

Supporting Information for

Ferrocene-based Conjugated Macrocycles: Shotgun Synthesis, Size-dependent Properties and Tunable Fluorescence Intensity

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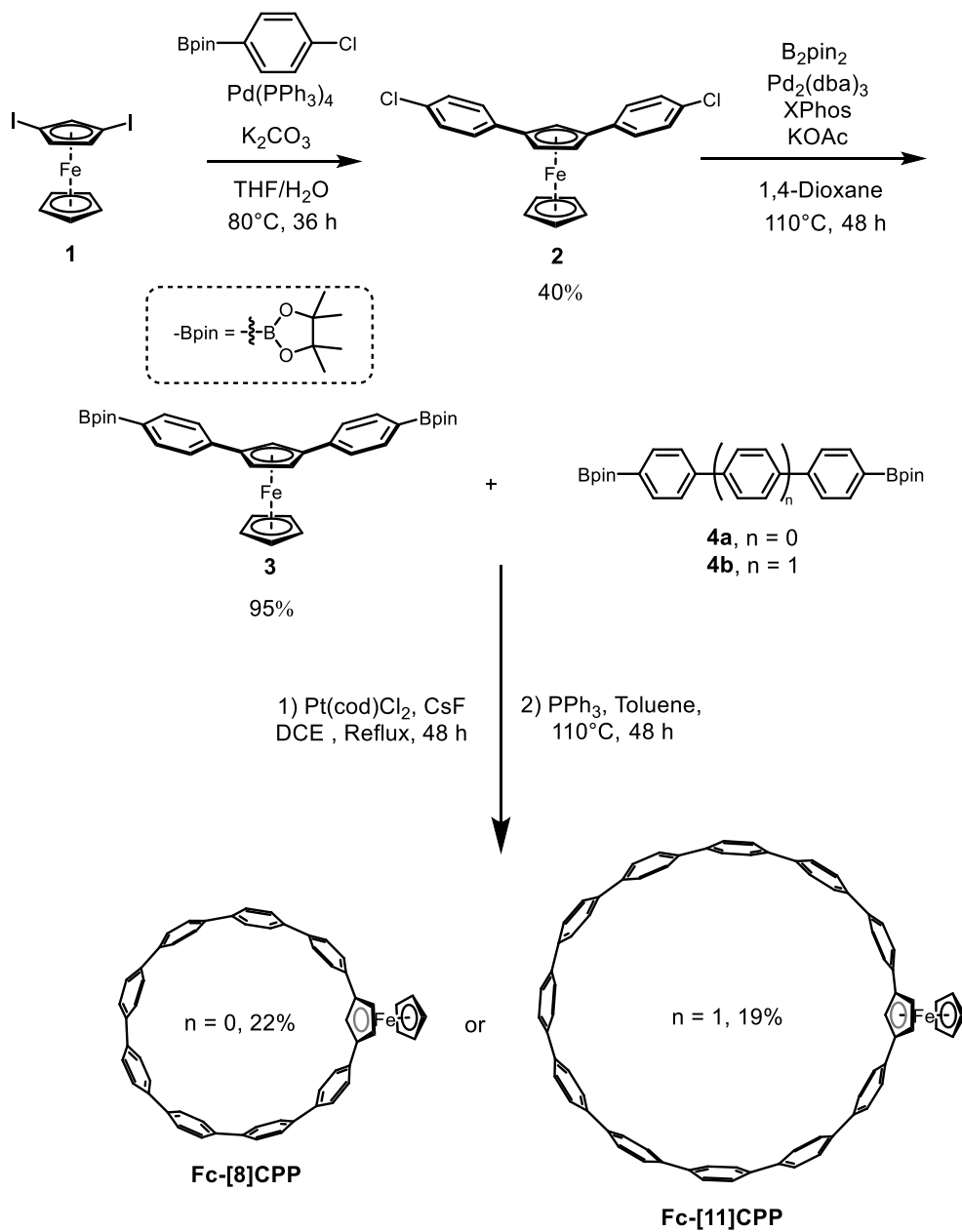
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1. General

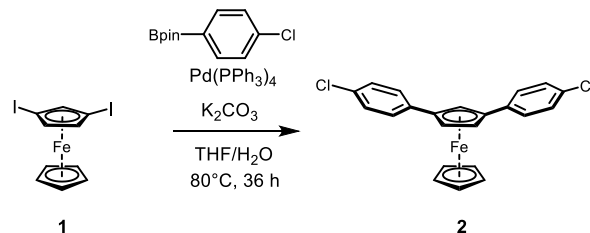
1,3-diiodoferrocene (**1**) was synthesized as reported^[S1], and other materials were purchased from commercial without further purification. ¹H and ¹³C NMR spectra were recorded at 298 K on a JNM-ECZ500R and JNM-ECZ600R instrument. The residual deuterated solvent signal was used as the internal reference in NMR spectra (CDCl₃ δ [ppm] = 7.26 for ¹H NMR, δ [ppm] = 77.16 for ¹³C NMR). High-resolution mass spectra (HRMS) were acquired on the Thermo Scientific Exactive Plus Mass spectrometer equipped with an electrospray ionization (ESI) source. Matrix-assisted laser desorption ionization–time of flight mass spectrometry (MALDI-TOF MS) was acquired on Bruker autoflex maX MALDI-TOF MS spectrometer. Electron Paramagnetic Resonance (EPR) Spectroscopy was recorded at 298 K on a Bruker A300 instrument. Single-crystal X-ray data were collected at 100 K on a Synergy Custom (Liquid MetalJet D2+) diffractometer equipped with Ga-Kα (λ = 1.34050) and reduction was performed by using the program CrysAlisPro.^[S2] The structures were solved by the direct method and refined by full-matrix least-squares on F² using SHELXTL and OLEX2.^[S3] The UV-Vis spectra were recorded on a UV 2700 spectrometer and steady-state emission spectra were acquired using Hitachi Instruments, F-7000 spectrometer. Transient emission spectra were acquired using Edinburgh Instruments, FLS980 spectrometer equipped with a 340 nm laser. The UV-Vis-NIR spectra were recorded on Perkins Elmer Lambda 900 spectrometer. The fluorescence quantum yields were determined using a Hamamatsu absolute PL quantum yield spectrometer C11347 Quantaaurus-QY (Hamamatsu, Japan). The CV and DPV were recorded on Matrohm Autolab and CHI 760E potentiostat (Chinstruments), working electrode: glassy carbon; counter electrode: Pt; reference electrode: Ag/AgCl, scan ratio: 100 mV/s, concentration: 0.1 mM unless otherwise specified. The measurements were carried out in Bu₄NPF₆ (0.1 M) as a supporting electrolyte. Oxidation titrations were measured 30 minutes after the addition of the oxidizing reagent (AgSbF₆).

2. Synthesis



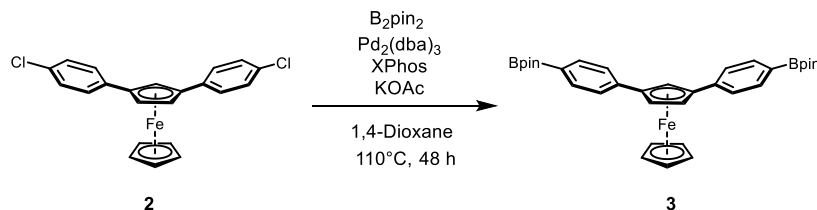
Scheme S1. The synthetic route of **Fc-[8]CPP** and **Fc-[11]CPP**.

2.1 Synthesis of 1,3-bis(4-chlorophenyl)ferrocene (**2**)



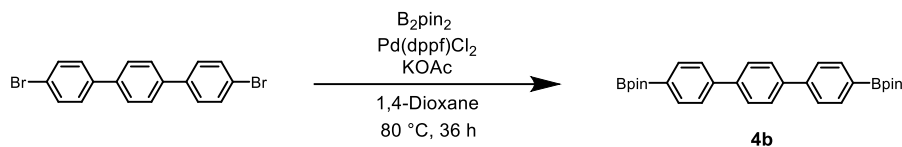
A mixture solution of 1,3-diiodoferrocene (3.50 g, 8.0 mmol, 1.0 equiv), 2-(4-chlorophenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (7.63 g, 32.0 mmol, 4.0 equiv), K₂CO₃ (11.06 g, 80.0 mmol, 10.0 equiv) in THF (180 mL) and H₂O (60 mL) was degassed with Ar for 30 min. Then Pd(PPh₃)₄ (0.93 g, 0.8 mmol, 0.1 equiv) was added and degassed with Ar for 5 min. After stirring at 80 °C for 36 h, the resulting mixture was cooled to room temperature, and concentrated under a vacuum. Then water (100 mL) was added and extracted with DCM (3 × 20 mL). The combined organic layers were dried over anhydrous Na₂SO₄, filtered, and concentrated under a vacuum. The crude residue was purified via column chromatography on silica gel (100% PE) to afford red solid (1.31 g, 40%). ¹H NMR (500 MHz, Chloroform-*d*) δ 7.47 – 7.43 (m, 4H), 7.30 – 7.26 (m, 4H), 5.08 (t, *J* = 1.5 Hz, 1H), 4.78 (d, *J* = 1.4 Hz, 2H), 3.92 (s, 5H). ¹³C{¹H} NMR (126 MHz, Chloroform-*d*) δ 137.5, 131.9, 128.7, 127.3, 85.4, 71.5, 67.6, 65.0. HRMS (ESI) *m/z* calculated for C₂₂H₁₆Cl₂Fe [M]⁺ 405.9973, Found: 405.9966.

2.2 Synthesis of 1,3-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ferrocene (**3**)



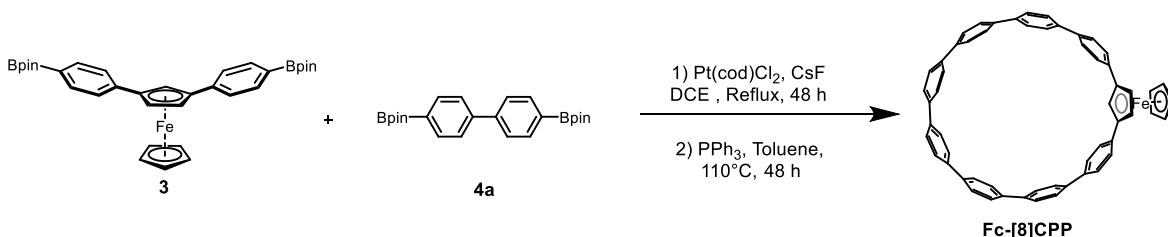
To 90 mL of dry 1,4-dioxane were added 1,3-bis(4-chlorophenyl)ferrocene **2** (1.83 g, 4.5 mmol, 1.0 equiv), bis(pinacolato)diboron (6.85 g, 27.0 mmol, 6.0 equiv), potassium acetate (2.65 g, 27.0 mmol, 6.0 equiv) and Pd₂(dba)₃ (0.08 g, 0.09 mmol, 0.02 equiv), Xphos (0.13 g, 0.27 mmol, 0.06 equiv). The mixture was degassed with Ar for 30 min and heated to 110 °C for 48 h under the protection of nitrogen. After cooling to room temperature, 100 mL DCM was added, and then filtered with Celite. The filtrate was washed with water and brine. The combined organic layers were dried over anhydrous Na₂SO₄, filtered, and concentrated under a vacuum. The residue was dissolved with 30 mL DCM and 100 mL methanol, then concentrated under a vacuum until most of the solid precipitated. The precipitate was filtered and washed with methanol, then dried under vacuum to afford red solid (2.52 g, 95%). ¹H NMR (500 MHz, Chloroform-*d*) δ 7.76 (d, *J* = 7.7 Hz, 4H), 7.55 (d, *J* = 7.7 Hz, 4H), 5.24 (s, 1H), 4.87 (s, 2H), 3.89 (s, 5H), 1.37 (s, 24H). ¹³C{¹H} NMR (126 MHz, Chloroform-*d*) δ 142.3, 135.0, 125.4, 86.0, 83.9, 71.5, 67.9, 65.4, 25.0. HRMS (ESI) *m/z* calculated for C₃₄H₄₁B₂FeO₄ [M+H]⁺ 591.2535, Found: 591.2526.

2.3 Synthesis of **4b**



4,4'-Dibromodiphenyl ether (3.88 g, 10.0 mmol, 1.0 equiv.), bis(pinacolato)diboron (5.59 g, 22.0 mmol, 2.2 equiv.), KOAc (3.92 g, 40.0 mmol, 4.0 equiv.) and 80 mL of 1,4-dioxane were placed in a 250 mL Schlenk flask under an argon atmosphere and then Pd(dppf)Cl₂ (439.0 mg, 0.6 mmol, 0.06 equiv.) was added to the flask. The flask was evacuated and backfilled with argon three times and then refluxed for 36 h. The mixture was filtered through Celite (washed with chloroform) and the solvent was removed under vacuum affording the crude product as a brown solid. The crude product was washed with a small amount of DCM to give a pure product **4b** as a white solid (3.48 g, 80%). ¹H NMR (600 MHz, Chloroform-*d*) δ 7.90 (d, *J* = 8.3 Hz, 4H), 7.71 (s, 4H), 7.66 (d, *J* = 8.3 Hz, 4H), 1.37 (s, 24H). ¹³C{¹H} NMR (151 MHz, Chloroform-*d*) δ 143.4, 140.4, 135.5, 127.8, 126.5, 84.0, 25.0. HRMS (ESI) *m/z* calculated for C₃₀H₃₆B₂O₄ [M]⁺ 482.2794, Found: 482.2779.

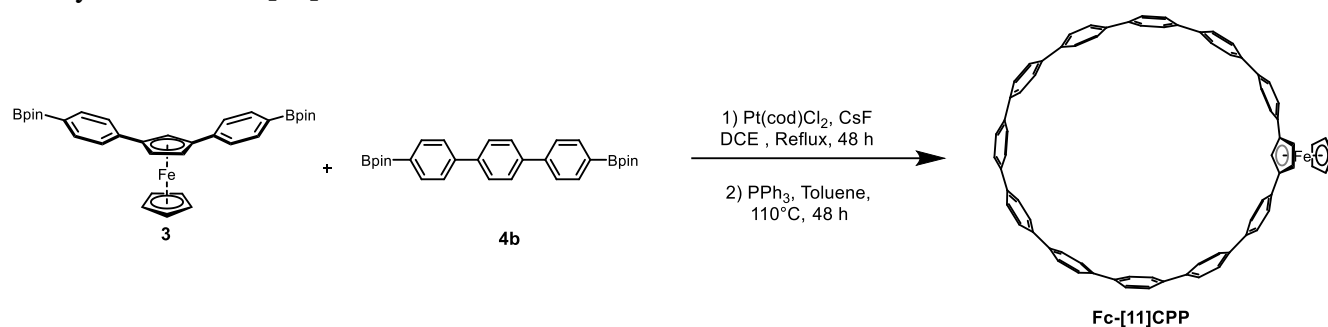
2.4 Synthesis of Fc-[8]CPP



1,3-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ferrocene (**3**) (59.0 mg, 0.1 mmol, 1.0 equiv), 4,4'-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,1'-biphenyl (**4a**) (162.5 mg, 0.4 mmol, 4.0 equiv), Pt(cod)Cl₂ (187.1 mg, 0.5 mmol, 5.0 equiv) and CsF (455.7 mg, 3.0 mmol, 30.0 equiv) and DCE (80 mL) were placed in a 250 mL Schlenk flask then heated at 85 °C for 48 h. The most of solvent was removed under reduced pressure after the reaction was completed. After the addition of methanol (75 mL) to the residue, the precipitates were collected and washed further with methanol (50 mL). The crude material was dried under vacuum and then placed in a 100 mL Schlenk flask. Triphenylphosphine (1.31 g, 5.0 mmol, 50.0 equiv) and toluene (32 mL) were added to the flask. The inhomogeneous mixture was stirred at ambient temperature for 30 min, and then at 110 °C stirred for 48 h. The mixture was passed through column chromatography on silica gel (PE/DCM = 20%-50%) and the solvent was removed under reduced pressure. The crude product was purified by GPC to afford the product as a red solid (17.5 mg, 22%). ¹H NMR (600 MHz, Chloroform-*d*) δ 7.58 – 7.54 (m, 20H), 7.49 (d, *J* = 8.7 Hz, 4H), 7.41 (d, *J* = 8.6 Hz, 4H), 7.37 (d, *J* = 8.6 Hz, 4H), 4.51 (d, *J* = 1.5 Hz, 2H), 4.33 (s, 5H), 3.63 (t, *J* = 1.6 Hz, 1H). ¹³C{¹H} NMR (151 MHz, Chloroform-*d*) δ 138.8, 138.7, 138.3, 138.1, 138.0, 138.0, 128.7, 127.6, 127.6, 127.5, 127.5, 127.4, 127.0, 89.2, 80.3, 70.1, 63.9. HRMS (ESI) *m/z* calculated for C₅₈H₄₀Fe [M]⁺ 792.2474, Found: 792.2471.

[8]CPP was also obtained as a yellow solid (5.8 mg, 1%), ¹H NMR (600 MHz, Chloroform-*d*) 7.48 (s, 32 H), this is in accordance with the results reported in the existing literature^[S4]; **di-Fc-CPPs** and **tri-Fc-CPPs** could also be monitored by MALDI-TOF MS (See Figure S28), but can not be effectively separated due to low conversion rate.

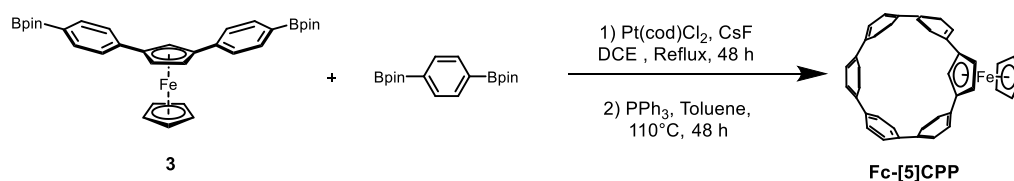
2.5 Synthesis of **Fc-[11]CPP**



Fc-[11]CPP was prepared according to **Fc-[8]CPP** with **4b** (144.5 mg, 0.3 mmol, 3.0 equiv), $\text{Pt}(\text{cod})\text{Cl}_2$ (149.7 mg, 0.4 mmol, 4.0 equiv) and CsF (364.5 mg, 2.4 mmol, 24.0 equiv). Purified by silica gel chromatography (PE/DCM=20%-50%) gave **Fc-[11]CPP** as an orange-red solid (19.5 mg, 19%). ^1H NMR (600 MHz, Chloroform-*d*) δ 7.64 (q, $J = 1.9$ Hz, 4H), 7.63 – 7.60 (m, 28H), 7.58 – 7.56 (m, 4H), 7.47 (s, 8H), 4.62 (d, $J = 1.5$ Hz, 2H), 4.22 (s, 5H), 4.21 (t, $J = 1.5$ Hz, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, Chloroform-*d*) δ 139.5, 138.8, 138.8, 138.7, 138.7, 138.7, 138.6, 138.6, 138.1, 128.2, 127.5, 127.5, 127.5, 127.4, 127.4, 127.1, 88.8, 76.5, 70.8, 64.8. HRMS (ESI) m/z calculated for $\text{C}_{76}\text{H}_{52}\text{Fe}$ $[\text{M}]^+$ 1020.3413, Found: 1020.3465.

[12]CPP was also obtained as a yellowish-white solid (8.9 mg, 1%), ^1H NMR (600 MHz, Chloroform-*d*) 7.61 (s, 48 H), which is consistent with the results reported in the existing literature ^[S4].

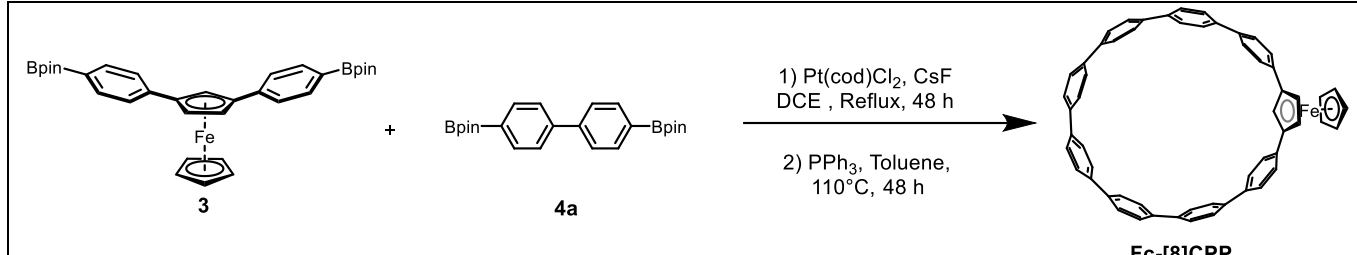
2.6 Synthesis of **Fc-[5]CPP**



Fc-[5]CPP was prepared according to **Fc-[8]CPP** with 1,4-Benzenediboronic acid bis(pinacolate) ester (99.0 mg, 0.3 mmol, 3.0 equiv), $\text{Pt}(\text{cod})\text{Cl}_2$ (149.7 mg, 0.4 mmol, 4.0 equiv) and CsF (364.5 mg, 2.4 mmol, 24 equiv), but it failed.

2.7 The optimization of the synthesis of **Fc-[8]CPP**

Table S1. The optimization of the synthesis of **Fc-[8]CPP**



Entries	3:4a	Cat. (eq.)	Solvent (Step 1)	Concentration (mM)	Yield
1	1:3.0	4.2	THF	3.50	0.4%
2	1:3.0	4.2	DCE	3.50	9%
3	1:3.0	4.4	DCE	3.50	5%
4	1:3.0	4.4	DCE	1.25	11%
5	1:3.0	4.4	DCE	1.00	10%
6	1:3.0	4.1	DCE	1.25	15%
7	1:3.0	4.0	DCE	1.25	16%
8	1:2.5	3.5	DCE	1.25	0.4%
9	1:2.5	4.0	DCE	1.25	7%
10	1:3.5	4.5	DCE	1.25	14%
11	1:4.0	5.0	DCE	1.25	22%
12	1:4.5	5.5	DCE	1.25	16%

3. X-Ray Crystallography

Table S2. Crystal data and structure refinement for **Fc-[8]CPP**

Sample	Fc-[8]CPP
CCDC number	2313391
Empirical formula	C ₅₈ H ₄₀ Fe
Formula weight	792.75
Temperature/K	121(30)
Crystal system	monoclinic
Space group	<i>P</i> 2 ₁ / <i>n</i>
<i>a</i> /Å	20.2138(7)
<i>b</i> /Å	12.8399(6)
<i>c</i> /Å	20.5547(11)
α /°	90
β /°	93.970(4)
γ /°	90
Volume/Å ³	5322.0(4)
<i>Z</i>	4
<i>F</i> (000)	1656.0
Reflections collected	30687
Independent reflections	9539 [<i>R</i> _{int} = 0.0640, <i>R</i> _{sigma} = 0.0593]
Data/restraints/parameters	9539/0/532
Goodness-of-fit on <i>F</i> ²	1.078
Final <i>R</i> indexes [<i>I</i> ≥ 2σ (<i>I</i>)]	<i>R</i> ₁ = 0.0685, <i>wR</i> ₂ = 0.1872
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.0938, <i>wR</i> ₂ = 0.2039

The weak intermolecular interaction

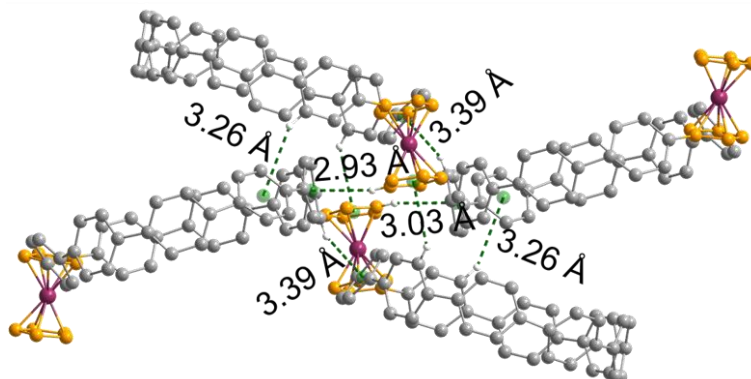


Figure S1. The C-H... π interactions in **Fc-[8]CPP**.

Table S3 Four kinds of C-H... π interactions in the packing model of **Fc-[8]CPP**

$d_{\text{C-H}\cdots\pi}$ ($\angle\text{C-H}\cdots\pi$)	π (Cp)	π (Ph)
C-H (Cp)	-	2.93 Å (167.4°)
C-H (Ph)	3.03 Å (141.7°)	3.26 Å (151.9°) 3.39 Å (152.9°)

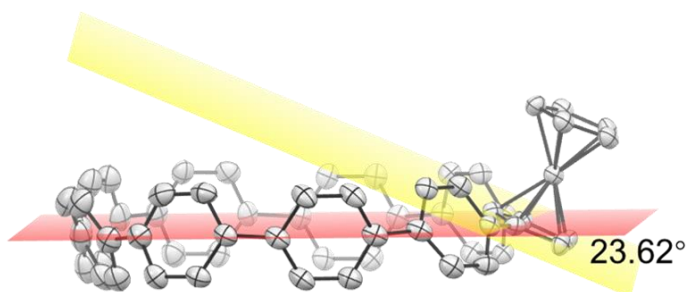


Figure S2. The angle between the plane of Cp and the plane of CPP in **Fc-[8]CPP**.

4. Density Functional Theory (DFT) Computational Details

The geometry optimizations and frontier molecular orbital were performed by the Gaussian 16 package^[S5] at the B3LYP-D3(BJ)/6-31G(d) (C, H) and SDD (Fe) level of theory.^[S6] The geometry optimizations, frontier molecular orbital and strain energies of **Fc-[*n*]CPP** ($n = 5-12$) were calculated at B3LYP/6-31G(d) (C, H, Fe) level of theory for comparison with [*n*]CPP and *m*[*n*]CPP. In the calculations of the rotation process, geometry optimizations were performed by the Gaussian 16 package at the PBE0-D3(BJ)/6-31G(d,p) level of theory. Specifically, iron atoms in the system were treated with the SDD basis set and pseudopotential. Intrinsic reaction coordinate (IRC) calculations were used to ensure that each transition state connected the correct two minima. Highly accurate electronic energies were computed by ORCA 5.0.4 package^[S7] at the RI- ω B97M-V/Def2-TZVP level of theory.^[S8] Def2/J auxiliary basis sets were used for the RI-J approximation.^[S9] Solvation effects were included using the solvation model based on density (SMD) with a standard state of 1 M.^[S10] Grimme' s quasiharmonic correction and harmonic vibrational frequency scale factors for the PBE0/6-31G(d,p) level of theory were applied by using the Shermo 2.4 package.^[S11] Optimized structures were illustrated using CYLview.^[S12] Vibrational frequency calculations were carried out at the same level to confirm whether the structure is a minimum (no imaginary frequency) or a transition state (only one imaginary frequency). Spin densities were drawn by combining Multiwfn 3.8^[S13] and VMD^[S14]. The strain energies were calculated based on the homodesmotic reaction schemes.^[S15]

4.1 TD-DFT calculation

The measured and calculated UV-Vis absorption spectra at different functional theory, basis set was 6-31G(d) for C, H; SDD for Fe.

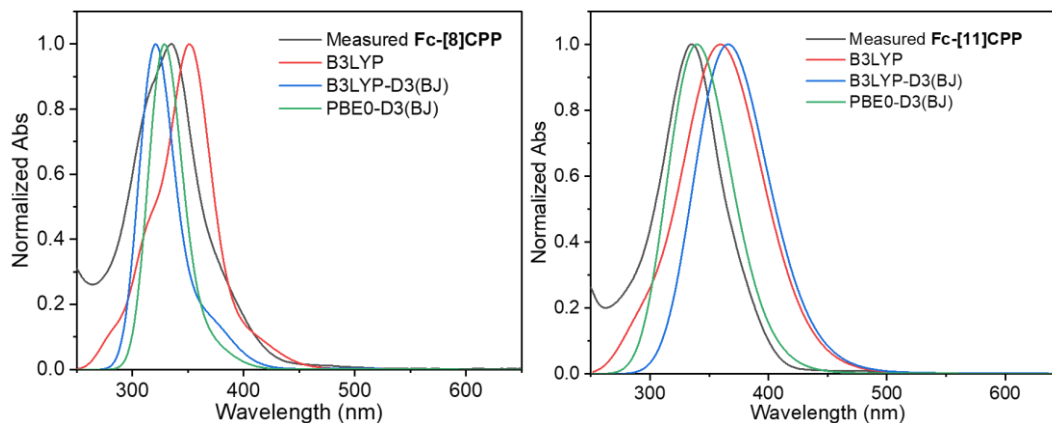


Figure S3. The measured and calculated UV-Vis absorption spectra.

Table S4. Major electronic transitions for **Fc-[8]CPP** by TD-DFT calculated at the B3LYP/6-31G(d) (C, H) and SDD (Fe) level of theory.

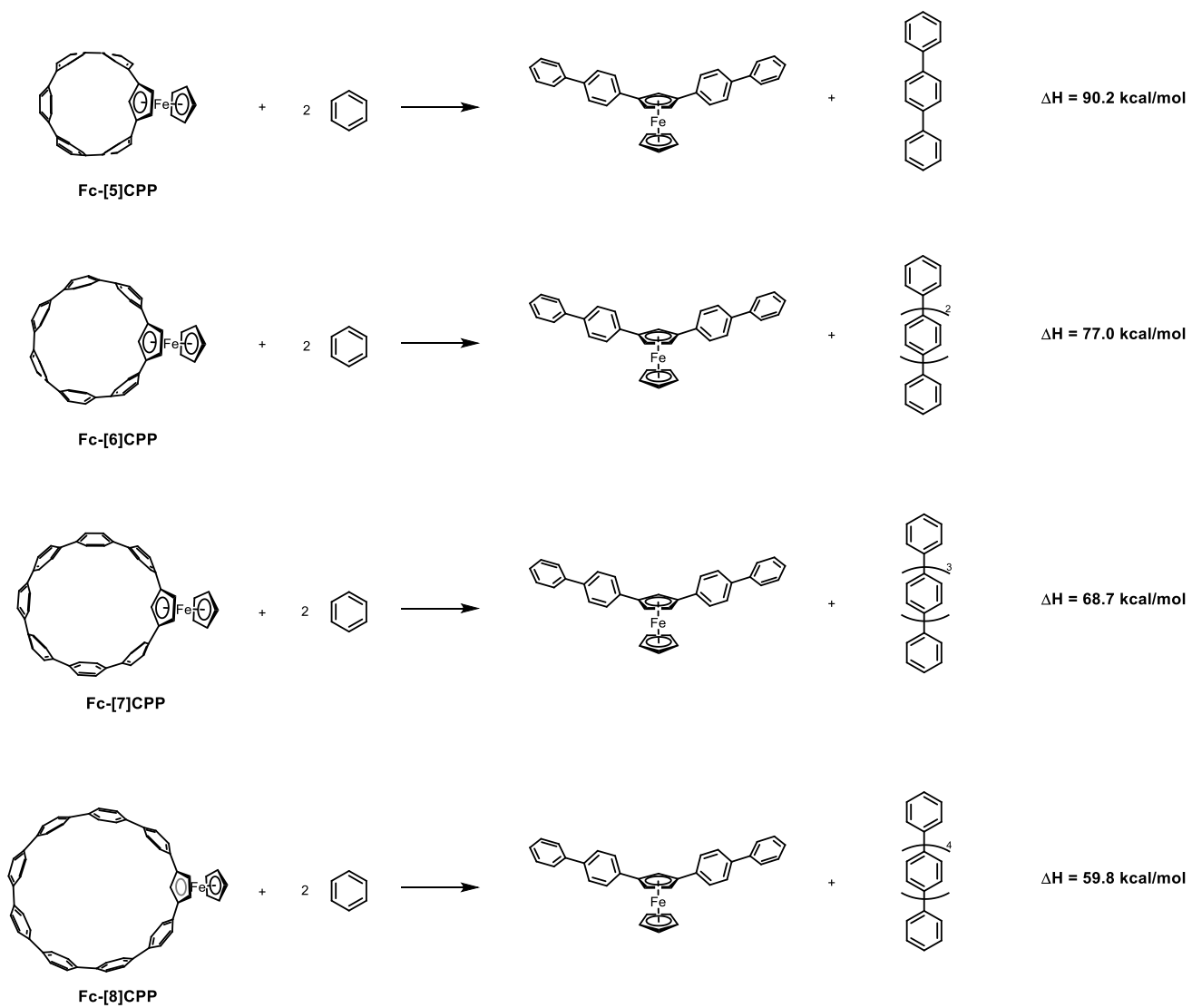
Excited states	Energy (eV)	Excitation [nm]	Oscillator strength (f)	Contribution
S1	2.4188	512.59	0.00050	H-1 → L+12 12.7%, H-2 → L+13 10.6%, H-3 → L+13 9.5%, H-2 → L+3 8.7%, H-2 → L+12 5.6%
S2	2.4249	511.30	0.00500	H-2 → L+12 12.6%, H-1 → L+13 11.1%, H-3 → L+12 10.8%, H-1 → L+3 7.4%, H-2 → L+13 5.3%
S3	2.8092	441.35	0.00060	H-6 → L+13 13.5%, H-1 → L+12 10.4%, H-6 → L+3 8.4%, H-2 → L+13 5.5%
S4	2.8608	433.39	0.00160	H-6 → L+12 20.8%, H-2 → L+12 10.3%, H-3 → L+12 8.0%
S5	3.0600	405.18	0.21020	H → L 93.4%
S6	3.5004	354.20	1.26680	H-1 → L 61.0%, H → L+1 31.3%
S7	3.5198	352.25	0.71600	H → L+1 41.1%, H-1 → L 28.9%, H-2 → L 22.9%
S8	3.5380	350.44	0.02940	H-2 → L 69.3%, H → L+1 20.9%
S9	3.6356	341.03	0.11630	H-3 → L 59.0%, H-2 → L+1 9.1%
S10	3.6577	338.97	0.03500	H-3 → L 28.0%, H-2 → L+1 7.6%, H-1 → L+1 6.3%, H-1 → L+12 5.4%

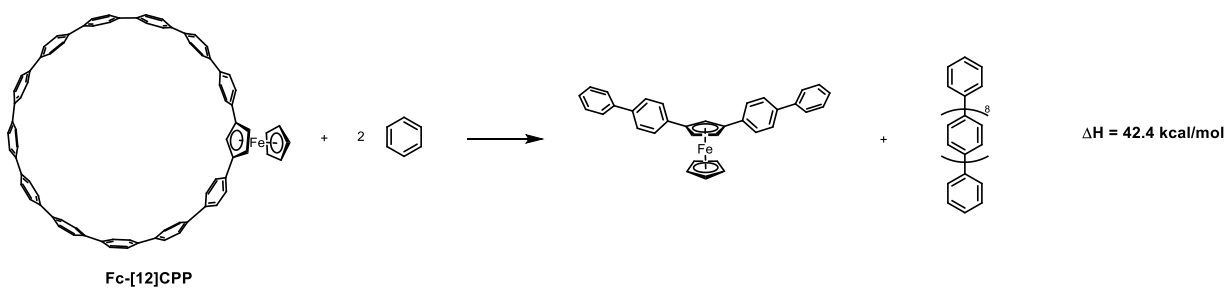
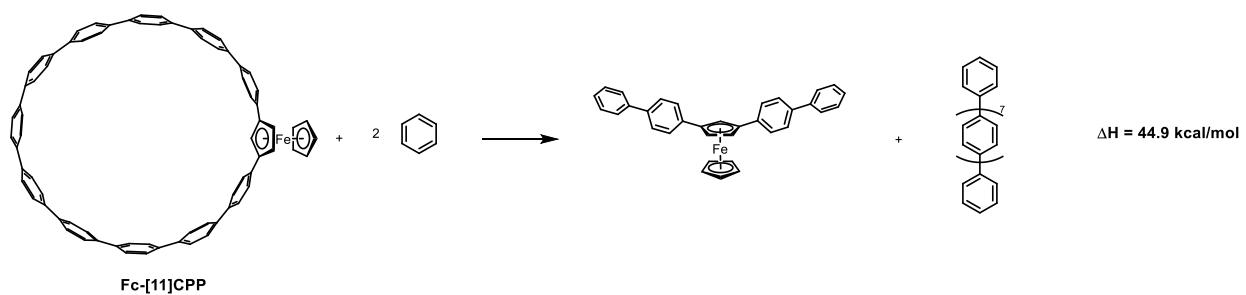
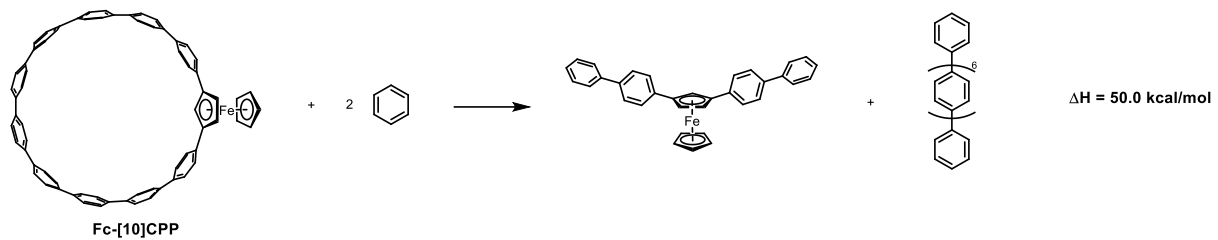
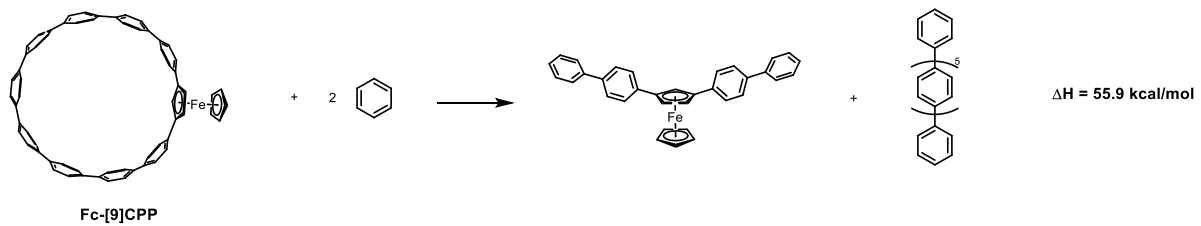
Table S5. Major electronic transitions for **Fc-[11]CPP** by TD-DFT calculated at the B3LYP/6-31G(d) for C, H, SDD for Fe.

Excited states	Energy (eV)	Excitation [nm]	Oscillator strength (f)	Contribution
S1	2.0578	602.51	0.00120	H-1 → L+5 15.3%, H → L+14 12.8%, H-1 → L+20 11.6%, H-2 → L+14 11.3%
S2	2.0637	600.79	0.00510	H-1 → L+14 23.9%, H-3 → L+14 8.3%, H → L+5 7.9%, H- 2 → L+5 7.2%, H → L+20 6.0%
S3	2.5126	493.45	0.00450	H-7 → L+5 15.0%, H-7 → L+20 12.7%, H → L+14 11.8%, H-2 → L+14 10.2%
S4	2.5735	481.77	0.00120	H-7 → L+14 33.5%, H-1 → L+14 22.3%, H-3 → L+14 9.9%
S5	3.1396	394.90	0.01670	H → L 71.8%, H-2 → L 10.8%
S6	3.3491	370.20	0.35280	H-2 → L 26.8%, H-7 → L+5 9.6%, H-7 → L+20 6.8%, H-1 → L+1 6.8%, H → L+2 6.0%, H-7 → L+3 5.8%
S7	3.3602	368.98	2.12310	H → L+1 66.0%, H-1 → L 11.0%, H-3 → L 10.7%
S8	3.3952	365.17	0.49410	H-2 → L 44.2%, H → L 9.5%, H-1 → L+1 8.8%, H → L+2 6.4%
S9	3.3995	364.71	0.26630	H-1 → L 53.3%, H-7 → L+14 14.6%, H-1 → L+2 8.9%, H-2 → L+1 5.1%
S10	3.5238	351.85	0.19510	H-1 → L 23.2%, H-7 → L+14 19.5%, H-2 → L+1 16.1%, H- 1 → L+14 10.9%, H-3 → L 5.9%

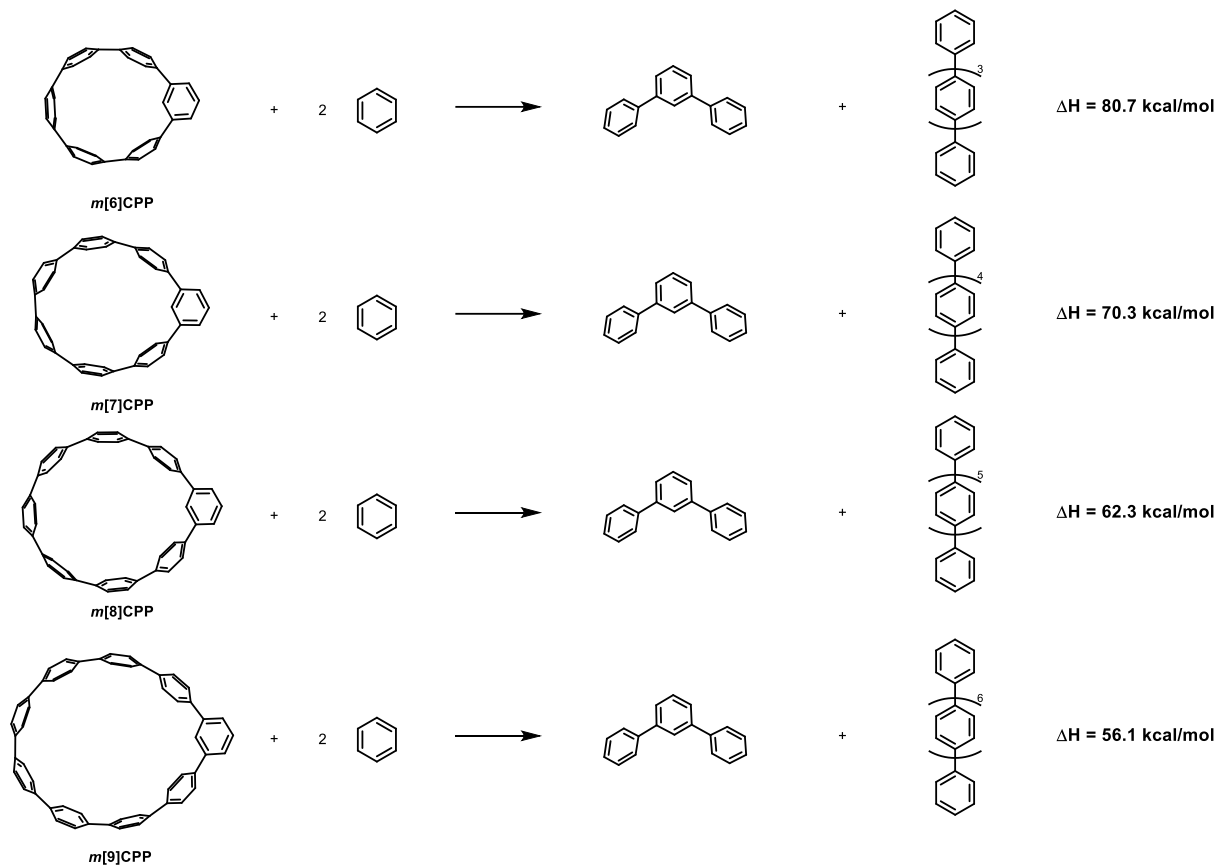
4.2 Strain energy calculation

The strain energy of **Fc-[n]CPP** calculated at the B3LYP/6-31G(d) level of theory





Strain energy of $m[n]$ CPP calculated at the B3LYP/6-31G(d) level of theory



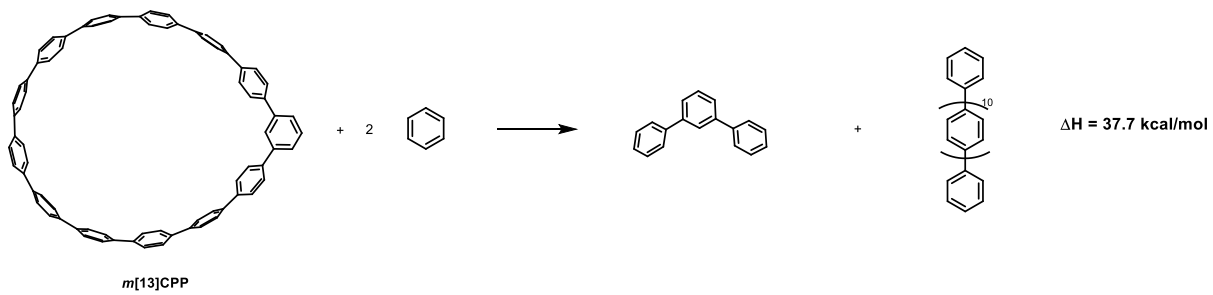
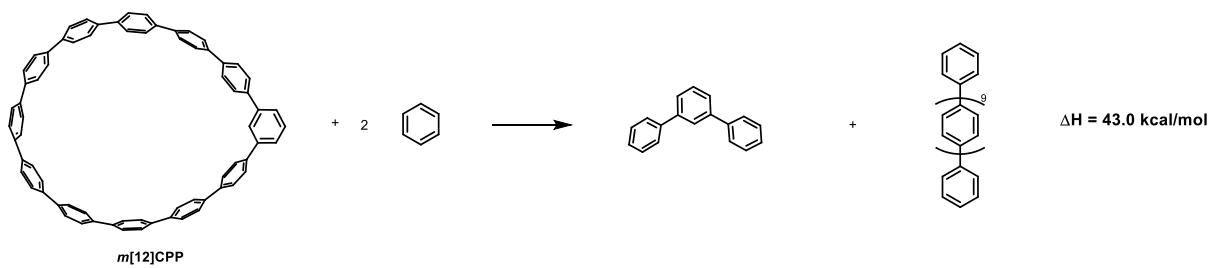
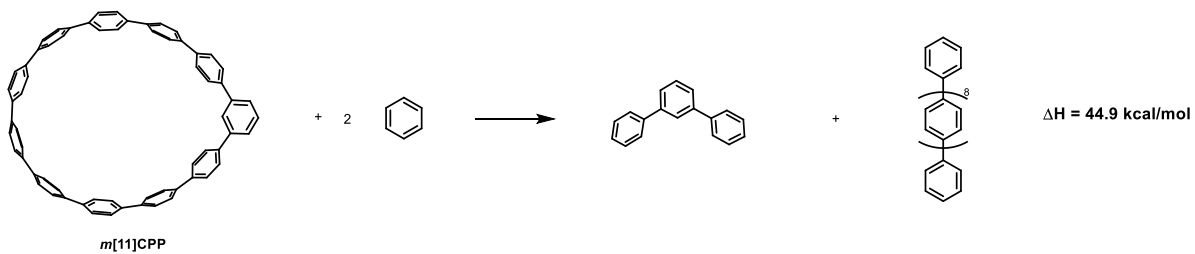
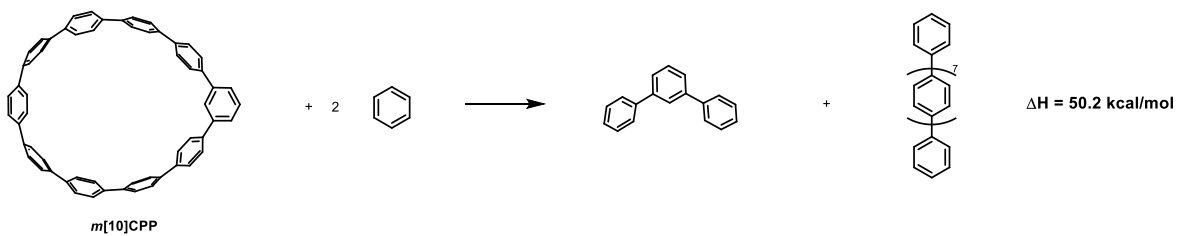


Table S6. HOMO, LUMO energy and strain energy of **Fc-[*n*]CPP**, [*n*]CPP,^[S16, S17] and *m*[*n*]CPP calculated at the B3LYP/6-31G(d) level of theory.

Compound	HOMO (eV)	LUMO (eV)	Energy gap (eV)	Strain energy (kcal/mol)
[6]CPP	-4.92	-1.78	3.14	96.0
[7]CPP	-4.97	-1.80	3.17	84.0
[8]CPP	-5.11	-1.70	3.41	72.2
[9]CPP	-5.13	-1.72	3.41	65.6
[10]CPP	-5.20	-1.67	3.53	57.7
[11]CPP	-5.21	-1.68	3.53	53.7
[12]CPP	-5.26	-1.63	3.63	48.1
[13]CPP	-5.26	-1.65	3.61	45.5
<i>m</i> [6]CPP	-5.09	-1.58	3.51	80.7
<i>m</i> [7]CPP	-5.07	-1.67	3.40	70.3
<i>m</i> [8]CPP	-5.14	-1.65	3.49	62.3
<i>m</i> [9]CPP	-5.15	-1.67	3.48	56.1
<i>m</i> [10]CPP	-5.18	-1.66	3.50	50.2
<i>m</i> [11]CPP	-5.24	-1.62	3.62	44.9
<i>m</i> [12]CPP	-5.23	-1.65	3.58	43.0
<i>m</i> [13]CPP	-5.27	-1.62	3.65	37.7
Fc-[5]CPP	-4.93	-1.60	3.33	90.2
Fc-[6]CPP	-4.90	-1.66	3.30	77.0
Fc-[7]CPP	-5.00	-1.69	3.11	68.7
Fc-[8]CPP	-5.09	-1.63	3.46	59.8
Fc-[9]CPP	-5.08	-1.65	3.43	55.9
Fc-[10]CPP	-5.14	-1.59	3.55	50.0
Fc-[11]CPP	-5.12	-1.62	3.50	44.9
Fc-[12]CPP	-5.15	-1.62	3.54	42.4

The HOMO and LUMO data of [*n*]CPP were taken from ref S4; the strain energy data of [*n*]CPP were taken from ref S16.

4.3 Relative energy in the rotation process of **Fc-[8]CPP**

Table S7. Relative energy in the rotation process of **Fc-[8]CPP**

Conformation	Energy (Hartree)	Relative energy (Hartree)	Relative energy (kal/mol)
A	-3497.2494931	0.0000000	0
B	-3497.242339	0.0071545	4.4895167
TS-1	-3497.246698	0.0027949	1.7538263
TS-2	-3497.197146	0.0523467	32.848052

4.4 Oxidation state optimization of **Fc-CPPs**

Comparison between the ground station and oxidation state of **Fc-[8]CPP**

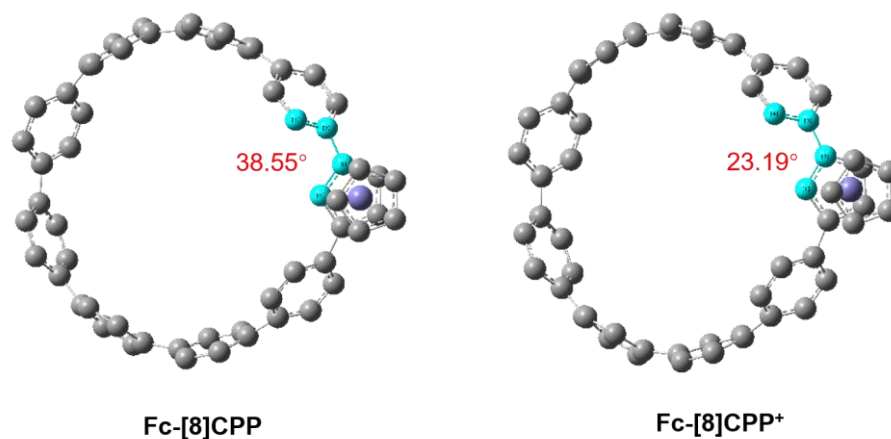


Figure S4. The geometry optimizations of ground station and oxidation state of **Fc-[8]CPP**

As shown in Figure S4, the oxidation of **Fc-[8]CPP** (named **Fc-[8]CPP⁺**) has smaller torsion angel between Fc and adjacent benzene units, which means the conformation of **Fc-[8]CPP** could be adjusted by oxidation.

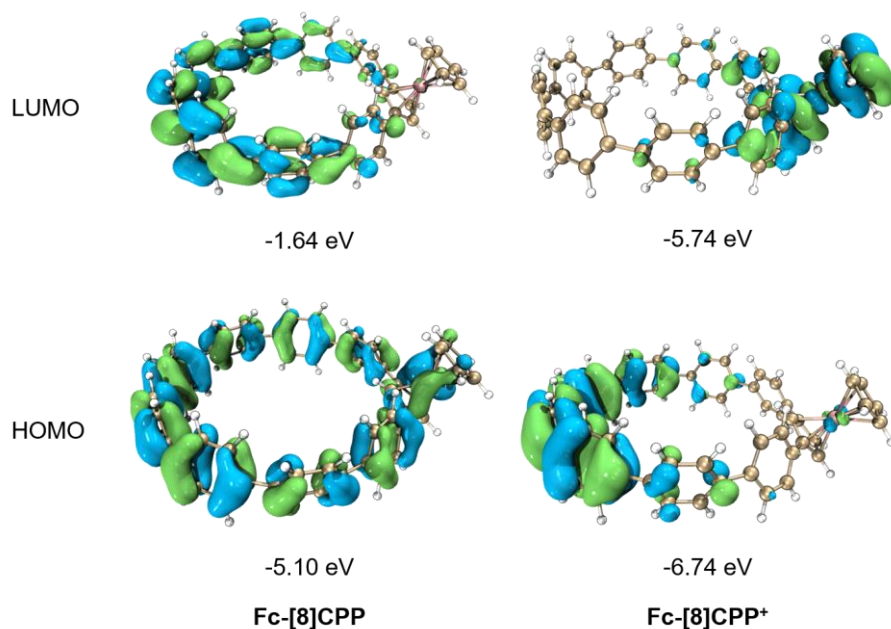


Figure S5. The frontier molecular orbit of the ground station and oxidation state of **Fc-[8]CPP**

As shown in Figure S5, after oxidation, the electron density had obvious separation, the electron was mainly delocalized at the CPP part at HOMO, and the electron was mainly delocalized at the Fc⁺ part at LUMO. The oxidation state of **Fc-[11]CPP** (named **Fc-[11]CPP⁺**) was similar, see below.

Comparison between the ground station and oxidation state of **Fc-[11]CPP**

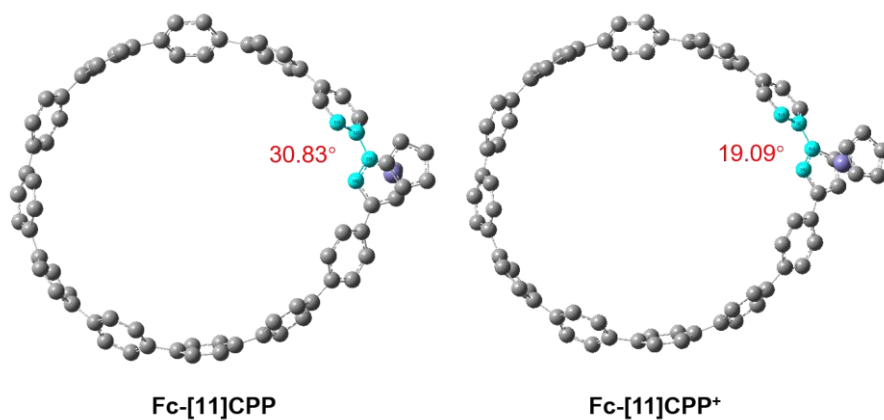


Figure S6. The geometry optimizations of the ground station and oxidation state of **Fc-[11]CPP**

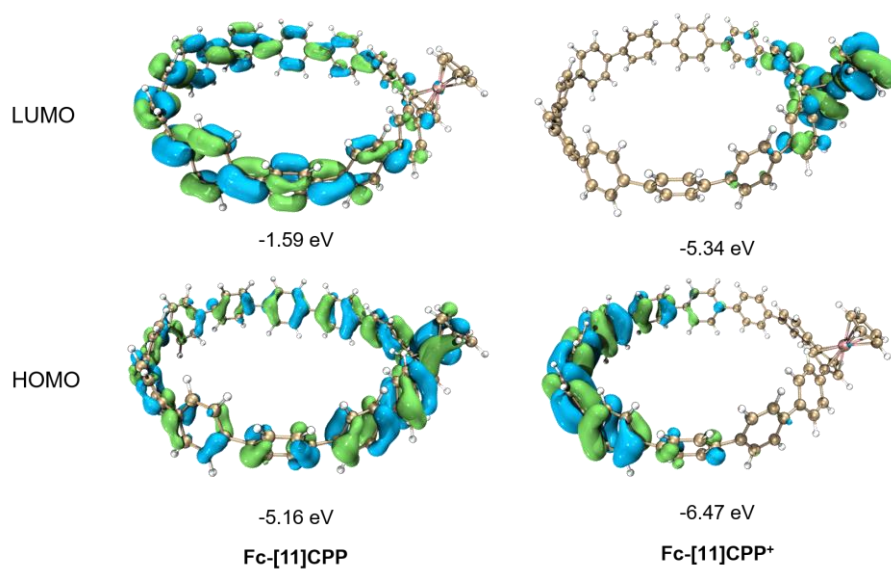


Figure S7. The frontier molecular orbitals of the ground station and oxidation state of **Fc-[11]CPP**

5. Variable temperature NMR (VT-NMR) of Fc-[8]CPP

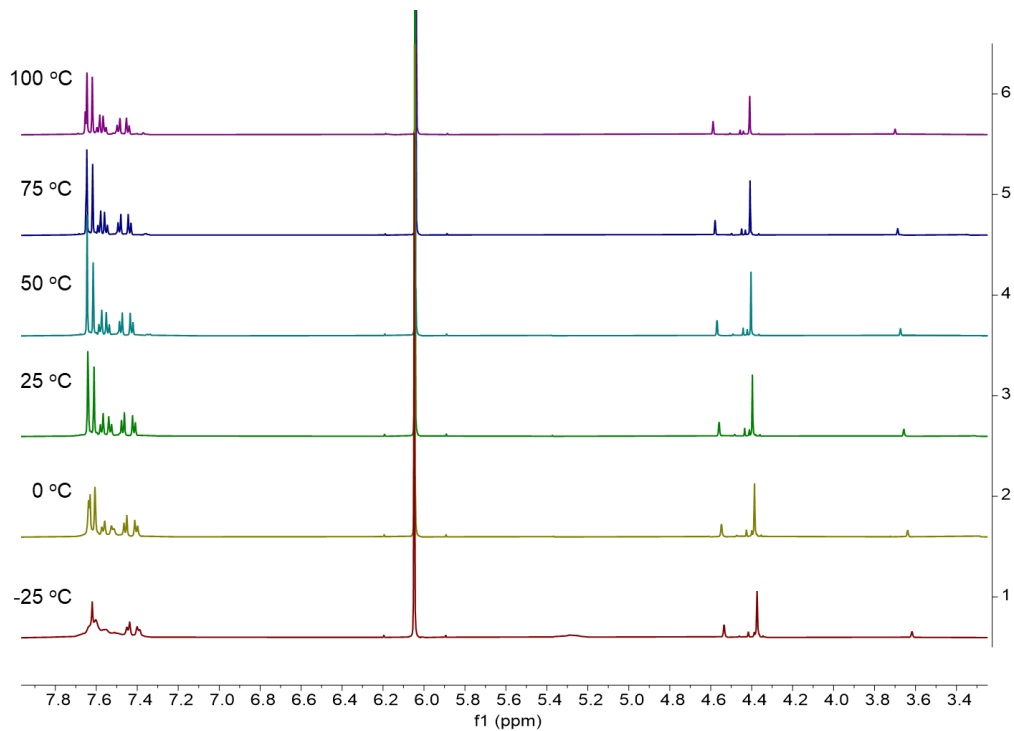


Figure S8 VT-NMR of Fc-[8]CPP in 1,1,2,2-tetrachloroethane-*d*₂ (600 MHz)

6. Redox property of Fc-[8]CPP

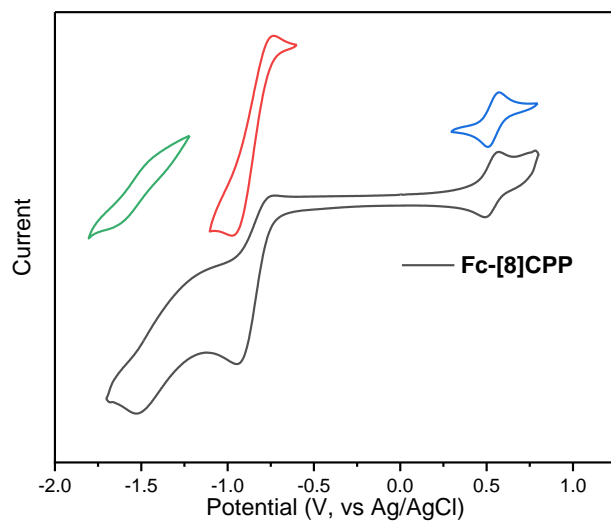


Figure S9. The CV curves of Fc-[8]CPP in CH₂Cl₂ solution (0.1 mM) containing 0.1 M *n*-Bu₄NPF₆ at room temperature, scan rate: 100 mV/s.

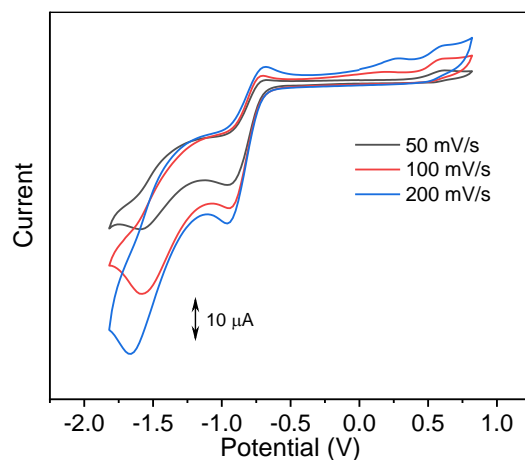


Figure S10. The CV curves of **Fc-[8]CPP** in CH_2Cl_2 solution (0.1 mM) containing 0.1 M $n\text{-Bu}_4\text{NPF}_6$ at room temperature at different scan rates.

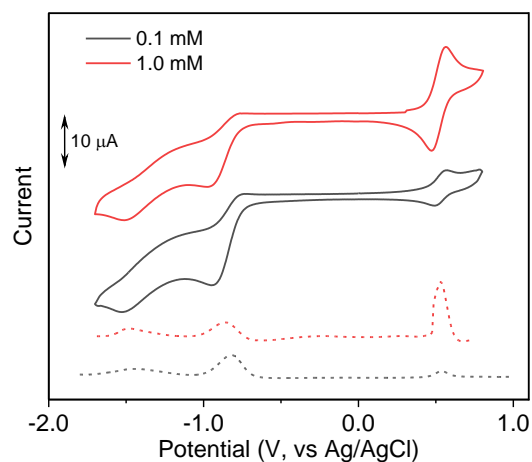


Figure S11. The CV (solid) and DPV (dashed) curves of **Fc-[8]CPP** in CH_2Cl_2 solution containing 0.1 M $n\text{-Bu}_4\text{NPF}_6$ at room temperature at different concentrations.

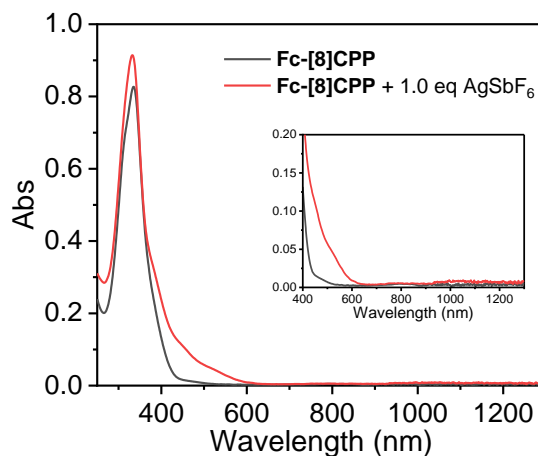


Figure S12. The UV-Vis-NIR absorption of **Fc-[8]CPP** (1.0×10^{-5} M) in the presence of AgSbF_6 in CH_2Cl_2 solution.

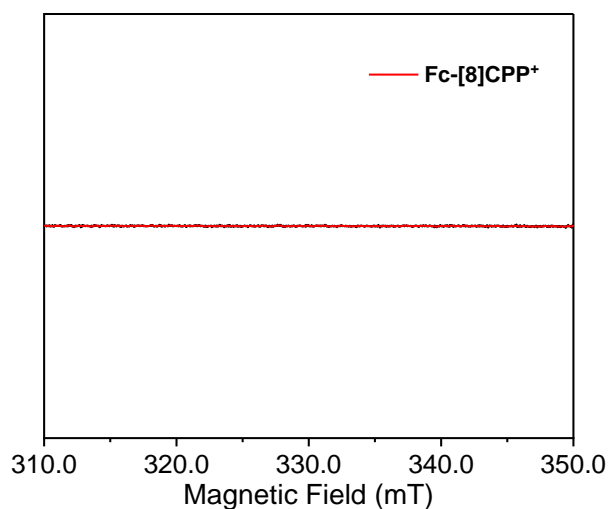


Figure S13. The EPR spectra of **Fc-[8]CPP⁺** (1.0×10^{-3} M) in the presence of AgSbF_6 in CH_2Cl_2 solution.

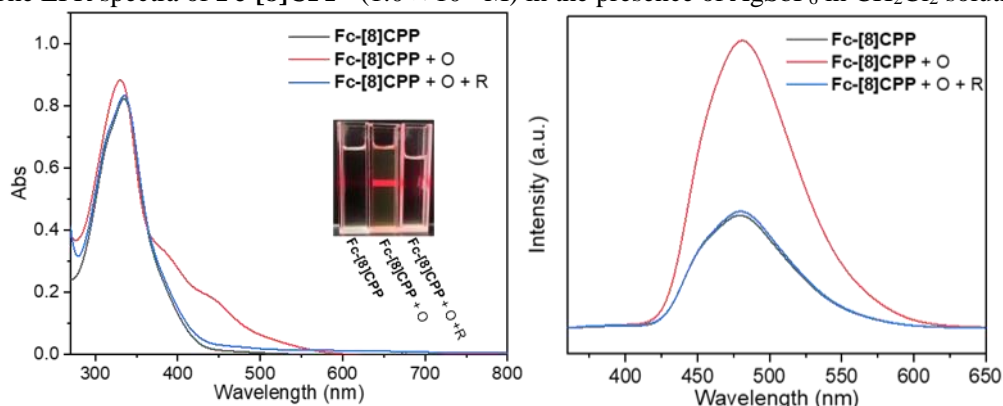


Figure S14. UV-Vis (left) and fluorescence (right) spectra curves of **Fc-[8]CPP** (1.0×10^{-5} M) in the presence of oxidation (O, 1.0 eq AgSbF_6) and reductant (R, excess Et_3N) in CH_2Cl_2 solution, $\lambda_{\text{ex}} = 340$ nm. (Inset) images of **Fc-[8]CPP** (left) in the presence of oxidation (middle) and excess reductant (right) under red laser irradiation.

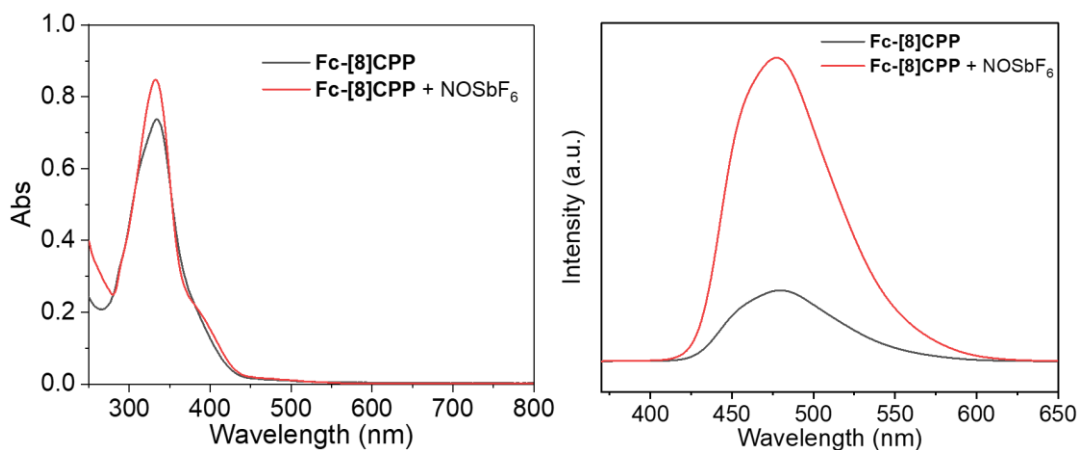


Figure S15. UV-Vis (left) and fluorescence (right) spectra curves of **Fc-[8]CPP** (1.0×10^{-5} M) in the presence of oxidation (O, 1.0 eq NOSbF_6) in THF solution, $\lambda_{\text{ex}} = 340$ nm.

7. Oxidation titration of Fc-[11]CPP

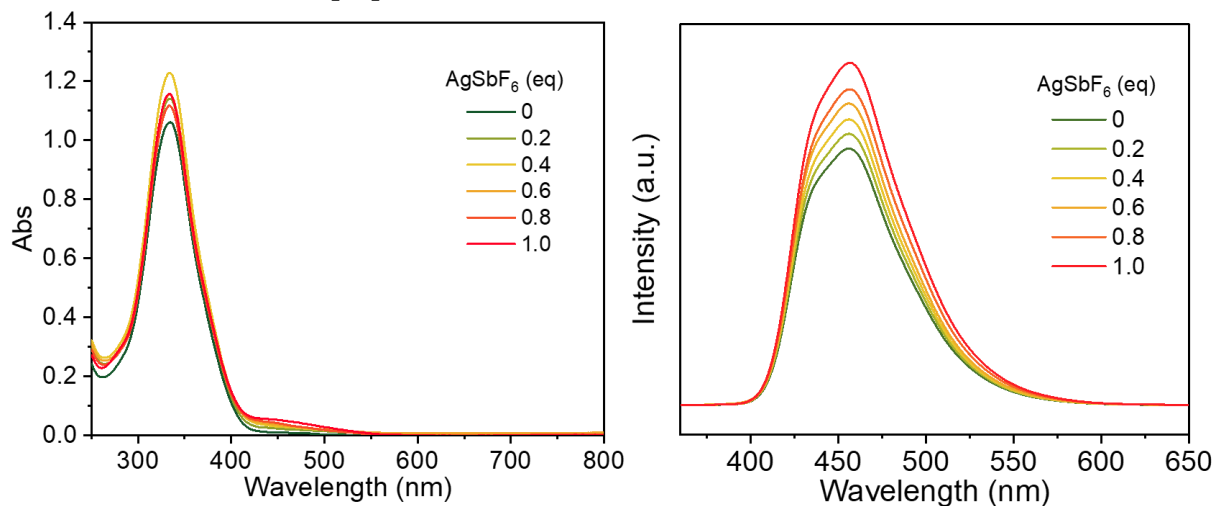


Figure S16. UV-Vis (left) and fluorescence (right) spectra curves of **Fc-[11]CPP** (1.0×10^{-5} M) in the presence of AgSbF_6 , $\lambda_{\text{ex}} = 340$ nm.

8. UV-Vis spectra titration of fullerenes to Fc-CPPs

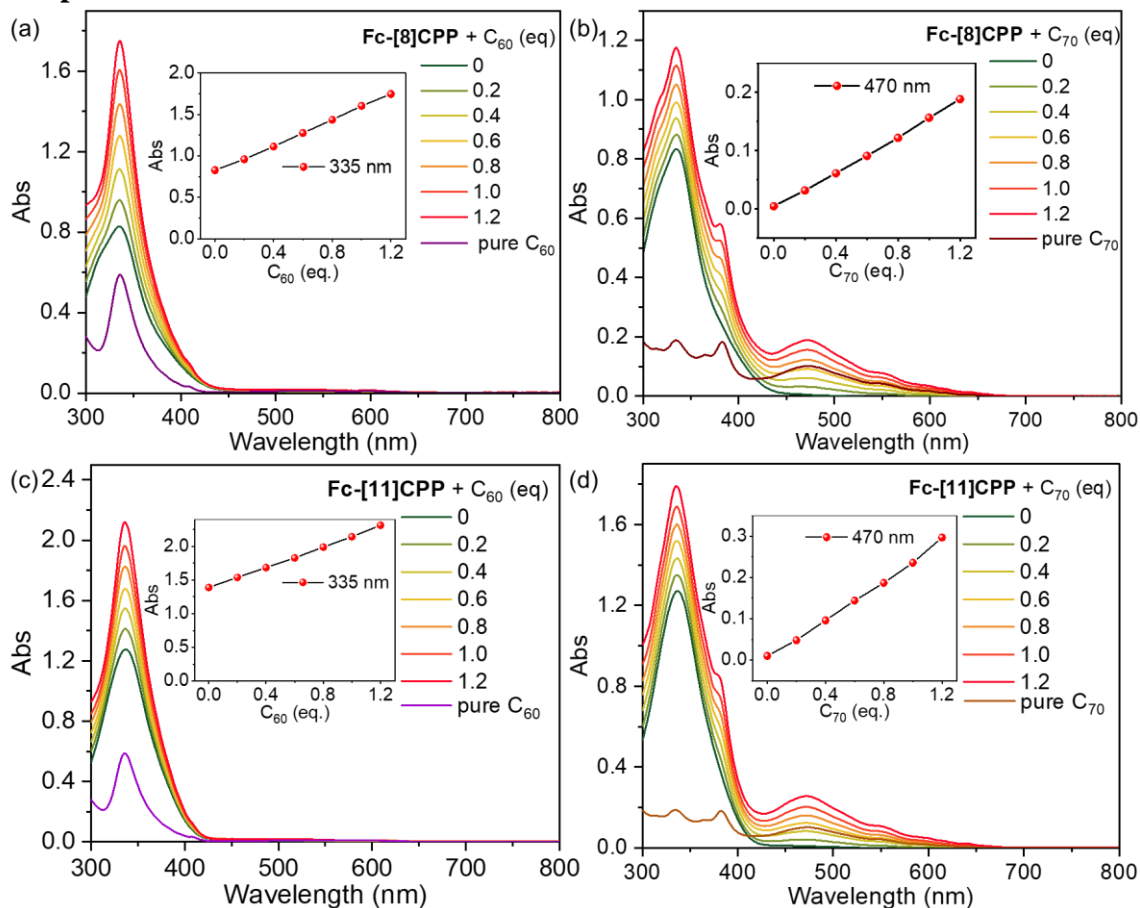


Figure S17. UV-Vis spectra of **Fc-[8]CPP** (a, b) and **Fc-[11]CPP** (c, d) in the presence of C₆₀ (a, c) and C₇₀ (b, d) in toluene solution, concentration: 1.0×10^{-5} M. Inset: the plot of absorption of **Fc-CPPs** with the addition of C₆₀ (at 335 nm) and C₇₀ (at 470 nm).

9. K_{SV} curve in titration process of Fc-CPPs with fullerenes

The Stern-Volmer equation: $F_0/F = 1 + K_{SV}[Q]$

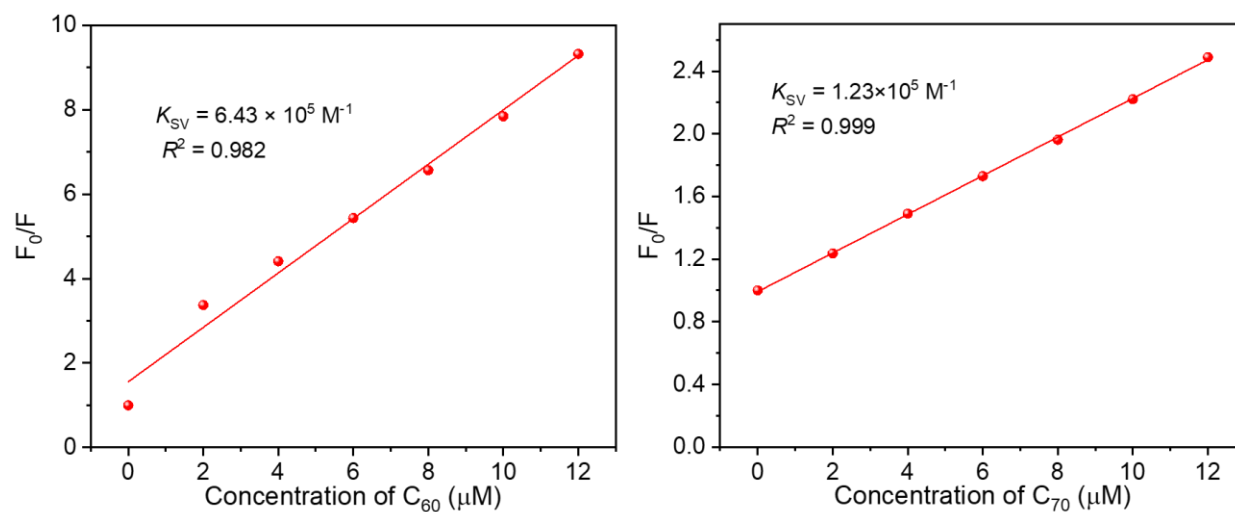


Figure S18. Correlation of concentration of C₆₀ (left) and C₇₀ (right) on the fluorescent intensity of Fc-[8]CPP in toluene (1.0×10^{-5} M) for obtaining the K_{sv} . R^2 is the standard deviation.

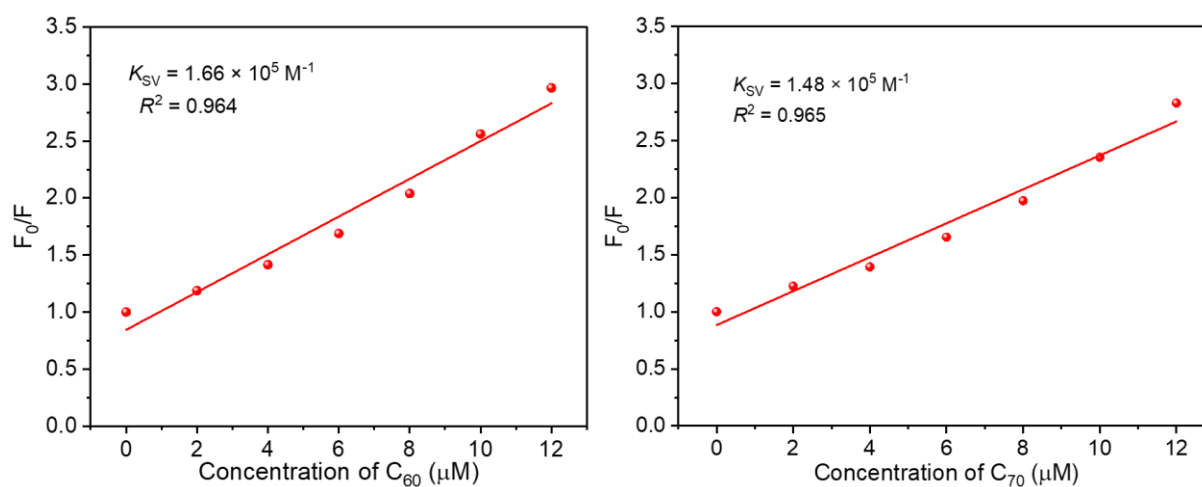


Figure S19. Correlation of concentration of C₆₀ (left) and C₇₀ (right) on the fluorescent intensity of Fc-[11]CPP in toluene (1.0×10^{-5} M) for obtaining the K_{sv} . R^2 is the standard deviation.

10. Cartesian coordinates of optimized structures

The geometry optimizations were calculated at the B3LYP/6-31G(d) level of theory unless otherwise specified.

Fc-[5]CPP							
C	-3.67969	0.716224	1.763264	C	-2.01193	2.446871	0.587099
C	-2.2185	0.000125	0.14893	C	-1.24887	2.921419	1.667501
C	-2.75179	-1.17282	0.771683	C	-0.06061	3.613482	1.450333
C	-3.67961	-0.71591	1.763369	C	1.878983	3.937033	-0.10388
C	-4.657	-0.0006	-2.09615	C	-2.75195	1.173106	0.771528
C	-5.21719	1.154517	-1.47097	H	-4.28719	1.347385	2.40024
C	-6.12262	0.713958	-0.45896	H	-1.43332	0.000157	-0.59512
C	-6.12294	-0.7134	-0.45846	H	-4.28708	-1.34709	2.400346
C	-5.2177	-1.15507	-1.47018	H	-3.92829	-0.00098	-2.89631
C	1.878844	-3.93707	-0.10389	H	-4.98692	2.184475	-1.7106
C	2.381766	-3.44533	-1.32373	H	-6.69789	1.351111	0.200047
C	3.624718	-2.82921	-1.39668	H	-6.69845	-1.34989	0.200969
C	4.428502	-2.67097	-0.25166	H	-4.98774	-2.18526	-1.7091
C	4.067567	-3.44991	0.866999	H	1.732122	-3.36898	-2.18905
C	2.822677	-4.07124	0.936994	H	3.87703	-2.29651	-2.30818
C	-0.51182	-3.65847	-0.89813	H	4.711181	-3.47198	1.742906
C	-1.68765	-2.94172	-0.68664	H	2.544048	-4.56347	1.864663
C	-2.01191	-2.44664	0.587301	H	-0.25794	-3.94295	-1.91511
C	-1.24881	-2.92123	1.667657	H	-2.3006	-2.66305	-1.53988
C	-0.06061	-3.61338	1.450424	H	-1.49499	-2.5982	2.675804
C	4.428615	2.670865	-0.25156	H	0.581626	-3.80032	2.305164
C	3.624998	2.829318	-1.39662	H	3.877349	2.296747	-2.30818
C	2.382031	3.44549	-1.32371	H	1.73253	3.369261	-2.18915
C	2.822733	4.071016	0.937149	H	2.543999	4.563168	1.864826
C	4.067579	3.449663	0.867206	H	4.711136	3.471617	1.743157
C	5.230744	-1.42063	-0.14633	H	5.87345	-1.21889	-2.20767
C	5.662268	-0.69627	-1.27805	H	5.87348	1.218834	-2.2076
C	5.66229	0.696165	-1.278	H	4.871402	1.20524	1.974859
C	5.230789	1.420478	-0.14624	H	4.871369	-1.20551	1.974789
C	5.148575	0.695077	1.057573	H	-0.25762	3.94291	-1.91522
C	5.148555	-0.6953	1.057532	H	-2.30043	2.663198	-1.54011
C	0.409368	-3.87426	0.147697	H	-1.49516	2.598449	2.675638
C	0.409497	3.874277	0.147641	H	0.581568	3.800414	2.305118
C	-0.51163	3.658505	-0.89826	Fe	-4.23358	-4E-06	-0.08596
C	-1.68754	2.94186	-0.68683				

Fe-[6]CPP

C	4.604679	0.67891	-1.63153	C	2.476216	3.188111	-1.7287
C	2.966199	-0.00924	-0.18345	C	2.896695	2.460717	-0.60206
C	3.567864	-1.19296	-0.71603	C	2.336856	2.814932	0.637049
C	4.60118	-0.75316	-1.60752	C	1.246199	3.673527	0.709954
C	5.754426	-1.1364	1.790267	C	-0.76589	4.603079	-0.41906
C	5.13909	0.037442	2.322005	C	3.574188	1.152919	-0.75485
C	5.778091	1.173165	1.737795	H	5.284817	1.297293	-2.20424
C	6.787977	0.70109	0.846313	H	2.102944	0.004473	0.467498
C	6.773328	-0.72602	0.878679	H	5.278174	-1.39352	-2.15945
C	-4.79036	-3.25664	0.137551	H	5.484333	-2.15853	2.022044
C	-5.0287	-2.74125	1.42681	H	4.325869	0.06191	3.035869
C	-5.66305	-1.5182	1.612301	H	5.529366	2.210082	1.92312
C	-6.0601	-0.72679	0.515273	H	7.440045	1.317778	0.24159
C	-6.09731	-1.38896	-0.72895	H	7.412294	-1.38274	0.302804
C	-5.4929	-2.62793	-0.91001	H	-4.58526	-3.2212	2.293763
C	-2.86567	-4.73294	0.912025	H	-5.7194	-1.12303	2.621627
C	-1.49898	-4.97399	0.790542	H	-6.47735	-0.87753	-1.60763
C	-0.79338	-4.60559	-0.37187	H	-5.46174	-3.04256	-1.91325
C	-1.57199	-4.2301	-1.48132	H	-3.34765	-4.95306	1.860643
C	-2.93314	-3.98449	-1.35769	H	-0.95914	-5.371	1.646572
C	-3.5926	-4.10196	-0.11899	H	-1.0843	-3.96242	-2.41346
C	1.402509	-4.12888	-1.55545	H	-3.44405	-3.53719	-2.20337
C	2.49409	-3.26494	-1.63564	H	1.070184	-4.63823	-2.45626
C	2.882997	-2.49191	-0.52822	H	2.967656	-3.09512	-2.59923
C	2.286927	-2.79513	0.707893	H	2.607066	-2.25907	1.597368
C	1.190541	-3.64641	0.783812	H	0.663542	-3.73463	1.729265
C	-3.55115	4.132901	-0.04614	H	-3.23407	5.031332	1.898785
C	-2.7845	4.785908	0.939951	H	-0.84693	5.435504	1.578048
C	-1.42292	5.015248	0.757506	H	-1.1351	3.89655	-2.427
C	-1.58709	4.200461	-1.4879	H	-3.50003	3.496468	-2.10993
C	-2.94608	3.971724	-1.30627	H	-5.22365	0.855574	2.591595
C	-6.0263	0.7616	0.580199	H	-4.12179	2.974363	2.326474
C	-5.38413	1.393029	1.66358	H	-5.73342	3.337299	-1.64215
C	-4.75139	2.620671	1.515763	H	-6.84387	1.194248	-1.38356
C	-4.7301	3.286244	0.276562	H	1.032437	4.532366	-2.56316
C	-5.61804	2.800692	-0.70384	H	2.9207	2.976846	-2.69796
C	-6.25344	1.571043	-0.55348	H	2.680858	2.31306	1.537441
C	0.649131	-4.24219	-0.37132	H	0.748037	3.80203	1.666226
C	0.673305	4.225805	-0.45168	Fe	4.945825	-0.00699	0.277457
C	1.389687	4.059227	-1.65218				

Fe-[7]CPP

C	5.476504	0.715462	-1.48219	C	2.442811	4.226706	-1.66512
C	3.741172	0.000011	-0.16257	C	3.454952	3.26814	-1.68176
C	4.385935	-1.17204	-0.67145	C	3.732432	2.493108	-0.54302
C	5.476425	-0.71545	-1.48228	C	3.095189	2.853913	0.655998
C	7.474778	0.713306	1.148128	C	2.082572	3.806599	0.670668
C	7.474454	-0.71427	1.148257	C	0.298508	5.023706	-0.56654
C	6.398124	-1.15534	1.975537	C	4.386078	1.17207	-0.67128
C	5.732967	0.000021	2.487531	H	6.192525	1.346326	-1.99423
C	6.398627	1.155019	1.975321	H	2.837896	0.000076	0.432358
C	-6.54664	-1.42933	0.646406	H	6.192354	-1.34636	-1.9944
C	-6.07084	-0.69344	1.747645	H	8.161145	1.349992	0.605214
C	-6.07082	0.693626	1.747628	H	8.160581	-1.35129	0.605438
C	-6.54658	1.429506	0.64637	H	6.123566	-2.18509	2.164293
C	-7.24403	0.696784	-0.3355	H	4.870771	0.00029	3.141859
C	-7.24406	-0.6966	-0.33548	H	6.124543	2.184915	2.163969
C	-5.74728	-3.24337	-0.89204	H	-5.54582	-1.19981	2.550308
C	-4.75673	-4.18333	-1.15525	H	-5.54578	1.199997	2.550278
C	-3.94291	-4.69598	-0.12592	H	-7.72366	1.216238	-1.16084
C	-4.38152	-4.44435	1.189	H	-7.72371	-1.21605	-1.16082
C	-5.39586	-3.53128	1.453415	H	-6.23181	-2.75826	-1.73406
C	-6.00182	-2.79344	0.417721	H	-4.5436	-4.42812	-2.19129
C	-1.724	-5.69088	0.624466	H	-3.84263	-4.86669	2.031353
C	-0.33531	-5.62016	0.539435	H	-5.6347	-3.30988	2.489502
C	0.298277	-5.02366	-0.5666	H	-2.16644	-6.10097	1.527885
C	-0.5204	-4.69871	-1.66214	H	0.262189	-5.96991	1.377648
C	-1.90491	-4.75805	-1.5712	H	-0.07712	-4.2508	-2.54643
C	-2.54986	-5.15234	-0.38341	H	-2.48339	-4.35155	-2.39351
C	2.082335	-3.80649	0.670531	H	1.522766	-3.9653	1.587927
C	3.094959	-2.85381	0.655832	H	3.324728	-2.30472	1.565016
C	3.732214	-2.49304	-0.54319	H	3.958783	-3.0411	-2.61778
C	3.454707	-3.2681	-1.68191	H	2.196112	-4.75006	-2.58549
C	2.442548	-4.22664	-1.66525	H	-2.48309	4.351288	-2.39346
C	-2.54964	5.152354	-0.38348	H	-0.0768	4.250589	-2.54629
C	-1.90463	4.757906	-1.57119	H	0.262322	5.970165	1.377607
C	-0.52013	4.698599	-1.66207	H	-2.16631	6.101192	1.527727
C	-0.33512	5.620301	0.539403	H	-6.23169	2.758392	-1.73411
C	-1.72383	5.691011	0.624367	H	-4.54343	4.428191	-2.19137
C	-6.00169	2.793594	0.417667	H	-3.84236	4.866745	2.031258
C	-5.74714	3.243492	-0.8921	H	-5.63452	3.310014	2.489446
C	-4.75655	4.18342	-1.15533	H	2.196376	4.750112	-2.58537
C	-3.9427	4.69603	-0.12601	H	3.959025	3.0411	-2.61762
C	-4.3813	4.444427	1.188925	H	3.324965	2.304832	1.565181
C	-5.39568	3.531409	1.453354	H	1.522985	3.965453	1.588046
C	1.665938	-4.44452	-0.51262	Fe	5.685496	-0.00012	0.434213
C	1.666196	4.444611	-0.51251				

Fe-[8]CPP

C	-6.18667	-0.64949	-1.59611	C	3.859324	5.874668	-1.00718
C	-5.14284	-1.13236	-0.74021	C	5.096235	5.237285	-0.97139
C	-4.51301	0.022638	-0.17631	C	-4.50329	2.535913	-0.4859
C	-5.12404	1.210381	-0.69042	C	-3.88083	2.84271	0.736024
C	-6.17567	0.780406	-1.56528	C	-2.93858	3.859877	0.826061
C	-8.29602	0.756831	0.966612	C	-2.58204	4.626214	-0.29901
C	-7.25475	1.151509	1.859489	C	-3.3366	4.433175	-1.47025
C	-6.63831	-0.03169	2.368783	C	-4.27534	3.406655	-1.56424
C	-7.29874	-1.15747	1.789129	H	-6.88136	-1.26324	-2.15599
C	-8.32324	-0.66987	0.92321	H	-3.64215	0.001127	0.464661
C	-3.96218	-2.84736	0.63899	H	-6.86046	1.428109	-2.09847
C	-3.0348	-3.87935	0.708039	H	-8.94141	1.423377	0.409473
C	-2.65096	-4.59492	-0.44143	H	-6.96958	2.169425	2.091794
C	-3.36383	-4.33408	-1.62546	H	-5.8107	-0.06849	3.065413
C	-4.28854	-3.2927	-1.69773	H	-7.05274	-2.1977	1.958908
C	-4.54271	-2.47429	-0.58478	H	-8.99289	-1.27627	0.327322
C	5.067265	-5.2954	-0.78011	H	-4.17566	-2.26055	1.528243
C	3.825393	-5.91491	-0.89943	H	-2.52013	-4.05993	1.647072
C	2.84578	-5.78336	0.102152	H	-3.1422	-4.90528	-2.5232
C	3.245258	-5.16835	1.301246	H	-4.74653	-3.05154	-2.65352
C	4.478347	-4.53984	1.413856	H	5.769543	-5.37757	-1.60489
C	5.385324	-4.49856	0.338158	H	3.590897	-6.45519	-1.81316
C	6.787106	-2.71344	1.455954	H	2.527271	-5.05374	2.107786
C	7.293563	-1.42142	1.372369	H	4.671598	-3.95696	2.307873
C	7.496658	-0.7893	0.130548	H	6.580248	-3.12293	2.440062
C	7.389217	-1.61257	-1.00698	H	7.417099	-0.85997	2.293173
C	6.849693	-2.8913	-0.92554	H	7.631752	-1.21813	-1.98904
C	6.421524	-3.43255	0.301771	H	6.651652	-3.42308	-1.85098
C	-0.49541	-5.25839	-1.51099	H	-0.8409	-4.81001	-2.43776
C	0.856146	-5.55914	-1.37831	H	1.525209	-5.33622	-2.20439
C	1.393374	-5.96896	-0.14535	H	0.842953	-6.65117	1.830959
C	0.479771	-6.25289	0.887	H	-1.53892	-6.13207	1.593473
C	-0.87342	-5.95553	0.752503	H	-0.84566	4.895847	-2.34487
C	-1.37518	-5.35655	-0.41857	H	1.528361	5.392241	-2.18765
C	-1.29519	5.368856	-0.28709	H	1.021501	6.562415	1.918741
C	-0.45974	5.304955	-1.41599	H	-1.36888	6.060461	1.760422
C	0.897748	5.58988	-1.32616	H	5.999465	2.968952	-2.02462
C	1.489442	5.953653	-0.10325	H	6.848606	0.708531	-2.04
C	0.619907	6.200206	0.975885	H	8.130862	1.156203	2.045298
C	-0.74004	5.914043	0.886032	H	7.245238	3.427953	2.063127
C	6.47525	3.363957	0.043108	H	4.94233	3.977771	2.171632
C	6.503177	2.599659	-1.13642	H	2.778285	5.087259	2.107505
C	6.992015	1.299991	-1.14231	H	3.563496	6.402213	-1.91021
C	7.487954	0.694439	0.027624	H	5.737476	5.27758	-1.84819
C	7.664027	1.539339	1.142287	H	-4.0737	2.215918	1.602464
C	7.162719	2.838803	1.153218	H	-2.39225	3.988668	1.755819
C	5.485704	4.467154	0.140956	H	-3.13686	5.046357	-2.34509

C	4.673614	4.546296	1.286114	H	-4.76607	3.21846	-2.51564
C	3.436325	5.180262	1.248696	Fe	-6.48703	0.027716	0.321518
C	2.953747	5.768035	0.065874				

Fe-[8]CPP (B3LYP-D3(BJ)/6-31G(d) for C, H, SDD for Fe)

C	0.428177	6.255531	0.896673	C	-5.11003	1.117434	-0.82529
C	0.606141	-6.19578	0.985998	C	-6.19345	-0.79486	-1.57711
C	0.81384	5.595233	-1.37918	C	-6.20874	0.635265	-1.60815
C	0.886924	-5.61472	-1.32517	C	-6.35481	0.010966	2.406886
C	1.342624	5.989122	-0.13838	C	-7.01791	-1.16855	1.948635
C	1.473987	-5.96298	-0.09641	C	-7.05863	1.142252	1.891202
C	2.789623	5.795782	0.114117	C	-8.13242	-0.76584	1.15265
C	2.93367	-5.76941	0.073971	C	-8.15753	0.661591	1.117122
C	3.173723	5.156795	1.304749	H	0.791244	6.637437	1.846814
C	3.406862	-5.16757	1.252592	H	1.010151	-6.54198	1.933199
C	3.773362	5.93909	-0.88035	H	1.489377	5.383064	-2.20221
C	3.83818	-5.87841	-0.99856	H	1.521571	-5.4239	-2.18458
C	4.403121	4.522841	1.416085	H	2.445235	5.028461	2.099008
C	4.639873	-4.52676	1.287085	H	2.74293	-5.06912	2.105575
C	5.011831	5.314149	-0.76203	H	3.542983	6.492539	-1.78664
C	5.069983	-5.23282	-0.96642	H	3.543019	-6.41273	-1.89717
C	5.3178	4.502223	0.347437	H	4.588547	3.918937	2.297095
C	5.451771	-4.45579	0.142398	H	4.905405	-3.94509	2.164446
C	6.351067	3.438651	0.304896	H	5.712775	-5.26963	-1.84163
C	6.429989	-3.34786	0.037922	H	5.721648	5.403306	-1.57897
C	6.433295	-2.58147	-1.13951	H	5.916649	-2.95369	-2.01847
C	6.717463	2.718246	1.456867	H	6.509943	3.126856	2.440671
C	6.770318	2.902117	-0.92643	H	6.561899	3.436359	-1.8476
C	6.912096	-1.27887	-1.1474	H	6.749948	-0.68183	-2.03754
C	7.122124	-2.82228	1.143482	H	7.213572	-3.41428	2.050102
C	7.223645	1.427348	1.368157	H	7.347218	0.859638	2.284466
C	7.311672	1.625287	-1.0129	H	7.549363	1.229931	-1.99521
C	7.421659	-0.67735	0.017804	H	8.087853	-1.13291	2.027102
C	7.425981	0.80278	0.123419	H	-0.85866	-4.93415	-2.35239
C	7.614732	-1.52037	1.129864	H	-0.8808	4.853484	-2.45107
C	-0.47034	-5.33399	-1.42096	H	-1.38489	-6.04162	1.765131
C	-0.53602	5.293161	-1.52034	H	-1.59304	6.111877	1.594822
C	-0.75309	-5.91205	0.890808	H	-2.35928	-3.94515	1.715784
C	-0.92269	5.955799	0.754273	H	-2.50646	4.008347	1.605587
C	-1.30447	-5.38637	-0.29162	H	-3.15471	-5.11758	-2.34118
C	-1.41605	5.374443	-0.42792	H	-3.19142	4.966322	-2.52733
C	-2.58504	-4.6401	-0.31437	H	-3.53466	-0.01002	0.28596
C	-2.68046	4.601155	-0.46177	H	-4.03056	-2.1538	1.522769
C	-2.91878	-3.83776	0.791642	H	-4.13951	2.179745	1.450336
C	-3.03495	3.846602	0.671317	H	-4.77465	-3.27602	-2.55091
C	-3.34602	-4.47723	-1.48467	H	-4.77529	3.08876	-2.69389
C	-3.39965	4.366168	-1.64596	H	-5.45578	0.041604	3.008315
C	-3.85085	-2.81478	0.679987	H	-6.7031	-2.1875	2.130786
C	-3.94562	2.802816	0.582323	H	-6.78023	2.179452	2.022352

C	-4.27614	-3.4454	-1.60039	H	-6.92317	-1.44593	-2.04058
C	-4.30955	3.313583	-1.73824	H	-6.95189	1.250174	-2.09886
C	-4.43573	-0.03329	-0.31041	H	-8.81402	-1.42737	0.634907
C	-4.48308	-2.54436	-0.54498	H	-8.86159	1.272248	0.567891
C	-4.53633	2.462837	-0.64574	Fe	-6.37356	-0.0408	0.344006
C	-5.0847	-1.21949	-0.77489				

Fe-[9]CPP

C	7.079595	0.715414	-1.30474	C	-5.82214	-5.03271	-0.0299
C	5.256384	0.00013	-0.10817	C	-6.11969	-4.68938	1.301915
C	5.937386	-1.17183	-0.56733	C	-6.96142	-3.62311	1.601594
C	7.079664	-0.71511	-1.30466	C	-1.8358	-6.51859	-0.64519
C	8.894169	-0.71379	1.456877	C	-2.62943	-7.05147	0.388666
C	7.762555	-1.15519	2.206355	C	-3.96849	-6.69247	0.533247
C	7.063476	0.000201	2.670902	C	-4.58133	-5.78349	-0.34997
C	7.762832	1.155435	2.206473	C	-3.8306	-5.38724	-1.47154
C	8.894307	0.713899	1.456946	C	-2.49732	-5.74373	-1.61462
C	-7.52781	2.832614	0.583819	H	7.830053	1.34554	-1.76551
C	-6.96165	3.622747	1.601706	H	4.31692	0.000155	0.42711
C	-6.11998	4.689081	1.302074	H	7.830276	-1.34518	-1.76526
C	-5.82247	5.032504	-0.02973	H	9.616344	-1.35063	0.962751
C	-6.5775	4.39374	-1.03079	H	7.472724	-2.18469	2.372359
C	-7.40072	3.313166	-0.73285	H	6.158165	0.000273	3.264248
C	-8.76052	0.696569	-0.06264	H	7.473186	2.184993	2.372523
C	-8.76047	-0.69699	-0.06265	H	9.616671	1.350615	0.962933
C	-7.94696	-1.42828	0.824267	H	-7.10232	3.34401	2.642244
C	-7.28781	-0.69406	1.826661	H	-5.59562	5.183831	2.114594
C	-7.28786	0.6937	1.826681	H	-6.44861	4.682876	-2.07001
C	-7.94706	1.427897	0.824301	H	-7.85498	2.763474	-1.55203
C	0.405985	-6.27891	-1.78434	H	-9.35656	1.220945	-0.80502
C	1.718959	-5.82661	-1.71218	H	-9.35647	-1.22139	-0.80505
C	2.352606	-5.61084	-0.47445	H	-6.64877	-1.2083	2.537056
C	1.664443	-6.05021	0.671677	H	-6.64887	1.207962	2.537092
C	0.343013	-6.47948	0.60155	H	-0.062	-6.37097	-2.76029
C	-0.35086	-6.51518	-0.6218	H	2.220461	-5.53806	-2.63118
C	4.437044	-4.52862	-1.45435	H	2.139672	-5.98117	1.646003
C	5.308697	-3.43947	-1.47716	H	-0.18691	-6.68822	1.526419
C	5.337922	-2.51404	-0.42137	H	4.408464	-5.19386	-2.31312
C	4.566662	-2.8093	0.715707	H	5.9133	-3.26028	-2.3625
C	3.688196	-3.88308	0.730475	H	4.601907	-2.13925	1.570106
C	-0.35129	6.515203	-0.62182	H	3.031591	-4.00485	1.585988
C	0.405507	6.278937	-1.7844	H	-0.06254	6.370982	-2.76032
C	1.718493	5.826658	-1.7123	H	2.219927	5.538106	-2.63133
C	1.664077	6.050244	0.671557	H	2.139347	5.981238	1.645864
C	0.342633	6.479489	0.601494	H	-0.18725	6.688191	1.526393
C	-4.58168	5.783344	-0.34979	H	-4.53028	7.086716	1.376481
C	-3.96884	6.69231	0.533432	H	-2.18326	7.717886	1.122062

C	-2.6298	7.051383	0.388792	H	-1.93149	5.303899	-2.42902
C	-1.83622	6.518578	-0.64514	H	-4.25487	4.681798	-2.17874
C	-2.49775	5.743728	-1.61456	H	4.407925	5.193876	-2.3134
C	-3.83101	5.387187	-1.47143	H	5.912844	3.260407	-2.36279
C	3.547497	-4.73243	-0.38353	H	4.601844	2.139551	1.570019
C	3.54715	4.732553	-0.38369	H	3.031472	4.005055	1.585908
C	4.436614	4.528703	-1.45458	H	-7.8548	-2.76374	-1.55211
C	5.308334	3.439605	-1.47738	H	-6.44833	-4.68305	-2.07017
C	5.337716	2.514258	-0.42154	H	-5.59531	-5.18415	2.114407
C	4.566532	2.809545	0.715578	H	-7.10212	-3.34443	2.642145
C	3.688009	3.883288	0.730347	H	-2.18293	-7.71798	1.121953
C	2.352221	5.610911	-0.47459	H	-4.52998	-7.08692	1.376247
C	5.93726	1.172071	-0.5675	H	-4.25443	-4.68183	-2.17884
C	-7.52761	-2.83296	0.583734	H	-1.93103	-5.30382	-2.42901
C	-7.4005	-3.31345	-0.73295	Fe	7.158837	0.000218	0.619652
C	-6.57721	-4.39396	-1.03094				

Fe-[10]CPP

C	-7.86524	-0.82299	-1.2732	C	8.945338	-1.47925	1.629278
C	-6.69887	-1.25001	-0.55588	C	8.892582	-0.61277	0.522181
C	-6.0423	-0.06127	-0.1041	C	8.608825	-1.1884	-0.72824
C	-6.76409	1.092419	-0.54745	C	8.216598	-2.51785	-0.83638
C	-7.90486	0.606485	-1.26835	C	8.836298	0.864125	0.660952
C	-8.48155	-1.29409	2.244275	C	8.088314	1.412585	1.716866
C	-7.80307	-0.12444	2.703585	C	7.635422	2.725386	1.67343
C	-8.53814	1.01583	2.257624	C	7.91544	3.562424	0.57798
C	-9.67106	0.550689	1.524742	C	8.817028	3.067107	-0.38406
C	-9.63617	-0.87659	1.516568	C	9.26041	1.747476	-0.34829
C	-5.27771	-2.85849	0.708642	H	-8.60577	-1.47235	-1.72309
C	-4.42229	-3.95013	0.730621	H	-5.0956	-0.03637	0.41771
C	-4.33731	-4.83939	-0.35746	H	-8.67996	1.217064	-1.71432
C	-5.24167	-4.63897	-1.41591	H	-8.16314	-2.31697	2.398585
C	-6.09068	-3.53217	-1.44628	H	-6.88793	-0.10541	3.281363
C	-6.08084	-2.58331	-0.41131	H	-8.27057	2.051285	2.424069
C	3.019736	-6.48025	-1.51074	H	-10.4169	1.172215	1.046432
C	1.641153	-6.61581	-1.61758	H	-10.3508	-1.52825	1.030909
C	0.875401	-7.17584	-0.57887	H	-5.27853	-2.16683	1.546327
C	1.584385	-7.72872	0.50509	H	-3.74709	-4.06467	1.572552
C	2.964298	-7.57962	0.620224	H	-5.25061	-5.32947	-2.25497
C	3.705327	-6.88583	-0.35293	H	-6.71611	-3.36487	-2.31937
C	5.999011	-6.14478	-1.14067	H	3.555582	-5.9388	-2.28492
C	7.07858	-5.28158	-0.97662	H	1.144351	-6.17122	-2.47382
C	7.268729	-4.57067	0.223647	H	1.045824	-8.24268	1.296415
C	6.434629	-4.91023	1.30394	H	3.468343	-7.97011	1.500698
C	5.362964	-5.78188	1.144287	H	5.846754	-6.62775	-2.10252
C	5.067134	-6.34908	-0.10694	H	7.750914	-5.11457	-1.81378
C	-2.54118	-6.24087	0.730963	H	6.544428	-4.3901	2.250597
C	-1.2694	-6.79915	0.671558	H	4.670419	-5.9205	1.969635
C	-0.59427	-6.9608	-0.55233	H	-3.00154	-6.0933	1.703584
C	-1.32913	-6.68143	-1.71936	H	-0.75907	-7.02602	1.602664
C	-2.59112	-6.09909	-1.65902	H	-0.88277	-6.85667	-2.69388
C	-3.19753	-5.78869	-0.4282	H	-3.07011	-5.79723	-2.58587
C	-3.45119	5.756206	-0.44371	H	-3.32969	5.708739	-2.60111
C	-2.85243	6.04198	-1.68428	H	-1.14757	6.783925	-2.73987
C	-1.5963	6.633148	-1.76214	H	-1.02161	7.08073	1.547683
C	-0.86423	6.94969	-0.60329	H	-3.25794	6.118046	1.679365
C	-1.53493	6.820968	0.626242	H	4.694964	6.580985	1.979733
C	-2.8007	6.248425	0.702643	H	6.652317	5.201685	2.426567
C	4.82935	6.445861	-0.17288	H	7.269946	4.721246	-1.8035
C	5.277432	6.212635	1.139996	H	5.393257	6.204354	-2.24577
C	6.381126	5.404114	1.394405	H	3.221891	8.220282	1.276188
C	7.077716	4.768175	0.349918	H	0.791967	8.432948	1.091798
C	6.740975	5.155375	-0.96059	H	0.847581	5.921565	-2.39888
C	5.652955	5.982096	-1.21469	H	3.25426	5.710778	-2.21646
C	3.443192	6.910352	-0.4306	H	-5.40157	2.082543	1.562738

C	2.709488	7.71262	0.463076	H	-3.9498	4.044075	1.581499
C	1.324734	7.833514	0.358182	H	-5.50136	5.226449	-2.25284
C	0.604946	7.158043	-0.64515	H	-6.88541	3.203245	-2.30862
C	1.357497	6.470467	-1.61371	H	8.570161	-3.43841	2.407078
C	2.735725	6.350174	-1.50941	H	9.236072	-1.08999	2.601685
C	-6.21605	2.45559	-0.3986	H	8.563103	-0.55451	-1.60909
C	-5.42944	2.770706	0.722599	H	7.874115	-2.88097	-1.8005
C	-4.61984	3.897313	0.740264	H	7.74319	0.76571	2.518107
C	-4.56748	4.780576	-0.35451	H	6.947424	3.058554	2.443706
C	-5.46563	4.541164	-1.41022	H	9.132871	3.703402	-1.20622
C	-6.26827	3.400498	-1.43589	H	9.90306	1.382698	-1.14558
C	8.097176	-3.33987	0.298444	Fe	-7.93296	-0.11598	0.654332
C	8.562611	-2.8131	1.518391				

Fe-[11]CPP

C	8.616034	0.7173	-1.28112	C	-9.02868	2.845324	0.326631
C	7.45601	1.173461	-0.57124	C	-8.91341	3.712058	1.428763
C	6.762304	0.001591	-0.13057	C	-8.1898	4.898501	1.340802
C	7.456958	-1.16959	-0.5716	C	-7.54252	5.272209	0.148264
C	8.616607	-0.71227	-1.28138	C	-7.78963	4.480834	-0.98729
C	8.497737	-0.00062	2.691351	C	-8.51553	3.299043	-0.90088
C	9.210564	-1.15454	2.24457	C	-8.51107	-3.30164	-0.90093
C	10.36152	-0.71084	1.526754	C	-7.78453	-4.48299	-0.98728
C	10.35992	0.716866	1.528669	C	-7.53859	-5.2751	0.148047
C	9.207956	1.156055	2.247606	C	-8.1873	-4.90252	1.340099
C	6.075419	2.818213	0.692273	C	-8.91168	-3.71648	1.428003
C	5.291855	3.961959	0.730239	H	9.377851	1.347744	-1.72218
C	5.29566	4.890771	-0.32746	H	5.811969	0.001024	0.385102
C	6.205454	4.660968	-1.37493	H	9.378884	-1.34207	-1.72256
C	6.981924	3.50278	-1.42177	H	7.576327	-0.00234	3.259362
C	6.891125	2.528398	-0.41495	H	8.916244	-2.18451	2.399458
C	-1.86155	7.396556	-1.49315	H	11.09757	-1.34618	1.051494
C	-0.47629	7.330831	-1.57575	H	11.09456	1.355223	1.055302
C	0.343725	7.769291	-0.52041	H	8.911242	2.1849	2.405385
C	-0.29668	8.400169	0.563247	H	6.013131	2.104433	1.508743
C	-1.68545	8.452943	0.653655	H	4.605852	4.095972	1.560553
C	-2.50168	7.892667	-0.34466	H	6.279514	5.375522	-2.19029
C	-4.37699	7.085149	1.090761	H	7.617412	3.322512	-2.28493
C	-5.60459	6.442091	1.211261	H	-2.45719	6.949484	-2.28372
C	-6.45903	6.286283	0.105522	H	-0.03246	6.829112	-2.42964
C	-6.09363	6.944218	-1.08392	H	0.297306	8.821801	1.36937
C	-4.8615	7.578827	-1.20784	H	-2.14361	8.904536	1.52993
C	-3.94175	7.595906	-0.1439	H	-3.69533	7.082362	1.936635
C	3.618357	6.41091	0.788415	H	-5.84695	5.950682	2.148845
C	2.412275	7.100268	0.736415	H	-6.762	6.917123	-1.94025
C	1.774464	7.372574	-0.48756	H	-4.58874	8.029408	-2.15863
C	2.485383	7.047175	-1.65729	H	4.051095	6.187251	1.75919

C	3.680079	6.336335	-1.60517	H	1.91751	7.352483	1.669465
C	4.240506	5.933847	-0.37946	H	2.069313	7.297394	-2.62887
C	4.244446	-5.9319	-0.38024	H	4.136892	6.014656	-2.53658
C	3.623241	-6.41002	0.787688	H	4.056405	-6.18672	1.758358
C	2.417499	-7.10002	0.73598	H	1.92356	-7.35304	1.669236
C	1.779028	-7.37191	-0.48776	H	2.072794	-7.29526	-2.62921
C	2.489162	-7.04541	-1.65768	H	4.139562	-6.01148	-2.53734
C	3.683492	-6.33396	-1.60584	H	-4.58382	-8.03182	-2.15806
C	-3.9371	-7.5977	-0.14337	H	-6.75735	-6.91998	-1.94018
C	-4.85675	-7.5811	-1.20739	H	-5.84332	-5.95293	2.148965
C	-6.08912	-6.94685	-1.08373	H	-3.69115	-7.08377	1.937167
C	-6.45486	-6.28895	0.105579	H	-2.45296	-6.95379	-2.28448
C	-5.60053	-6.44433	1.211475	H	-0.02854	-6.83255	-2.43085
C	-4.37271	-7.08698	1.09122	H	0.302563	-8.81938	1.371159
C	-2.49696	-7.89406	-0.34398	H	-2.13811	-8.90317	1.531963
C	-1.85712	-7.39945	-1.49327	H	7.618652	-3.31767	-2.28645
C	-0.4719	-7.33316	-1.57608	H	6.281992	-5.37152	-2.19203
C	0.3485	-7.76948	-0.52015	H	4.610061	-4.09496	1.560606
C	-0.29159	-8.39913	0.564455	H	6.016156	-2.10255	1.508913
C	-1.6803	-8.45248	0.655039	H	-8.59414	1.217652	2.438349
C	6.893078	-2.52498	-0.41558	H	-8.59311	-1.2215	2.438177
C	6.983816	-3.49877	-1.42298	H	-10.3761	-1.22803	-1.47347
C	6.208065	-4.65744	-1.37624	H	-10.3772	1.223138	-1.47328
C	5.299068	-4.88831	-0.32831	H	-9.35873	3.432957	2.38018
C	5.295433	-3.96009	0.729903	H	-8.08852	5.521486	2.225496
C	6.078324	-2.81587	0.692034	H	-7.30739	4.728343	-1.92801
C	-9.42868	1.422046	0.458537	H	-8.57973	2.659211	-1.77594
C	-9.02819	0.693393	1.591959	H	-8.57461	-2.66112	-1.77554
C	-9.02756	-0.69744	1.59186	H	-7.30097	-4.72976	-1.92753
C	-9.42745	-1.42627	0.458361	H	-8.08656	-5.52602	2.224501
C	-9.98378	-0.69813	-0.60945	H	-9.35819	-3.43811	2.379085
C	-9.98438	0.693512	-0.60936	Fe	8.64824	0.002139	0.643844
C	-9.02613	-2.84919	0.326285				

Fe-[11]CPP (B3LYP-D3/6-31G(d) for C, H, SDD for Fe)

C	-7.38748	-1.1689	-0.66322	C	8.122974	-4.89481	1.326303
C	-8.59621	-0.71477	-1.28666	C	7.472775	-5.2716	0.137492
C	-8.59621	0.714803	-1.28666	C	7.702066	-4.47993	-1.00061
C	-7.38748	1.168925	-0.66321	C	8.421675	-3.29469	-0.92028
C	-6.6579	0.000011	-0.28054	C	8.94351	-2.84208	0.303073
C	-8.91713	-1.15617	2.305325	C	9.339827	1.42096	0.430833
C	-8.17204	-9.2E-05	2.691935	C	8.943119	0.695054	1.566329
C	-8.917	1.156102	2.30542	C	8.943117	-0.69507	1.56633
C	-10.1235	0.714219	1.683421	C	9.339823	-1.42098	0.430834
C	-10.1235	-0.71411	1.683362	C	9.886157	-0.69542	-0.64267
C	-6.97796	3.532685	-1.44079	C	9.886159	0.695396	-0.64267
C	-6.21963	4.701243	-1.36554	Fe	-8.48131	0.000008	0.65191

C	-5.29	4.901174	-0.33103	H	-7.63253	3.372289	-2.29314
C	-5.24024	3.931775	0.687781	H	-6.32135	5.448362	-2.14747
C	-6.00406	-2.77744	0.621674	H	-4.5331	4.047195	1.502476
C	-5.24025	-3.93176	0.687775	H	-5.91395	-2.02792	1.401955
C	-5.29001	-4.90116	-0.33104	H	-4.53312	-4.04719	1.502472
C	-6.21964	-4.70122	-1.36555	H	-6.32136	-5.44834	-2.14749
C	-6.97796	-3.53266	-1.4408	H	-7.63253	-3.37226	-2.29316
C	-6.00405	2.777455	0.621681	H	-5.91393	2.027936	1.401959
C	-6.84363	2.523642	-0.47609	H	4.534786	8.056698	-2.14646
C	-6.84364	-2.52362	-0.4761	H	6.703891	6.923616	-1.94005
C	4.810497	7.600063	-1.19998	H	5.793058	5.941532	2.143363
C	6.0372	6.955413	-1.08318	H	3.644732	7.092585	1.942766
C	6.399112	6.291432	0.102858	H	2.117997	8.909341	1.563012
C	5.550208	6.443864	1.212249	H	-0.32872	8.83405	1.409323
C	4.327836	7.096467	1.098687	H	-0.01647	6.891941	-2.41412
C	3.896955	7.61859	-0.13186	H	2.414409	7.003738	-2.27394
C	2.461731	7.92508	-0.32662	H	8.474748	2.65089	-1.79263
C	1.652879	8.473688	0.682959	H	7.209764	4.731906	-1.93439
C	0.264548	8.425397	0.596641	H	8.027663	5.518712	2.210396
C	-0.3778	7.811627	-0.49447	H	9.290323	3.418903	2.354691
C	0.434733	7.383578	-1.55877	H	-4.17604	6.089583	-2.51871
C	1.819754	7.444328	-1.47965	H	-2.11289	7.392268	-2.59838
C	8.421683	3.294666	-0.92029	H	-1.9173	7.334399	1.695557
C	7.702077	4.479912	-1.00062	H	-4.04677	6.148795	1.776244
C	7.47279	5.271583	0.137486	H	2.414393	-7.00374	-2.27394
C	8.12299	4.894789	1.326298	H	-0.01648	-6.89194	-2.41412
C	8.840377	3.705066	1.408129	H	-0.32875	-8.83404	1.409321
C	8.943518	2.842056	0.30307	H	2.117969	-8.90934	1.563015
C	-3.7106	6.394556	-1.58642	H	3.644708	-7.09259	1.942769
C	-2.52188	7.114658	-1.63172	H	5.793038	-5.94154	2.143367
C	-1.80434	7.412891	-0.45982	H	6.703875	-6.92364	-1.94005
C	-2.42447	7.104953	0.763833	H	4.534766	-8.05671	-2.14646
C	-3.62445	6.406155	0.809706	H	-4.04679	-6.14879	1.776234
C	-4.2527	5.957904	-0.36522	H	-1.91733	-7.33439	1.695552
C	1.819735	-7.44433	-1.47965	H	-2.11291	-7.39226	-2.59838
C	0.434714	-7.38358	-1.55878	H	-4.17605	-6.08957	-2.51871
C	-0.37782	-7.81162	-0.49447	H	9.290311	-3.41892	2.354696
C	0.264523	-8.42539	0.59664	H	8.027644	-5.51873	2.210402
C	1.652853	-8.47369	0.68296	H	7.209755	-4.73193	-1.93439
C	2.461709	-7.92508	-0.32662	H	8.474744	-2.65091	-1.79263
C	3.896933	-7.6186	-0.13186	H	8.512188	1.222345	2.411835
C	4.327814	-7.09647	1.098691	H	8.512185	-1.22236	2.411836
C	5.550188	-6.44387	1.212253	H	10.26981	-1.22804	-1.50826
C	6.399094	-6.29145	0.102863	H	10.26982	1.228009	-1.50826
C	6.037181	-6.95543	-1.08317	H	-5.68041	0.00001	0.179953
C	4.810478	-7.60007	-1.19998	H	-9.39775	1.347546	-1.64463
C	-3.62447	-6.40614	0.809698	H	-9.39775	-1.34751	-1.64463
C	-2.42449	-7.10495	0.763826	H	-8.59775	2.184062	2.414737
C	-1.80436	-7.41288	-0.45983	H	-7.19728	-0.00017	3.16181

C	-2.5219	-7.11465	-1.63173	H	-8.59799	-2.18418	2.414555
C	-3.71062	-6.39454	-1.58643	H	-10.8834	-1.35056	1.249921
C	-4.25272	-5.95789	-0.36523	H	-10.8833	1.350796	1.250032
C	8.840365	-3.70509	1.408134				

Fe-[12]CPP

C	9.402897	0.642988	-1.14545	C	1.292493	-8.18044	-0.68841
C	7.499773	-0.06776	-0.07394	C	0.725514	-8.92299	0.364518
C	8.191725	-1.23963	-0.51814	C	-0.6491	-9.12811	0.447743
C	9.381529	-0.78547	-1.17817	C	-1.52196	-8.61487	-0.52751
C	9.862082	-1.31541	2.349973	C	-0.94236	-7.99447	-1.64714
C	9.143447	-0.16766	2.803405	C	0.428341	-7.77736	-1.72224
C	9.875416	0.99439	2.412158	C	-5.67346	-7.60987	-0.00401
C	11.0466	0.564676	1.718889	C	-4.78898	-7.67126	1.08758
C	11.0384	-0.86259	1.680567	C	-3.48028	-8.11546	0.934957
C	-5.48289	7.714068	-0.18721	C	-2.98735	-8.50962	-0.32034
C	-4.68578	7.807211	0.966563	C	-3.90781	-8.57876	-1.38102
C	-3.36315	8.235145	0.895625	C	-5.22163	-8.14666	-1.22413
C	-2.77792	8.58909	-0.3322	H	10.1888	1.270721	-1.54617
C	-3.62176	8.643582	-1.45642	H	6.533497	-0.06535	0.411257
C	-4.94341	8.216367	-1.3855	H	10.14856	-1.4177	-1.60739
C	-6.97004	6.017095	-1.23161	H	9.555726	-2.34662	2.469249
C	-7.92241	5.012078	-1.13016	H	8.204418	-0.17654	3.34169
C	-8.69018	4.842045	0.036094	H	9.580808	2.021189	2.586429
C	-8.5379	5.811313	1.045522	H	11.80027	1.209046	1.285235
C	-7.57487	6.813562	0.948743	H	11.7848	-1.49138	1.21279
C	-6.72523	6.902819	-0.16827	H	-5.06752	7.430007	1.911135
C	3.368491	-7.25271	-1.7989	H	-2.74395	8.182475	1.786711
C	4.5156	-6.46871	-1.72386	H	-3.22401	8.984604	-2.40855
C	5.047512	-6.06601	-0.48583	H	-5.55509	8.230831	-2.28364
C	4.447878	-6.60081	0.668361	H	-6.32871	6.044828	-2.10743
C	3.290525	-7.36708	0.593785	H	-7.99164	4.282936	-1.93083
C	2.681584	-7.65843	-0.64033	H	-9.15648	5.762435	1.937547
C	6.995608	-4.72396	-1.41857	H	-7.45998	7.518691	1.768017
C	7.754099	-3.55316	-1.42497	H	2.97136	-7.50644	-2.77759
C	7.615768	-2.59421	-0.40876	H	4.956954	-6.09692	-2.64414
C	6.759691	-2.90501	0.661602	H	4.86167	-6.3697	1.645715
C	5.995662	-4.06274	0.660317	H	2.808521	-7.6739	1.517145
C	2.892708	7.651416	-0.42859	H	7.11025	-5.42953	-2.23712
C	3.618497	7.29449	-1.57947	H	8.41845	-3.35353	-2.26169
C	4.748484	6.48712	-1.50143	H	6.65611	-2.20087	1.482238
C	4.590165	6.499016	0.890259	H	5.283155	-4.21987	1.464047
C	3.448934	7.289532	0.811445	H	3.263273	7.60509	-2.55787
C	-1.30132	8.665413	-0.45721	H	5.218459	6.154458	-2.42242
C	-0.46398	9.136534	0.569419	H	4.961582	6.210988	1.869524
C	0.910147	8.909678	0.541269	H	2.935693	7.558909	1.729863
C	1.512308	8.191288	-0.50867	H	-0.89723	9.663034	1.415983

C	0.687402	7.826616	-1.58756	H	1.519602	9.270526	1.365341
C	-0.68131	8.060987	-1.5644	H	1.103116	7.25752	-2.41306
C	6.059126	-4.98321	-0.40251	H	-1.29413	7.671536	-2.3719
C	6.207709	4.901015	-0.2055	H	7.319652	5.405972	-1.98863
C	7.16296	4.664532	-1.20978	H	8.56338	3.294519	-2.08907
C	7.885274	3.472313	-1.2585	H	6.676333	2.012683	1.55113
C	7.691973	2.467587	-0.29694	H	5.36502	4.070125	1.60258
C	6.821394	2.752517	0.769097	H	-9.27553	3.571978	2.387935
C	6.092286	3.931984	0.808651	H	-9.973	1.260583	2.678467
C	5.224068	6.010853	-0.26653	H	-10.4266	0.868018	-1.58134
C	8.226461	1.102218	-0.46479	H	-9.86496	3.216029	-1.85714
C	-9.44187	3.577021	0.232653	H	-11.3147	-1.07345	-1.10713
C	-9.56433	3.001249	1.510276	H	-10.7247	-3.44641	-1.19515
C	-9.93787	1.671462	1.673793	H	-8.47943	-3.02155	2.443351
C	-10.1824	0.837578	0.56716	H	-9.02394	-0.65293	2.511496
C	-10.2152	1.45844	-0.69509	H	-8.95177	-5.3937	2.452767
C	-9.86798	2.794761	-0.85612	H	-7.31746	-7.20019	2.189543
C	-10.1733	-0.64335	0.680609	H	-6.88731	-6.19139	-1.96941
C	-10.6842	-1.48654	-0.32478	H	-8.54205	-4.41855	-1.71187
C	-10.3544	-2.8386	-0.37346	H	1.363936	-9.31752	1.150122
C	-9.514	-3.41797	0.593261	H	-1.05531	-9.66866	1.298865
C	-9.132	-2.61106	1.678191	H	-1.58512	-7.57832	-2.41761
C	-9.44701	-1.25847	1.716587	H	0.816717	-7.19233	-2.55
C	-8.84104	-4.72642	0.401712	H	-5.09149	-7.26271	2.046922
C	-8.50597	-5.56835	1.476912	H	-2.7982	-8.04704	1.777697
C	-7.57363	-6.59082	1.327245	H	-3.57981	-8.94212	-2.35152
C	-6.91988	-6.80947	0.100024	H	-5.89511	-8.18918	-2.07569
C	-7.36504	-6.0599	-1.00334	Fe	9.359396	-0.11394	0.762163
C	-8.30687	-5.04722	-0.85769				

Fe-[8]CPP⁺

C	-1.35951	5.98347	0.070336	C	-6.81659	2.961945	0.994586
C	4.371091	-2.6038	0.370589	C	-6.82175	2.784145	-1.39034
C	2.66056	4.565548	0.322165	C	-5.0195	5.350341	0.798566
C	2.791338	-3.89044	-0.95692	C	-7.01599	-1.22933	1.214926
C	4.536195	-0.09065	-0.02191	C	-7.3427	1.499085	-1.29266
C	3.03097	3.835767	-0.82774	C	-7.74307	-1.45355	-1.05654
C	4.508121	2.411847	0.475615	C	-7.3683	1.689424	1.090919
C	5.050595	1.059905	0.666647	C	-7.26076	-2.75947	-1.08217
C	-0.46457	6.228259	-0.99129	Fe	6.648954	-0.06434	-0.18627
C	4.956717	-1.29059	0.63241	H	2.233708	-4.00142	-1.88099
C	1.40574	5.351928	0.302575	H	3.799499	-0.04798	-0.81164
C	0.884848	5.912356	-0.88081	H	2.522826	4.026143	-1.76732
C	3.924899	2.779097	-0.75236	H	-0.84302	6.609418	-1.93546
C	-2.81754	5.814733	-0.14133	H	1.532188	6.058768	-1.74148
C	-3.95512	-5.8497	0.992617	H	4.113746	2.183591	-1.64226
C	4.180663	-3.51957	1.425587	H	-3.64835	-6.38817	1.88525

C	3.714446	-2.86413	-0.85037	H	4.694943	-3.37202	2.371353
C	7.276384	0.030051	-2.22403	H	3.878389	-2.21188	-1.7041
C	-0.79841	5.614498	1.306902	H	6.596452	0.036844	-3.06619
C	5.89965	-0.882	1.633039	H	-1.44978	5.433773	2.1563
C	1.176445	-5.43361	0.148714	H	6.467433	-1.54492	2.273836
C	-1.61783	-5.97037	0.016721	H	3.184641	4.897401	2.394652
C	3.383026	4.308194	1.504581	H	-2.5573	5.079261	-2.15604
C	-3.08048	-5.76127	-0.10889	H	7.708066	-2.14999	-1.95206
C	-3.25084	5.199571	-1.32928	H	7.454365	2.205487	-1.69501
C	7.878058	-1.12504	-1.64711	H	6.539018	1.138716	2.355484
C	7.727384	1.17695	-1.4985	H	-4.71551	4.00177	-2.29741
C	5.945662	0.547274	1.669678	H	4.73974	3.014923	2.542411
C	-4.49162	4.581503	-1.40883	H	9.246442	-1.35254	0.103694
C	-5.37068	4.55076	-0.30924	H	1.181027	-6.01734	-1.93815
C	2.453479	-4.68914	0.158109	H	-1.58532	-5.5365	2.13326
C	4.28325	3.249169	1.584367	H	0.794922	-5.08251	2.249715
C	8.68376	-0.70467	-0.55627	H	0.911257	4.888992	2.357398
C	0.580719	-5.90449	-1.03918	H	3.069155	-5.18802	2.172007
C	-0.98468	-5.68829	1.242478	H	-1.21138	-6.49951	-2.04345
C	0.378162	-5.42796	1.308475	H	-3.51069	6.50218	1.790379
C	0.551806	5.303734	1.420437	H	-5.80095	-5.22686	1.882568
C	3.242679	-4.54031	1.318253	H	-2.95609	-5.0858	-2.1597
C	-0.78034	-6.17934	-1.09947	H	9.098681	1.33745	0.271213
C	-3.76936	5.956818	0.886412	H	-5.0984	-3.93902	-2.15945
C	-5.18106	-5.19235	0.990889	H	-6.03497	-2.91758	2.073792
C	-3.58572	-5.16398	-1.2787	H	-6.59038	3.492903	1.913898
C	-5.58658	-4.41212	-0.11045	H	-6.64163	3.193698	-2.37956
C	8.595582	0.718076	-0.4599	H	-5.70302	5.445758	1.637031
C	-6.41753	3.497831	-0.24529	H	-6.84884	-0.64349	2.111984
C	-6.55793	-3.29702	0.012999	H	-7.50462	0.941634	-2.20966
C	-4.81117	-4.50757	-1.28023	H	-8.22882	-1.06288	-1.94584
C	-6.54771	-2.53664	1.195771	H	-7.59169	1.298686	2.07873
C	-7.51772	0.869286	-0.04467	H	-7.3765	-3.34645	-1.98965
C	-7.52754	-0.61414	0.056365				

Fc-[11]CPP+

C	0.218682	8.390047	0.660342	C	-6.86867	2.449423	-0.36611
C	0.385571	7.379765	-1.51082	C	-6.96206	3.41792	-1.38082
C	0.446868	-8.40247	0.683845	C	-7.29366	-1.2685	-0.57973
C	0.57683	-7.42194	-1.50469	C	-7.37933	1.084318	-0.55738
C	1.606893	8.456811	0.735388	C	-8.36949	-0.83694	-1.41998
C	1.770444	7.455258	-1.44007	C	-8.41136	0.591744	-1.42394
C	1.835895	-8.43787	0.749818	C	-9.06393	-0.36516	2.522042
C	1.96332	-7.46379	-1.44133	C	-9.39845	0.986711	2.192553
C	2.417884	7.926459	-0.28466	C	-9.95496	-1.22162	1.805143
C	2.628575	-7.90115	-0.28217	C	-10.4886	0.95741	1.279657
C	3.862543	7.643086	-0.10545	C	-10.8264	-0.40215	1.036855

C	4.065311	-7.57956	-0.11083	Fe	-8.77959	-0.06842	0.494623
C	4.318075	7.128461	1.120344	H	0.113455	-6.96478	-2.37315
C	4.513632	-7.05766	1.114941	H	2.070217	8.895201	1.6151
C	4.766977	7.641178	-1.18274	H	2.314516	-8.85493	1.631554
C	4.964084	-7.54912	-1.19283	H	2.361789	7.036749	-2.24881
C	5.55291	6.496329	1.219928	H	2.5395	-7.04338	-2.25985
C	5.7315	-6.39367	1.210984	H	3.649653	7.115303	1.976624
C	6.006775	7.019048	-1.07879	H	3.849992	-7.06493	1.9749
C	6.187409	-6.89516	-1.09227	H	4.479574	8.09824	-2.12604
C	6.393348	6.355662	0.101355	H	4.68519	-8.0108	-2.1364
C	6.562437	-6.22611	0.088797	H	5.814322	6.003741	2.151563
C	7.488759	5.354409	0.123603	H	5.984374	-5.89823	2.143367
C	7.631708	-5.1976	0.110863	H	6.665474	7.006993	-1.94261
C	7.728144	4.572443	-1.02009	H	6.841485	-6.86299	-1.95901
C	7.849196	-4.40704	-1.03142	H	7.232134	4.820768	-1.95342
C	8.156501	4.982515	1.305393	H	7.359183	-4.66614	-1.965
C	8.290871	-4.81103	1.292924	H	8.063013	5.600925	2.194068
C	8.468273	3.398581	-0.95022	H	8.215398	-5.43399	2.180116
C	8.557626	-3.21394	-0.95928	H	8.529492	2.765347	-1.83016
C	8.895662	3.804956	1.376218	H	8.601098	-2.5771	-1.83763
C	8.998581	-3.61465	1.365762	H	8.640794	1.30858	2.386793
C	9.003994	2.94491	0.267756	H	8.674613	-1.12987	2.383221
C	9.06003	0.791531	1.528676	H	9.360824	3.528042	2.318531
C	9.07932	-0.5989	1.526606	H	9.457659	-3.32783	2.308046
C	9.081897	-2.74882	0.259468	H	-0.06109	6.898678	-2.37505
C	9.424324	1.526793	0.387238	H	-0.12701	-8.80277	1.514923
C	9.463649	-1.32031	0.382872	H	-0.36939	8.788663	1.482297
C	9.966066	0.807754	-0.69449	H	-1.7487	-7.34922	1.79028
C	9.984896	-0.58344	-0.69684	H	-1.98145	7.324495	1.762396
C	-0.21817	-7.82505	-0.41568	H	-1.99149	-7.44875	-2.50475
C	-0.42594	7.782881	-0.43463	H	10.33465	1.343706	-1.56499
C	-1.6463	-7.43461	-0.36877	H	10.36778	-1.10632	-1.56915
C	-1.84898	7.367275	-0.3958	H	-2.16391	7.328613	-2.53575
C	-2.262	-7.1257	0.86074	H	-3.87653	-6.1824	1.886911
C	-2.38715	-7.16154	-1.53567	H	-4.06483	-6.18199	-2.41833
C	-2.47713	7.073661	0.830126	H	-4.09378	6.129857	1.853668
C	-2.56769	7.055556	-1.5659	H	-4.21165	6.02341	-2.45127
C	-3.46404	-6.43517	0.914542	H	-4.46941	-4.13336	1.645575
C	-3.58519	-6.4596	-1.4844	H	-4.67932	4.076589	1.663705
C	-3.67103	6.366601	0.881576	H	-5.83603	-2.13262	1.543127
C	-3.7531	6.331479	-1.51631	H	-5.91265	-0.05495	0.682004
C	-4.11675	-6.01117	-0.25962	H	-6.01261	2.050675	1.584163
C	-4.29762	5.903916	-0.29095	H	-6.168	-5.50264	-2.06766
C	-5.15454	-4.01384	0.813799	H	-6.28902	5.301419	-2.13597
C	-5.16213	-4.96865	-0.22672	H	-7.50237	-3.46216	-2.20859
C	-5.32972	4.843593	-0.25144	H	-7.56921	3.225025	-2.26129
C	-5.33731	3.921377	0.815892	H	-8.29117	-0.68137	3.210221
C	-5.92023	-2.86474	0.745069	H	-8.90521	1.876766	2.561054
C	-6.08516	2.757179	0.761337	H	-9.03635	-1.48449	-1.97515

C	-6.08551	-4.76627	-1.27447	H	-9.10533	1.195019	-1.99541
C	-6.21595	4.591695	-1.3179	H	-9.95521	-2.30385	1.826926
C	-6.75006	-2.608	-0.36495	H	-10.954	1.819062	0.818346
C	-6.76143	-0.08014	0.014221	H	-11.5956	-0.7525	0.360357
C	-6.85972	-3.61374	-1.34561				

m[6]CPP

C	-0.05182	-4.19649	1.420428	C	-0.05463	-0.8213	3.895904
C	1.152168	-4.11561	0.694961	C	-1.27168	-1.35341	3.43222
C	1.152168	-4.11561	-0.69496	C	-1.32437	-2.60556	2.830636
C	-0.05182	-4.19649	-1.42043	C	-0.16226	-3.38294	2.663569
C	-1.18067	-4.63608	-0.69622	C	0.962992	-2.98639	3.416784
C	-1.18067	-4.63608	0.696223	C	1.016654	-1.73047	4.016356
C	-0.16226	-3.38294	-2.66357	H	2.07006	-3.8381	1.20357
C	0.962992	-2.98639	-3.41678	H	2.07006	-3.8381	-1.20357
C	1.016654	-1.73047	-4.01636	H	-2.10986	-4.85129	-1.21782
C	-0.05463	-0.8213	-3.8959	H	-2.10986	-4.85129	1.217819
C	-1.27168	-1.35341	-3.43222	H	1.85314	-3.6102	-3.43127
C	-1.32437	-2.60556	-2.83064	H	1.945617	-1.41255	-4.48308
C	0.143358	0.65232	-3.80451	H	-2.14567	-0.71348	-3.35963
C	-0.91936	1.573665	-3.87537	H	-2.23638	-2.88374	-2.31208
C	-0.86717	2.787064	-3.18741	H	-1.84424	1.293704	-4.37308
C	0.25454	3.128873	-2.41281	H	-1.75729	3.409976	-3.14451
C	1.39893	2.326621	-2.55515	H	2.306458	2.595198	-2.02071
C	1.346149	1.116832	-3.23771	H	2.207291	0.457272	-3.19216
C	-0.39263	5.336261	-1.22089	H	-0.62444	5.842532	-2.15448
C	-0.62935	5.977421	0	H	-1.02664	6.989314	0
C	-0.39263	5.336261	1.220887	H	-0.62444	5.842532	2.154476
C	0.134392	4.037127	1.234333	H	0.756897	2.403375	0
C	0.416886	3.432983	0	H	2.306458	2.595198	2.020713
C	0.134392	4.037127	-1.23433	H	2.207291	0.457272	3.192155
C	0.25454	3.128873	2.412811	H	-1.84424	1.293704	4.373081
C	1.39893	2.326621	2.555151	H	-1.75729	3.409976	3.14451
C	1.346149	1.116832	3.237707	H	-2.14567	-0.71348	3.359632
C	0.143358	0.65232	3.80451	H	-2.23638	-2.88374	2.312078
C	-0.91936	1.573665	3.875368	H	1.85314	-3.6102	3.431273
C	-0.86717	2.787064	3.18741	H	1.945617	-1.41255	4.483078

m[7]CPP

C	5.121097	0.777026	0.06504000	C	0.62564	-4.78219	1.07987
C	5.162271	1.613937	-1.07058500	C	5.15556	-0.70811	-0.03363
C	4.483248	2.829227	-1.09620000	C	5.007873	-1.52796	1.103695
C	3.73881	3.270551	0.01613200	C	4.337997	-2.74399	1.031081
C	3.96039	2.582935	1.22327000	C	3.810538	-3.22154	-0.18602
C	4.634302	1.369002	1.24681000	C	4.277481	-2.56999	-1.34554
C	2.502222	4.087096	-0.10672200	C	4.917516	-1.33842	-1.27136
C	1.723599	3.944007	-1.27020100	H	5.63372	1.267475	-1.98598
C	0.3473	4.1411	-1.24540100	H	4.445981	3.387924	-2.02793
C	-0.31576	4.488942	-0.05531600	H	3.448733	2.902389	2.125807
C	0.493678	4.877143	1.02992600	H	4.618502	0.803267	2.171875
C	1.872573	4.685601	1.00319700	H	2.165998	3.508622	-2.16089
C	-1.74101	4.093733	0.10391500	H	-0.23307	3.857592	-2.1184
C	-2.65226	4.054189	-0.96711400	H	0.030767	5.251215	1.939657
C	-3.77703	3.229201	-0.92581400	H	2.451816	4.91521	1.893836
C	-4.03259	2.412481	0.18834600	H	-2.43463	4.604266	-1.87907
C	-3.23164	2.603228	1.32607900	H	-4.39966	3.134388	-1.81199
C	-2.1136	3.428141	1.28672000	H	-3.43502	2.023566	2.222635
C	-6.20166	1.162641	-0.41993300	H	-1.4487	3.451499	2.14497
C	-6.83499	-0.06758	-0.62193300	H	-6.72188	2.08764	-0.65508
C	-6.17629	-1.27414	-0.36742900	H	-7.8542	-0.08637	-0.99947
C	-4.8666	-1.26385	0.13447300	H	-6.67763	-2.21885	-0.56184
C	-4.26546	-0.01956	0.37565200	H	-3.23001	-0.00086	0.698464
C	-4.89343	1.20007	0.08321100	H	-4.41002	-3.29902	-1.65974
C	-3.98148	-2.45351	0.27926500	H	-2.42774	-4.74345	-1.71356
C	-3.75403	-3.33212	-0.79343300	H	-1.3107	-3.33865	2.194917
C	-2.61891	-4.14235	-0.82831000	H	-3.31713	-1.9407	2.265235
C	-1.66647	-4.10435	0.20684500	H	-0.26236	-4.02265	-2.09682
C	-2.00658	-3.37582	1.36215500	H	2.109438	-3.65745	-2.28754
C	-3.1365	-2.56707	1.39565600	H	2.612052	-4.73185	1.852791
C	-0.24336	-4.48759	0.01199100	H	0.216276	-5.09324	2.037683
C	0.360115	-4.22331	-1.22992600	H	5.294385	-1.15952	2.084076
C	1.728789	-4.00959	-1.33529000	H	4.105505	-3.24986	1.962773
C	2.569927	-4.04623	-0.20574400	H	4.021785	-2.95119	-2.32905
C	1.997996	-4.57441	0.97102400	H	5.092021	-0.80087	-2.19804

m[8]CPP

C	-0.14848	-5.06063	2.76022300	C	1.172083	-5.46741	-0.69543
C	-1.32631	-4.34004	3.02783300	C	1.172083	-5.46741	0.695429
C	-1.33857	-3.28792	3.93394200	C	-0.17653	-2.90203	-4.62787
C	-0.17653	-2.90203	4.62787300	C	-1.33857	-3.28792	-3.93394
C	0.921457	-3.7828	4.54154500	C	-1.32631	-4.34004	-3.02783
C	0.938347	-4.83228	3.62589400	C	-0.14848	-5.06063	-2.76022
C	-0.04994	-1.50003	5.10983900	C	0.938347	-4.83228	-3.62589
C	-1.16871	-0.65412	5.23972000	C	0.921457	-3.7828	-4.54155
C	-1.04727	0.727618	5.13498300	H	-2.20112	-4.49385	2.403633
C	0.20294	1.340965	4.93132900	H	-2.22827	-2.66926	3.978833
C	1.332426	0.512343	5.06934600	H	1.812594	-3.59918	5.135188
C	1.209487	-0.87051	5.14086900	H	1.84206	-5.42829	3.525985
C	0.295118	2.689212	4.31134500	H	-2.16499	-1.07827	5.319846
C	-0.74827	3.633589	4.35047100	H	-1.95438	1.323132	5.092703
C	-0.80975	4.685847	3.43562800	H	2.328606	0.942463	5.023457
C	0.175788	4.845485	2.44743300	H	2.114941	-1.46777	5.09997
C	1.301198	4.008135	2.52386100	H	-1.56419	3.508501	5.057111
C	1.357692	2.956405	3.42717800	H	-1.68272	5.333792	3.431308
C	-0.56524	6.976951	1.21860600	H	2.111607	4.140099	1.812405
C	-0.81706	7.61386	0.00000000	H	2.196039	2.270476	3.367775
C	-0.56524	6.976951	-1.21860600	H	-0.77767	7.489243	2.15346
C	-0.03117	5.679746	-1.23295700	H	-1.21904	8.623824	0
C	0.233462	5.066103	0.00000000	H	-0.77767	7.489243	-2.15346
C	-0.03117	5.679746	1.23295700	H	0.573838	4.036599	0
C	0.175788	4.845485	-2.44743300	H	-1.68272	5.333792	-3.43131
C	-0.80975	4.685847	-3.43562800	H	-1.56419	3.508501	-5.05711
C	-0.74827	3.633589	-4.35047100	H	2.196039	2.270476	-3.36778
C	0.295118	2.689212	-4.31134500	H	2.111607	4.140099	-1.81241
C	1.357692	2.956405	-3.42717800	H	-1.95438	1.323132	-5.0927
C	1.301198	4.008135	-2.52386100	H	-2.16499	-1.07827	-5.31985
C	0.20294	1.340965	-4.93132900	H	2.114941	-1.46777	-5.09997
C	-1.04727	0.727618	-5.13498300	H	2.328606	0.942463	-5.02346
C	-1.16871	-0.65412	-5.23972000	H	-2.02327	-6.46504	1.223184
C	-0.04994	-1.50003	-5.10983900	H	-2.02327	-6.46504	-1.22318
C	1.209487	-0.87051	-5.14086900	H	2.060074	-5.11815	-1.21389
C	1.332426	0.512343	-5.06935	H	2.060074	-5.11815	1.213891
C	-0.01138	-5.69188	1.421778	H	-2.22827	-2.66926	-3.97883
C	-1.11758	-6.17631	0.695923	H	-2.20112	-4.49385	-2.40363
C	-1.11758	-6.17631	-0.69592	H	1.84206	-5.42829	-3.52599
C	-0.01138	-5.69188	-1.42178	H	1.812594	-3.59918	-5.13519

m[9]CPP

C	4.629061	-4.30687	-0.10012	C	4.280408	4.516046	-0.30125
C	4.188601	-5.14498	0.940728	C	3.878376	5.389121	0.728364
C	2.949631	-5.77781	0.87982	C	2.602322	5.949459	0.745519
C	2.082851	-5.58824	-0.21519	C	6.564122	0.943089	0.122375
C	2.6174	-4.917	-1.33036	C	6.457319	1.569506	-1.13492
C	3.860175	-4.29807	-1.27713	C	5.893149	2.832248	-1.27126
C	0.613694	-5.79768	-0.1218	C	5.377106	3.524306	-0.15945
C	-0.02927	-5.75061	1.129694	C	5.711657	3.00739	1.10608
C	-1.39166	-5.49758	1.237383	C	6.305814	1.756986	1.242759
C	-2.1819	-5.25062	0.100002	H	4.791925	-5.24888	1.839134
C	-1.57924	-5.48925	-1.14856	H	2.625464	-6.37057	1.73059
C	-0.22047	-5.77016	-1.25556	H	2.001763	-4.752	-2.20839
C	-3.47839	-4.53164	0.197127	H	4.168877	-3.67406	-2.11066
C	-3.6657	-3.61273	1.246476	H	0.557673	-5.80595	2.041142
C	-4.69606	-2.68371	1.219883	H	-1.82962	-5.41176	2.227606
C	-5.59059	-2.61586	0.138946	H	-2.15474	-5.35086	-2.05931
C	-5.48925	-3.6146	-0.84372	H	0.208176	-5.88448	-2.24681
C	-4.457	-4.55327	-0.81362	H	-2.94101	-3.56167	2.052492
C	-7.78549	-1.44682	-0.47554	H	-4.77698	-1.95771	2.023966
C	-8.48349	-0.25117	-0.66492	H	-6.17763	-3.60949	-1.6851
C	-7.88161	0.985582	-0.41892	H	-4.38345	-5.27852	-1.61961
C	-6.55668	1.042159	0.039875	H	-8.27268	-2.39786	-0.67447
C	-5.87806	-0.16909	0.237466	H	-9.51433	-0.28383	-1.00825
C	-6.4601	-1.41949	-0.016	H	-8.44288	1.903259	-0.57465
C	-5.78101	2.29482	0.240163	H	-4.83161	-0.13495	0.520225
C	-5.77719	3.34134	-0.69693	H	-6.48335	3.322952	-1.52322
C	-4.81345	4.349047	-0.64755	H	-4.81168	5.110904	-1.42245
C	-3.80695	4.35096	0.335862	H	-3.16007	3.347132	2.137715
C	-3.90644	3.381078	1.350745	H	-4.88056	1.621097	2.080002
C	-4.87032	2.383576	1.30626	H	-2.63087	5.33266	-1.92945
C	-2.55591	5.144987	0.223168	H	-0.29937	5.975371	-2.195
C	-2.02184	5.46155	-1.03952	H	0.245369	5.749619	2.065024
C	-0.68293	5.805292	-1.19306	H	-2.1179	5.237897	2.339373
C	0.197325	5.82385	-0.09497	H	6.521943	-3.24235	-1.87059
C	-0.38384	5.704048	1.18095	H	7.3848	-0.96588	-1.75495
C	-1.72873	5.384898	1.335979	H	5.836925	-0.60299	2.246653
C	5.620762	-3.219	0.094754	H	5.017598	-2.87358	2.137475
C	6.377881	-2.67077	-0.9571	H	1.45855	4.70671	-2.19122
C	6.86467	-1.36811	-0.89044	H	3.66545	3.733942	-2.2198
C	6.598491	-0.54172	0.220755	H	4.54753	5.586157	1.561876
C	6.04332	-1.1753	1.348795	H	2.313621	6.568455	1.590988
C	5.571521	-2.48083	1.2898	H	6.702471	1.020158	-2.0382
C	1.664393	5.666581	-0.26643	H	5.758785	3.236689	-2.27036
C	2.137535	4.951402	-1.38105	H	5.388883	3.527273	2.003407
C	3.407267	4.392969	-1.39775	H	6.465221	1.371067	2.244926

m[10]CPP

C	0.393403	-3.58028	5.695284	C	-1.50288	-6.61248	-0.69376
C	-0.56283	-3.02865	6.569129	C	-0.42763	-7.14473	-1.42797
C	-0.55563	-1.67148	6.885941	C	0.546289	-7.8522	-0.69676
C	0.409191	-0.79969	6.348302	C	0.546289	-7.8522	0.696764
C	1.453689	-1.38589	5.612047	C	0.205367	-4.86902	-4.98123
C	1.445284	-2.7367	5.293931	C	1.279021	-5.53171	-4.35787
C	0.248307	0.67572	6.305946	C	1.067483	-6.40725	-3.29831
C	-1.03192	1.244162	6.176768	C	-0.22929	-6.68325	-2.82599
C	-1.20013	2.552388	5.734941	C	-1.29909	-6.21231	-3.6102
C	-0.09734	3.352316	5.38541	C	-1.08784	-5.31689	-4.65338
C	1.179496	2.840017	5.677915	H	-1.3551	-3.65677	6.967946
C	1.347499	1.536873	6.135134	H	-1.34278	-1.27618	7.523612
C	-0.24901	4.561942	4.537152	H	2.219482	-0.7549	5.172134
C	-1.26764	4.589273	3.567208	H	2.203854	-3.11053	4.614109
C	-1.28125	5.544907	2.560232	H	-1.91137	0.624263	6.325692
C	-0.27449	6.520024	2.465906	H	-2.20745	2.933639	5.592722
C	0.675732	6.568817	3.499406	H	2.060657	3.433648	5.451794
C	0.687539	5.610856	4.513305	H	2.354732	1.160714	6.291108
C	0.208253	8.694735	1.21632	H	-2.01338	3.800641	3.550617
C	0.378429	9.360006	0	H	-2.05923	5.507759	1.802876
C	0.208253	8.694735	-1.21632	H	1.459816	7.321144	3.470119
C	-0.15244	7.338625	-1.23111	H	1.465457	5.654595	5.270981
C	-0.33135	6.691238	0	H	0.344309	9.230309	2.152228
C	-0.15244	7.338625	1.231108	H	0.644725	10.41386	0
C	-0.27449	6.520024	-2.46591	H	0.344309	9.230309	-2.15223
C	0.675732	6.568817	-3.49941	H	-0.5397	5.626639	0
C	0.687539	5.610856	-4.51331	H	1.459816	7.321144	-3.47012
C	-0.24901	4.561942	-4.53715	H	1.465457	5.654595	-5.27098
C	-1.26764	4.589273	-3.56721	H	-2.01338	3.800641	-3.55062
C	-1.28125	5.544907	-2.56023	H	-2.05923	5.507759	-1.80288
C	-0.09734	3.352316	-5.38541	H	2.060657	3.433648	-5.45179
C	1.179496	2.840017	-5.67792	H	2.354732	1.160714	-6.29111
C	1.347499	1.536873	-6.13513	H	-1.91137	0.624263	-6.32569
C	0.248307	0.67572	-6.30595	H	-2.20745	2.933639	-5.59272
C	-1.03192	1.244162	-6.17677	H	2.29969	-5.28824	4.638911
C	-1.20013	2.552388	-5.73494	H	1.929338	-6.78424	2.755559
C	0.205367	-4.86902	4.981232	H	-2.3197	-6.47002	3.341816
C	1.279021	-5.53171	4.357869	H	-1.951	-4.87084	5.138844
C	1.067483	-6.40725	3.298311	H	2.219482	-0.7549	-5.17213
C	-0.22929	-6.68325	2.825993	H	2.203854	-3.11053	-4.61411
C	-1.29909	-6.21231	3.610201	H	-1.3551	-3.65677	-6.96795
C	-1.08784	-5.31689	4.653376	H	-1.34278	-1.27618	-7.52361
C	0.409191	-0.79969	-6.3483	H	-2.28389	-6.06113	1.206893
C	1.453689	-1.38589	-5.61205	H	-2.28389	-6.06113	-1.20689
C	1.445284	-2.7367	-5.29393	H	1.354024	-8.35664	-1.22063
C	0.393403	-3.58028	-5.69528	H	1.354024	-8.35664	1.220629

C	-0.56283	-3.02865	-6.56913	H	2.29969	-5.28824	-4.63891
C	-0.5563	-1.67148	-6.88594	H	1.929338	-6.78424	-2.75556
C	-0.42763	-7.14473	1.427969	H	-2.3197	-6.47002	-3.34182
C	-1.50288	-6.61248	0.693764	H	-1.951	-4.87084	-5.13884

m[11]CPP

C	2.35275	6.772621	-0.33977	C	5.008406	-6.02968	-1.24594
C	1.58332	6.204667	-1.37132	C	6.115745	-5.18835	-1.18566
C	0.197247	6.271843	-1.36401	C	6.424273	-4.47162	-0.01388
C	-0.50006	6.907903	-0.32228	C	5.68092	-4.78408	1.138422
C	0.269776	7.587787	0.639405	C	4.580806	-5.63239	1.081329
C	1.662019	7.523842	0.62947	C	8.091918	-0.52888	0.122371
C	-1.95473	6.652395	-0.17575	C	8.250819	-1.39523	1.2196
C	-2.7757	6.399461	-1.28933	C	7.856236	-2.72814	1.146798
C	-4.02283	5.800307	-1.14568	C	7.274284	-3.25354	-0.02272
C	-4.51625	5.436886	0.120027	C	7.29334	-2.43508	-1.1661
C	-3.76663	5.841116	1.239091	C	7.696038	-1.10615	-1.09652
C	-2.51392	6.428935	1.095056	H	2.067761	5.602051	-2.13269
C	-5.65209	4.488611	0.24273	H	-0.35459	5.722717	-2.12051
C	-6.69879	4.416692	-0.69353	H	-0.22698	8.147432	1.427746
C	-7.58952	3.343635	-0.70193	H	2.217398	8.036303	1.410594
C	-7.47224	2.295854	0.226307	H	-2.40724	6.615931	-2.2882
C	-6.49597	2.425961	1.227994	H	-4.58091	5.528377	-2.0371
C	-5.60723	3.49274	1.234904	H	-4.14102	5.637327	2.238415
C	-9.58868	0.957701	-0.25883	H	-1.92277	6.631513	1.983673
C	-10.206	-0.28321	-0.42995	H	-6.7955	5.189214	-1.45181
C	-9.49176	-1.47188	-0.26543	H	-8.34376	3.284908	-1.48247
C	-8.13352	-1.43402	0.086364	H	-6.40726	1.655411	1.988618
C	-7.53334	-0.17875	0.26177	H	-4.81577	3.511826	1.977779
C	-8.23189	1.025497	0.093521	H	-10.1624	1.872026	-0.38542
C	-7.27824	-2.64226	0.215842	H	-11.2607	-0.32465	-0.68933
C	-7.32912	-3.70545	-0.70101	H	-9.99151	-2.42805	-0.39637
C	-6.36983	-4.71782	-0.68575	H	-6.46832	-0.13611	0.463784
C	-5.3164	-4.71121	0.2457	H	-8.09105	-3.70738	-1.47624
C	-5.32782	-3.69755	1.220901	H	-6.42242	-5.50585	-1.43229
C	-6.28546	-2.69277	1.208446	H	-4.53219	-3.65373	1.958026
C	-4.13425	-5.60358	0.145376	H	-6.24302	-1.90971	1.960115
C	-3.62911	-5.99993	-1.10577	H	-4.19986	-5.78973	-2.00588
C	-2.36101	-6.55983	-1.22973	H	-1.99307	-6.80891	-2.22104
C	-1.52607	-6.7349	-0.11122	H	-1.49132	-6.60873	2.045879
C	-2.08978	-6.4709	1.150369	H	-3.74194	-5.70004	2.267991
C	-3.36347	-5.92835	1.275714	H	3.823	6.50025	1.953001
C	3.774645	6.368279	-0.20389	H	5.86989	5.212091	2.225095
C	4.345326	6.157266	1.064485	H	6.139165	4.752158	-2.04377
C	5.501919	5.399695	1.220534	H	4.170463	6.151814	-2.31845
C	6.132067	4.791943	0.118572	H	0.060915	-6.0199	-2.18353

C	5.666968	5.163347	-1.15684	H	2.486032	-5.81936	-2.19473
C	4.526065	5.941462	-1.3139	H	2.674151	-7.74038	1.645055
C	-0.06451	-6.96182	-0.24328	H	0.236559	-7.97031	1.646471
C	0.621455	-6.44501	-1.35683	H	6.266734	3.097499	2.225028
C	2.006269	-6.329	-1.36426	H	7.126426	0.828772	2.224762
C	2.776917	-6.71494	-0.25399	H	8.903202	1.487598	-1.63255
C	2.106382	-7.36539	0.797327	H	8.06878	3.785916	-1.62144
C	0.719603	-7.49113	0.799287	H	4.763845	-6.51834	-2.18558
C	7.031409	3.619108	0.271415	H	6.715422	-5.0422	-2.08004
C	6.885371	2.780759	1.391685	H	5.883687	-4.25797	2.066228
C	7.375631	1.480973	1.392923	H	3.959985	-5.7475	1.965184
C	8.028687	0.947013	0.268716	H	8.631392	-1.00555	2.160315
C	8.332018	1.838189	-0.77662	H	7.944182	-3.35251	2.031862
C	7.85164	3.145329	-0.77112	H	6.861388	-2.7987	-2.09345
C	4.165101	-6.2037	-0.13344	H	7.568147	-0.47318	-1.96989

m[12]CPP

C	1.689806	-7.51429	0.055316	C	8.808247	-1.25288	-0.10717
C	0.909418	-7.56065	1.225309	C	8.867901	-0.6358	1.156611
C	-0.47693	-7.46687	1.17854	C	8.825953	0.746492	1.291794
C	-1.16793	-7.35468	-0.04193	C	8.693652	1.586215	0.170946
C	-0.39744	-7.48197	-1.21214	C	8.829358	0.979858	-1.0911
C	0.990539	-7.54373	-1.16537	C	8.899168	-0.40331	-1.22567
C	-2.59326	-6.93795	-0.08333	C	6.51891	5.300833	0.261342
C	-3.09212	-6.23484	-1.19553	C	6.477704	4.389763	1.33134
C	-4.33599	-5.6157	-1.16736	C	7.277279	3.256203	1.347888
C	-5.13929	-5.6482	-0.01609	C	8.166542	2.968099	0.296872
C	-4.68875	-6.42657	1.063129	C	8.314399	3.952761	-0.69806
C	-3.45264	-7.06679	1.02435	C	7.5094	5.090445	-0.71611
C	-6.31484	-4.74625	0.078597	H	1.391524	-7.61117	2.196818
C	-7.20923	-4.56619	-0.98956	H	-1.02068	-7.40146	2.115838
C	-8.15622	-3.54366	-0.97018	H	-0.88265	-7.4762	-2.18337
C	-8.23105	-2.64929	0.109594	H	1.538159	-7.53318	-2.10254
C	-7.39379	-2.88189	1.212442	H	-2.46457	-6.08986	-2.06868
C	-6.46195	-3.91501	1.201881	H	-4.64898	-5.01618	-2.01767
C	-10.4054	-1.40954	-0.34899	H	-5.30785	-6.51717	1.952053
C	-11.0916	-0.20031	-0.47744	H	-3.1427	-7.65383	1.883967
C	-10.4461	1.016709	-0.25405	H	-7.13958	-5.21446	-1.85927
C	-9.09301	1.042264	0.119881	H	-8.80089	-3.39348	-1.83235
C	-8.42777	-0.18356	0.273676	H	-7.45262	-2.22097	2.073178
C	-9.05596	-1.4136	0.033853	H	-5.78598	-4.0343	2.04421
C	-8.3134	2.298785	0.262833	H	-10.9171	-2.35018	-0.53469
C	-8.45591	3.362888	-0.64361	H	-12.142	-0.20643	-0.75668
C	-7.57255	4.440602	-0.63575	H	-10.9945	1.948701	-0.36224
C	-6.50671	4.502328	0.278624	H	-7.36734	-0.18064	0.505529
C	-6.42636	3.483577	1.244829	H	-9.22869	3.315471	-1.40631

C	-7.30864	2.410215	1.238144	H	-7.69327	5.229281	-1.37361
C	-5.40241	5.486812	0.159252	H	-5.61711	3.49555	1.968829
C	-4.9374	5.886676	-1.10615	H	-7.19555	1.624929	1.980324
C	-3.73579	6.572324	-1.25025	H	-5.48246	5.586041	-1.99641
C	-2.93625	6.884556	-0.13679	H	-3.38718	6.824022	-2.24809
C	-3.4646	6.598355	1.134463	H	-2.88384	6.836879	2.021088
C	-4.67022	5.918821	1.278889	H	-5.02406	5.676782	2.27727
C	3.147757	-7.23051	0.092674	H	3.629325	-7.97176	-1.8838
C	3.983228	-7.40426	-1.02798	H	5.832494	-6.91934	-2.00023
C	5.242142	-6.81285	-1.0936	H	5.322944	-5.41323	1.990808
C	5.738226	-6.03865	-0.03042	H	3.110334	-6.40977	2.093689
C	4.973473	-6.00237	1.147756	H	-1.40667	8.592376	1.439793
C	3.708905	-6.57505	1.204028	H	1.031615	8.816728	1.398988
C	-1.51924	7.298272	-0.28707	H	1.191617	6.315364	-2.09621
C	-0.84258	8.089902	0.658289	H	-1.23057	6.106737	-2.06306
C	0.544736	8.216644	0.634834	H	6.257627	-4.4932	-2.16628
C	1.323406	7.552151	-0.33076	H	7.548359	-2.43521	-2.20192
C	0.632881	6.858829	-1.34088	H	9.117464	-3.34979	1.700411
C	-0.75008	6.737237	-1.32109	H	7.773454	-5.39163	1.751767
C	6.859322	-5.07802	-0.17987	H	2.823883	7.518589	1.946916
C	6.90996	-4.26884	-1.32708	H	5.075577	6.617596	2.208814
C	7.652124	-3.09389	-1.34597	H	5.404256	6.201975	-2.05815
C	8.39493	-2.67557	-0.2264	H	3.19874	7.211941	-2.3258
C	8.488162	-3.58366	0.846438	H	8.840616	-1.24247	2.056288
C	7.729014	-4.75022	0.875182	H	8.812882	1.173829	2.29029
C	2.792142	7.375103	-0.20902	H	8.772443	1.58836	-1.9891
C	3.39559	7.270812	1.057263	H	8.940803	-0.82601	-2.22517
C	4.670262	6.73558	1.207815	H	5.723639	4.503454	2.103578
C	5.397392	6.2598	0.10153	H	7.117843	2.523848	2.132442
C	4.864246	6.524985	-1.1727	H	9.039017	3.809062	-1.49527
C	3.596614	7.077451	-1.32395	H	7.625813	5.80493	-1.5269

m[13]CPP

C	-0.64743	-8.32145	-0.25392	C	-9.56171	-2.70944	-0.73232
C	0.000962	-7.74284	-1.35832	C	-5.70118	6.868039	-0.27387
C	1.373707	-7.52329	-1.35531	C	-5.92438	6.004333	-1.35967
C	2.169224	-7.87904	-0.25191	C	-6.93169	5.049482	-1.32752
C	1.53758	-8.57284	0.796828	C	-7.77887	4.911771	-0.21299
C	0.161711	-8.78424	0.798656	C	-7.64359	5.868416	0.810974
C	3.559284	-7.37003	-0.14482	C	-6.62529	6.818857	0.784914
C	4.34441	-7.09063	-1.27756	C	-8.59473	3.679772	-0.06861
C	5.52097	-6.35353	-1.17873	C	-8.96945	2.906843	-1.18278
C	5.977945	-5.86977	0.059739	C	-9.3655	1.581686	-1.04372
C	5.259354	-6.25788	1.204	C	-9.4367	0.964609	0.218878
C	4.077571	-6.98274	1.103909	C	-9.25272	1.797597	1.337966
C	7.068194	-4.86623	0.138983	C	-8.82919	3.11488	1.19829
C	6.981203	-3.82613	1.08143	H	-0.59185	-7.36405	-2.18596
C	7.879305	-2.76739	1.074437	H	1.816764	-6.97587	-2.18172
C	8.907593	-2.68808	0.120597	H	2.126613	-8.92753	1.638154
C	9.0419	-3.76103	-0.77623	H	-0.29676	-9.29217	1.643185
C	8.142222	-4.82623	-0.76719	H	4.008655	-7.41631	-2.25812
C	11.11192	-1.48279	-0.26918	H	6.054317	-6.08863	-2.08742
C	11.82361	-0.28727	-0.38194	H	5.607992	-5.95136	2.186089
C	11.19027	0.944489	-0.20873	H	3.509738	-7.18618	2.006936
C	9.818739	0.997136	0.086285	H	6.16219	-3.81627	1.794071
C	9.120756	-0.21432	0.196334	H	7.769528	-1.97341	1.807555
C	9.739736	-1.46119	0.026209	H	9.82948	-3.73706	-1.5249
C	9.065838	2.268948	0.235044	H	8.264741	-5.62821	-1.49031
C	8.030695	2.368177	1.179689	H	11.6244	-2.43315	-0.39201
C	7.196275	3.477175	1.222815	H	12.88874	-0.31626	-0.59668
C	7.358024	4.550208	0.328423	H	11.76342	1.864585	-0.28507
C	8.445062	4.488344	-0.56109	H	8.047954	-0.18403	0.355475
C	9.279676	3.372656	-0.60739	H	7.862108	1.550295	1.874337
C	6.322251	5.6111	0.266314	H	6.366163	3.483361	1.922547
C	5.92921	6.168306	-0.96325	H	8.627156	5.313148	-1.24483
C	4.790011	6.960416	-1.06662	H	10.076	3.335504	-1.34618
C	3.979016	7.224315	0.051534	H	6.479666	5.918038	-1.86574
C	4.439151	6.765134	1.298471	H	4.50104	7.341768	-2.04196
C	5.584905	5.984329	1.403799	H	3.850519	6.956541	2.190954
C	-2.12467	-8.23481	-0.14819	H	5.886824	5.62127	2.382118
C	-2.70876	-7.83002	1.063941	H	-2.08625	-7.72909	1.948409
C	-4.03548	-7.41879	1.122407	H	-4.41179	-7.00256	2.051893
C	-4.84751	-7.40037	-0.0255	H	-4.91677	-8.01511	-2.09735
C	-4.30224	-7.94243	-1.20418	H	-2.57132	-8.71672	-2.20558
C	-2.97085	-8.34399	-1.26599	H	2.301817	6.941297	-2.0467
C	2.613392	7.788676	-0.08524	H	-0.08409	7.425965	-2.13627
C	1.848507	7.488815	-1.22605	H	0.133105	9.262542	1.743873
C	0.487936	7.764563	-1.27756	H	2.535625	8.788674	1.829562
C	-0.1815	8.350652	-0.18929	H	-6.65537	-7.03543	2.042108
C	0.602504	8.752469	0.906687	H	-8.34394	-5.26513	2.186418

C	1.967567	8.48054	0.955926	H	-7.65838	-4.2785	-1.93937
C	-6.11919	-6.6342	-0.01391	H	-5.95443	-6.01835	-2.07741
C	-6.86384	-6.43158	1.16318	H	-1.95774	8.790108	-2.25276
C	-7.82639	-5.42982	1.24486	H	-4.32769	8.158428	-2.28925
C	-8.09942	-4.5926	0.148449	H	-4.15045	7.264455	1.911132
C	-7.47254	-4.90316	-1.07024	H	-1.78701	7.890168	1.947011
C	-6.50227	-5.89642	-1.14789	H	-7.9138	-2.90082	2.222378
C	-1.66493	8.336324	-0.16092	H	-8.45832	-0.53333	2.253301
C	-2.43166	8.453547	-1.33457	H	-10.4572	-0.94091	-1.53606
C	-3.77581	8.096672	-1.35507	H	-9.86692	-3.3144	-1.58237
C	-4.41659	7.607075	-0.20247	H	-5.22789	6.003904	-2.19281
C	-3.68973	7.635739	1.000046	H	-6.9861	4.329234	-2.13723
C	-2.34438	7.991501	1.020107	H	-8.31955	5.847598	1.661436
C	-8.79766	-3.29156	0.294426	H	-6.52616	7.512233	1.616196
C	-8.50432	-2.48845	1.409399	H	-8.8833	3.322827	-2.18226
C	-8.81929	-1.13564	1.426093	H	-9.52958	0.993978	-1.9417
C	-9.45705	-0.51598	0.335898	H	-9.37159	1.393093	2.338756
C	-9.89188	-1.35679	-0.70676	H	-8.58711	3.680037	2.093426

Cartesian coordinates for the rotation process of **Fe-[8]CPP**

Fe-[8]CPP-A (PBE0-D3(BJ)/6-31G(d,p) for C, H, SDD for Fe)

C	-0.63799	6.271578	-1.06812	C	-4.94519	5.184919	1.136919
C	0.719451	5.979657	-1.11935	C	-5.42577	4.469365	0.029381
C	1.347453	5.257486	-0.09252	C	-2.90682	-5.71126	0.086255
C	0.592932	5.006304	1.061915	C	-3.3785	-5.11575	1.263511
C	-0.75639	5.312266	1.121773	C	-3.81146	-5.832	-0.97974
C	-1.42163	5.871375	0.023	C	-4.61737	-4.49513	1.304495
C	-6.41469	2.618011	1.334337	C	-5.05124	-5.20848	-0.93987
C	-6.92556	1.33009	1.351148	C	-5.43743	-4.44133	0.169376
C	-7.46478	0.75053	0.194876	H	-1.10847	6.770042	-1.91157
C	-7.66029	1.590897	-0.91188	H	1.286488	6.26814	-1.99988
C	-7.14895	2.88184	-0.92834	H	1.032036	4.444915	1.879984
C	-6.42094	3.384402	0.161042	H	-1.33397	4.984985	1.981103
C	-7.10275	-2.84906	1.210507	H	-5.86539	2.973109	2.200777
C	-7.61082	-1.55717	1.214674	H	-6.76129	0.713719	2.229676
C	-7.47396	-0.72396	0.093601	H	-8.1536	1.203924	-1.79948
C	-7.00719	-1.31268	-1.08927	H	-7.25246	3.482181	-1.82822
C	-6.50235	-2.60381	-1.09436	H	-7.15267	-3.44366	2.118795
C	-6.44114	-3.36011	0.083652	H	-8.05114	-1.16242	2.126374
C	-0.86711	-5.51984	-1.30261	H	-6.89169	-0.70187	-1.97948
C	0.485897	-5.23268	-1.39252	H	-6.00635	-2.96958	-1.98837
C	1.316793	-5.3014	-0.26648	H	-1.50434	-5.31738	-2.15807
C	0.769449	-5.84399	0.905436	H	0.874546	-4.81486	-2.31632
C	-0.58554	-6.13418	0.99467	H	1.402795	-5.98524	1.777153
C	-1.4498	-5.89038	-0.08324	H	-0.99031	-6.49796	1.935249
C	5.153655	1.168466	-0.80017	H	3.640401	0.074732	0.416725
C	4.499002	0.032078	-0.2396	H	6.853078	-1.41321	-2.1162
C	5.100173	-1.15987	-0.74412	H	6.905417	1.280772	-2.18952
C	6.159915	-0.75186	-1.6127	H	4.768625	2.580492	1.506949
C	6.189836	0.6741	-1.65017	H	3.14171	4.395653	1.813062
C	4.291239	3.028568	0.640514	H	2.496122	4.502664	-2.43155
C	3.357308	4.041021	0.809446	H	4.189376	2.76219	-2.73039
C	2.632378	4.548041	-0.27974	H	4.783009	-3.20013	-2.51342
C	3.027428	4.1334	-1.55978	H	3.160604	-5.03731	-2.30857
C	3.982825	3.140796	-1.73317	H	2.368852	-3.8748	1.745262
C	4.565022	2.508562	-0.62941	H	4.047607	-2.09008	1.559502
C	4.284323	-3.37181	-1.56341	H	8.76462	-1.576	0.394891
C	3.354098	-4.3985	-1.45111	H	9.031022	1.103033	0.219159
C	2.595262	-4.56036	-0.2841	H	7.168452	2.231169	1.797121
C	2.930379	-3.76564	0.821996	H	5.745055	0.249818	2.957143
C	3.864743	-2.74807	0.71421	H	6.729332	-2.10246	2.075601
C	4.493707	-2.47696	-0.50778	H	-2.86616	5.133551	-2.1067
C	8.187675	-0.84171	0.940559	H	-3.31627	6.274261	2.003073
C	8.32772	0.572888	0.846945	H	-5.0467	4.04175	-2.04711
C	7.340971	1.169448	1.682575	H	-5.52065	5.198252	2.058551
C	6.589952	0.122897	2.293373	H	-2.70896	-5.00609	2.111231

C	7.113578	-1.12036	1.833719	H	-3.51226	-6.36276	-1.8795
C	-2.8905	5.725393	-0.03805	H	-4.8851	-3.91471	2.182255
C	-3.46349	5.197064	-1.20177	H	-5.70062	-5.25862	-1.80981
C	-3.69955	5.796019	1.105605	Fe	6.459333	-0.00176	0.262774
C	-4.70454	4.578443	-1.16743				

Fe-[8]CPP-B (PBE0-D3(BJ)/6-31G(d,p) for C, H, SDD for Fe)

C	0.049216	6.315462	-1.46016	C	-4.14066	5.395375	1.01347
C	1.396904	5.998222	-1.56043	C	-4.66892	4.643338	-0.04679
C	2.083956	5.418229	-0.48375	C	-2.58621	-5.72961	0.025662
C	1.415903	5.353308	0.74622	C	-2.92665	-5.03544	1.195536
C	0.068413	5.666159	0.844868	C	-3.58705	-5.857	-0.95116
C	-0.66697	6.061664	-0.28066	C	-4.12364	-4.34726	1.302086
C	-5.62595	2.829419	1.334425	C	-4.78193	-5.15565	-0.85172
C	-6.17279	1.557445	1.397021	C	-5.03442	-4.31005	0.238244
C	-6.79514	0.980633	0.281552	H	-0.47207	6.703202	-2.33123
C	-7.02188	1.810522	-0.82701	H	1.908982	6.139407	-2.50849
C	-6.47263	3.08421	-0.89046	H	1.919144	4.915005	1.603338
C	-5.67609	3.580501	0.1527	H	-0.45101	5.461304	1.776156
C	-6.54437	-2.61496	1.343846	H	-5.02129	3.181591	2.16466
C	-6.9838	-1.29847	1.352995	H	-5.98022	0.948082	2.274663
C	-6.87518	-0.49349	0.208504	H	-7.57544	1.42772	-1.6802
C	-6.51509	-1.12644	-0.98895	H	-6.60533	3.676015	-1.79218
C	-6.08155	-2.44376	-0.99985	H	-6.56459	-3.1904	2.265528
C	-5.98555	-3.18051	0.18786	H	-7.34534	-0.86534	2.28169
C	-0.66702	-5.93842	-1.55548	H	-6.42537	-0.53811	-1.89715
C	0.677233	-5.71262	-1.80799	H	-5.66487	-2.85391	-1.91509
C	1.587579	-5.5149	-0.75935	H	-1.35936	-5.9392	-2.3917
C	1.131333	-5.80074	0.535809	H	1.004568	-5.59118	-2.83638
C	-0.20819	-6.06051	0.785501	H	1.809978	-5.70351	1.378142
C	-1.16004	-6.01268	-0.24417	H	-0.52938	-6.20558	1.812646
C	5.526885	0.987179	-0.58359	H	3.914036	-0.03418	-1.72837
C	4.817638	-0.11902	-1.1423	H	7.106891	-1.67443	0.731411
C	5.387106	-1.34456	-0.67698	H	7.264586	1.001588	0.838741
C	6.470874	-0.9869	0.190053	H	5.718058	3.084553	1.197107
C	6.5553	0.43743	0.247911	H	4.244609	5.049016	1.23044
C	5.08765	3.293709	0.337241	H	2.712498	3.954532	-2.62489
C	4.240615	4.394088	0.363099	H	4.241242	2.041663	-2.68892
C	3.309562	4.612706	-0.66464	H	3.766614	-1.99234	-2.71391
C	3.402598	3.79934	-1.80083	H	2.092209	-3.75637	-2.71499
C	4.251925	2.703372	-1.82797	H	3.953984	-5.52895	0.724536
C	5.027416	2.366776	-0.71305	H	5.564955	-3.68707	0.789888
C	3.812263	-2.76218	-1.95019	H	4.949674	1.440202	3.146744
C	2.876285	-3.78251	-1.96534	H	2.9369	1.86645	1.40777
C	2.838527	-4.75325	-0.95526	H	1.964804	-0.53394	0.654921
C	3.896088	-4.7498	-0.03077	H	3.404258	-2.43736	1.88294
C	4.823928	-3.71569	-0.00457	H	5.244759	-1.22446	3.441755
C	4.734851	-2.64394	-0.90472	H	-2.19387	5.20403	-2.30354

C	4.333614	0.67804	2.688618	H	-2.48632	6.526056	1.76817
C	3.259296	0.903694	1.78124	H	-4.37161	4.130518	-2.11654
C	2.752601	-0.36321	1.376097	H	-4.67829	5.444093	1.956591
C	3.510609	-1.37175	2.034455	H	-2.18827	-4.9081	1.980097
C	4.489777	-0.73061	2.844769	H	-3.40327	-6.45817	-1.83718
C	-2.13499	5.892521	-0.26418	H	-4.28582	-3.7062	2.163303
C	-2.75309	5.310253	-1.37894	H	-5.50229	-5.21398	-1.66345
C	-2.89903	6.007543	0.906958	Fe	4.729831	-0.19616	0.886035
C	-3.99285	4.699446	-1.27283				

Fe-[8]CPP-TS-1 (PBE0-D3(BJ)/6-31G(d,p) for C, H, SDD for Fe)

C	0.426865	-6.0839	-1.69598	C	4.389686	-5.28459	1.156865
C	-0.90741	-5.7536	-1.88757	C	5.011649	-4.52697	0.153504
C	-1.69064	-5.27765	-0.82708	C	2.701141	5.730577	-0.2214
C	-1.13599	-5.32218	0.457901	C	3.04761	5.23045	1.040279
C	0.202963	-5.63412	0.645274	C	3.694592	5.72985	-1.21131
C	1.037408	-5.92924	-0.44164	C	4.252115	4.572657	1.240358
C	5.826668	-2.68906	1.593546	C	4.904669	5.081623	-1.00663
C	6.346407	-1.406	1.675854	C	5.163508	4.39577	0.190372
C	7.059264	-0.84572	0.607384	H	1.022069	-6.39862	-2.54861
C	7.411193	-1.7	-0.44891	H	-1.33383	-5.8025	-2.88601
C	6.889471	-2.98348	-0.53228	H	-1.72221	-4.96756	1.301133
C	5.997446	-3.46368	0.438614	H	0.635549	-5.50854	1.633143
C	6.62742	2.788704	1.486054	H	5.148694	-3.03222	2.369354
C	7.098769	1.486747	1.592009	H	6.060991	-0.77727	2.513908
C	7.098668	0.626487	0.483622	H	8.038398	-1.32722	-1.25426
C	6.801783	1.19009	-0.76454	H	7.115609	-3.59501	-1.40171
C	6.327706	2.487805	-0.86919	H	6.575477	3.407549	2.377746
C	6.132209	3.281889	0.268894	H	7.403775	1.109435	2.564447
C	0.770924	5.33154	-1.70194	H	6.793384	0.556883	-1.64643
C	-0.58057	5.063526	-1.84765	H	5.96162	2.833095	-1.83104
C	-1.499	5.384456	-0.83877	H	1.467735	4.949909	-2.44228
C	-1.02116	6.141033	0.24266	H	-0.90364	4.476142	-2.70104
C	0.335476	6.395726	0.398145	H	-1.71256	6.483745	1.007317
C	1.269572	5.921058	-0.53307	H	0.681891	6.921064	1.284276
C	-5.38151	-0.99735	-0.84642	H	-3.52328	0.225213	-1.04253
C	-4.59398	0.189886	-0.89084	H	-7.59965	1.437026	-0.1509
C	-5.41002	1.325676	-0.62225	H	-7.56678	-1.2466	-0.40009
C	-6.73562	0.836011	-0.40137	H	-5.70817	-3.37888	0.55996
C	-6.71778	-0.58915	-0.53394	H	-4.10278	-5.24669	0.570109
C	-4.90939	-3.40233	-0.1737	H	-2.01994	-3.461	-2.72609
C	-4.00023	-4.45474	-0.16727	H	-3.62886	-1.60232	-2.73323
C	-2.90688	-4.46601	-1.04415	H	-4.69919	2.688432	-2.81596
C	-2.84939	-3.46813	-2.02489	H	-3.03478	4.484212	-2.95473
C	-3.74664	-2.41154	-2.01835	H	-2.96991	4.722487	1.33229
C	-4.74033	-2.31299	-1.03721	H	-4.69835	3.000942	1.447262
C	-4.34363	3.160073	-1.90378	H	-7.39361	-0.09512	2.997463

C	-3.38914	4.165724	-1.97867	H	-6.00679	-2.32977	2.435644
C	-2.81087	4.700319	-0.81736	H	-3.44718	-1.6343	1.966331
C	-3.37984	4.328187	0.407434	H	-3.24109	1.036434	2.291088
C	-4.35296	3.339711	0.479573	H	-5.69371	1.976611	2.95064
C	-4.78479	2.670528	-0.66733	H	2.740733	-5.04701	-2.31397
C	-6.33012	-0.15332	2.809214	H	2.677382	-6.42132	1.752217
C	-5.59559	-1.33283	2.507411	H	4.897206	-3.99441	-1.92883
C	-4.23943	-0.96563	2.275558	H	4.841436	-5.34194	2.143643
C	-4.1336	0.444183	2.441999	H	2.303055	5.221914	1.83102
C	-5.42641	0.943602	2.774678	H	3.487657	6.182945	-2.17723
C	2.499142	-5.76167	-0.29559	H	4.418308	4.061374	2.18363
C	3.214633	-5.16951	-1.3452	H	5.629376	5.043475	-1.8153
C	3.161089	-5.89315	0.935102	Fe	-5.46463	-0.00725	0.95317
C	4.443902	-4.56906	-1.12684				

Fe-[8]CPP-TS-2 (PBE0-D3(BJ)/6-31G(d,p) for C, H, SDD for Fe)

C	-7.06965	-0.16789	0.456462	C	-5.41178	4.24452	-1.07593
C	-6.82752	-1.53039	0.337687	C	-4.66476	4.433742	0.097167
C	-6.12579	-2.04583	-0.76465	C	6.259499	2.1592	-0.20971
C	-5.92396	-1.17749	-1.84724	C	5.639473	2.77058	-1.30861
C	-6.17573	0.18066	-1.7339	C	6.21127	2.845182	1.013955
C	-6.63533	0.730929	-0.53018	C	4.845153	3.89541	-1.15094
C	-2.66109	5.389525	-1.00481	C	5.411632	3.969527	1.172968
C	-1.3397	5.801697	-0.92636	C	4.632153	4.459334	0.113846
C	-0.75456	6.129182	0.303978	H	-7.52304	0.213066	1.367854
C	-1.59944	6.19025	1.422069	H	-7.09866	-2.18706	1.159926
C	-2.92418	5.781346	1.342484	H	-5.39946	-1.5331	-2.72826
C	-3.45957	5.288606	0.142693	H	-5.84627	0.840794	-2.53063
C	2.883818	6.097157	-0.68972	H	-3.03776	5.012756	-1.95089
C	1.556641	6.502239	-0.64528	H	-0.71551	5.7399	-1.81281
C	0.719167	6.122616	0.414234	H	-1.1984	6.512451	2.379303
C	1.314785	5.472782	1.503391	H	-3.53762	5.791639	2.239333
C	2.640025	5.066252	1.458015	H	3.491328	6.359665	-1.5516
C	3.429192	5.292603	0.322146	H	1.146856	7.075466	-1.47253
C	6.254064	-0.12117	0.750062	H	0.696827	5.162064	2.340635
C	5.985531	-1.46477	0.535692	H	3.027338	4.444883	2.259965
C	6.047103	-2.01564	-0.75204	H	6.02081	0.307434	1.720021
C	6.645161	-1.2337	-1.75256	H	5.547339	-2.04581	1.341834
C	6.917862	0.110488	-1.53619	H	6.800706	-1.65479	-2.74242
C	6.600338	0.723588	-0.31331	H	7.291854	0.713843	-2.35902
C	-1.23731	-4.2392	-0.52663	H	-0.01583	-6.1022	-0.81905
C	-0.0575	-5.02353	-0.74631	H	1.181603	-1.91427	-0.62098
C	1.062391	-4.12908	-0.82847	H	-1.51009	-2.0418	-0.2812
C	0.560646	-2.79956	-0.65178	H	-2.89811	-4.69731	-2.64408
C	-0.83287	-2.86563	-0.46239	H	-5.13755	-3.7182	-2.779
C	-3.40765	-4.40865	-1.72852	H	-5.12339	-3.14512	1.476746
C	-4.67087	-3.83351	-1.80452	H	-2.93086	-4.20639	1.605131

C	-5.26108	-3.24575	-0.67296	H	3.146927	-5.29676	0.679377
C	-4.68168	-3.54268	0.568004	H	5.409896	-4.33735	0.709039
C	-3.42824	-4.13474	0.645802	H	4.542587	-2.22462	-2.92516
C	-2.70868	-4.43925	-0.51331	H	2.299309	-3.19407	-2.94922
C	3.461617	-4.64766	-0.13138	H	0.768729	-1.75035	2.60761
C	4.742608	-4.10043	-0.11588	H	-1.63955	-2.90024	2.913143
C	5.116634	-3.12747	-1.05515	H	-1.31047	-5.58239	2.749952
C	4.272501	-2.9458	-2.15968	H	1.304557	-6.07118	2.360404
C	2.996251	-3.48613	-2.16853	H	2.589434	-3.69189	2.267143
C	2.522076	-4.23023	-1.08095	H	-5.76336	1.705108	1.796375
C	0.573041	-2.81376	2.635008	H	-6.71706	2.965397	-2.19216
C	-0.70174	-3.42519	2.792556	H	-4.36162	3.674892	2.089969
C	-0.52789	-4.83675	2.704443	H	-5.31217	4.951638	-1.89499
C	0.857413	-5.09546	2.496514	H	5.653374	2.272937	-2.27333
C	1.536459	-3.84395	2.45757	H	6.748098	2.451356	1.872807
C	-6.29697	2.141279	-0.24281	H	4.264425	4.249457	-1.99737
C	-5.71525	2.438918	0.997368	H	5.339111	4.435435	2.152078
C	-6.21072	3.121367	-1.24328	Fe	0.115406	-3.9334	0.984469
C	-4.91548	3.559477	1.163144				

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12. NMR spectra

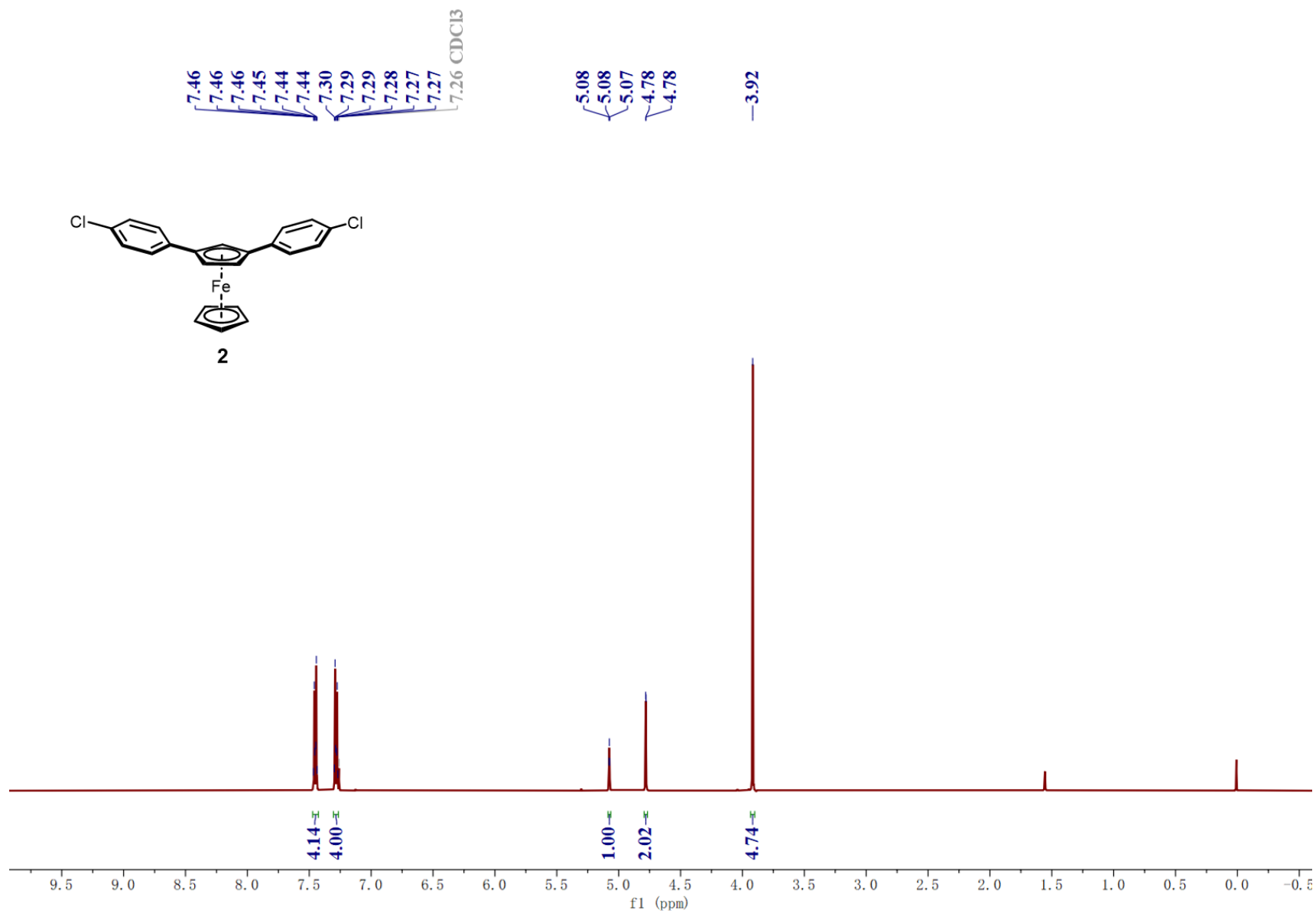


Figure S20. ¹H NMR (500 M) of 1,3-bis(4-chlorophenyl)ferrocene (2)

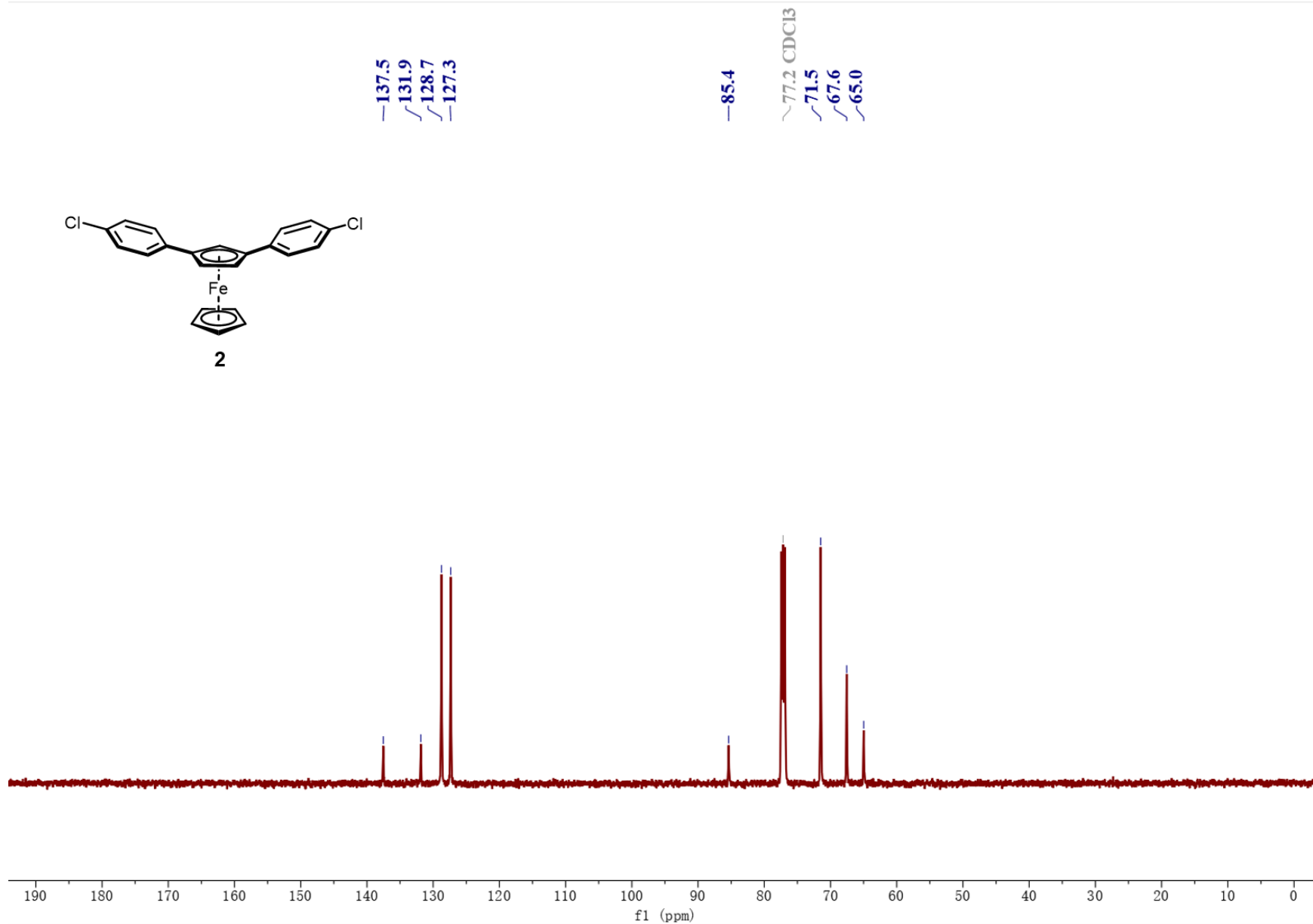


Figure S21. ¹³C NMR (126 M) of 1,3-bis(4-chlorophenyl)ferrocene (2)

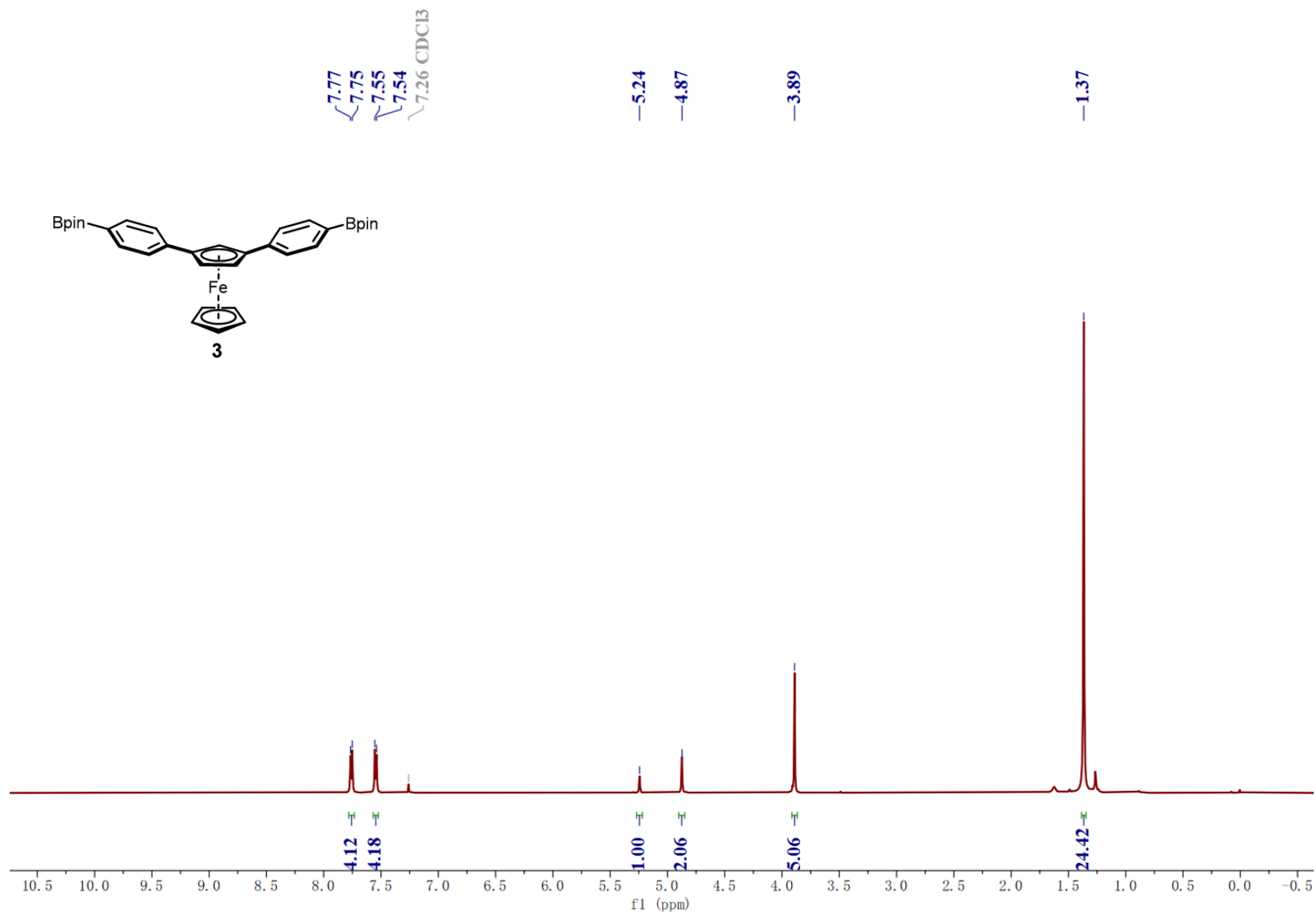


Figure S22. ¹H NMR (500 M) of 1,3-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ferrocene (3)

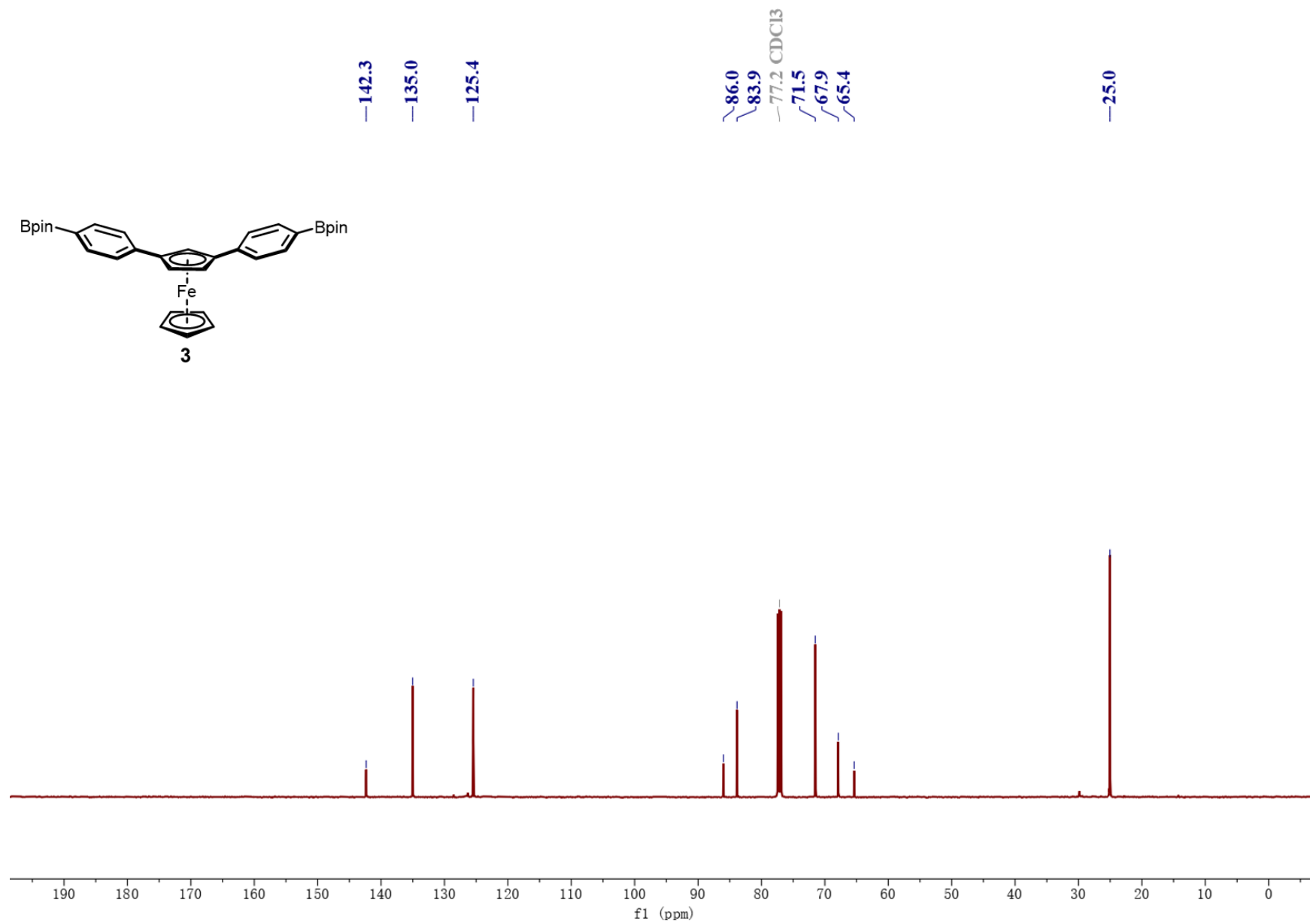


Figure S23. ¹³C NMR (126 M) of 1,3-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ferrocene (**3**)

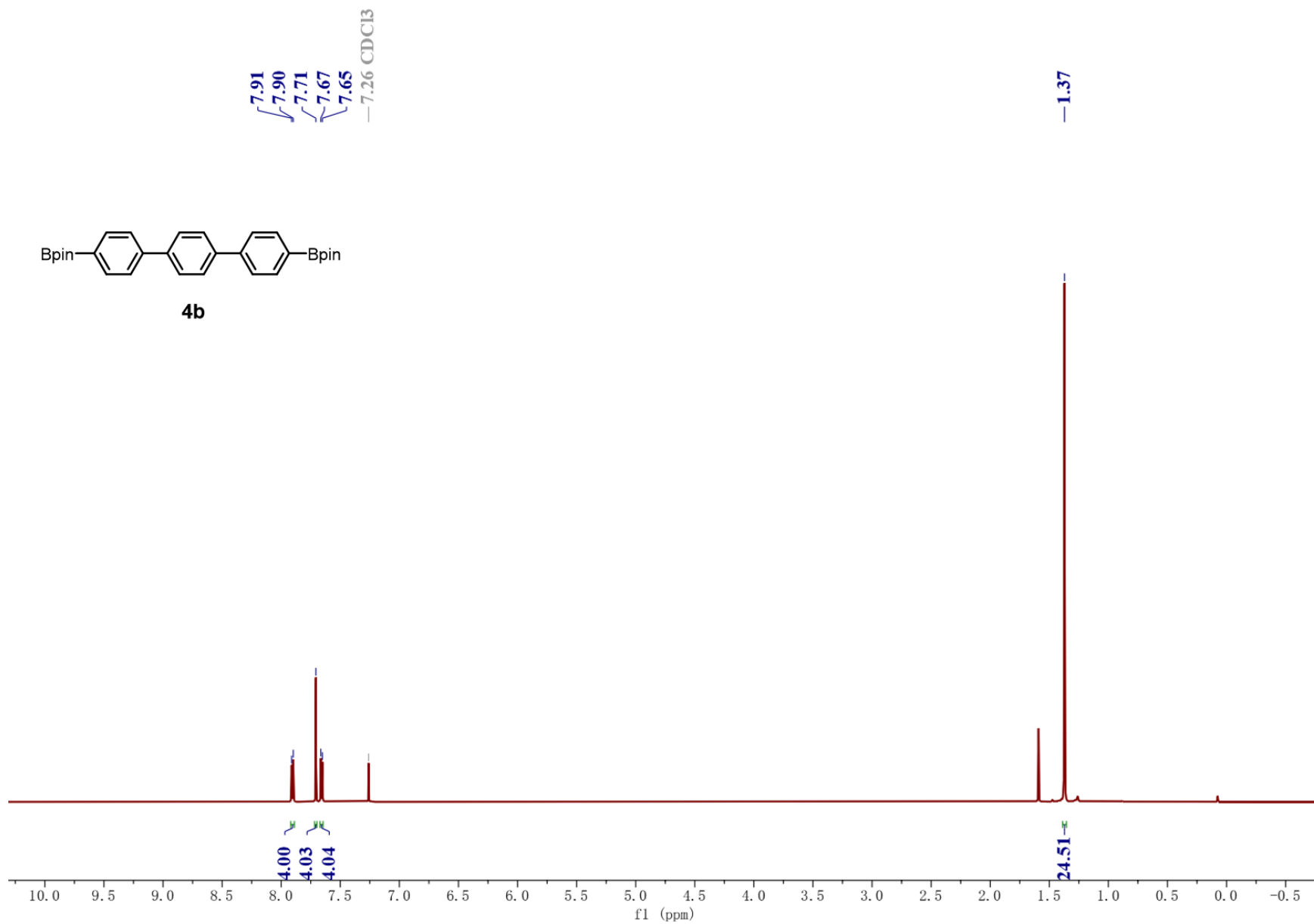


Figure S24. ¹H NMR (500 M) of **4b**

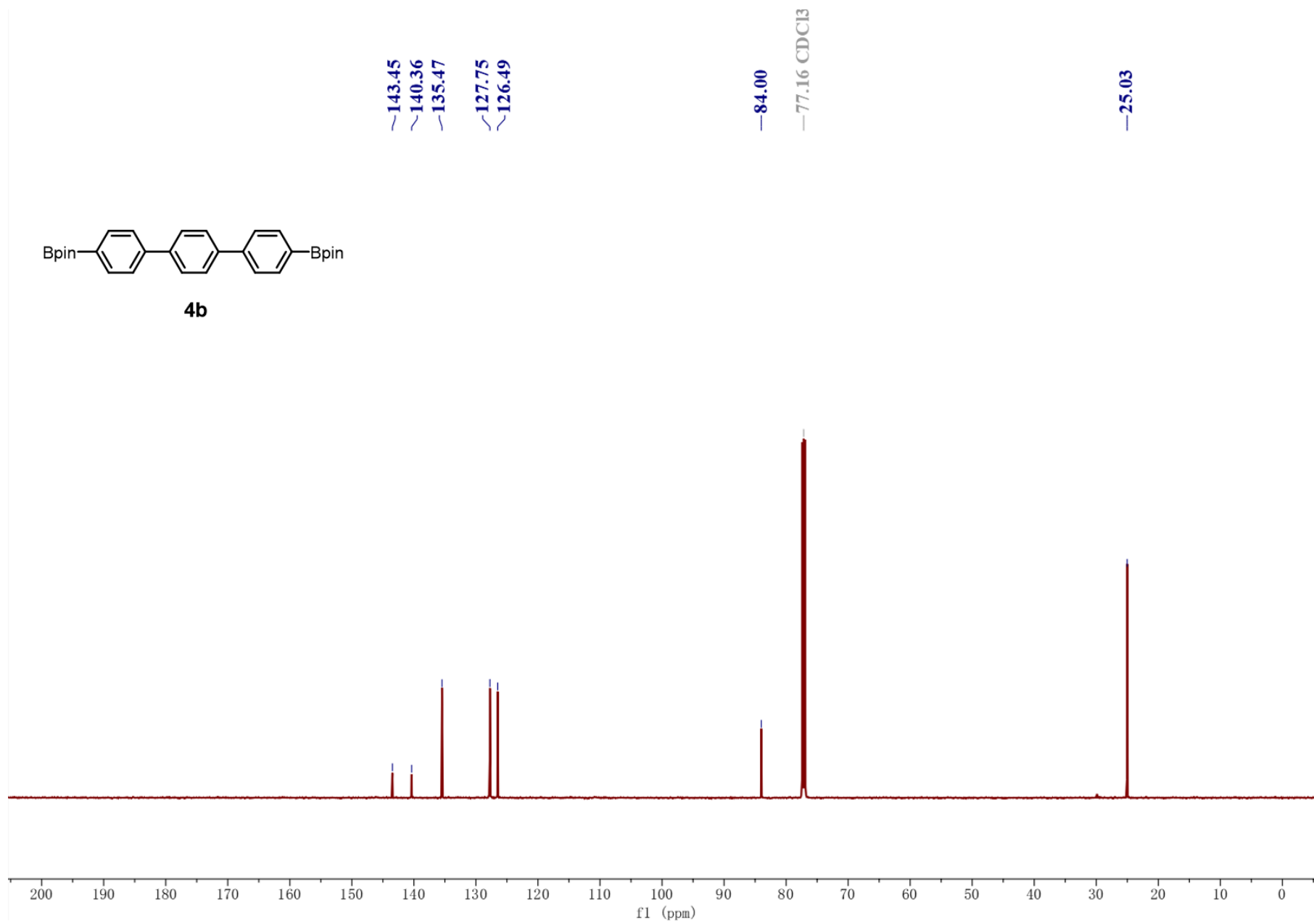


Figure S25. ¹³C NMR (126 M) of **4b**

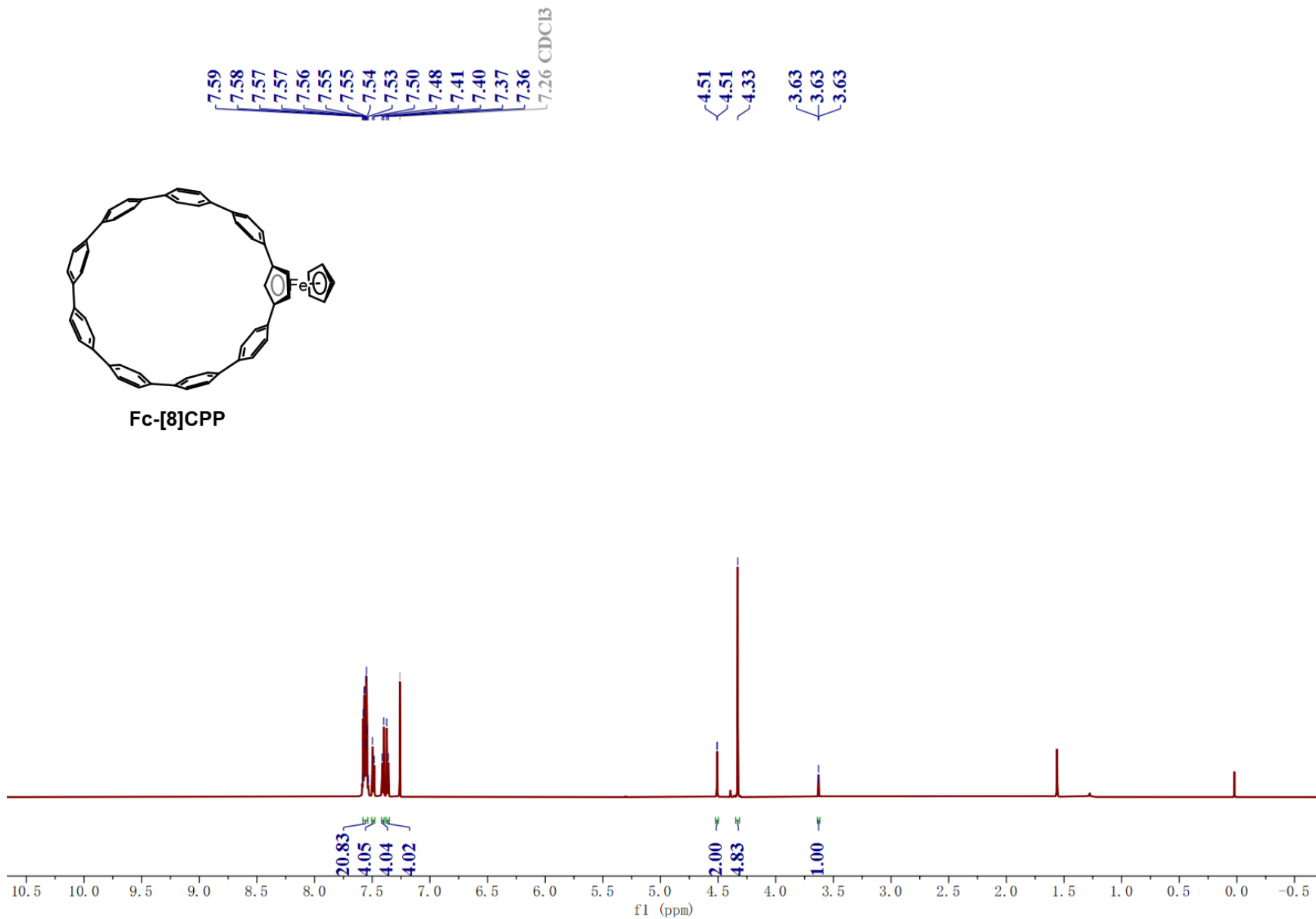


Figure S26. ^1H NMR (600 M) of Fc-[8]CPP

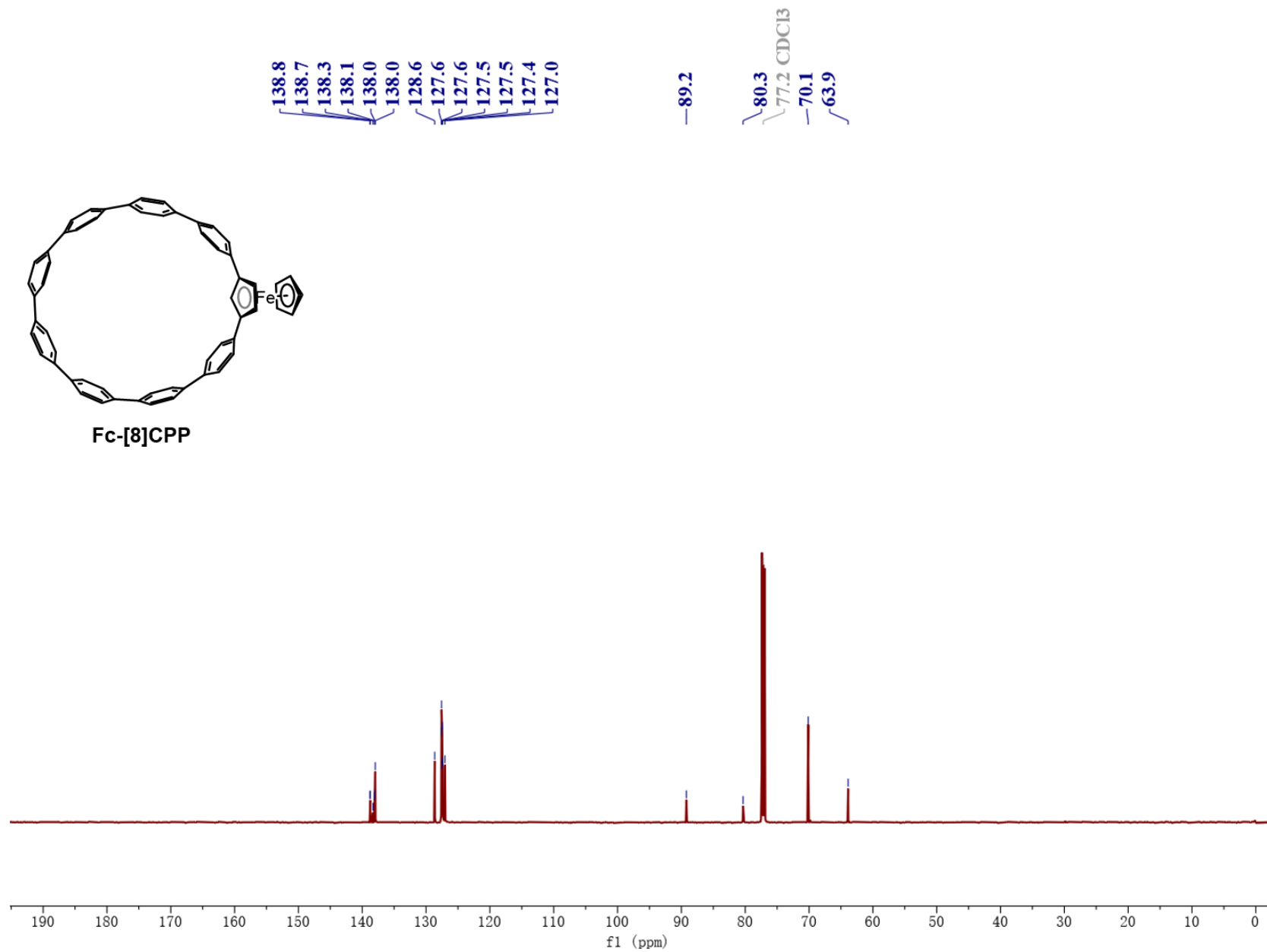


Figure S27. ¹³C NMR (151 M) of Fc-[8]CPP

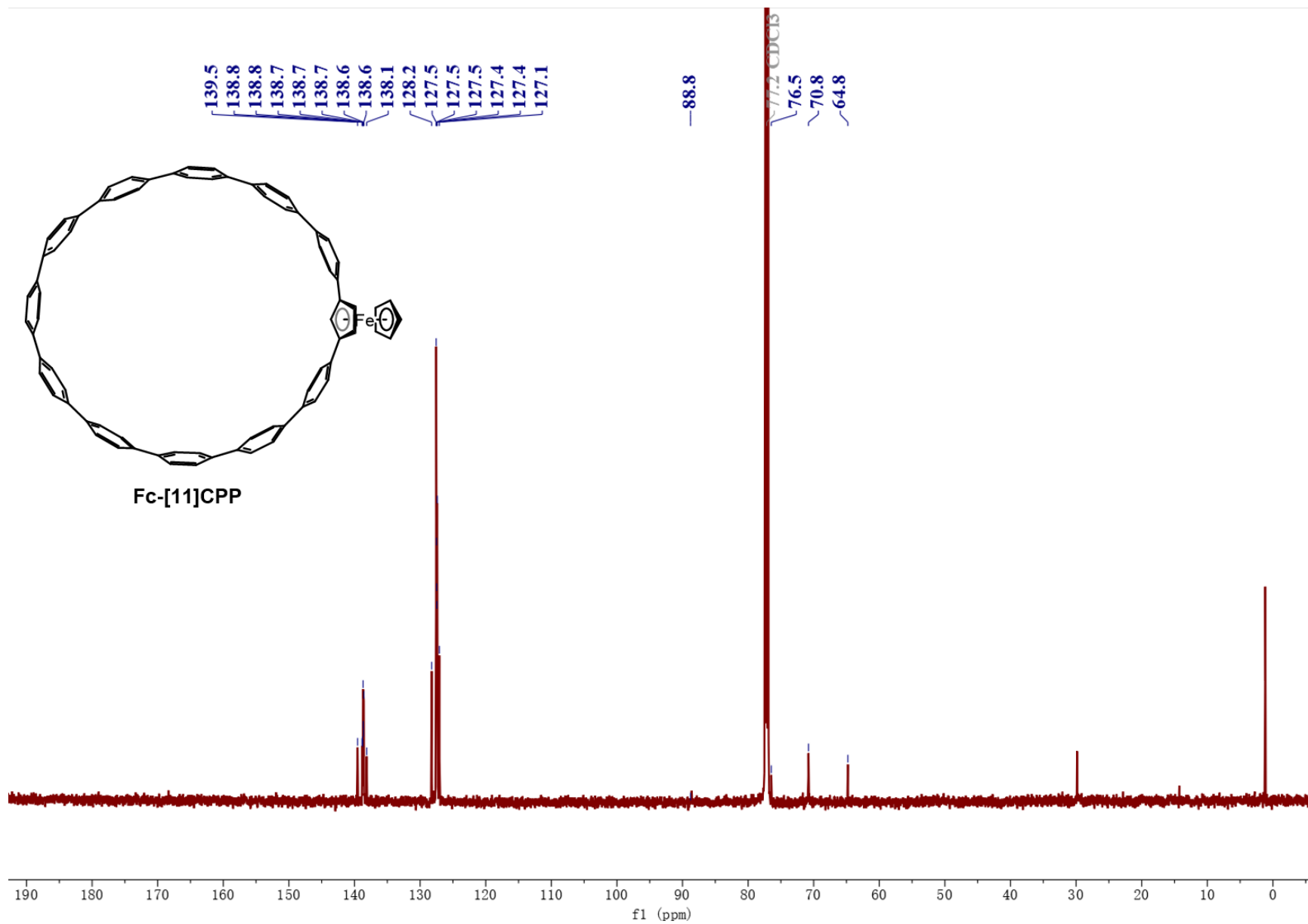


Figure S29. ¹³C NMR (151 M) of Fc-[11]CPP

13. High-resolution mass spectra (HRMS)

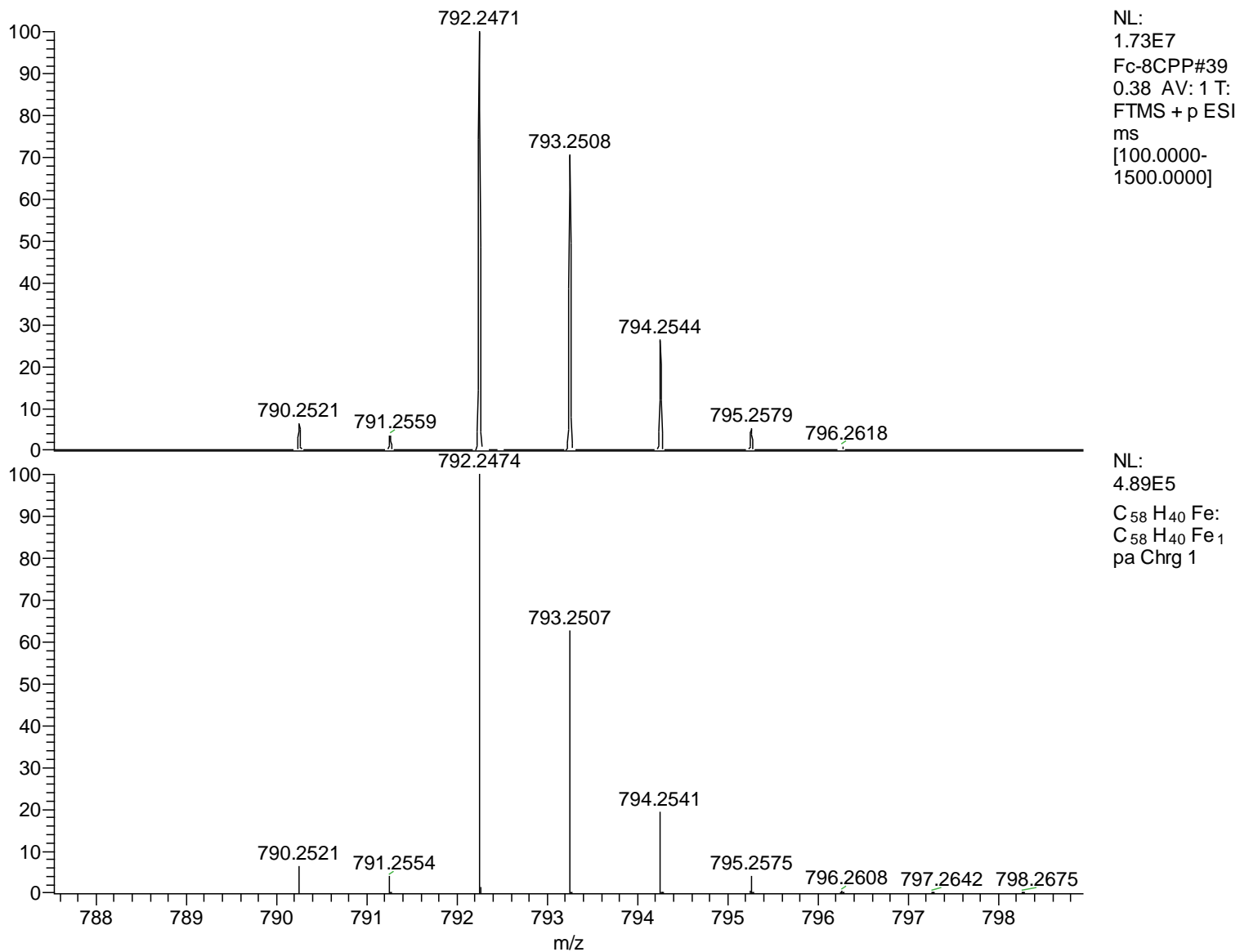


Figure S30. HRMS of Fc-[8]CPP (top, the measured; down, Simulated with C₅₈H₄₀Fe)

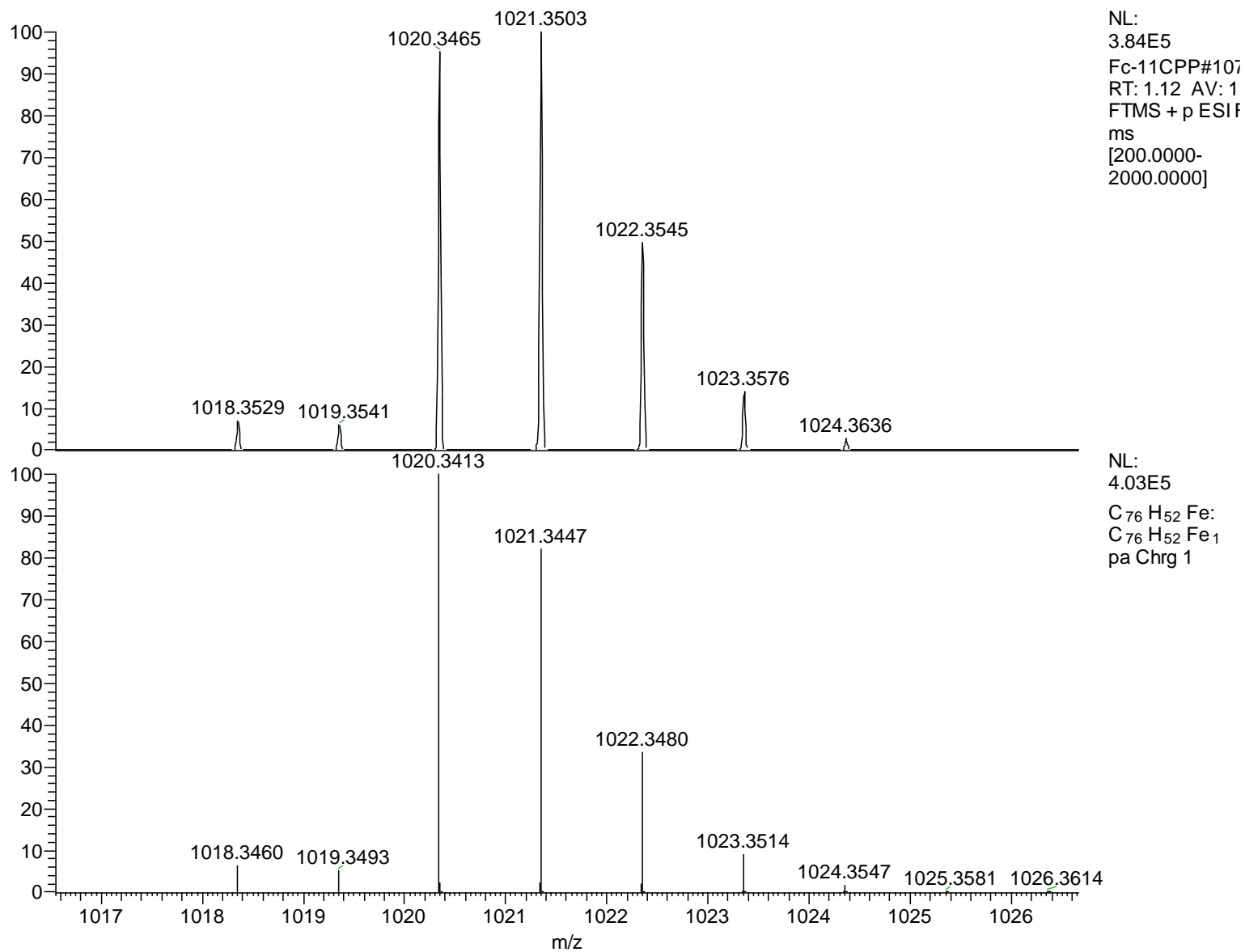


Figure S31. HRMS of Fc-[11]CPP (top, the measured; down, Simulated with C₇₆H₅₂Fe)

14. Maldi-tof mass spectra (HRMS)

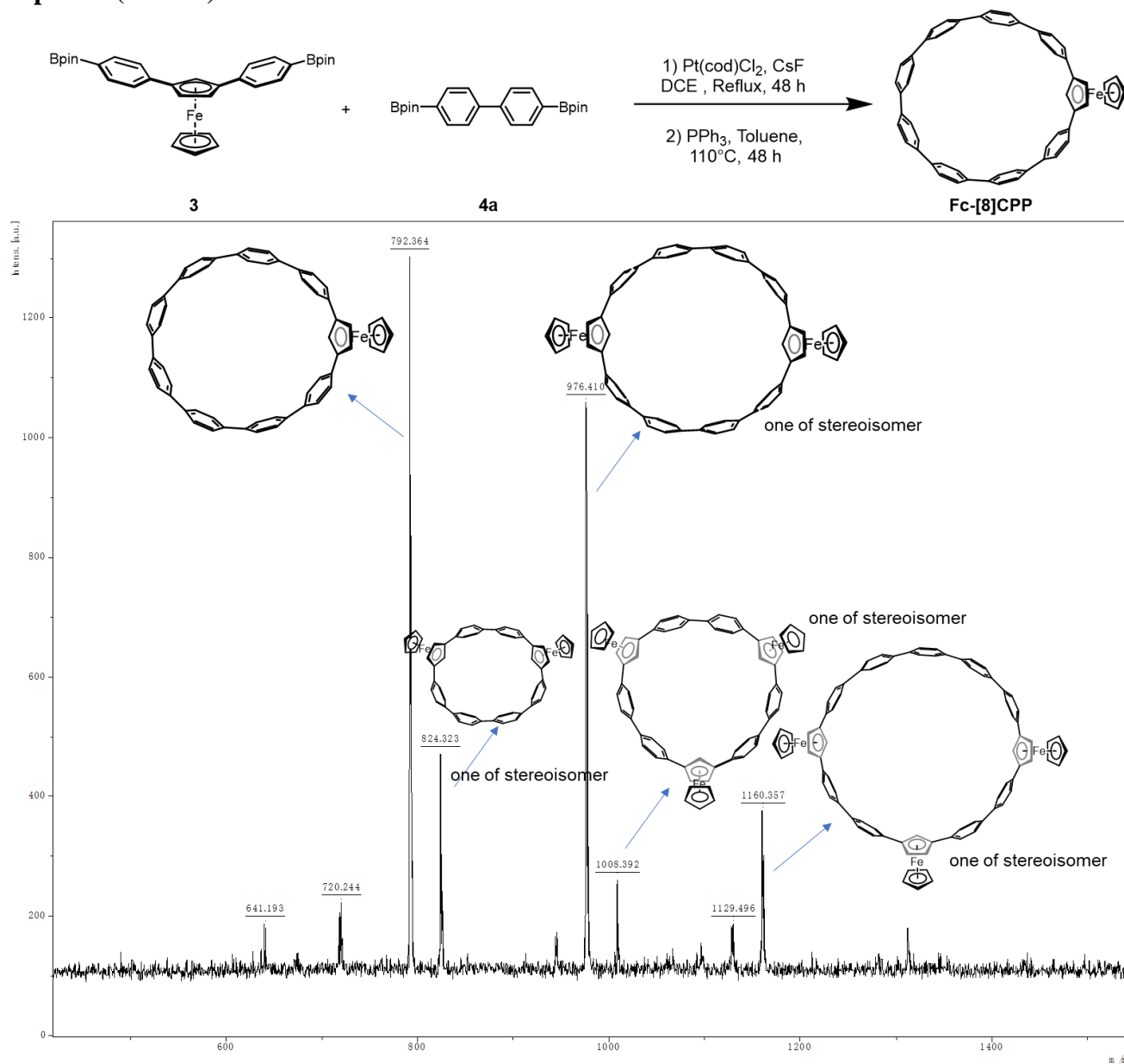


Figure S32. Maldi-tof MS of Fc-[8]CPP, di-Fc-CPPs and tri-Fc-CPPs