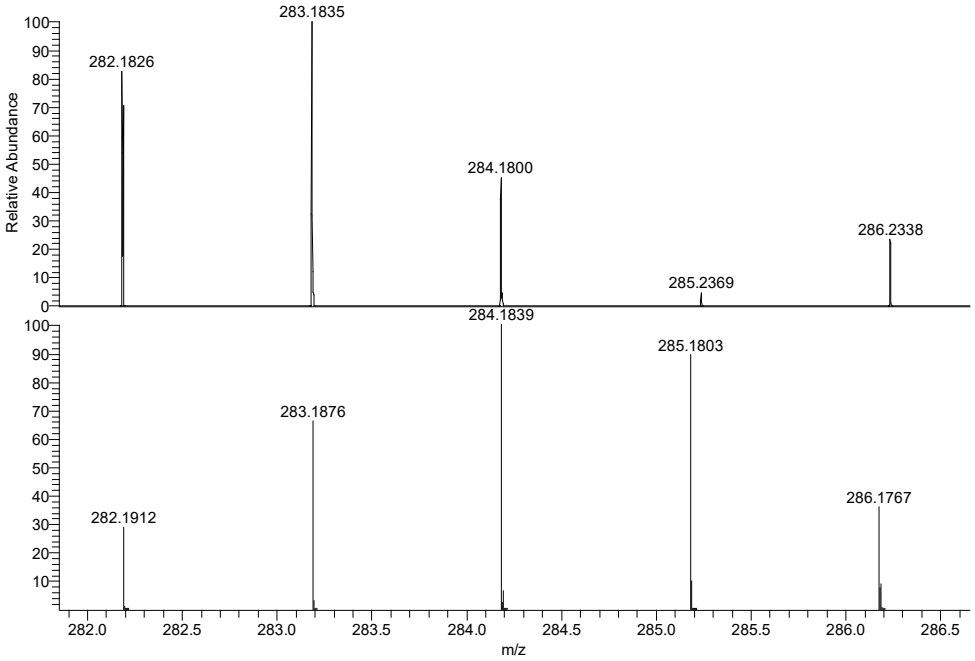


Fig. S35 MS of ***p*-OCBs**

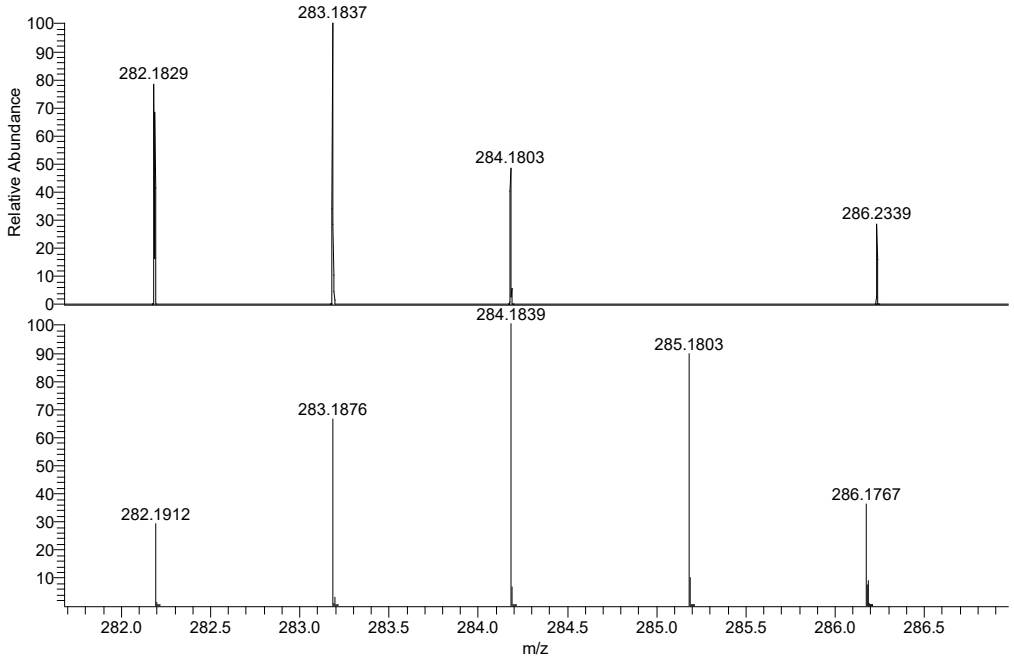


Fig. S36 MS of ***m*-OCBs**

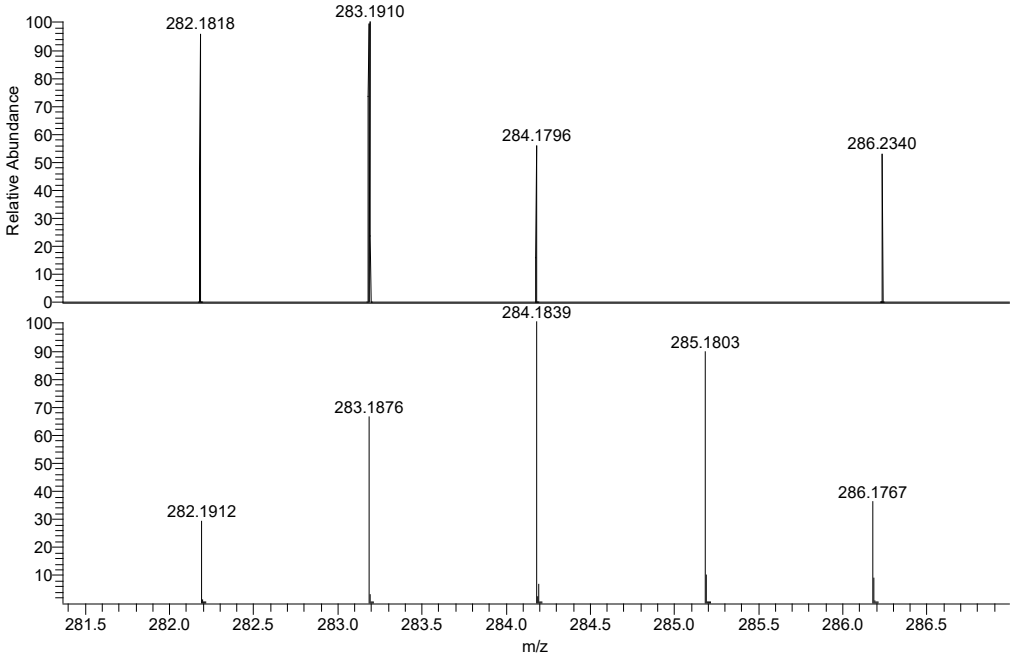


Fig. S37 MS of ***o*-OCBs**

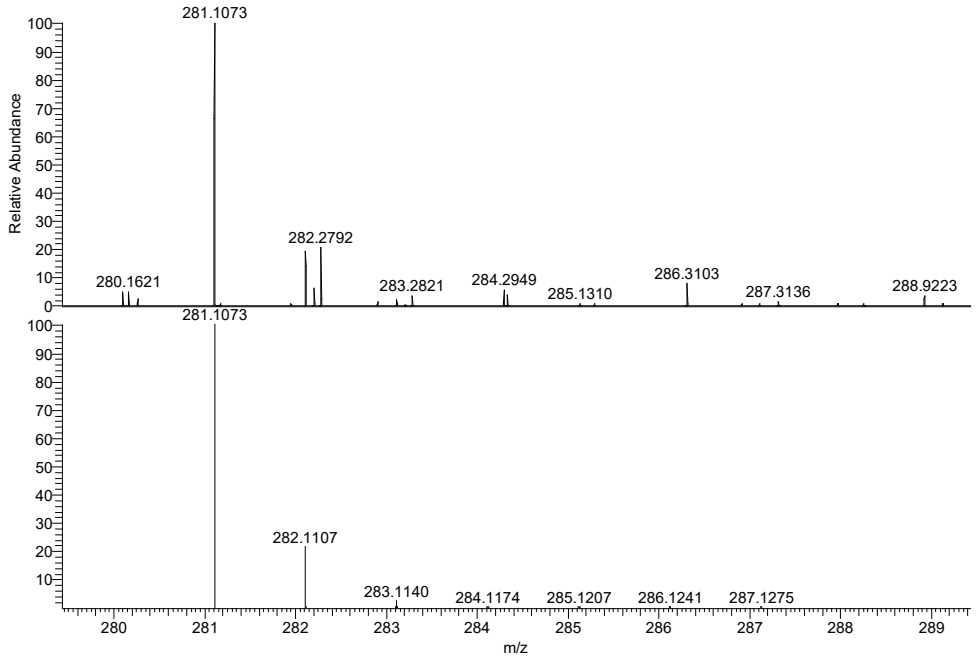


Fig. S38 MS of ***p*-3ph**

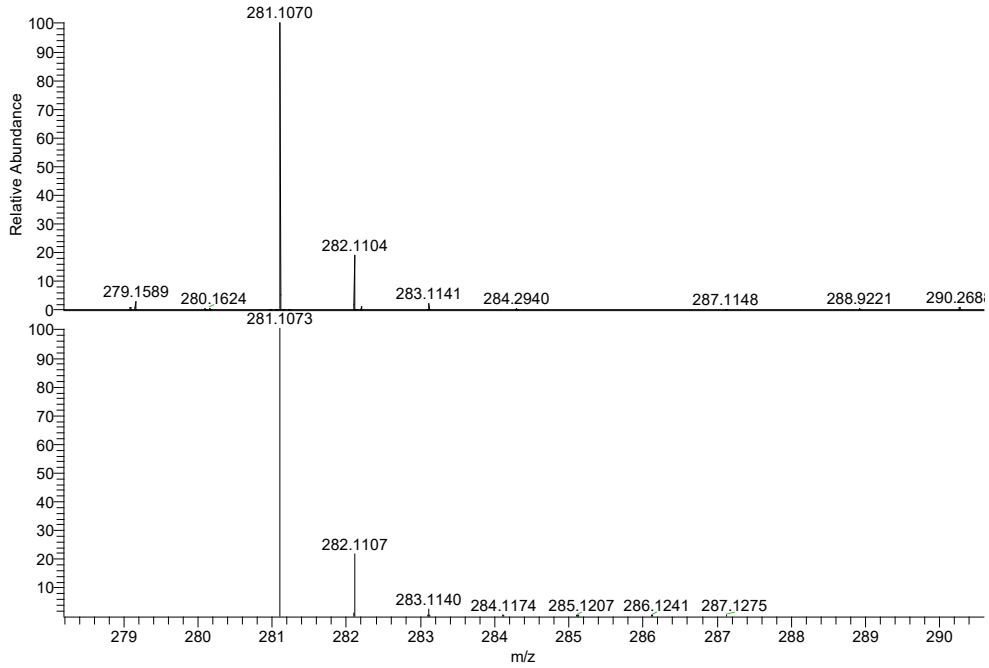


Fig. S39 MS of ***m*-3ph**

7. Single-crystal

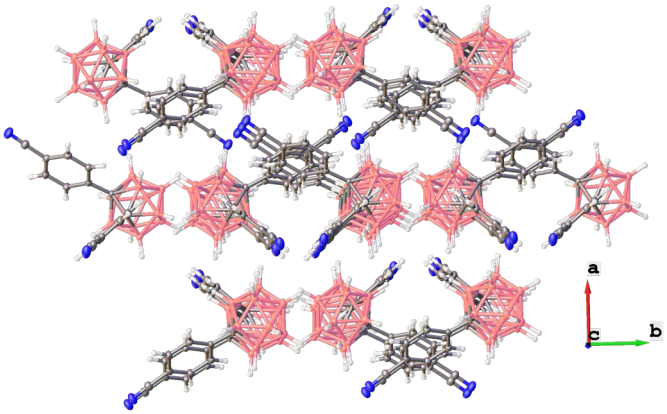


Fig. S40 The packing cell for the crystal structure of ***p*-OCB**, hydrogens are omitted for clarity. Atoms are coloured as follows: C in gray, N in blue, H in white and B in pink.

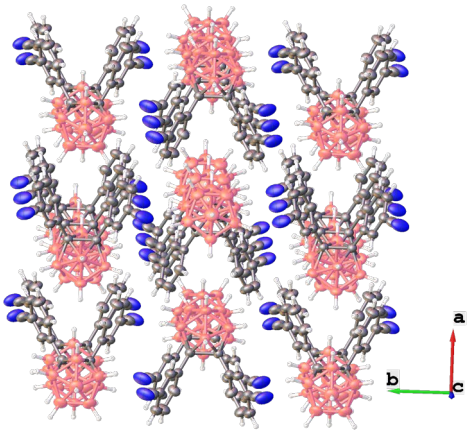


Fig. S41 The packing cell for the crystal structure of ***m*-OCB**, hydrogens are omitted for clarity. Atoms are coloured as follows: C in gray, N in blue, H in white and B in pink.

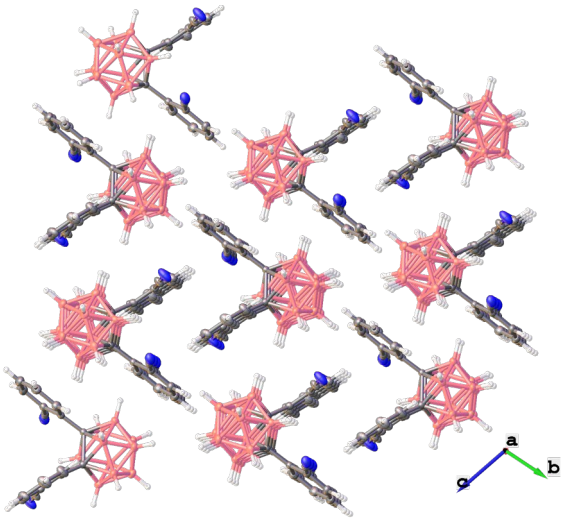


Fig. S42 The packing cell for the crystal structure of ***o*-OCB**, hydrogens are omitted for clarity. Atoms are coloured as follows: C in gray, N in blue, H in white and B in pink.

Table S2 Selected crystallographic data and collection parameters for wires

	***p*-OCB**	***m*-OCB**	***o*-OCB**	***p*-3ph**	***m*-3ph**
CCDC number	2132545	2125465	2132546	2214760	2214758
Empirical formula	$C_{16}H_{18}B_{10}N_2$	$C_{16}H_{18}B_{10}N_2$	$C_{16}H_{18}B_{10}N_2$	$C_{20}H_{12}N_2$	$C_{20}H_{12}N_2$
Formula weight	346.42	346.42	346.42	280.32	280.32
Temperature/K	100(2)	295.15	296.15	296.15	296(2)
Crystal system	Monoclinic	Orthorhombic	Triclinic	Monoclinic	Triclinic
Space group	$P2_1/c$	Pnma	P_{-1}	$I2/c$	P_{-1}
a/Å	14.0009(3)	15.7091(3)	8.1494(6)	8.774(6)	9.183(6)
b/Å	12.7944(2)	15.5322(3)	10.0960(8)	9.536(6)	9.523(8)
c/Å	10.7411(2)	8.0832(2)	12.6685(9)	18.164(12)	10.047(9)
α/°	90	90	104.041(2)	90	99.63(4)
β/°	97.2876(17)	90	91.846(2)	97.18(4)	116.10(3)
γ/°	90	90	108.764(3)	90	98.13(4)
Volume/Å^3	1908.53(6)	1972.28(7)	950.51(12)	1507.8(17)	754.6(11)
Z	4	4	2	4	2
μ/mm^{-1}	0.463	0.448	0.063	0.073	0.073
F(000)	712.0	712.0	356.0	584.0	292.0
2θ range/°	6.364 to 153.032	11.266 to 145.006	4.422 to 50.108	4.52 to 54.3	4.472 to 54.334
Reflections collected	13039	6159	21097	12198	14256
Independent reflections	3846	1970	3355	1672	3247
Data/restraints/parameters	3846/0/254	1970/0/134	3355/0/253	1672/0/100	3247/0/200
Goodness-of-fit on F^2	1.057	1.047	1.032	1.036	1.052
Final *R* indices	R_1 = 0.0408 wR_2 = 0.1094	R_1 = 0.0489 wR_2 = 0.1335	R_1 = 0.0426 wR_2 = 0.1091	R_1 = 0.0424 wR_2 = 0.0967	R_1 = 0.0439 wR_2 = 0.1090
R indices	R_1 = 0.0462 wR_2 = 0.1125	R_1 = 0.0559 wR_2 = 0.1413	R_1 = 0.0555 wR_2 = 0.1156	R_1 = 0.0713 wR_2 = 0.1078	R_1 = 0.0785 wR_2 = 0.1225

8. UV-vis of wires

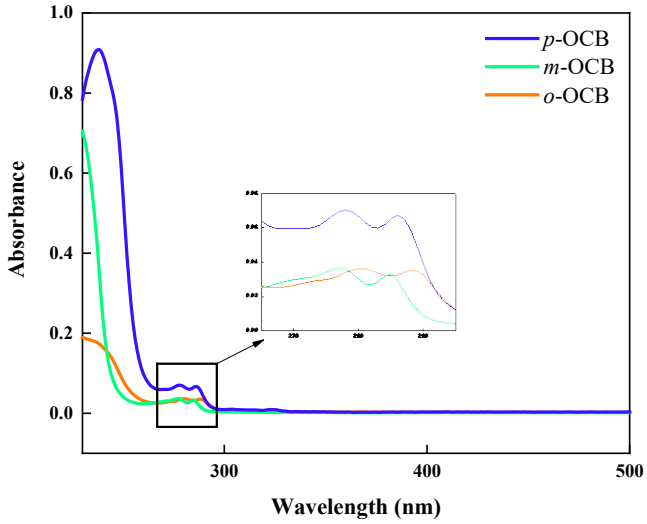


Fig. S43 UV-Vis absorption of wires (3.0×10^{-5} mol/L) in CH_2Cl_2 at room temperature.

9. Electrochemical Characterization of wires

The redox behavior of wires was characterized by cyclic voltammetry (CV) and differential pulse voltammetry (DPV) in acetonitrile with a scan rate of 100 mV s^{-1}. CV and DPV were performed by using 1.0×10^{-3} mol L^{-1} samples and using (n-$C_4H_9)_4NPF_6$ (0.1 mol L^{-1}) as the supporting electrolyte. The electrochemical behavior of wires has two reversible electrochemical redox processes. The first redox process is the formation of a stable carborane radical anion with a true 2n+3 cluster electron count.[6, 7] The second redox process is the formation of 12-vertex carboranes with 2n+4 (*nido*) skeletal electron counts.[6]

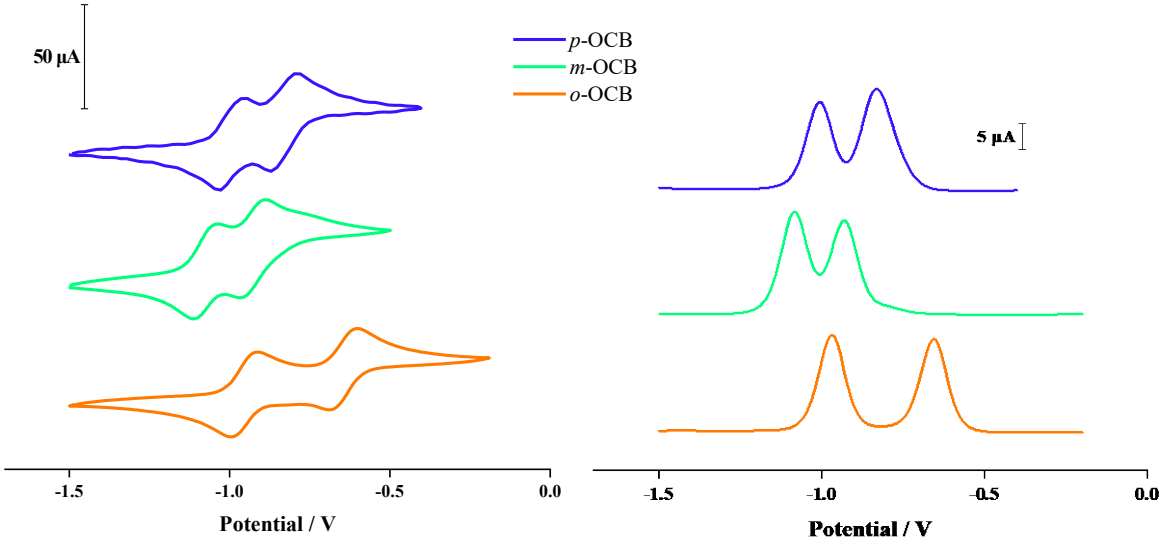


Fig. S44 CV (left) and DPV (right) curves of wires (1.0×10^{-3} mol L^{-1}) in acetonitrile at room temperature.

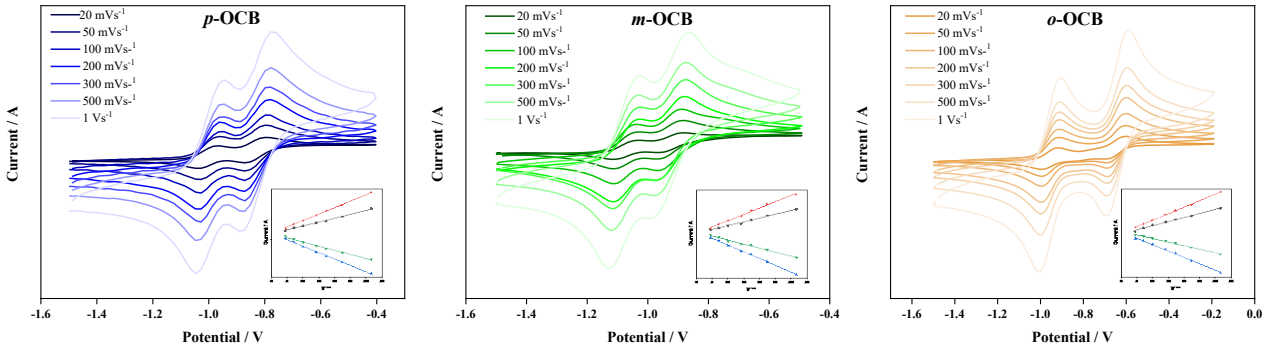


Fig. S45 CV of wires in acetonitrile at room temperature: (left) ***p*-OCB**, (middle) ***m*-OCB**, (right) ***o*-OCB**. The scan rates are 20, 50, 100, 200, 300 and 500 and 1000 mV s^{-1}, respectively. Inset: linear dependence of the peak currents as a function of scan rates.

Table S3 The ^{13}C NMR and ^{11}B NMR of wires in $CDCl_3$.

Wires	$\delta^{13}C$	$\delta^{11}B$
***p*-OCB**	83.2	–0.78, –1.96, –9.10, –10.10, –12.02
***m*-OCB**	82.9	–0.76, –1.95, –9.19, –10.17, –12.34
***o*-OCB**	84.9	–0.11, –1.08, –8.22, –9.47, –11.78

10. Blank solvent conductance test

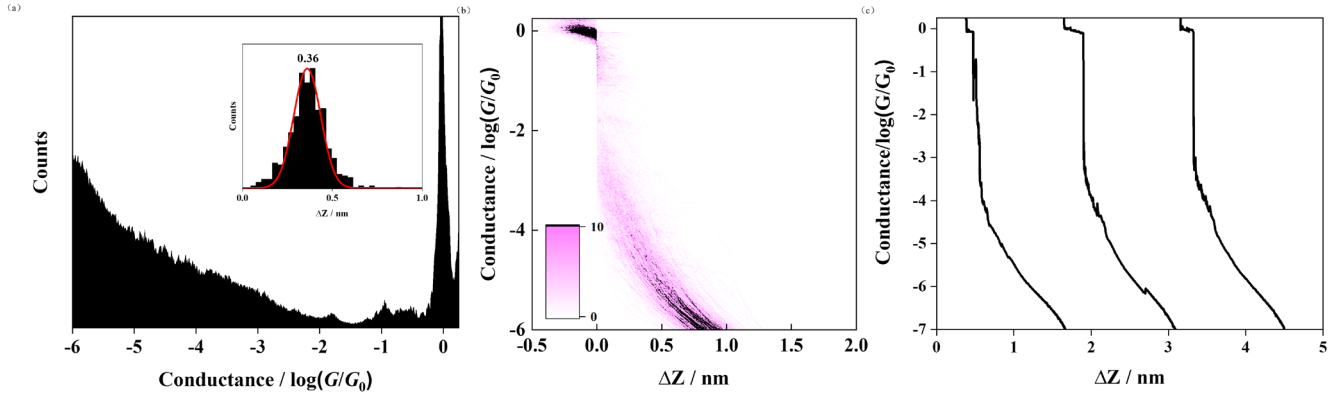


Fig. S46 The conductance testing of blank solvent. (a) 1D conductance histogram of blank solvent without molecular junction peak. Inset: The relative stretching displacement histogram from $10^{-3.0}$ G_0 to $10^{-5.0}$ G_0. (b) 2D conductance histogram of blank solvent. (C) The typical individual traces of blank solvent.

11. The flicker noise measurement

The flicker noise measurements were carried out according to the same process as previous studies.[8] When the conductance reached the range of the molecular platform, it indicated that the molecular junction has been formed. The conductance platform of ***m*-OCB** was set as $10^{-2.2\sim-3.3}$ and that of ***p*-OCB** was $10^{-2.5\sim-3.5}$, which can be distinguished from the most possible conductance in the 1D histograms. We suspended the tip during the retracting process for 100 ms after the formation of molecular junctions. The noise spectrums were obtained by the fast Fourier transform. We calculated the noise power according to the noise spectrum integration from 100 Hz to 1000 Hz and plotted the noise power against the average conductance.

12. Conductance of the rest of the molecules

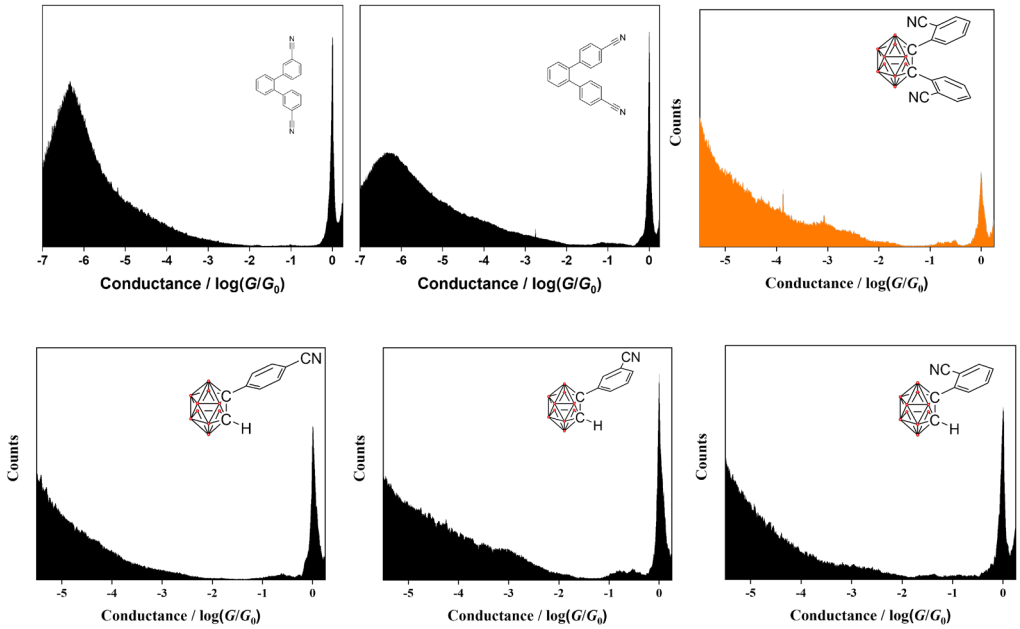


Fig. S47 The conductance testing of the rest of molecules.

13. Single crystals of *p*-3ph and *m*-3ph

Single crystal of ***p*-3ph** were obtained by slow diffusion of *n*-hexane into a solution of the compound in $CHCl_3$ at room temperature and analyzed by X-ray diffraction crystallography. Single crystal of ***m*-3ph** were obtained by slow diffusion of *n*-hexane into a solution of the compound in $CDCl_3$ at room temperature and analyzed by X-ray diffraction crystallography.

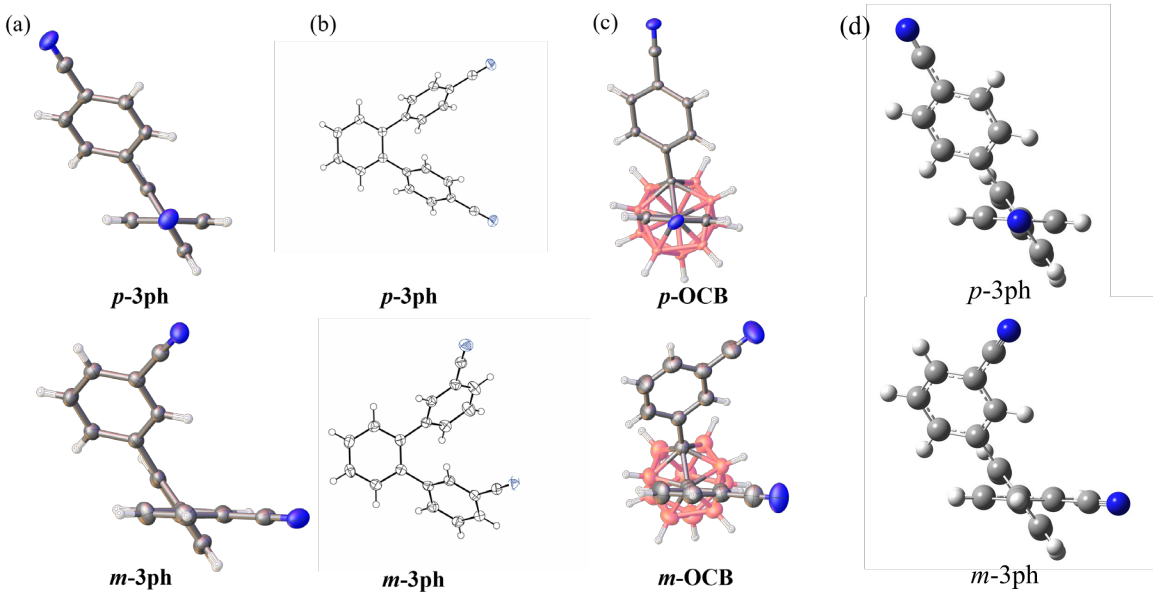


Fig. S48 Structures of phenyl-centered molecules (a) single crystal structures (b) ORTEP diagram (50% probability level). And (c) single crystal structure of *o*-carborane-based molecules. Atoms are coloured as follows: C in gray, N in blue, H in white and B in pink. (d) The optimized structures of phenyl-centered molecules.

14. The XYZ file of the junction geometries

***p*-OCB**

Au	1.441879e+00	8.324693e-01	1.177289e+00
Au	4.325637e+00	8.324693e-01	1.177289e+00
Au	7.209396e+00	8.324693e-01	1.177289e+00
Au	1.009315e+01	8.324693e-01	1.177289e+00
Au	1.297691e+01	8.324693e-01	1.177289e+00
Au	1.586067e+01	8.324693e-01	1.177289e+00
Au	0.000000e+00	3.329877e+00	1.177289e+00
Au	2.883758e+00	3.329877e+00	1.177289e+00
Au	5.767516e+00	3.329877e+00	1.177289e+00
Au	8.651275e+00	3.329877e+00	1.177289e+00
Au	1.153503e+01	3.329877e+00	1.177289e+00
Au	1.441879e+01	3.329877e+00	1.177289e+00
Au	-1.441879e+00	5.827285e+00	1.177289e+00
Au	1.441879e+00	5.827285e+00	1.177289e+00
Au	4.325637e+00	5.827285e+00	1.177289e+00
Au	7.209396e+00	5.827285e+00	1.177289e+00
Au	1.009315e+01	5.827285e+00	1.177289e+00
Au	1.297691e+01	5.827285e+00	1.177289e+00
Au	-2.883758e+00	8.324693e+00	1.177289e+00
Au	0.000000e+00	8.324693e+00	1.177289e+00
Au	2.883758e+00	8.324693e+00	1.177289e+00
Au	5.767516e+00	8.324693e+00	1.177289e+00
Au	8.651275e+00	8.324693e+00	1.177289e+00
Au	1.153503e+01	8.324693e+00	1.177289e+00
Au	-4.325637e+00	1.082210e+01	1.177289e+00
Au	-1.441879e+00	1.082210e+01	1.177289e+00
Au	1.441879e+00	1.082210e+01	1.177289e+00
Au	4.325637e+00	1.082210e+01	1.177289e+00
Au	7.209396e+00	1.082210e+01	1.177289e+00
Au	1.009315e+01	1.082210e+01	1.177289e+00
Au	-5.767516e+00	1.331951e+01	1.177289e+00
Au	-2.883758e+00	1.331951e+01	1.177289e+00
Au	0.000000e+00	1.331951e+01	1.177289e+00
Au	2.883758e+00	1.331951e+01	1.177289e+00
Au	5.767516e+00	1.331951e+01	1.177289e+00
Au	8.651275e+00	1.331951e+01	1.177289e+00
Au	0.000000e+00	1.664939e+00	3.531868e+00
Au	2.883758e+00	1.664939e+00	3.531868e+00
Au	5.767516e+00	1.664939e+00	3.531868e+00
Au	8.651275e+00	1.664939e+00	3.531868e+00
Au	1.153503e+01	1.664939e+00	3.531868e+00
Au	1.441879e+01	1.664939e+00	3.531868e+00
Au	-1.441879e+00	4.162346e+00	3.531868e+00
Au	1.441879e+00	4.162346e+00	3.531868e+00
Au	4.325637e+00	4.162346e+00	3.531868e+00

Au	7.209396e+00	4.162346e+00	3.531868e+00
Au	1.009315e+01	4.162346e+00	3.531868e+00
Au	1.297691e+01	4.162346e+00	3.531868e+00
Au	-2.883758e+00	6.659754e+00	3.531868e+00
Au	0.000000e+00	6.659754e+00	3.531868e+00
Au	2.883758e+00	6.659754e+00	3.531868e+00
Au	5.767516e+00	6.659754e+00	3.531868e+00
Au	8.651275e+00	6.659754e+00	3.531868e+00
Au	1.153503e+01	6.659754e+00	3.531868e+00
Au	-4.325637e+00	9.157162e+00	3.531868e+00
Au	-1.441879e+00	9.157162e+00	3.531868e+00
Au	1.441879e+00	9.157162e+00	3.531868e+00
Au	4.325637e+00	9.157162e+00	3.531868e+00
Au	7.209396e+00	9.157162e+00	3.531868e+00
Au	1.009315e+01	9.157162e+00	3.531868e+00
Au	-5.767516e+00	1.165457e+01	3.531868e+00
Au	-2.883758e+00	1.165457e+01	3.531868e+00
Au	0.000000e+00	1.165457e+01	3.531868e+00
Au	2.883758e+00	1.165457e+01	3.531868e+00
Au	5.767516e+00	1.165457e+01	3.531868e+00
Au	8.651275e+00	1.165457e+01	3.531868e+00
Au	-7.209396e+00	1.415198e+01	3.531868e+00
Au	-4.325637e+00	1.415198e+01	3.531868e+00
Au	-1.441879e+00	1.415198e+01	3.531868e+00
Au	1.441879e+00	1.415198e+01	3.531868e+00
Au	4.325637e+00	1.415198e+01	3.531868e+00
Au	7.209396e+00	1.415198e+01	3.531868e+00
Au	0.000000e+00	0.000000e+00	5.886447e+00
Au	2.883758e+00	0.000000e+00	5.886447e+00
Au	5.767516e+00	0.000000e+00	5.886447e+00
Au	8.651275e+00	0.000000e+00	5.886447e+00
Au	1.153503e+01	0.000000e+00	5.886447e+00
Au	1.441879e+01	0.000000e+00	5.886447e+00
Au	-1.441879e+00	2.497408e+00	5.886447e+00
Au	1.441879e+00	2.497408e+00	5.886447e+00
Au	4.325637e+00	2.497408e+00	5.886447e+00
Au	7.209396e+00	2.497408e+00	5.886447e+00
Au	1.009315e+01	2.497408e+00	5.886447e+00
Au	1.297691e+01	2.497408e+00	5.886447e+00
Au	-2.883758e+00	4.994816e+00	5.886447e+00
Au	0.000000e+00	4.994816e+00	5.886447e+00
Au	2.883758e+00	4.994816e+00	5.886447e+00
Au	5.767516e+00	4.994816e+00	5.886447e+00
Au	8.651275e+00	4.994816e+00	5.886447e+00
Au	1.153503e+01	4.994816e+00	5.886447e+00

Au	-4.325637e+00	7.492224e+00	5.886447e+00
Au	-1.441879e+00	7.492224e+00	5.886447e+00
Au	1.441879e+00	7.492224e+00	5.886447e+00
Au	4.325637e+00	7.492224e+00	5.886447e+00
Au	7.209396e+00	7.492224e+00	5.886447e+00
Au	1.009315e+01	7.492224e+00	5.886447e+00
Au	-5.767516e+00	9.989632e+00	5.886447e+00
Au	-2.883758e+00	9.989632e+00	5.886447e+00
Au	0.000000e+00	9.989632e+00	5.886447e+00
Au	2.883758e+00	9.989632e+00	5.886447e+00
Au	5.767516e+00	9.989632e+00	5.886447e+00
Au	8.651275e+00	9.989632e+00	5.886447e+00
Au	-7.209396e+00	1.248704e+01	5.886447e+00
Au	-4.325637e+00	1.248704e+01	5.886447e+00
Au	-1.441879e+00	1.248704e+01	5.886447e+00
Au	1.441879e+00	1.248704e+01	5.886447e+00
Au	4.325637e+00	1.248704e+01	5.886447e+00
Au	7.209396e+00	1.248704e+01	5.886447e+00
Au	1.441879e+00	8.324693e-01	8.241026e+00
Au	4.325637e+00	8.324693e-01	8.241026e+00
Au	7.209396e+00	8.324693e-01	8.241026e+00
Au	1.009315e+01	8.324693e-01	8.241026e+00
Au	1.297691e+01	8.324693e-01	8.241026e+00
Au	1.586067e+01	8.324693e-01	8.241026e+00
Au	-0.000000e+00	3.329877e+00	8.241026e+00
Au	2.883758e+00	3.329877e+00	8.241026e+00
Au	5.767516e+00	3.329877e+00	8.241026e+00
Au	8.651275e+00	3.329877e+00	8.241026e+00
Au	1.153503e+01	3.329877e+00	8.241026e+00
Au	1.441879e+01	3.329877e+00	8.241026e+00
Au	-1.441879e+00	5.827285e+00	8.241026e+00
Au	1.441879e+00	5.827285e+00	8.241026e+00
Au	4.325637e+00	5.827285e+00	8.241026e+00
Au	7.209396e+00	5.827285e+00	8.241026e+00
Au	1.009315e+01	5.827285e+00	8.241026e+00
Au	1.297691e+01	5.827285e+00	8.241026e+00
Au	-2.883758e+00	8.324693e+00	8.241026e+00
Au	0.000000e+00	8.324693e+00	8.241026e+00
Au	2.883758e+00	8.324693e+00	8.241026e+00
Au	5.767516e+00	8.324693e+00	8.241026e+00
Au	8.651275e+00	8.324693e+00	8.241026e+00
Au	1.153503e+01	8.324693e+00	8.241026e+00
Au	-4.325637e+00	1.082210e+01	8.241026e+00
Au	-1.441879e+00	1.082210e+01	8.241026e+00
Au	1.441879e+00	1.082210e+01	8.241026e+00

Au	4.325637e+00	1.082210e+01	8.241026e+00
Au	7.209396e+00	1.082210e+01	8.241026e+00
Au	1.009315e+01	1.082210e+01	8.241026e+00
Au	-5.767516e+00	1.331951e+01	8.241026e+00
Au	-2.883758e+00	1.331951e+01	8.241026e+00
Au	-0.000000e+00	1.331951e+01	8.241026e+00
Au	2.883758e+00	1.331951e+01	8.241026e+00
Au	5.767516e+00	1.331951e+01	8.241026e+00
Au	8.651275e+00	1.331951e+01	8.241026e+00
Au	2.883758e+00	1.165457e+01	1.059560e+01
Au	5.767516e+00	1.165457e+01	1.059560e+01
Au	4.325637e+00	1.415198e+01	1.059560e+01
Au	4.325637e+00	1.248704e+01	1.295018e+01
N	4.215518e+00	1.120385e+01	1.462114e+01
C	4.301070e+00	1.020959e+01	1.521932e+01
C	4.406601e+00	8.983235e+00	1.595762e+01
H	6.564956e+00	9.010442e+00	1.601895e+01
H	2.273941e+00	8.655284e+00	1.604238e+01
C	5.667212e+00	8.476203e+00	1.631041e+01
C	3.250409e+00	8.276169e+00	1.632361e+01
H	6.308578e+00	4.223570e+00	1.655439e+01
H	3.323177e+00	3.974888e+00	1.656885e+01
C	5.763543e+00	7.287054e+00	1.702697e+01
C	3.358663e+00	7.087996e+00	1.704010e+01
H	6.746066e+00	6.905703e+00	1.727413e+01
H	2.454945e+00	6.550528e+00	1.729754e+01
C	4.613480e+00	6.579726e+00	1.741311e+01
H	5.035597e+00	1.512629e+00	1.743374e+01
B	5.720114e+00	4.005391e+00	1.755641e+01
B	3.949246e+00	3.857873e+00	1.756499e+01
B	4.957199e+00	2.492187e+00	1.809593e+01
C	4.726367e+00	5.265710e+00	1.814713e+01
H	7.436893e+00	2.677978e+00	1.897313e+01
B	6.355604e+00	3.162284e+00	1.898557e+01
H	2.489495e+00	2.265793e+00	1.899707e+01
B	3.475806e+00	2.922359e+00	1.899950e+01
B	6.181123e+00	4.917970e+00	1.900861e+01
H	7.040705e+00	5.721412e+00	1.901359e+01
B	3.357573e+00	4.682730e+00	1.902228e+01
H	2.376983e+00	5.332863e+00	1.903625e+01
B	4.967667e+00	2.469877e+00	1.987451e+01
C	4.736674e+00	5.243778e+00	1.989560e+01
B	5.737107e+00	3.969204e+00	2.044279e+01
B	3.966242e+00	3.821648e+00	2.045136e+01
H	5.053720e+00	1.474030e+00	2.051094e+01

C	4.632347e+00	6.538929e+00	2.066363e+01
H	6.766249e+00	6.864024e+00	2.078305e+01
H	2.475519e+00	6.504132e+00	2.080641e+01
C	5.786663e+00	7.237836e+00	2.105238e+01
C	3.382004e+00	7.036147e+00	2.106548e+01
H	6.337358e+00	4.162293e+00	2.144297e+01
H	3.351966e+00	3.913528e+00	2.145743e+01
C	5.698533e+00	8.408606e+00	2.179961e+01
C	3.281954e+00	8.205906e+00	2.181278e+01
H	6.599489e+00	8.936536e+00	2.209266e+01
H	2.308869e+00	8.576643e+00	2.211605e+01
C	4.442146e+00	8.905074e+00	2.218129e+01
C	4.345065e+00	1.011248e+01	2.295131e+01
N	4.266350e+00	1.109138e+01	2.357522e+01
Au	4.325637e+00	1.248704e+01	2.516777e+01
Au	2.883758e+00	1.165457e+01	2.752234e+01
Au	5.767516e+00	1.165457e+01	2.752234e+01
Au	4.325637e+00	1.415198e+01	2.752234e+01
Au	1.441879e+00	8.324693e-01	2.987692e+01
Au	4.325637e+00	8.324693e-01	2.987692e+01
Au	7.209396e+00	8.324693e-01	2.987692e+01
Au	1.009315e+01	8.324693e-01	2.987692e+01
Au	1.297691e+01	8.324693e-01	2.987692e+01
Au	1.586067e+01	8.324693e-01	2.987692e+01
Au	-0.000000e+00	3.329877e+00	2.987692e+01
Au	2.883758e+00	3.329877e+00	2.987692e+01
Au	5.767516e+00	3.329877e+00	2.987692e+01
Au	8.651275e+00	3.329877e+00	2.987692e+01
Au	1.153503e+01	3.329877e+00	2.987692e+01
Au	1.441879e+01	3.329877e+00	2.987692e+01
Au	-1.441879e+00	5.827285e+00	2.987692e+01
Au	1.441879e+00	5.827285e+00	2.987692e+01
Au	4.325637e+00	5.827285e+00	2.987692e+01
Au	7.209396e+00	5.827285e+00	2.987692e+01
Au	1.009315e+01	5.827285e+00	2.987692e+01
Au	1.297691e+01	5.827285e+00	2.987692e+01
Au	-2.883758e+00	8.324693e+00	2.987692e+01
Au	0.000000e+00	8.324693e+00	2.987692e+01
Au	2.883758e+00	8.324693e+00	2.987692e+01
Au	5.767516e+00	8.324693e+00	2.987692e+01
Au	8.651275e+00	8.324693e+00	2.987692e+01
Au	1.153503e+01	8.324693e+00	2.987692e+01
Au	-4.325637e+00	1.082210e+01	2.987692e+01
Au	-1.441879e+00	1.082210e+01	2.987692e+01
Au	1.441879e+00	1.082210e+01	2.987692e+01

Au	4.325637e+00	1.082210e+01	2.987692e+01
Au	7.209396e+00	1.082210e+01	2.987692e+01
Au	1.009315e+01	1.082210e+01	2.987692e+01
Au	-5.767516e+00	1.331951e+01	2.987692e+01
Au	-2.883758e+00	1.331951e+01	2.987692e+01
Au	-0.000000e+00	1.331951e+01	2.987692e+01
Au	2.883758e+00	1.331951e+01	2.987692e+01
Au	5.767516e+00	1.331951e+01	2.987692e+01
Au	8.651275e+00	1.331951e+01	2.987692e+01
Au	0.000000e+00	0.000000e+00	3.223150e+01
Au	2.883758e+00	0.000000e+00	3.223150e+01
Au	5.767516e+00	0.000000e+00	3.223150e+01
Au	8.651275e+00	0.000000e+00	3.223150e+01
Au	1.153503e+01	0.000000e+00	3.223150e+01
Au	1.441879e+01	0.000000e+00	3.223150e+01
Au	-1.441879e+00	2.497408e+00	3.223150e+01
Au	1.441879e+00	2.497408e+00	3.223150e+01
Au	4.325637e+00	2.497408e+00	3.223150e+01
Au	7.209396e+00	2.497408e+00	3.223150e+01
Au	1.009315e+01	2.497408e+00	3.223150e+01
Au	1.297691e+01	2.497408e+00	3.223150e+01
Au	-2.883758e+00	4.994816e+00	3.223150e+01
Au	0.000000e+00	4.994816e+00	3.223150e+01
Au	2.883758e+00	4.994816e+00	3.223150e+01
Au	5.767516e+00	4.994816e+00	3.223150e+01
Au	8.651275e+00	4.994816e+00	3.223150e+01
Au	1.153503e+01	4.994816e+00	3.223150e+01
Au	-4.325637e+00	7.492224e+00	3.223150e+01
Au	-1.441879e+00	7.492224e+00	3.223150e+01
Au	1.441879e+00	7.492224e+00	3.223150e+01
Au	4.325637e+00	7.492224e+00	3.223150e+01
Au	7.209396e+00	7.492224e+00	3.223150e+01
Au	1.009315e+01	7.492224e+00	3.223150e+01
Au	-5.767516e+00	9.989632e+00	3.223150e+01
Au	-2.883758e+00	9.989632e+00	3.223150e+01
Au	0.000000e+00	9.989632e+00	3.223150e+01
Au	2.883758e+00	9.989632e+00	3.223150e+01
Au	5.767516e+00	9.989632e+00	3.223150e+01
Au	8.651275e+00	9.989632e+00	3.223150e+01
Au	-7.209396e+00	1.248704e+01	3.223150e+01
Au	-4.325637e+00	1.248704e+01	3.223150e+01
Au	-1.441879e+00	1.248704e+01	3.223150e+01
Au	1.441879e+00	1.248704e+01	3.223150e+01
Au	4.325637e+00	1.248704e+01	3.223150e+01
Au	7.209396e+00	1.248704e+01	3.223150e+01

Au	0.000000e+00	1.664939e+00	3.458608e+01
Au	2.883758e+00	1.664939e+00	3.458608e+01
Au	5.767516e+00	1.664939e+00	3.458608e+01
Au	8.651275e+00	1.664939e+00	3.458608e+01
Au	1.153503e+01	1.664939e+00	3.458608e+01
Au	1.441879e+01	1.664939e+00	3.458608e+01
Au	-1.441879e+00	4.162346e+00	3.458608e+01
Au	1.441879e+00	4.162346e+00	3.458608e+01
Au	4.325637e+00	4.162346e+00	3.458608e+01
Au	7.209396e+00	4.162346e+00	3.458608e+01
Au	1.009315e+01	4.162346e+00	3.458608e+01
Au	1.297691e+01	4.162346e+00	3.458608e+01
Au	-2.883758e+00	6.659754e+00	3.458608e+01
Au	0.000000e+00	6.659754e+00	3.458608e+01
Au	2.883758e+00	6.659754e+00	3.458608e+01
Au	5.767516e+00	6.659754e+00	3.458608e+01
Au	8.651275e+00	6.659754e+00	3.458608e+01
Au	1.153503e+01	6.659754e+00	3.458608e+01
Au	-4.325637e+00	9.157162e+00	3.458608e+01
Au	-1.441879e+00	9.157162e+00	3.458608e+01
Au	1.441879e+00	9.157162e+00	3.458608e+01
Au	4.325637e+00	9.157162e+00	3.458608e+01
Au	7.209396e+00	9.157162e+00	3.458608e+01
Au	1.009315e+01	9.157162e+00	3.458608e+01
Au	-5.767516e+00	1.165457e+01	3.458608e+01
Au	-2.883758e+00	1.165457e+01	3.458608e+01
Au	0.000000e+00	1.165457e+01	3.458608e+01
Au	2.883758e+00	1.165457e+01	3.458608e+01
Au	5.767516e+00	1.165457e+01	3.458608e+01
Au	8.651275e+00	1.165457e+01	3.458608e+01
Au	-7.209396e+00	1.415198e+01	3.458608e+01
Au	-4.325637e+00	1.415198e+01	3.458608e+01
Au	-1.441879e+00	1.415198e+01	3.458608e+01
Au	1.441879e+00	1.415198e+01	3.458608e+01
Au	4.325637e+00	1.415198e+01	3.458608e+01
Au	7.209396e+00	1.415198e+01	3.458608e+01
Au	1.441879e+00	8.324693e-01	3.694066e+01
Au	4.325637e+00	8.324693e-01	3.694066e+01
Au	7.209396e+00	8.324693e-01	3.694066e+01
Au	1.009315e+01	8.324693e-01	3.694066e+01
Au	1.297691e+01	8.324693e-01	3.694066e+01
Au	1.586067e+01	8.324693e-01	3.694066e+01
Au	0.000000e+00	3.329877e+00	3.694066e+01
Au	2.883758e+00	3.329877e+00	3.694066e+01
Au	5.767516e+00	3.329877e+00	3.694066e+01

Au	8.651275e+00	3.329877e+00	3.694066e+01
Au	1.153503e+01	3.329877e+00	3.694066e+01
Au	1.441879e+01	3.329877e+00	3.694066e+01
Au	-1.441879e+00	5.827285e+00	3.694066e+01
Au	1.441879e+00	5.827285e+00	3.694066e+01
Au	4.325637e+00	5.827285e+00	3.694066e+01
Au	7.209396e+00	5.827285e+00	3.694066e+01
Au	1.009315e+01	5.827285e+00	3.694066e+01
Au	1.297691e+01	5.827285e+00	3.694066e+01
Au	-2.883758e+00	8.324693e+00	3.694066e+01
Au	0.000000e+00	8.324693e+00	3.694066e+01
Au	2.883758e+00	8.324693e+00	3.694066e+01
Au	5.767516e+00	8.324693e+00	3.694066e+01
Au	8.651275e+00	8.324693e+00	3.694066e+01
Au	1.153503e+01	8.324693e+00	3.694066e+01
Au	-4.325637e+00	1.082210e+01	3.694066e+01
Au	-1.441879e+00	1.082210e+01	3.694066e+01
Au	1.441879e+00	1.082210e+01	3.694066e+01
Au	4.325637e+00	1.082210e+01	3.694066e+01
Au	7.209396e+00	1.082210e+01	3.694066e+01
Au	1.009315e+01	1.082210e+01	3.694066e+01
Au	-5.767516e+00	1.331951e+01	3.694066e+01
Au	-2.883758e+00	1.331951e+01	3.694066e+01
Au	0.000000e+00	1.331951e+01	3.694066e+01
Au	2.883758e+00	1.331951e+01	3.694066e+01
Au	5.767516e+00	1.331951e+01	3.694066e+01
Au	8.651275e+00	1.331951e+01	3.694066e+01

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Au	1.441879e+00	8.324693e-01	1.177289e+00
Au	4.325637e+00	8.324693e-01	1.177289e+00
Au	7.209396e+00	8.324693e-01	1.177289e+00
Au	1.009315e+01	8.324693e-01	1.177289e+00
Au	1.297691e+01	8.324693e-01	1.177289e+00
Au	1.586067e+01	8.324693e-01	1.177289e+00
Au	1.874443e+01	8.324693e-01	1.177289e+00
Au	-0.000000e+00	3.329877e+00	1.177289e+00
Au	2.883758e+00	3.329877e+00	1.177289e+00
Au	5.767516e+00	3.329877e+00	1.177289e+00
Au	8.651275e+00	3.329877e+00	1.177289e+00
Au	1.153503e+01	3.329877e+00	1.177289e+00
Au	1.441879e+01	3.329877e+00	1.177289e+00
Au	1.730255e+01	3.329877e+00	1.177289e+00
Au	-1.441879e+00	5.827285e+00	1.177289e+00
Au	1.441879e+00	5.827285e+00	1.177289e+00

Au	4.325637e+00	5.827285e+00	1.177289e+00
Au	7.209396e+00	5.827285e+00	1.177289e+00
Au	1.009315e+01	5.827285e+00	1.177289e+00
Au	1.297691e+01	5.827285e+00	1.177289e+00
Au	1.586067e+01	5.827285e+00	1.177289e+00
Au	-2.883758e+00	8.324693e+00	1.177289e+00
Au	0.000000e+00	8.324693e+00	1.177289e+00
Au	2.883758e+00	8.324693e+00	1.177289e+00
Au	5.767516e+00	8.324693e+00	1.177289e+00
Au	8.651275e+00	8.324693e+00	1.177289e+00
Au	1.153503e+01	8.324693e+00	1.177289e+00
Au	1.441879e+01	8.324693e+00	1.177289e+00
Au	-4.325637e+00	1.082210e+01	1.177289e+00
Au	-1.441879e+00	1.082210e+01	1.177289e+00
Au	1.441879e+00	1.082210e+01	1.177289e+00
Au	4.325637e+00	1.082210e+01	1.177289e+00
Au	7.209396e+00	1.082210e+01	1.177289e+00
Au	1.009315e+01	1.082210e+01	1.177289e+00
Au	1.297691e+01	1.082210e+01	1.177289e+00
Au	-5.767516e+00	1.331951e+01	1.177289e+00
Au	-2.883758e+00	1.331951e+01	1.177289e+00
Au	-0.000000e+00	1.331951e+01	1.177289e+00
Au	2.883758e+00	1.331951e+01	1.177289e+00
Au	5.767516e+00	1.331951e+01	1.177289e+00
Au	8.651275e+00	1.331951e+01	1.177289e+00
Au	1.153503e+01	1.331951e+01	1.177289e+00
Au	-7.209396e+00	1.581692e+01	1.177289e+00
Au	-4.325637e+00	1.581692e+01	1.177289e+00
Au	-1.441879e+00	1.581692e+01	1.177289e+00
Au	1.441879e+00	1.581692e+01	1.177289e+00
Au	4.325637e+00	1.581692e+01	1.177289e+00
Au	7.209396e+00	1.581692e+01	1.177289e+00
Au	1.009315e+01	1.581692e+01	1.177289e+00
Au	0.000000e+00	1.664939e+00	3.531868e+00
Au	2.883758e+00	1.664939e+00	3.531868e+00
Au	5.767516e+00	1.664939e+00	3.531868e+00
Au	8.651275e+00	1.664939e+00	3.531868e+00
Au	1.153503e+01	1.664939e+00	3.531868e+00
Au	1.441879e+01	1.664939e+00	3.531868e+00
Au	1.730255e+01	1.664939e+00	3.531868e+00
Au	-1.441879e+00	4.162346e+00	3.531868e+00
Au	1.441879e+00	4.162346e+00	3.531868e+00
Au	4.325637e+00	4.162346e+00	3.531868e+00
Au	7.209396e+00	4.162346e+00	3.531868e+00
Au	1.009315e+01	4.162346e+00	3.531868e+00

Au	1.297691e+01	4.162346e+00	3.531868e+00
Au	1.586067e+01	4.162346e+00	3.531868e+00
Au	-2.883758e+00	6.659754e+00	3.531868e+00
Au	-0.000000e+00	6.659754e+00	3.531868e+00
Au	2.883758e+00	6.659754e+00	3.531868e+00
Au	5.767516e+00	6.659754e+00	3.531868e+00
Au	8.651275e+00	6.659754e+00	3.531868e+00
Au	1.153503e+01	6.659754e+00	3.531868e+00
Au	1.441879e+01	6.659754e+00	3.531868e+00
Au	-4.325637e+00	9.157162e+00	3.531868e+00
Au	-1.441879e+00	9.157162e+00	3.531868e+00
Au	1.441879e+00	9.157162e+00	3.531868e+00
Au	4.325637e+00	9.157162e+00	3.531868e+00
Au	7.209396e+00	9.157162e+00	3.531868e+00
Au	1.009315e+01	9.157162e+00	3.531868e+00
Au	1.297691e+01	9.157162e+00	3.531868e+00
Au	-5.767516e+00	1.165457e+01	3.531868e+00
Au	-2.883758e+00	1.165457e+01	3.531868e+00
Au	-0.000000e+00	1.165457e+01	3.531868e+00
Au	2.883758e+00	1.165457e+01	3.531868e+00
Au	5.767516e+00	1.165457e+01	3.531868e+00
Au	8.651275e+00	1.165457e+01	3.531868e+00
Au	1.153503e+01	1.165457e+01	3.531868e+00
Au	-7.209396e+00	1.415198e+01	3.531868e+00
Au	-4.325637e+00	1.415198e+01	3.531868e+00
Au	-1.441879e+00	1.415198e+01	3.531868e+00
Au	1.441879e+00	1.415198e+01	3.531868e+00
Au	4.325637e+00	1.415198e+01	3.531868e+00
Au	7.209396e+00	1.415198e+01	3.531868e+00
Au	1.009315e+01	1.415198e+01	3.531868e+00
Au	-8.651275e+00	1.664939e+01	3.531868e+00
Au	-5.767516e+00	1.664939e+01	3.531868e+00
Au	-2.883758e+00	1.664939e+01	3.531868e+00
Au	0.000000e+00	1.664939e+01	3.531868e+00
Au	2.883758e+00	1.664939e+01	3.531868e+00
Au	5.767516e+00	1.664939e+01	3.531868e+00
Au	8.651275e+00	1.664939e+01	3.531868e+00
Au	0.000000e+00	0.000000e+00	5.886447e+00
Au	2.883758e+00	0.000000e+00	5.886447e+00
Au	5.767516e+00	0.000000e+00	5.886447e+00
Au	8.651275e+00	0.000000e+00	5.886447e+00
Au	1.153503e+01	0.000000e+00	5.886447e+00
Au	1.441879e+01	0.000000e+00	5.886447e+00
Au	1.730255e+01	0.000000e+00	5.886447e+00
Au	-1.441879e+00	2.497408e+00	5.886447e+00

Au	1.441879e+00	2.497408e+00	5.886447e+00
Au	4.325637e+00	2.497408e+00	5.886447e+00
Au	7.209396e+00	2.497408e+00	5.886447e+00
Au	1.009315e+01	2.497408e+00	5.886447e+00
Au	1.297691e+01	2.497408e+00	5.886447e+00
Au	1.586067e+01	2.497408e+00	5.886447e+00
Au	-2.883758e+00	4.994816e+00	5.886447e+00
Au	-0.000000e+00	4.994816e+00	5.886447e+00
Au	2.883758e+00	4.994816e+00	5.886447e+00
Au	5.767516e+00	4.994816e+00	5.886447e+00
Au	8.651275e+00	4.994816e+00	5.886447e+00
Au	1.153503e+01	4.994816e+00	5.886447e+00
Au	1.441879e+01	4.994816e+00	5.886447e+00
Au	-4.325637e+00	7.492224e+00	5.886447e+00
Au	-1.441879e+00	7.492224e+00	5.886447e+00
Au	1.441879e+00	7.492224e+00	5.886447e+00
Au	4.325637e+00	7.492224e+00	5.886447e+00
Au	7.209396e+00	7.492224e+00	5.886447e+00
Au	1.009315e+01	7.492224e+00	5.886447e+00
Au	1.297691e+01	7.492224e+00	5.886447e+00
Au	-5.767516e+00	9.989632e+00	5.886447e+00
Au	-2.883758e+00	9.989632e+00	5.886447e+00
Au	-0.000000e+00	9.989632e+00	5.886447e+00
Au	2.883758e+00	9.989632e+00	5.886447e+00
Au	5.767516e+00	9.989632e+00	5.886447e+00
Au	8.651275e+00	9.989632e+00	5.886447e+00
Au	1.153503e+01	9.989632e+00	5.886447e+00
Au	-7.209396e+00	1.248704e+01	5.886447e+00
Au	-4.325637e+00	1.248704e+01	5.886447e+00
Au	-1.441879e+00	1.248704e+01	5.886447e+00
Au	1.441879e+00	1.248704e+01	5.886447e+00
Au	4.325637e+00	1.248704e+01	5.886447e+00
Au	7.209396e+00	1.248704e+01	5.886447e+00
Au	1.009315e+01	1.248704e+01	5.886447e+00
Au	-8.651275e+00	1.498445e+01	5.886447e+00
Au	-5.767516e+00	1.498445e+01	5.886447e+00
Au	-2.883758e+00	1.498445e+01	5.886447e+00
Au	-0.000000e+00	1.498445e+01	5.886447e+00
Au	2.883758e+00	1.498445e+01	5.886447e+00
Au	5.767516e+00	1.498445e+01	5.886447e+00
Au	8.651275e+00	1.498445e+01	5.886447e+00
Au	1.441879e+00	8.324693e-01	8.241026e+00
Au	4.325637e+00	8.324693e-01	8.241026e+00
Au	7.209396e+00	8.324693e-01	8.241026e+00
Au	1.009315e+01	8.324693e-01	8.241026e+00

Au	1.297691e+01	8.324693e-01	8.241026e+00
Au	1.586067e+01	8.324693e-01	8.241026e+00
Au	1.874443e+01	8.324693e-01	8.241026e+00
Au	0.000000e+00	3.329877e+00	8.241026e+00
Au	2.883758e+00	3.329877e+00	8.241026e+00
Au	5.767516e+00	3.329877e+00	8.241026e+00
Au	8.651275e+00	3.329877e+00	8.241026e+00
Au	1.153503e+01	3.329877e+00	8.241026e+00
Au	1.441879e+01	3.329877e+00	8.241026e+00
Au	1.730255e+01	3.329877e+00	8.241026e+00
Au	-1.441879e+00	5.827285e+00	8.241026e+00
Au	1.441879e+00	5.827285e+00	8.241026e+00
Au	4.325637e+00	5.827285e+00	8.241026e+00
Au	7.209396e+00	5.827285e+00	8.241026e+00
Au	1.009315e+01	5.827285e+00	8.241026e+00
Au	1.297691e+01	5.827285e+00	8.241026e+00
Au	1.586067e+01	5.827285e+00	8.241026e+00
Au	-2.883758e+00	8.324693e+00	8.241026e+00
Au	0.000000e+00	8.324693e+00	8.241026e+00
Au	2.883758e+00	8.324693e+00	8.241026e+00
Au	5.767516e+00	8.324693e+00	8.241026e+00
Au	8.651275e+00	8.324693e+00	8.241026e+00
Au	1.153503e+01	8.324693e+00	8.241026e+00
Au	1.441879e+01	8.324693e+00	8.241026e+00
Au	-4.325637e+00	1.082210e+01	8.241026e+00
Au	-1.441879e+00	1.082210e+01	8.241026e+00
Au	1.441879e+00	1.082210e+01	8.241026e+00
Au	4.325637e+00	1.082210e+01	8.241026e+00
Au	7.209396e+00	1.082210e+01	8.241026e+00
Au	1.009315e+01	1.082210e+01	8.241026e+00
Au	1.297691e+01	1.082210e+01	8.241026e+00
Au	-5.767516e+00	1.331951e+01	8.241026e+00
Au	-2.883758e+00	1.331951e+01	8.241026e+00
Au	-0.000000e+00	1.331951e+01	8.241026e+00
Au	2.883758e+00	1.331951e+01	8.241026e+00
Au	5.767516e+00	1.331951e+01	8.241026e+00
Au	8.651275e+00	1.331951e+01	8.241026e+00
Au	1.153503e+01	1.331951e+01	8.241026e+00
Au	-7.209396e+00	1.581692e+01	8.241026e+00
Au	-4.325637e+00	1.581692e+01	8.241026e+00
Au	-1.441879e+00	1.581692e+01	8.241026e+00
Au	1.441879e+00	1.581692e+01	8.241026e+00
Au	4.325637e+00	1.581692e+01	8.241026e+00
Au	7.209396e+00	1.581692e+01	8.241026e+00
Au	1.009315e+01	1.581692e+01	8.241026e+00

Au	-1.441879e+00	4.162346e+00	1.059560e+01
Au	1.441879e+00	4.162346e+00	1.059560e+01
Au	-0.000000e+00	6.659754e+00	1.059560e+01
Au	-0.000000e+00	4.994816e+00	1.295018e+01
N	8.288277e-01	5.946304e+00	1.468560e+01
C	1.332872e+00	6.144396e+00	1.571539e+01
H	1.934460e+00	1.217099e+01	1.572430e+01
H	5.023653e+00	8.932924e+00	1.595217e+01
H	4.029963e+00	1.091719e+01	1.600059e+01
H	8.089989e+00	8.920210e+00	1.607673e+01
H	3.603579e+00	7.445300e+00	1.610798e+01
C	2.213651e+00	1.180654e+01	1.670752e+01
H	6.419803e+00	1.138890e+01	1.685170e+01
C	3.400486e+00	1.108968e+01	1.686490e+01
B	5.670917e+00	8.947219e+00	1.693482e+01
C	1.952587e+00	6.394793e+00	1.698654e+01
H	6.399233e+00	6.500909e+00	1.698760e+01
C	3.159010e+00	7.110961e+00	1.703573e+01
B	7.430033e+00	8.947345e+00	1.706035e+01
B	6.514392e+00	1.040506e+01	1.750044e+01
B	6.507432e+00	7.519552e+00	1.757811e+01
H	4.628347e-01	1.261029e+01	1.768698e+01
C	1.388662e+00	1.205697e+01	1.780102e+01
H	4.226770e-01	5.373884e+00	1.811978e+01
C	3.789914e+00	1.060436e+01	1.812450e+01
C	1.354675e+00	5.926580e+00	1.816716e+01
C	3.776684e+00	7.377576e+00	1.826274e+01
C	5.095475e+00	9.862621e+00	1.828371e+01
C	5.090666e+00	8.118383e+00	1.833098e+01
B	7.868798e+00	9.878258e+00	1.852264e+01
B	7.863700e+00	8.100461e+00	1.857309e+01
H	8.858273e+00	1.052707e+01	1.858731e+01
H	8.849031e+00	7.450866e+00	1.867966e+01
C	1.773232e+00	1.158763e+01	1.906688e+01
C	2.969575e+00	1.087064e+01	1.922647e+01
B	6.361968e+00	1.046037e+01	1.926932e+01
B	6.353118e+00	7.574810e+00	1.934682e+01
C	1.978401e+00	6.177278e+00	1.938666e+01
C	3.175083e+00	6.893332e+00	1.943637e+01
B	5.426007e+00	9.033397e+00	1.975884e+01
H	6.154481e+00	1.147914e+01	1.983243e+01
B	7.180470e+00	9.031834e+00	1.993804e+01
H	6.147344e+00	6.591089e+00	1.996947e+01
C	9.432972e-01	1.183775e+01	2.021197e+01
H	3.246885e+00	1.053544e+01	2.021685e+01

H	1.533209e+00	5.813674e+00	2.030703e+01
H	3.645839e+00	7.065983e+00	2.039637e+01
H	4.619326e+00	9.048332e+00	2.061544e+01
H	7.661250e+00	9.058518e+00	2.102060e+01
N	2.688141e-01	1.203514e+01	2.113926e+01
Au	-1.518480e+00	1.213864e+01	2.246011e+01
Au	-2.960359e+00	1.130618e+01	2.481469e+01
Au	-7.660065e-02	1.130618e+01	2.481469e+01
Au	-1.518480e+00	1.380358e+01	2.481469e+01
Au	1.365278e+00	4.840742e-01	2.716927e+01
Au	4.249037e+00	4.840742e-01	2.716927e+01
Au	7.132795e+00	4.840742e-01	2.716927e+01
Au	1.001655e+01	4.840742e-01	2.716927e+01
Au	1.290031e+01	4.840742e-01	2.716927e+01
Au	1.578407e+01	4.840742e-01	2.716927e+01
Au	1.866783e+01	4.840742e-01	2.716927e+01
Au	-7.660065e-02	2.981482e+00	2.716927e+01
Au	2.807158e+00	2.981482e+00	2.716927e+01
Au	5.690916e+00	2.981482e+00	2.716927e+01
Au	8.574674e+00	2.981482e+00	2.716927e+01
Au	1.145843e+01	2.981482e+00	2.716927e+01
Au	1.434219e+01	2.981482e+00	2.716927e+01
Au	1.722595e+01	2.981482e+00	2.716927e+01
Au	-1.518480e+00	5.478890e+00	2.716927e+01
Au	1.365278e+00	5.478890e+00	2.716927e+01
Au	4.249037e+00	5.478890e+00	2.716927e+01
Au	7.132795e+00	5.478890e+00	2.716927e+01
Au	1.001655e+01	5.478890e+00	2.716927e+01
Au	1.290031e+01	5.478890e+00	2.716927e+01
Au	1.578407e+01	5.478890e+00	2.716927e+01
Au	-2.960359e+00	7.976298e+00	2.716927e+01
Au	-7.660065e-02	7.976298e+00	2.716927e+01
Au	2.807158e+00	7.976298e+00	2.716927e+01
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Au	8.574674e+00	7.976298e+00	2.716927e+01
Au	1.145843e+01	7.976298e+00	2.716927e+01
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Au	4.249037e+00	1.047371e+01	2.716927e+01
Au	1.001655e+01	1.047371e+01	2.716927e+01
Au	1.290031e+01	1.047371e+01	2.716927e+01
Au	-5.844117e+00	1.297111e+01	2.716927e+01

Au -2.960359e+00 1.297111e+01 2.716927e+01
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Au	7.132795e+00	1.546852e+01	3.423300e+01
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