Electronic Supplementary Materials for

Copper(III) organometallic complexes of non (anti)aromatic and aromatic doubly N-confused porphyrinoids: syntheses and characterization

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Materials and Methods:

1.1 Electronic absorption spectra were measured with a Perkin Elmer Lambda 950 UV-visible-NIR spectrophotometer. ^{1}H NMR spectra were recorded on a Bruker AVIII 500 MHz spectrometer, Bruker AVIII 400 MHz, Bruker DPX-300 MHz spectrometer and chemical shifts were reported as the delta scale in ppm relative to $CHCl_3$ (δ = 7.26 ppm) and CH_2Cl_2 (δ = 5.32 ppm) as internal reference for ^{1}H and ^{13}C NMR $CHCl_3$ (δ = 77.00 ppm) and CH_2Cl_2 (δ = 55.00 ppm). MALDI-TOF MS data were recorded using Bruker Daltonics flex Analyser and ESI HR-MS data were recorded using Waters QTOF Micro YA263 spectrometer. Cyclic voltammograms were recorded using a platinum working electrode, a platinum wire counter electrode and a Ag/AgCl reference electrode in Bioanalytical Systems EC epsilon. The measurements were carried out in CH_2Cl_2 solution using 0.1 M Bu_4NPF_6 as the supporting electrolyte at a scan rate of 0.1 V/s. Peak potentials were determined from differential pulse voltammetry experiments. The Fc/Fc^{+} redox couple was used as an internal standard. All solvents and chemicals were of reagent grade quality, obtained commercially and used without further purification except as noted. For spectral measurements, anhydrous dichloromethane was obtained by refluxing and distillation over CaH_2. Dry THF was obtained by refluxing and distillation over pressed Sodium metal. Thin layer chromatography (TLC) was carried out on alumina sheets coated with silica gel 60 F_{254} (Merck 5554) and gravity column chromatography were performed using Merck Silica Gel 230-400 mesh. Aluminum Oxide (Basic) grade II was purchased from Sigma Aldrich.

1.2 Theoretical Calculation

All DFT calculations were performed using the Gaussian 16 suite of programs.[1] The geometries were optimized using the B3LYP functional with LACVP basis set comprising the LanL2DZ-Los Alamos effective core potential for Cu and a 6-31g(d,p) basis set for the other atoms.[2] Electronic absorption spectra, singlet vertical excitation energies, and oscillator strengths were computed using time-dependent density functional theory (TD-DFT) based on ground-state geometries. [3] Solvent effects were modeled using the polarized continuum model (PCM) with dichloromethane as the solvent.[4] Fragment contributions to the macrocycle were analyzed using QMForge.[5] Nucleus-independent chemical shift (NICS) values [6] were calculated along the π-conjugation pathway (1–8 Å above and below the molecular plane) following the Stranger method [7], with NMR shielding tensors determined using the Gauge-Independent Atomic Orbital (GIAO) method along the same trajectory [8]. Aromaticity indices, including the harmonic oscillator model of aromaticity (HOMA), electron localization function (ELF), multi-center index (MCI), AV1245, AVmin, and localized orbital locator (LOL) topology analyses, were evaluated alongside Wiberg bond index decomposition using natural bond orbital (NBO) analysis with Multiwfn.[9] The anisotropy of the induced current density (ACID) was visualized through ACID plots.[10]

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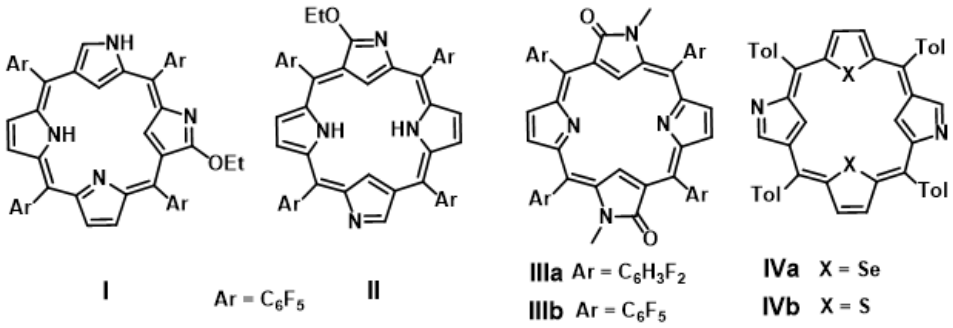
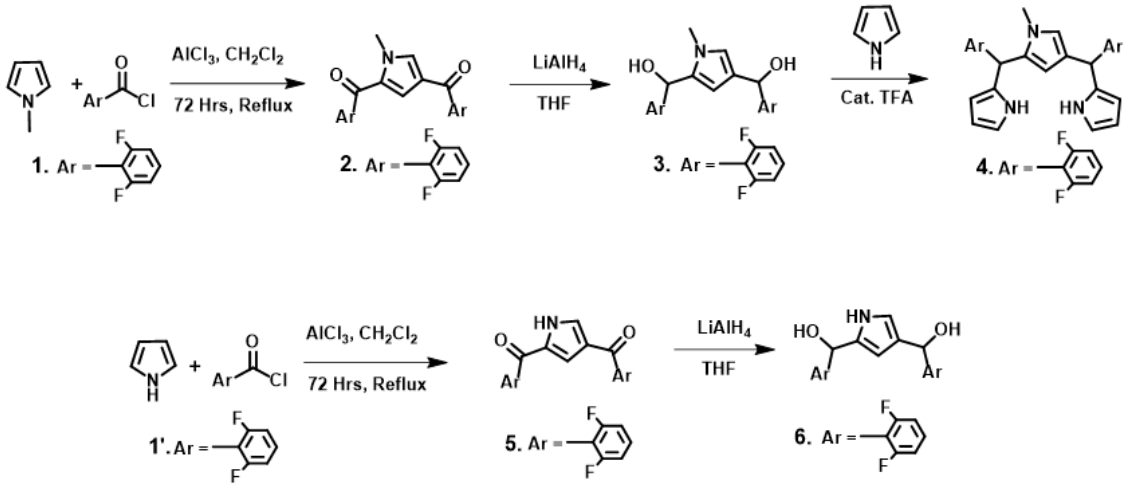
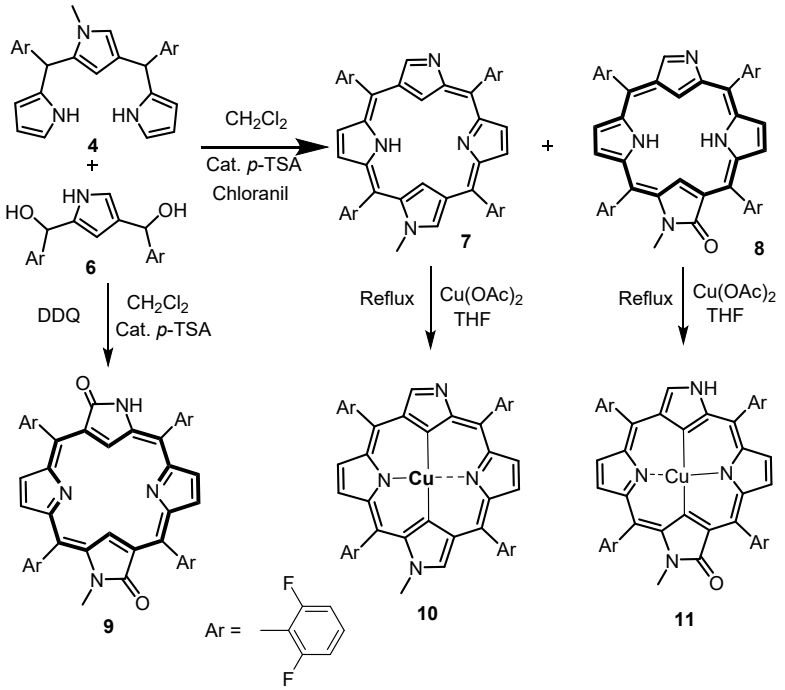


Chart S1 Literature known doubly N-confused porphyrinoids

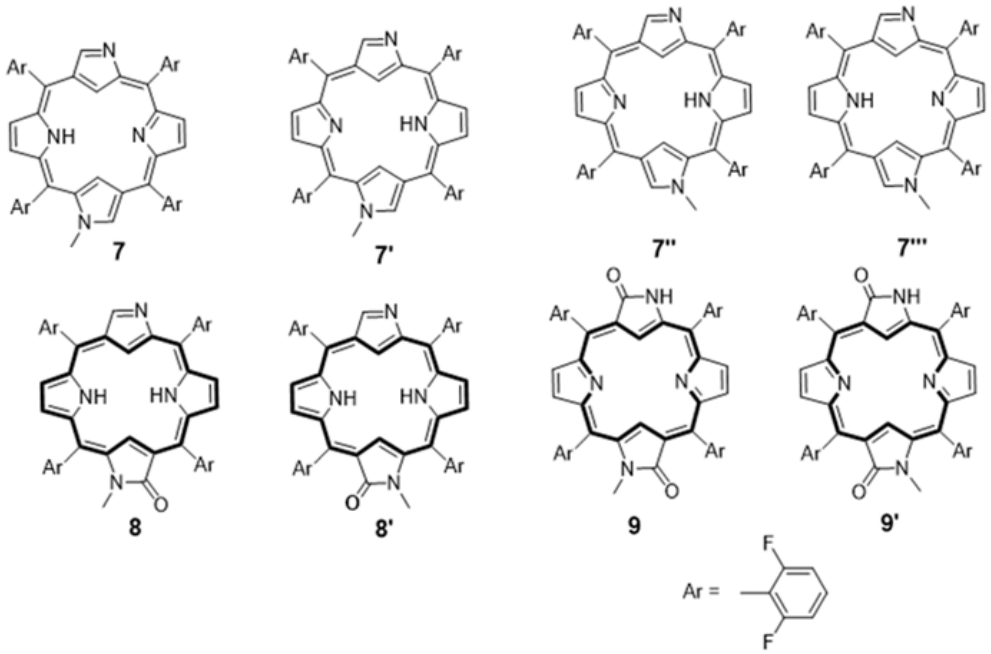
1.3 Synthesis



Scheme S1. Synthesis of all precursors used for the macrocycles reported in the manuscript



Scheme S2. Synthesis of macrocycles **7**-**11**



Scheme S3. Plausible isomers and Tautomers of macrocycles **7** - **9**

General Synthesis of 7-9:

Synthesis of 7-8: Tripyrrane **4** (0.463 g, 1 mmol) and diol **6** (0.380 g, 1 mmol) were taken in a round bottom flask, to it 100 mL of dry DCM was added and stirred for 15 minutes under nitrogen atmosphere to get a clear solution. After that *p*-Toluene sulfonic acid (0.035 g, 0.185 mmol) was added to the reaction mixture and stirred for 90 minutes under dark condition. Chloranil (735 mg, 2.5 mmol) was added to the reaction mixture and refluxed for 60 minutes. After complete removal of solvent from crude mixture by

rotary evaporator, the compound was purified using basic alumina followed by preparative thin layer chromatography (PTLC) leading to extra pure macrocycle **7** as an air-stable brown solids in 5% yields and extra pure macrocycle **8** as green solids in 15% yield.

[**7**] R_f = 0.4 (C_6H_{14}/CH_2Cl_2 = 80:20). Yield. ~40 mg (~5.2 %). Mp > 350°C.

HRMS (ESI-TOF) *m/z* calc. for $C_{45}H_{25}F_8N_4$ $[M+H]^+$, 773.1951; found, 773.1950.

UV-vis (CH_2Cl_2, λ [nm], (ϵ [$M^{-1}cm^{-1} \times 10^4$]), 298K): 454 (4.07), 524 (3.62). ^{1}H NMR ($CDCl_3$, 600 MHz): δ 14.17 (s, 1H), 7.38 (m, 2H), 7.20 (m, 2H), 7.00 (m, 2H), 6.93 (m, 4H), 6.84 (s, 1H), 6.66 (m, 2H), 6.24 (s, 1H), 6.19 (s, 1H), 6.15 (d, *J* = 4.8 Hz,1H), 6.10 (d, *J* = 4.8 Hz,1H), 5.81 (d, *J* = 4.8 Hz,1H), 5.75 (s, 1H), 5.74 (d, *J* = 4.8 Hz, 1H), 3.77 (s, 3H). ^{13}C {^{1}H} NMR ($CDCl_3$, 150 MHz): δ 162.46, 162.40, 161.81, 161.76, 161.68, 161.62, 161.57, 161.04, 160.85, 160.42, 159.77, 159.60, 159.05, 155.21, 154.17, 152.54, 151.81, 151.59, 145.71,145.52, 140.78, 139.52, 138.34, 137.06, 136.79, 133.95, 133.02, 129.46, 129.37, 128.19,124.32, 122.68, 121.28,120.46,119.29, 118.03, 113.30, 110.86, 110.71, 110.65, 110.27, 107.62, 107.43, 107.40, 34.05.

[**8**] R_f = 0.4 (C_6H_{14}/CH_2Cl_2 = 80:20). Yield. ~118 mg (~15 %). Mp > 350°C.

HRMS (ESI-TOF) *m/z* calc.for $C_{45}H_{25}F_8N_4O$ $[M+H]^+$, 789.1901; found, 789.1900.

UV-vis (CH_2Cl_2, λ [nm], (ϵ [$M^{-1}cm^{-1} \times 10^4$]), 298K): 438 (6.58), 652 (0.79), 717 (0.95). ^{1}H NMR ($CDCl_3$, 600 MHz): δ 8.90 (s, 1H), 7.54 (m, 4H), 7.45 (m, 2H), 7.37 (d, *J* = 5.4 Hz, 1H), 7.34 (d, *J* = 5.4 Hz, 1H), 7.17 (m, 4H), 7.10 (m, 2H), 7.05 (d, *J* = 5.4 Hz, 1H), 7.01 (d, *J* = 5.4 Hz, 1H), 3.46 (s, 3H), -2.37 (s, 1H), -2.59 (s, 1H), -3.91 (s, 1H), -3.96 (s, 1H). ^{13}C {^{1}H} NMR ($CDCl_3$, 150 MHz): δ 170.19, 164.80, 162.70,162.65,162.21,162.01, 161.96, 161.02, 160.56, 160.30, 153.54, 151.86, 146.49, 141.46, 139.31, 134.25, 131.02, 130.79, 130.75, 130.62, 129.49, 129.03, 128.49, 128.30, 125.17, 123.98,123.48, 118.77, 114.08, 114.08, 112.05, 111.99, 111.96, 111.85, 111.35, 111.21, 111.00, 114.08, 100.84, 101.13, 97.83, 96.56, 95.31, 37.18.

Synthesis of 9: Tripyrrane **4** (0.463 g, 1 mmol) and diol **6** (0.380 g, 1 mmol) were taken in a round bottom flask, to it 100 mL of dry DCM was added and stirred for 15 minutes under nitrogen atmosphere to get a clear solution. After that *p*-Toluenesulfonic acid (0.035 g, 0.185 mmol) was added to the reaction mixture and stirred for 90 minutes under dark condition. DDQ (765 mg, 2.5 mmol) was added to the reaction mixture and stirred for 60 minutes. After complete removal of solvent from crude mixture by rotary evaporator, the compound was purified using basic alumina followed by preparative thin layer chromatography (PTLC) leading to extra pure macrocycle **9** as green solids in 17% yield.

[**9**] R_f = 0.4 (C_6H_{14}/CH_2Cl_2 = 80:20). Yield. ~135 mg (~17 %). Mp > 350°C.

HRMS (ESI-TOF) *m/z* calc.for $C_{45}H_{23}F_8N_4O_2$ $[M+H]^+$, 803.1771; found, 803.1770.

UV-vis (CH_2Cl_2, λ [nm], (ϵ [$M^{-1}cm^{-1} \times 10^4$]), 298K): 475 (3.29), 599 (0.39), 1066(0.52). ^{1}H NMR (CD_2Cl_2, 600 MHz): δ 12.45 (s, 1H), 12.14 (s, 1H), 8.44 (s, 1H), 7.55 (m, 5H), 7.30 (m, 3H), 7.24 (m, 4H), 5.98 (d, *J* = 4.8 Hz, 1H), 5.92 (d, *J* = 4.8 Hz,1H), 5.55 (d, *J* = 4.8 Hz,1H), 5.53 (d, *J* = 4.8 Hz,1H), 3.51 (s, 3H). ^{13}C {1H} NMR (CD_2Cl_2, 150 MHz): δ 167.25, 162.52, 162.22, 162.00, 160.94,160.56, 160.30, 156.38, 151.91, 150.54, 148.23, 142.88, 140.93, 139.36, 136.30,135.10,

134.92, 133.52, 132.19, 132.12, 131.64, 131.77, 131.10, 130.89, 130.50, 129.20, 129.14, 128.71, 128.13, 126.92, 126.29, 123.96, 123.51, 123.03, 122.55, 116.91,115.82, 113.76, 112.35, 113.76, 112.35, 112.33, 97.17, 94.22, 38.00.

Synthesis of **10:** A mixture of compound **7** (20 mg, 25.9 µmol), $Cu(OAc)_2$ (23.5 mg, 129 µmol), and dry THF (20 mL) was refluxed for 8 hours under nitrogen atmosphere. The solvent was removed by evaporation. Silica gel column chromatography with (5% ethyl acetate/CH_2Cl_2) gave a brown red colored fraction. Concentration of the fraction and recrystallization of the residue from DCM- hexane afforded Cu-complex **10** as brown solids.

[**10**] Yield. 18 mg (84%). Mp > 350˚C, HRMS (ESI-TOF) m/z: Calc. for $C_{45}H_{21}CuF_8N_4$ $[M]^+$,832.0934; Found, 832.0933. UV-vis (CH_2Cl_2, λ [nm], (ϵ [$M^{-1}cm^{-1} \times 10^4$]), 298K): 425 (4.16), 455 (6.50). ^1H NMR ($CDCl_3$, 600 MHz): δ 7.54 (d, *J* = 2.4 Hz, 1H), 7.27 (d, *J* = 1.8 Hz, 1H), 7.15 (m, 4H), 7.05 (d, *J* = 1.8 Hz, 1H), 7.00 (d, *J* = 2.4 Hz, 1H), 6.82 (s, 1H), 6.65 (m, 8H), 6.52 (s, 1H), 2.76 (s, 3H).

Synthesis of **11: 11** was obtained by refluxing **8** (20 mg, 25.3 µmol) with an excess of Cu $(OAc)_2$ (23 mg, 126.6 µmol) in 5 mL THF for 1 hour. After that solvent was removed, and then hexane was added to extract a red residue that precipitated after solvent volume reduction. This was washed several times to remove unreacted salt. The residue was then purified by silica gel column chromatography (1% ethyl acetate/CH_2Cl_2) and recrystallized from DCM- hexane solution to obtain Cu (III) complex **11** as reddish-brown solids.

[**11**] Yield. 17.4 mg (81%). Mp > 350˚C, HRMS (ESI-TOF) m/z: Calc. for $C_{45}H_{21}CuF_8N_4O$ $[M]^+$,848.0884; Found, 848.0883. UV-vis (CH_2Cl_2, λ [nm], (ϵ [$M^{-1}cm^{-1} \times 10^4$]), 298K): 339 (8.25), 456 (6.66), 535 (2.56), 728 (1.53). ^1H NMR ($CDCl_3$, 600 MHz): δ 8.31 (s, 1H), 8.10 (s, 1H), 8.02 (d, *J* = 5.2 Hz, 1H), 7.94 (d, *J* = 5.6 Hz, 1H), 7.86 (d, *J* = 5.2 Hz, 1H), 7.79 (d, *J* = 5.2 Hz, 1H), 7.64 (m, 4H), 7.52 (m, 3H), 7.16 (m, 5H), 3.92 (s, 3H).

2. Supplementary Data:

2.1 Mass Spectra

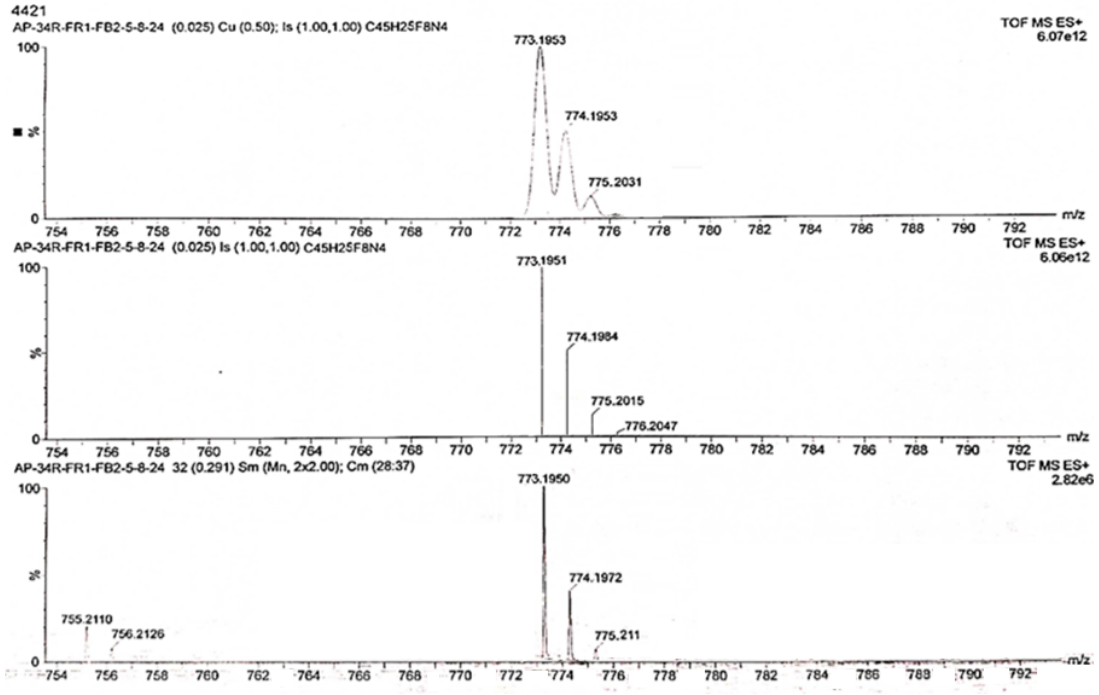


Fig. S1 HRMS Spectra of **7**

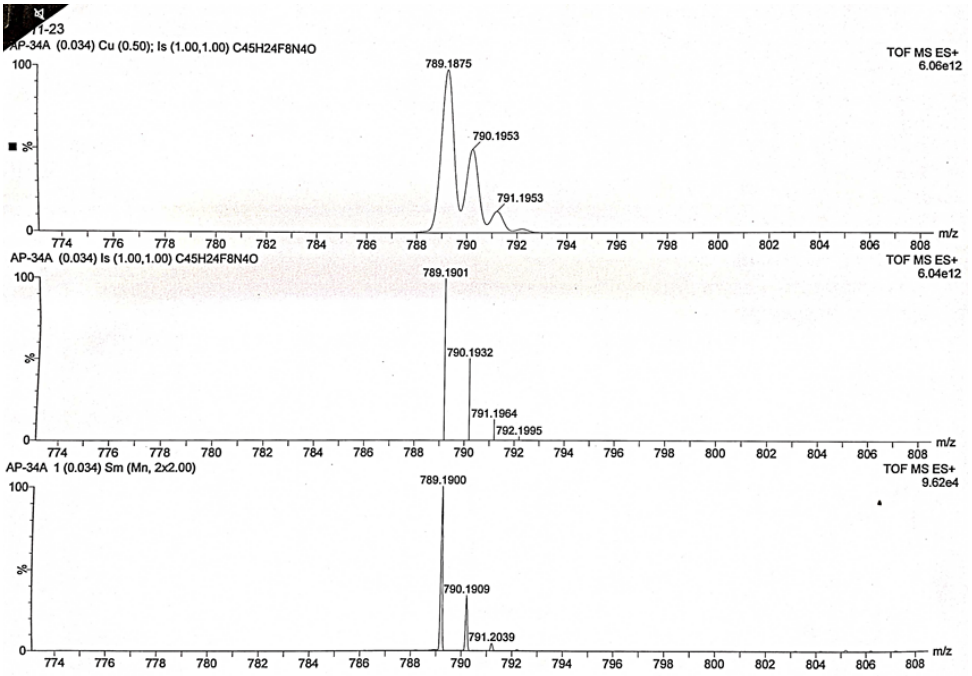


Fig. S2 HRMS Spectra of **8**

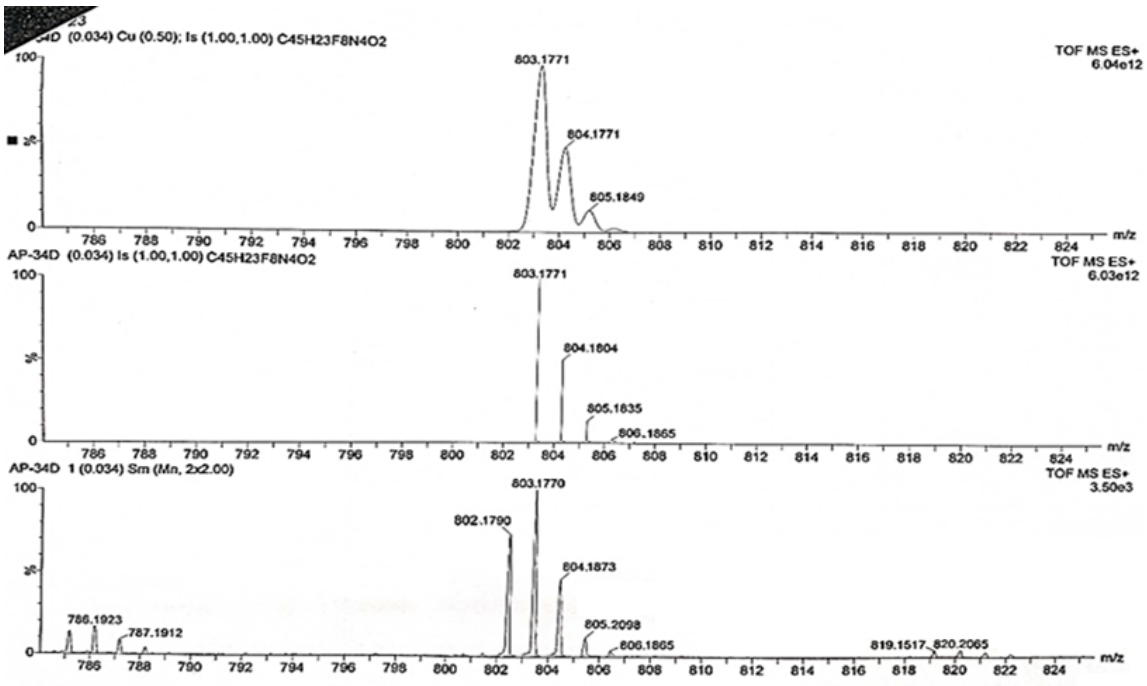


Fig. S3 HRMS Spectra of **9**

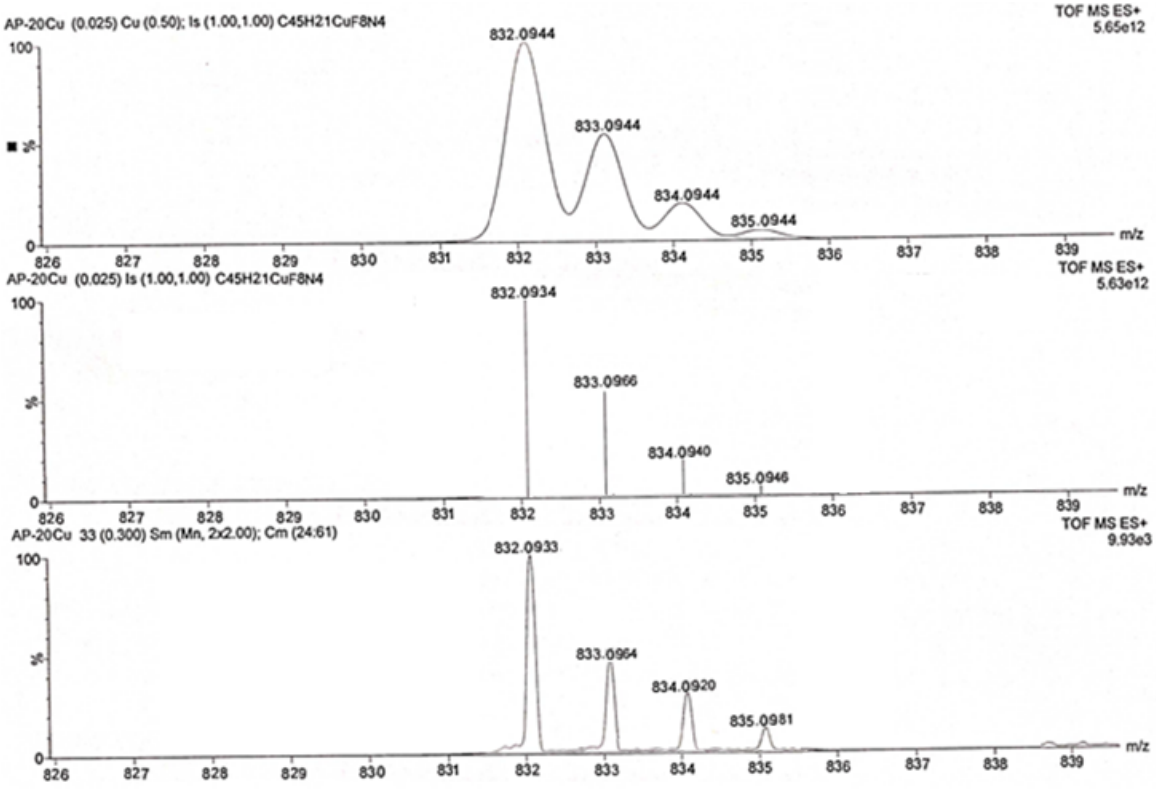


Fig. S4 HRMS Spectra of **10**

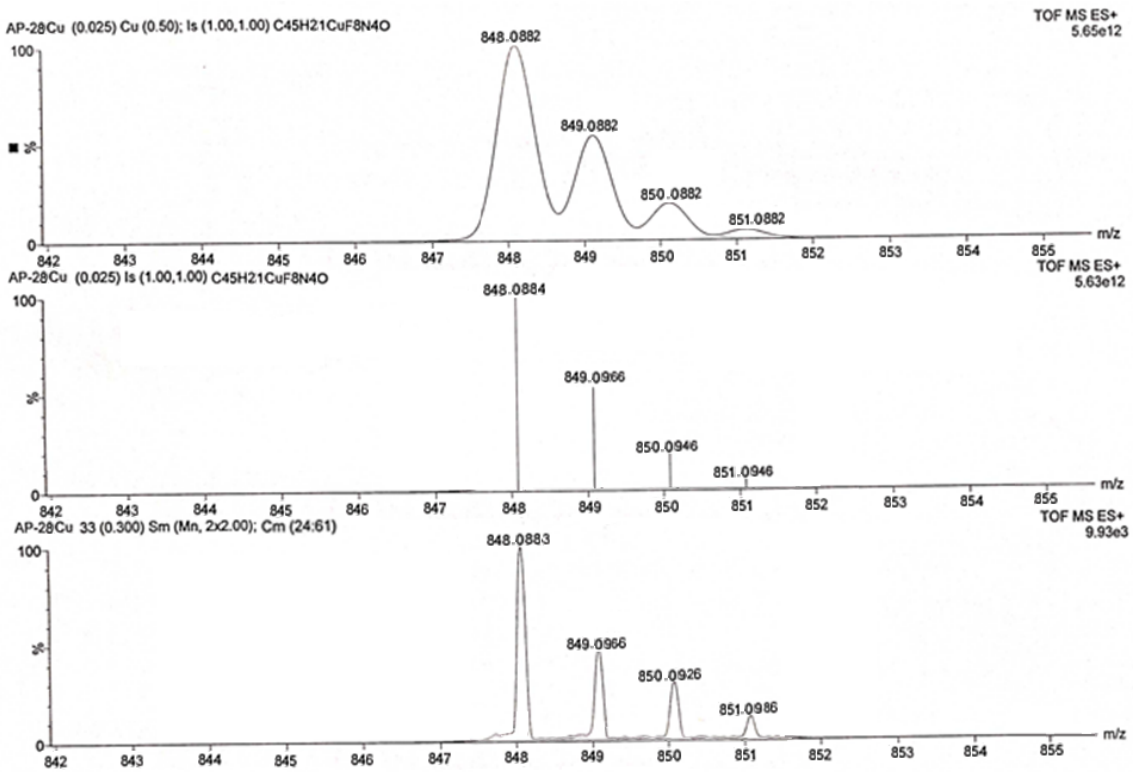


Fig. S5 HRMS Spectra of **11**

2.2 IR spectra:

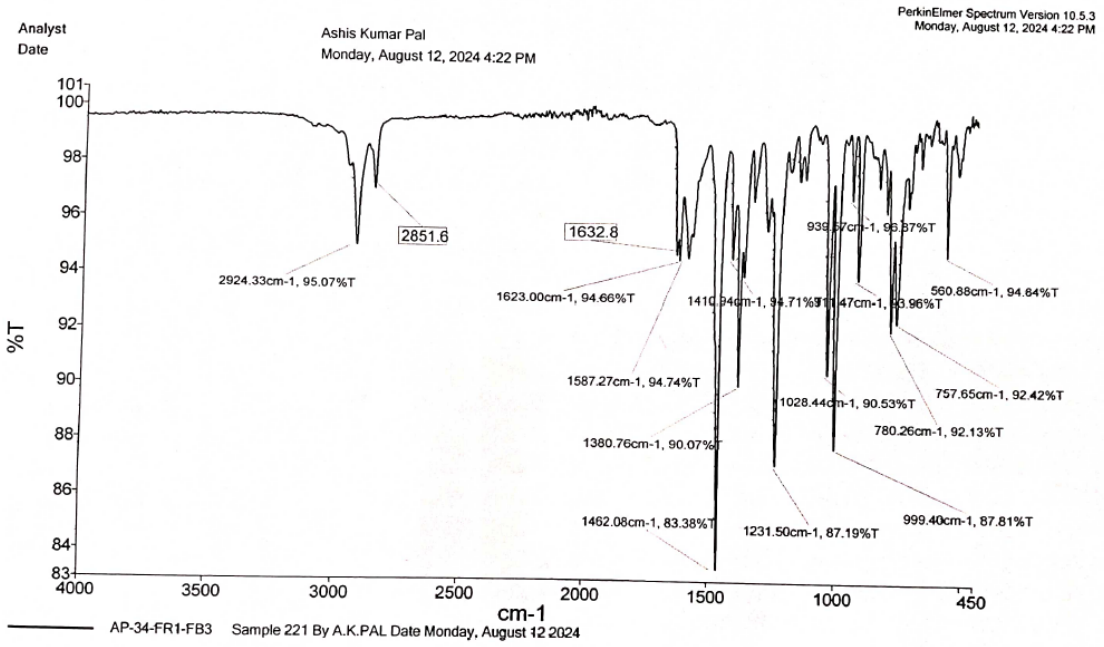


Fig. S6 IR Spectrum of **7**

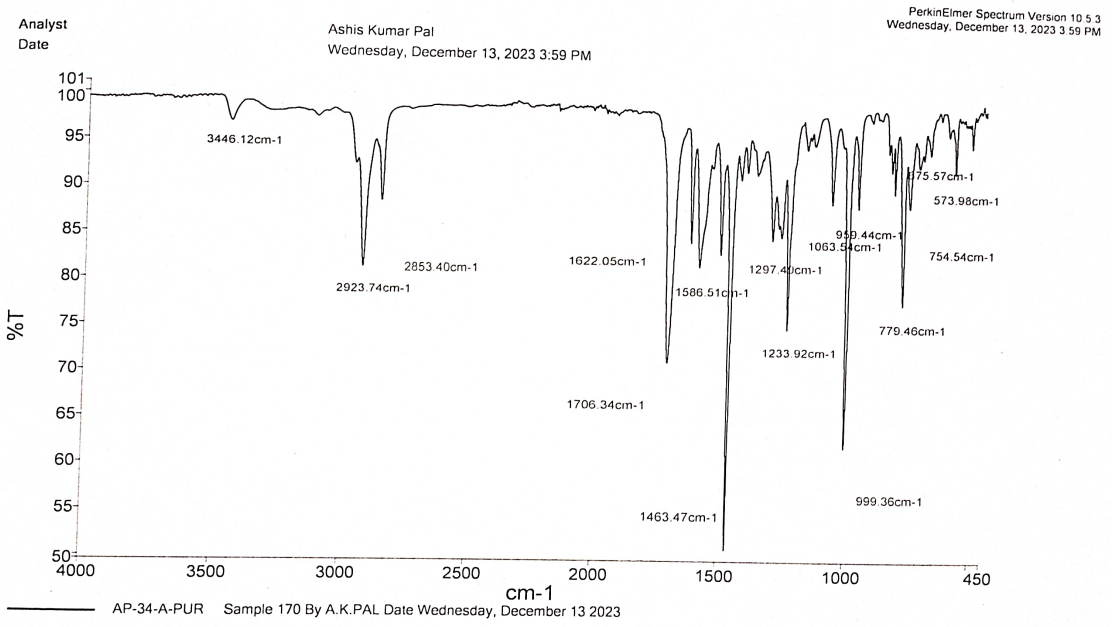


Fig. S7 IR Spectrum of **8**

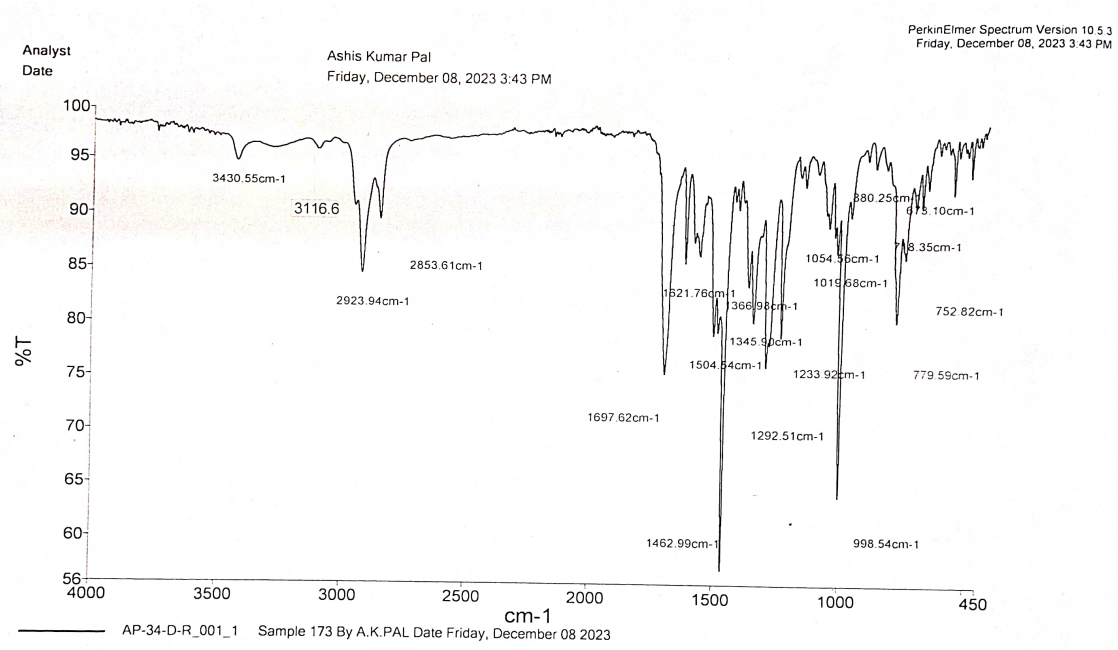


Fig. S8 IR Spectrum of **9**

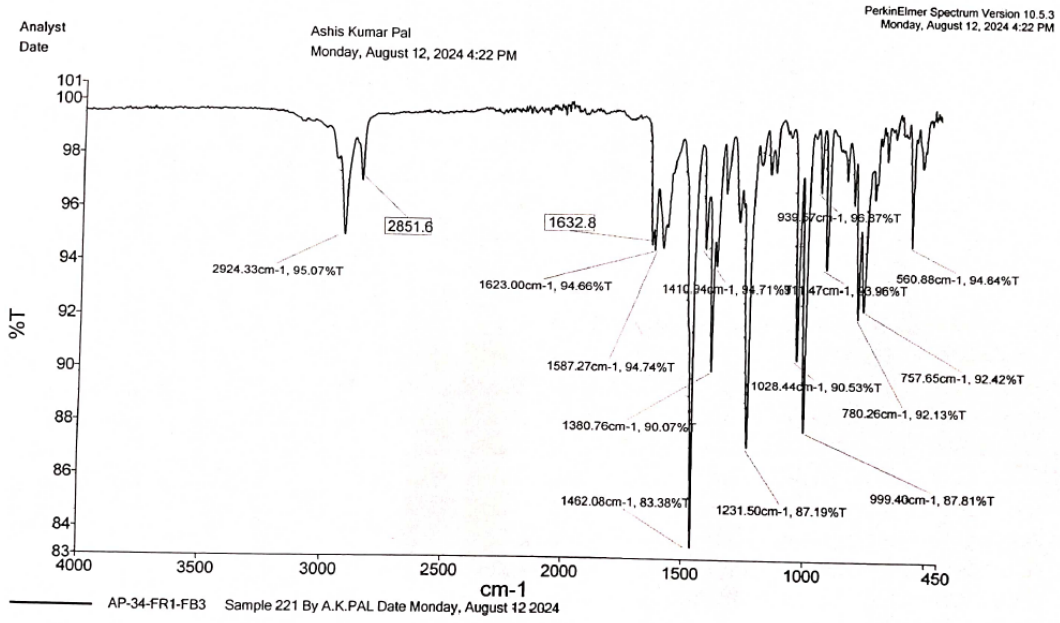


Fig. S9 IR Spectrum of **10**

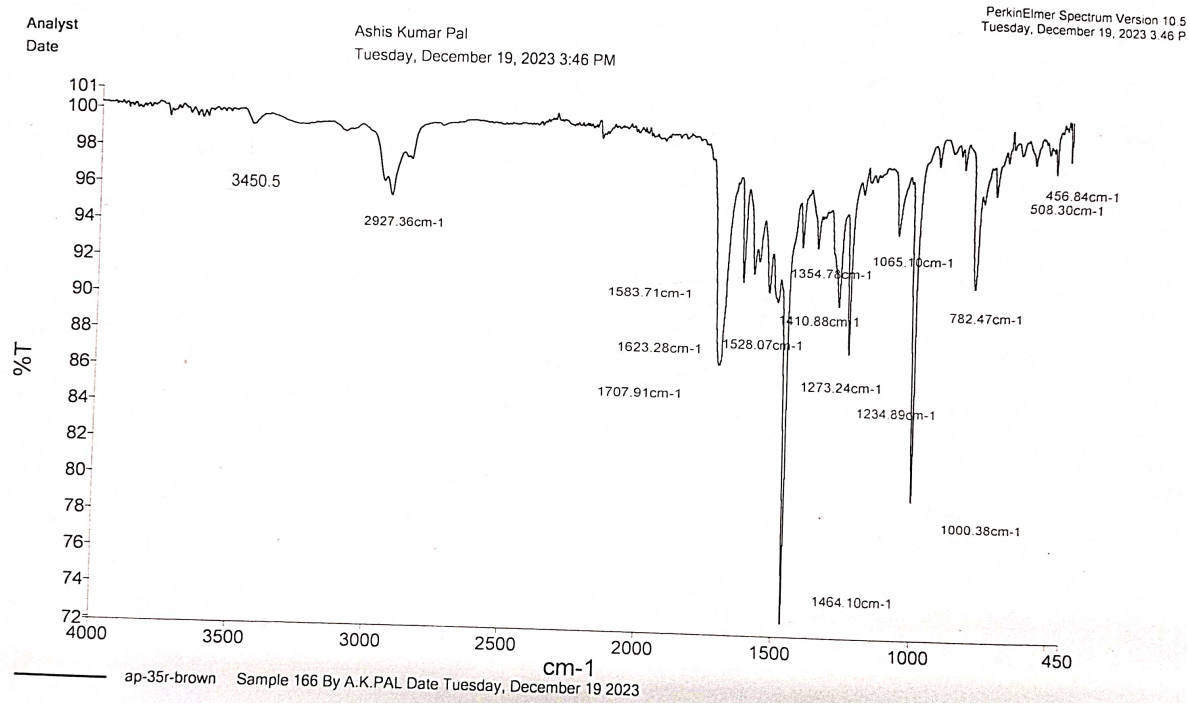


Fig. S10 IR Spectrum of **11**

2.3 UV-vis spectra:

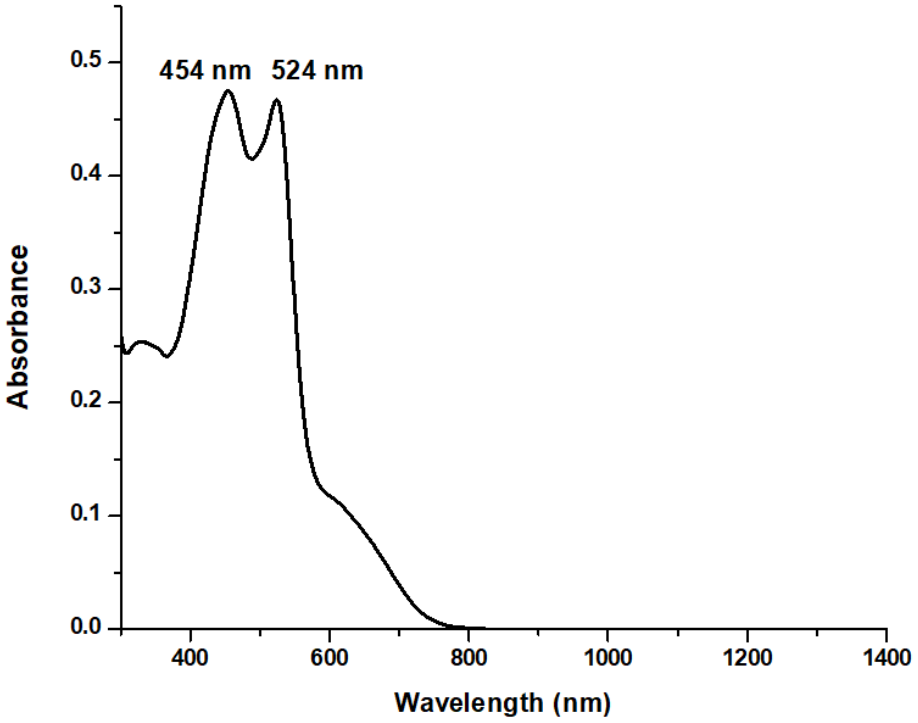


Fig. S11 UV-vis Spectra of **7** in CH_2Cl_2 at 298 K

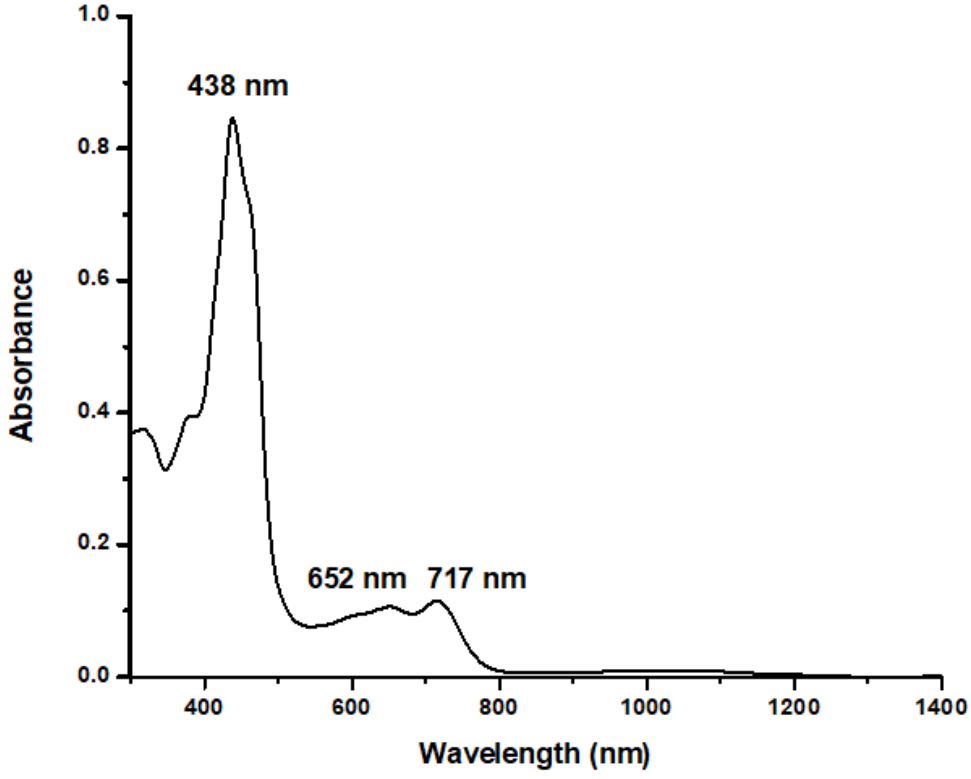


Fig. S12 UV-vis Spectrum of **8** in CH_2Cl_2 at 298 K

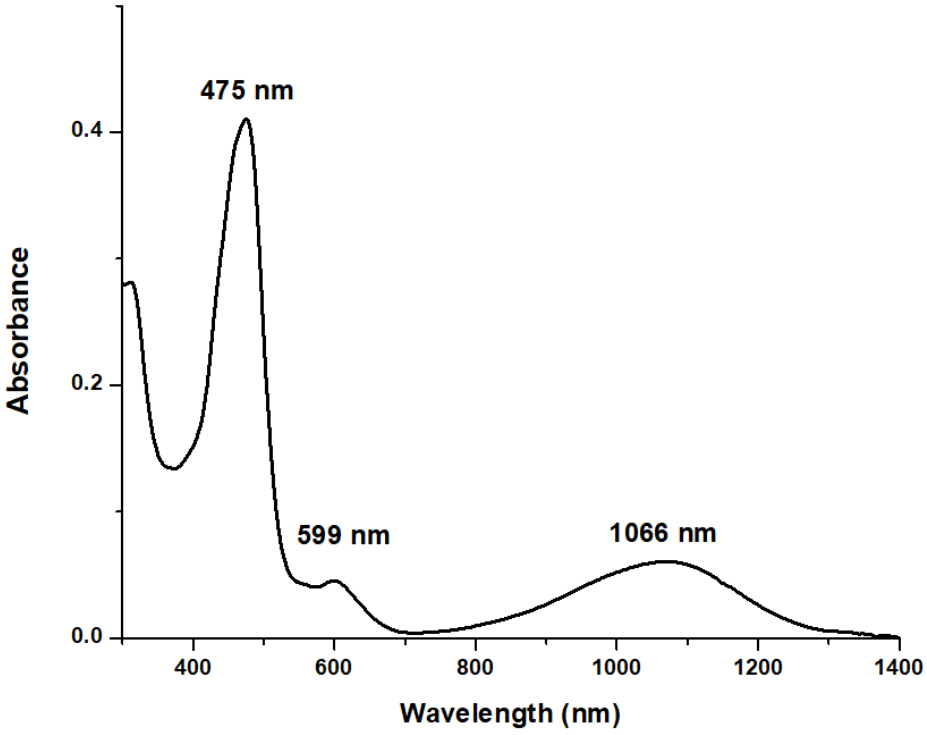


Fig. S13 UV-vis Spectra of **9** in CH_2Cl_2 at 298 K

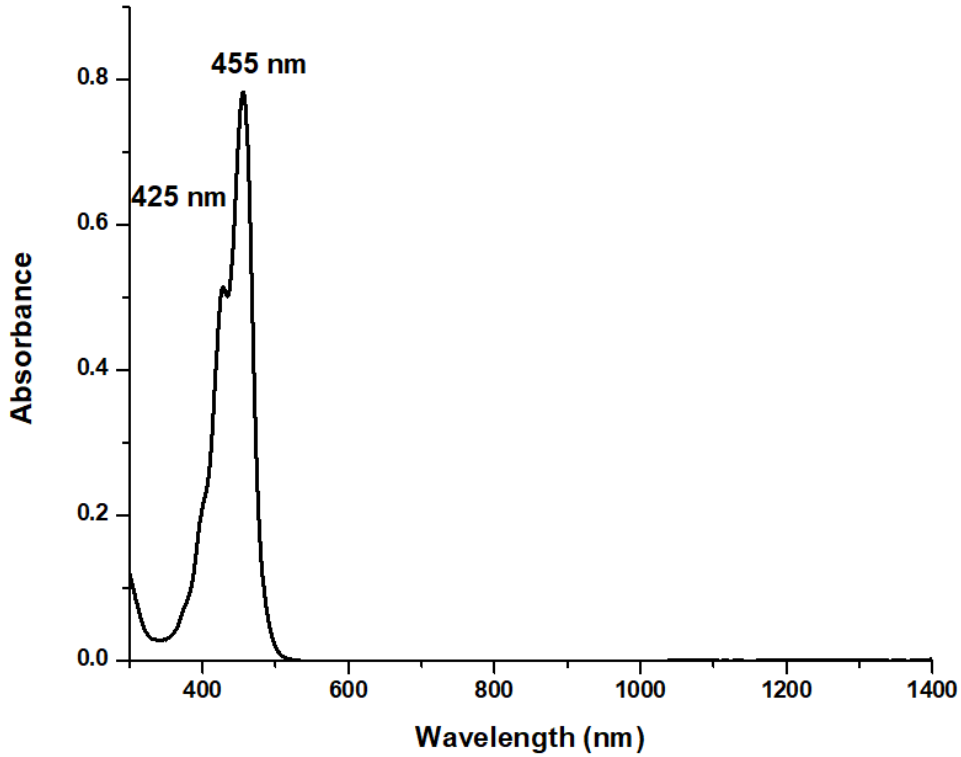


Fig. S14 UV-vis Spectra of **10** in CH_2Cl_2 at 298 K

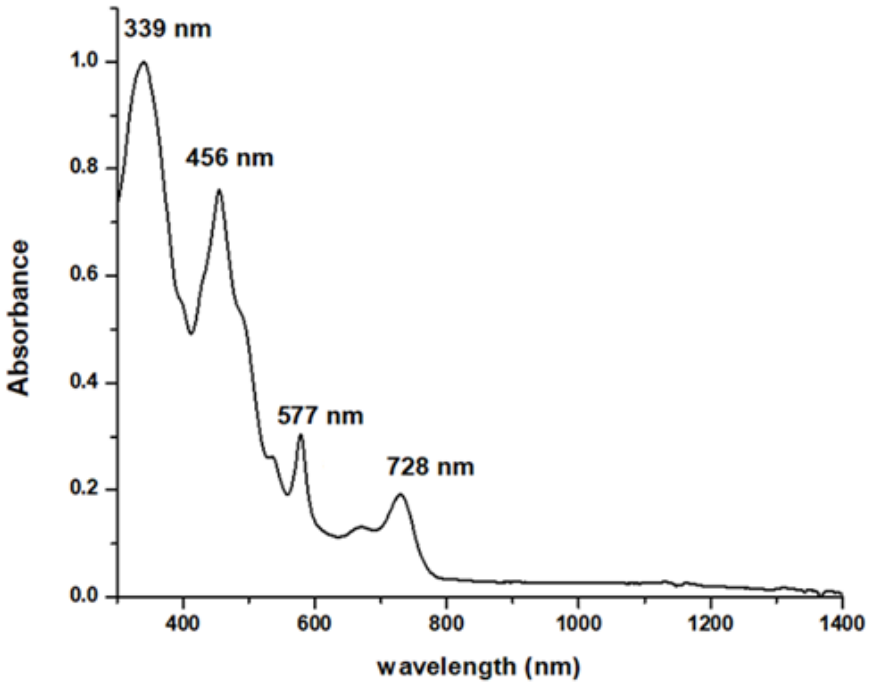


Fig. S15 UV-vis Spectra of **11** in CH_2Cl_2 at 298 K

2.4 NMR spectra:

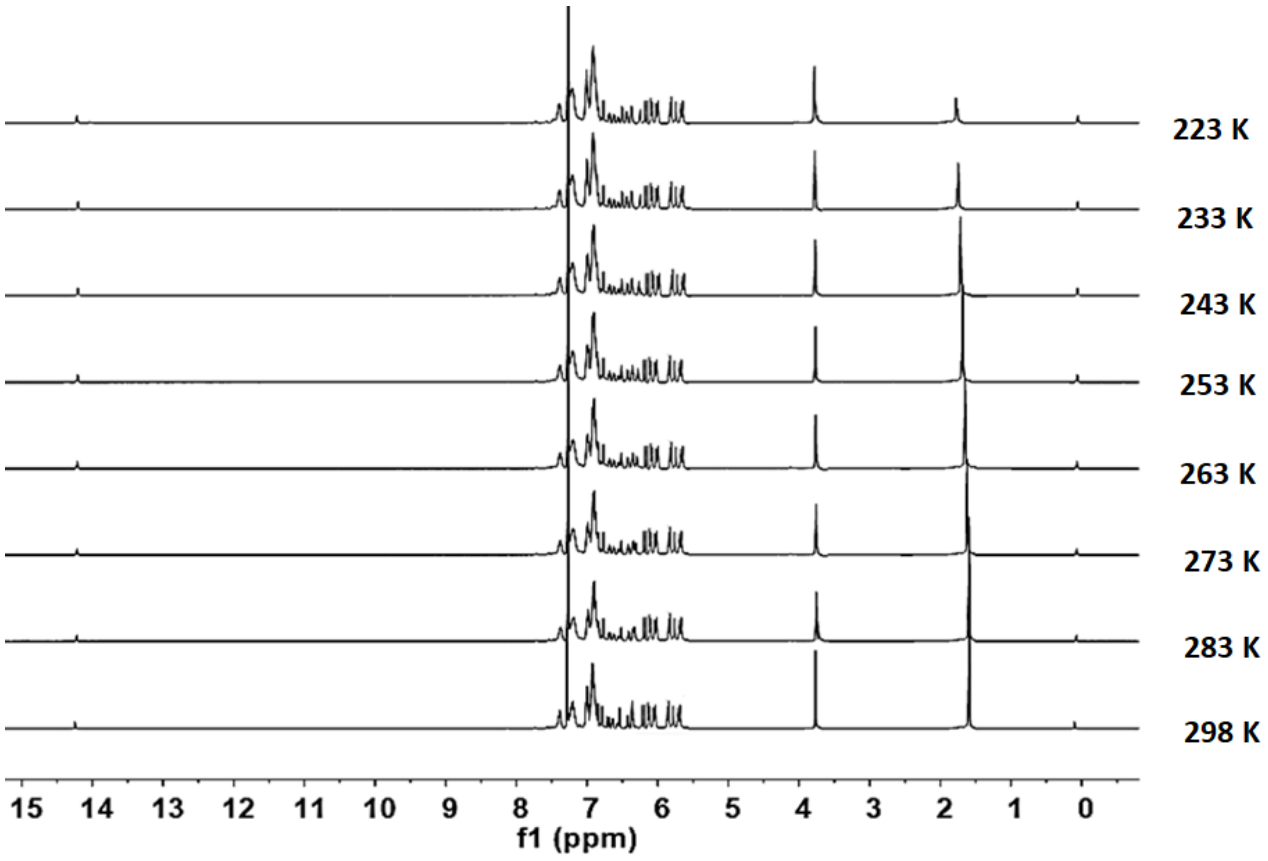


Fig. S16 Low VT ^1H NMR spectra of **7** in $CDCl_3$

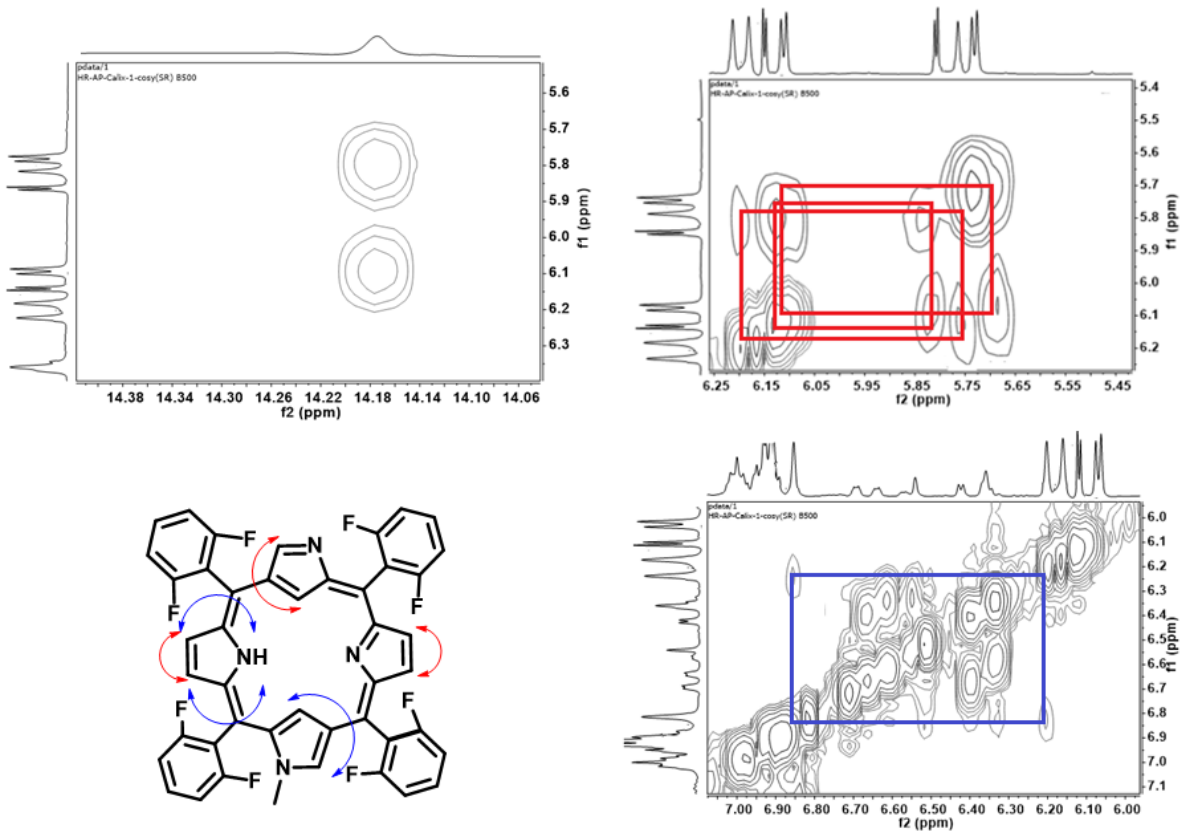


Fig. S17 ^{1}H -^{1}H 2D COSY NMR spectra of **7** in $CDCl_3$ at 298 K

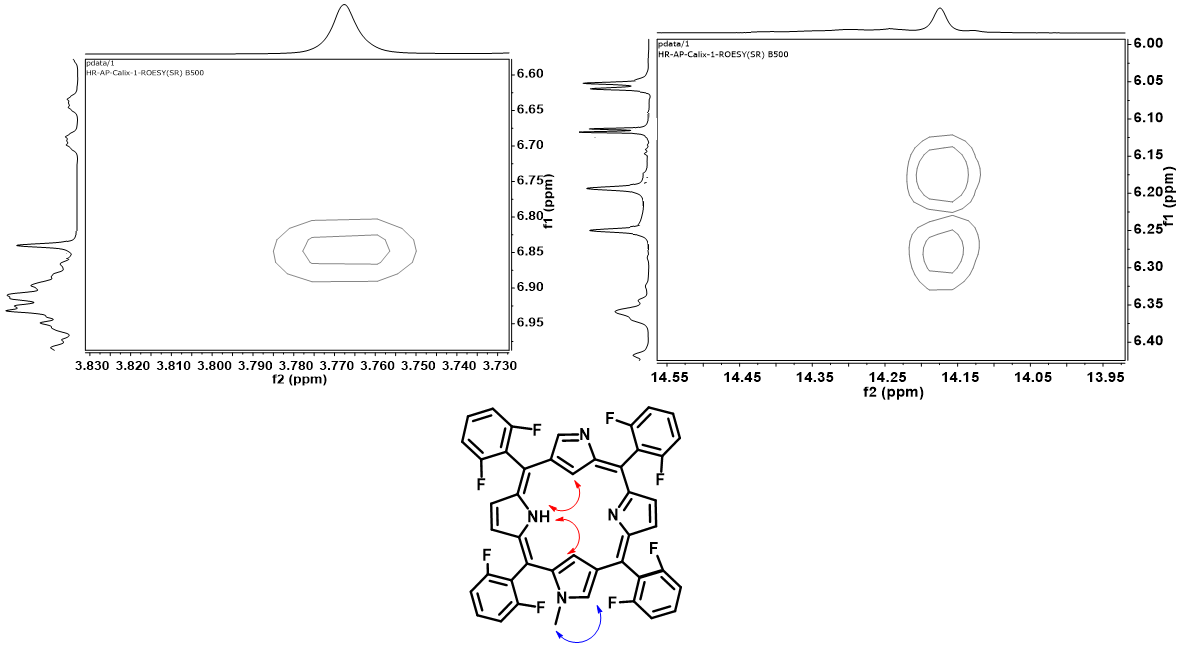


Fig. S18 ^{1}H -^{1}H 2D NOESY NMR spectra of **7** in $CDCl_3$ at 298 K

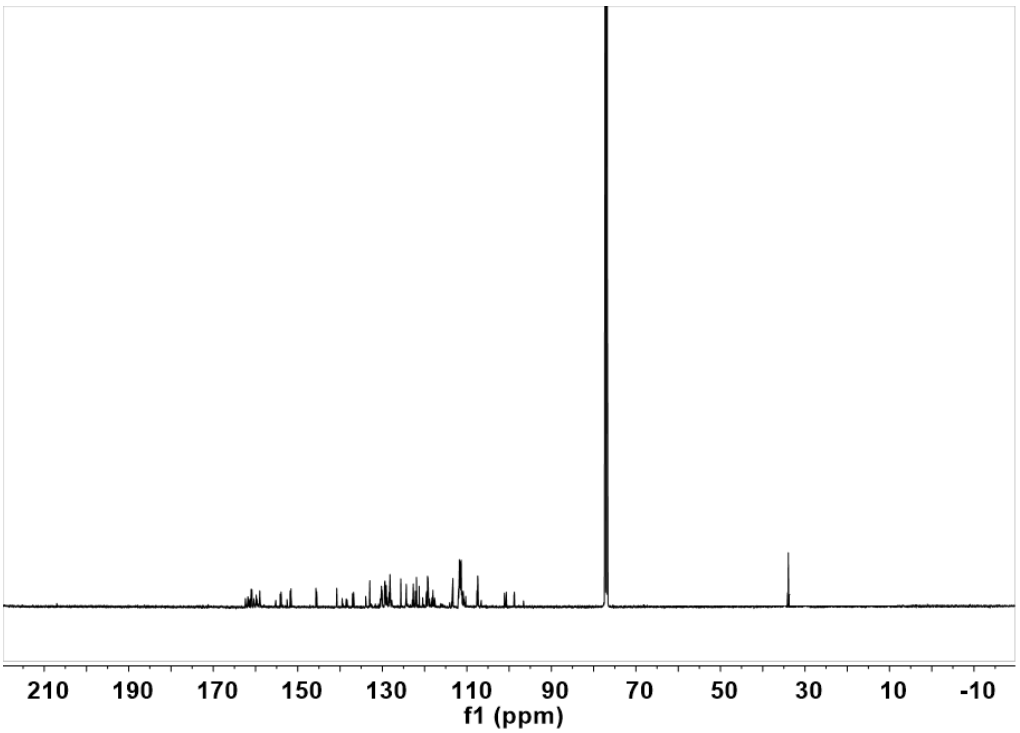
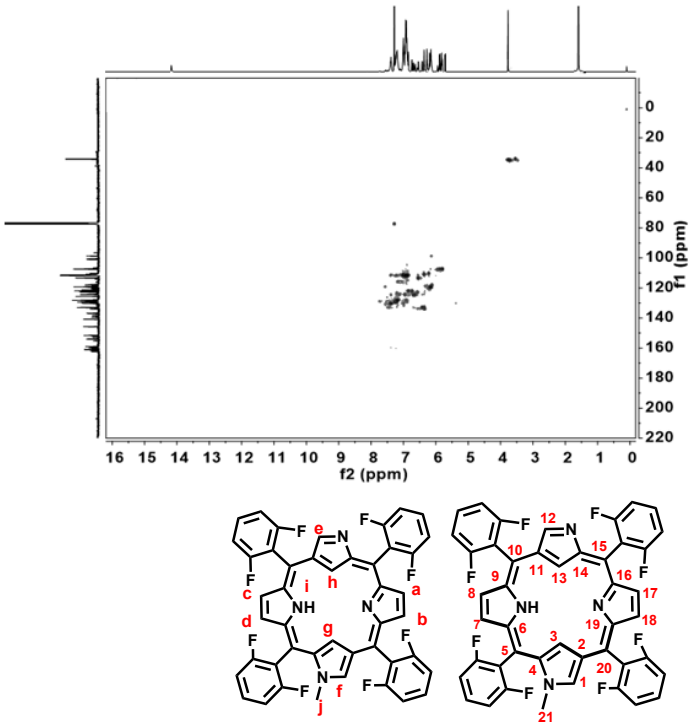
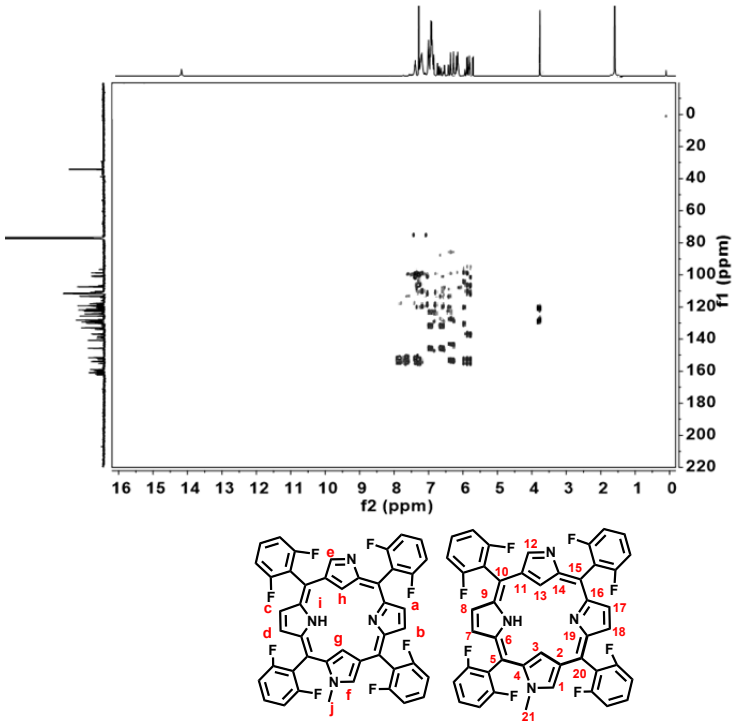


Fig. S19 ^{13}C NMR spectra of **7** in $CDCl_3$ at 298 K



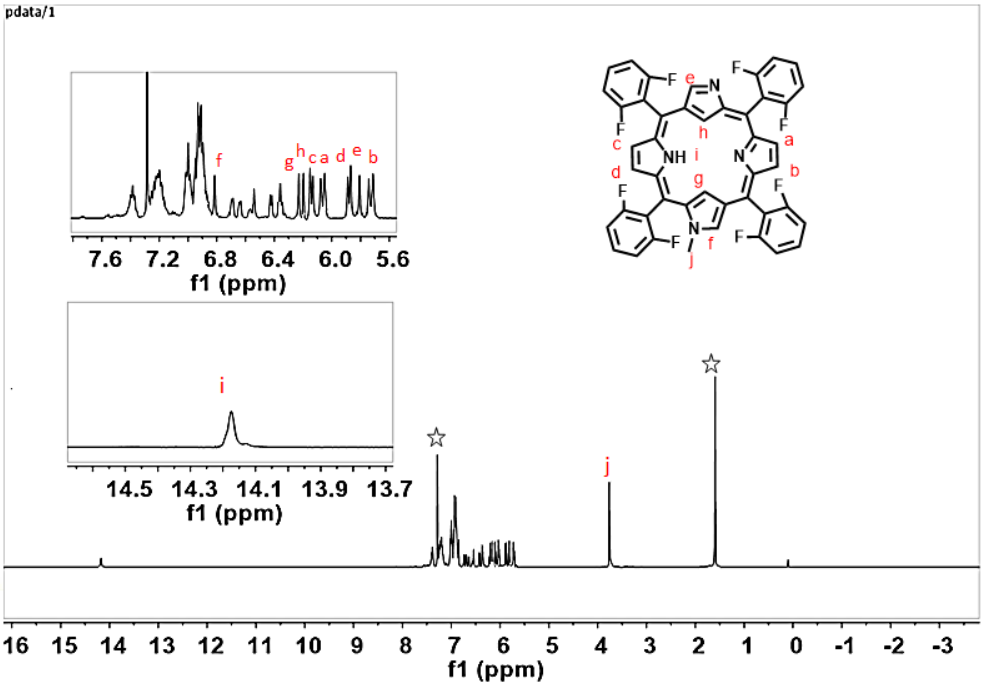
^{1}H ppm(Positions)	^{13}C ppm(Positions)
6.15 (c)	110.86 (8)
6.10 (a)	110.27 (17)
6.19 (h)	110.65 (13)
6.24 (g)	110.71 (3)
5.74 (b)	107.43 (18)
5.81 (d)	107.40 (7)
5.75 (e)	107.62 (12)
6.84 (f)	110.50 (1)
3.77 (j)	34.05 (21)
14.17 (i)	

Fig. S20 ^{1}H -^{13}C 2D HSQC NMR spectra of **7** in $CDCl_3$ at 298 K



^{1}H ppm(Positions)	^{13}C ppm(Positions)
6.10 (a)	107.43 (18), 140.83 (16)
6.15 (c)	107.40 (7), 158.99 (9)
6.19 (h)	138.34 (11),107.62 (12), 128.75 (14)
6.24 (g)	121.28 (4), 130.05 (2)
5.74 (b)	110.27 (17), 137.06 (19)
5.81 (d)	110.86 (8), 151.59 (6)
5.75 (e)	138.34 (11),110.65 (13), 128.75 (14)
6.84 (f)	130.05 (2)
3.77 (j)	121.28 (4), 130.05 (2)

Fig. S21 ^{1}H -^{13}C 2D HMBC NMR spectra of **7** in $CDCl_3$ at 298 K



^{1}H Positions	ppm
a	6.10 (d)
c	6.15 (d)
h	6.19 (s)
g	6.24 (s)
b	5.74 (d)
d	5.81 (d)
e	5.75 (s)
f	6.84 (s)
j	3.77 (s)
i	14.17 (s)

Fig. S22 Complete ^{1}H NMR spectral assignment of **7** in $CDCl_3$ at 298 K

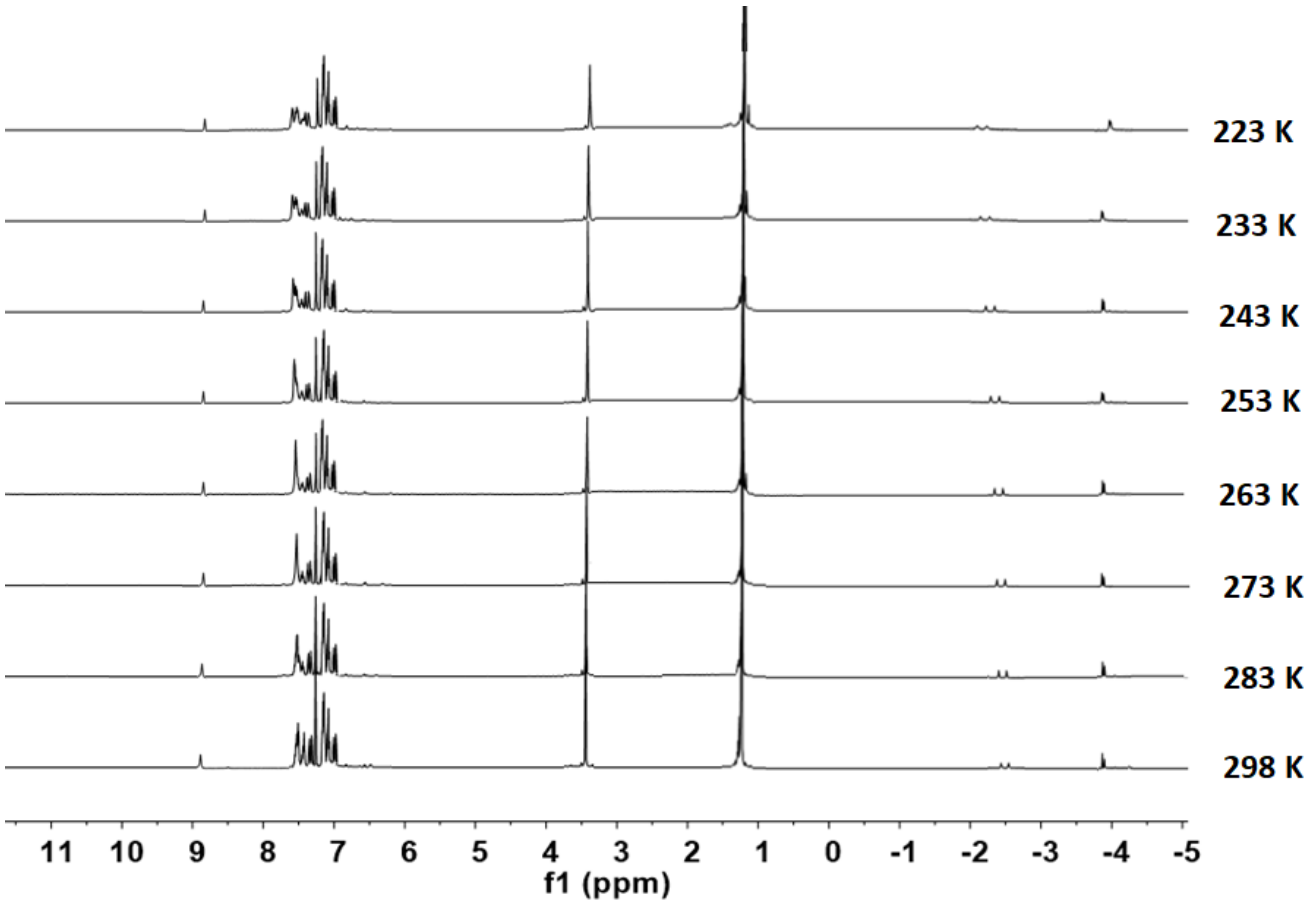


Fig. S23 Low VT ^{1}H NMR spectra of **8** in $CDCl_3$

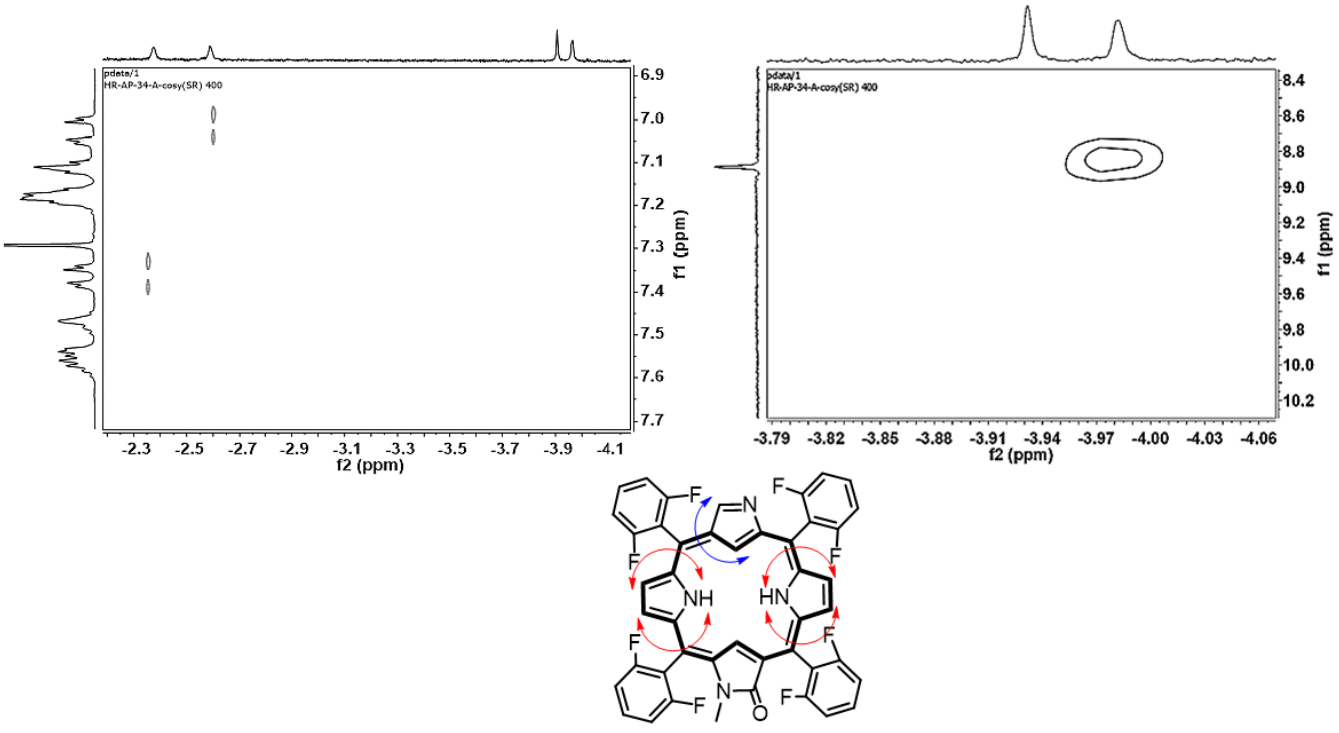


Fig. S24 ^{1}H -^{1}H 2D COSY NMR spectra of **8** in $CDCl_3$ at 298 K

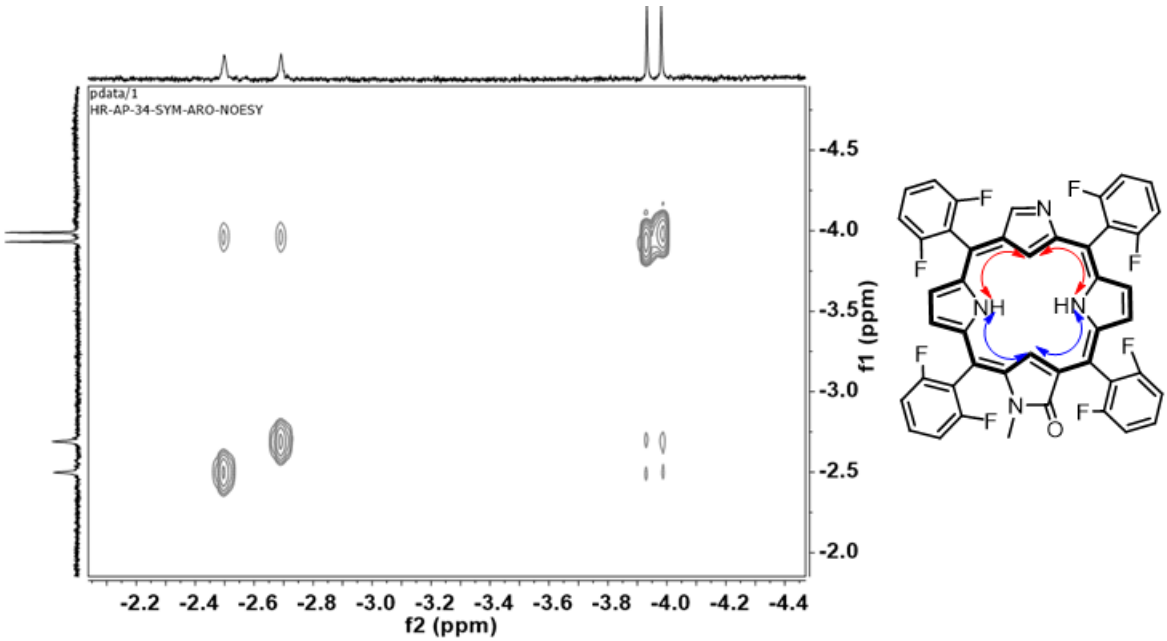


Fig. S25 ^{1}H -^{1}H 2D NOESY NMR spectra of **8** in $CDCl_3$ at 298 K

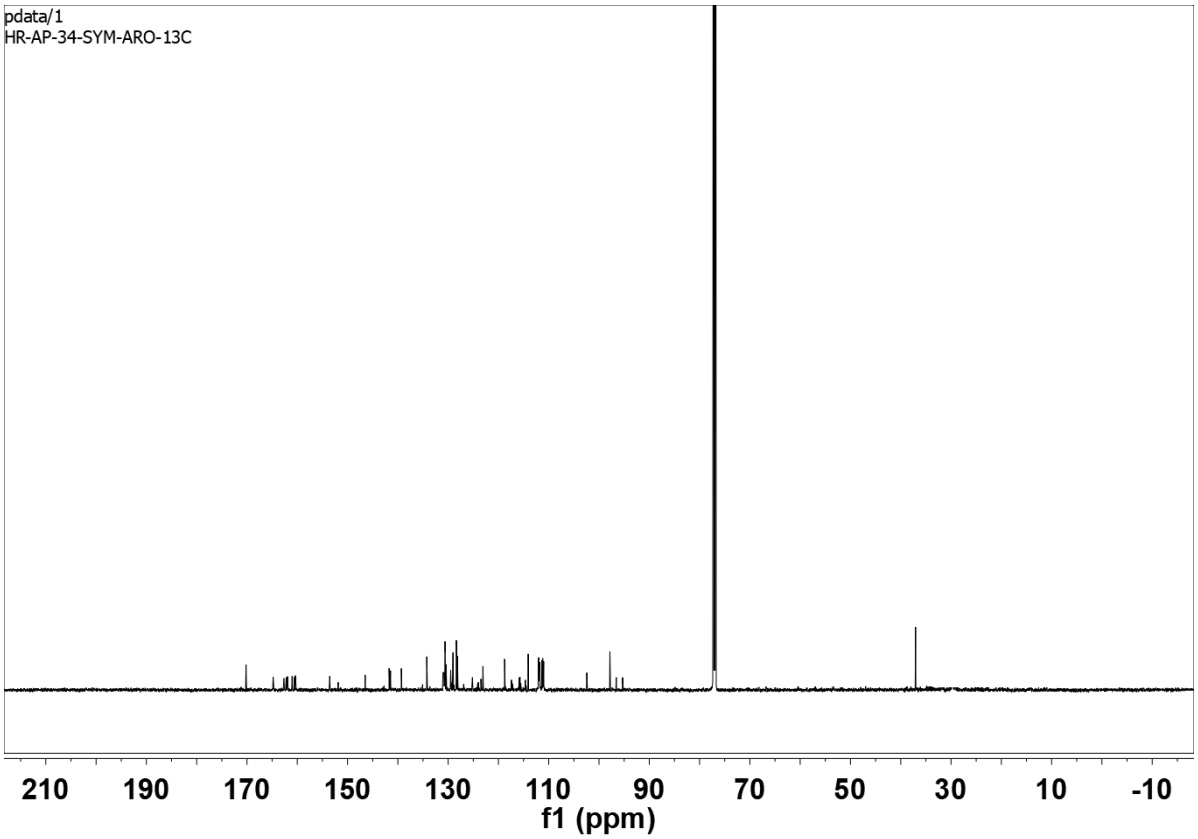
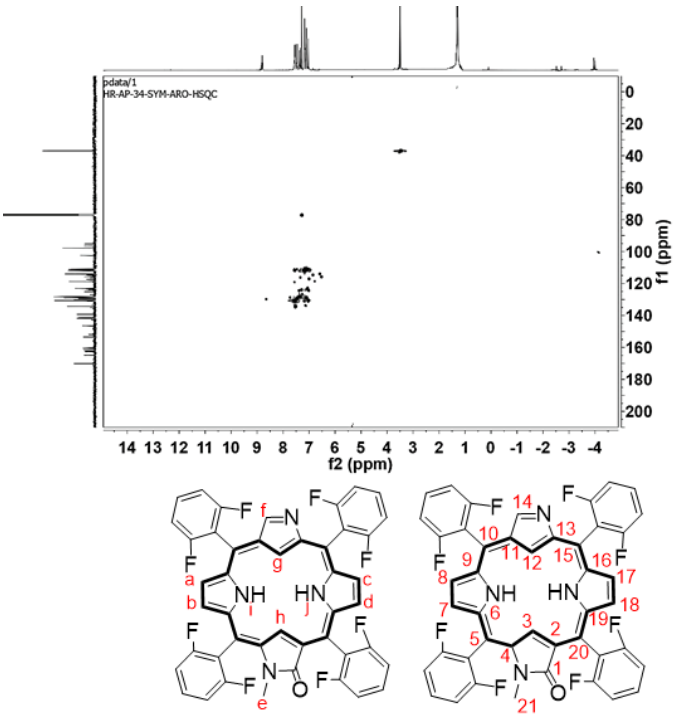
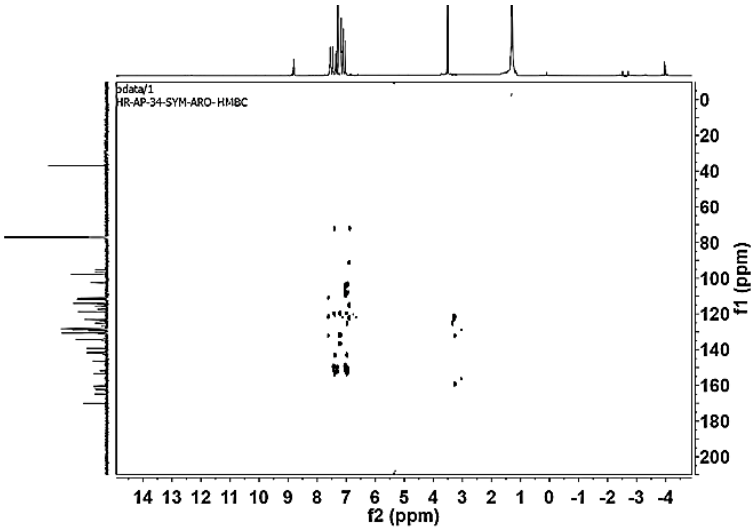


Fig. S26 ^{13}C NMR spectra of **8** in $CDCl_3$ at 298 K



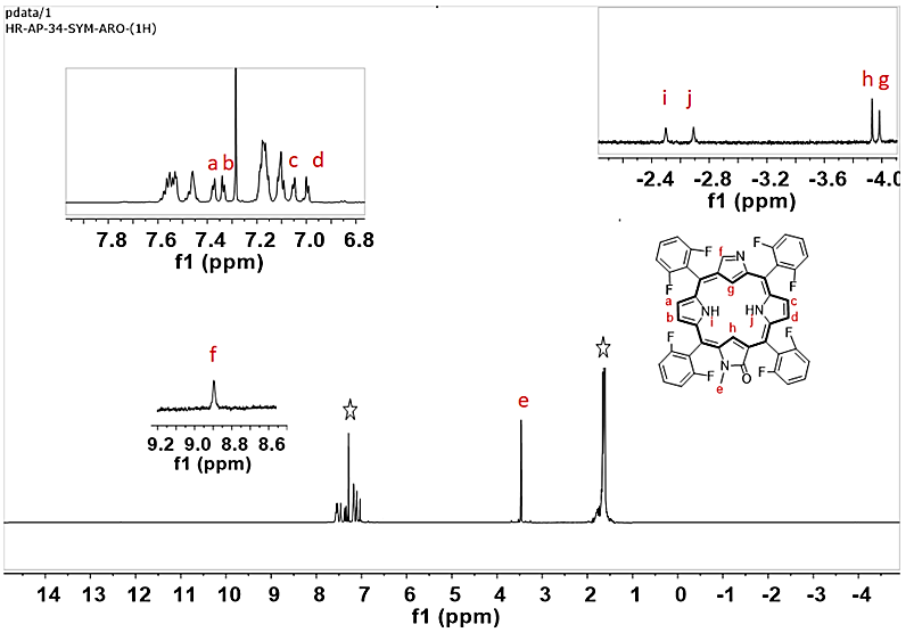
^{1}H ppm(Positions)	^{13}C ppm(Positions)
7.05 (c)	118.77 (17)
7.37 (a)	128.49 (8)
7.01 (d)	114.08 (18)
7.34 (b)	128.30 (7)
-3.96 (g)	100.84 (12)
-3.91 (h)	101.13 (3)
3.46 (e)	37.18 (21)
8.90 (f)	131.02 (14)
-2.37 (i)	
-2.59 (j)	

Fig. S27 ^{1}H -^{13}C 2D HSQC NMR spectra of **8** in $CDCl_3$ at 298 K



^{1}H ppm (Positions)	^{13}C ppm(Positions)
7.05 (c)	114.08 (18), 123.08 (16)
7.37 (a)	128.30 (7), 141.46 (9)
7.01 (d)	118.77 (17), 130.62 (19)
7.34 (b)	128.49 (8), 141.74 (6)
3.46 (e)	130.62 (4), 170.19 (1), 139.31 (2)

Fig. S28 ^{1}H -^{13}C 2D HMBC NMR spectra of **8** in $CDCl_3$ at 298 K



^{1}H Positions	ppm
c	7.05 (d)
a	7.37 (d)
d	7.01 (d)
b	7.34 (d)
f	8.90 (s)
e	3.46 (s)
g	-3.91 (s)
h	-3.96 (s)
i	-2.37 (s)
j	-2.59 (s)

Fig. S29 Complete ^{1}H NMR spectral assignment of **8** in $CDCl_3$ at 298 K

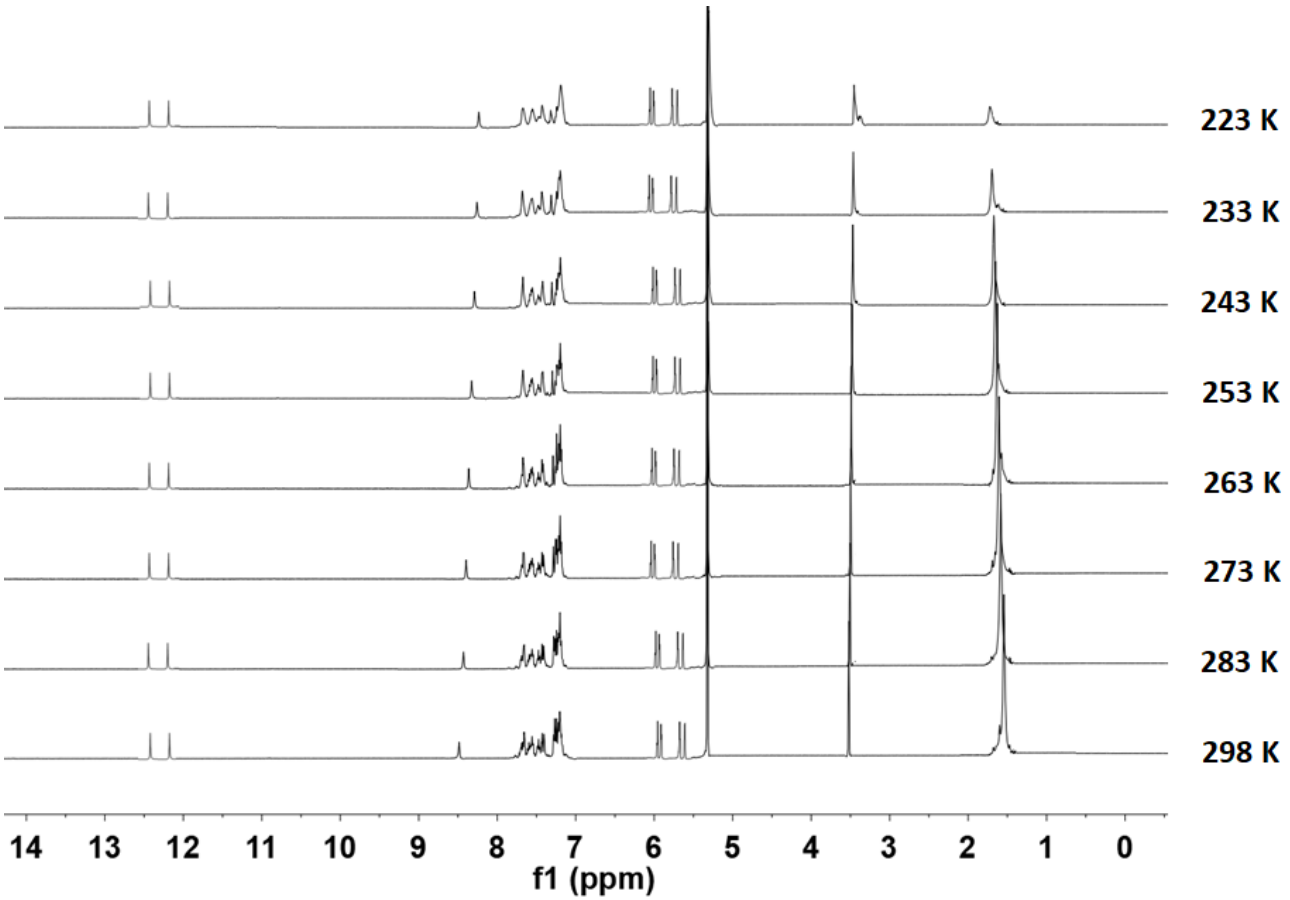


Fig. S30 Low VT ^{1}H NMR spectra of **9** in CD_2Cl_2

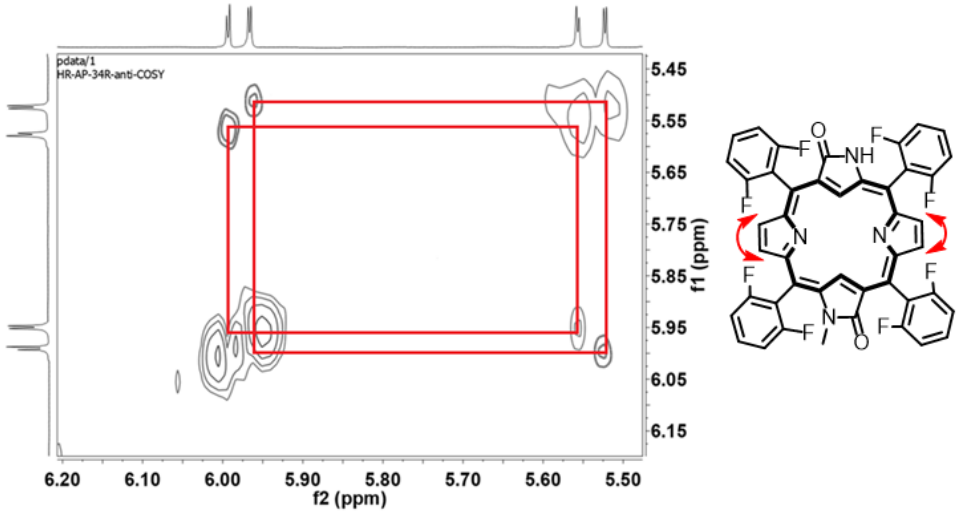


Fig. S31 ^{1}H -^{1}H 2D COSY NMR spectra of **9** in CD_2Cl_2 at 298 K

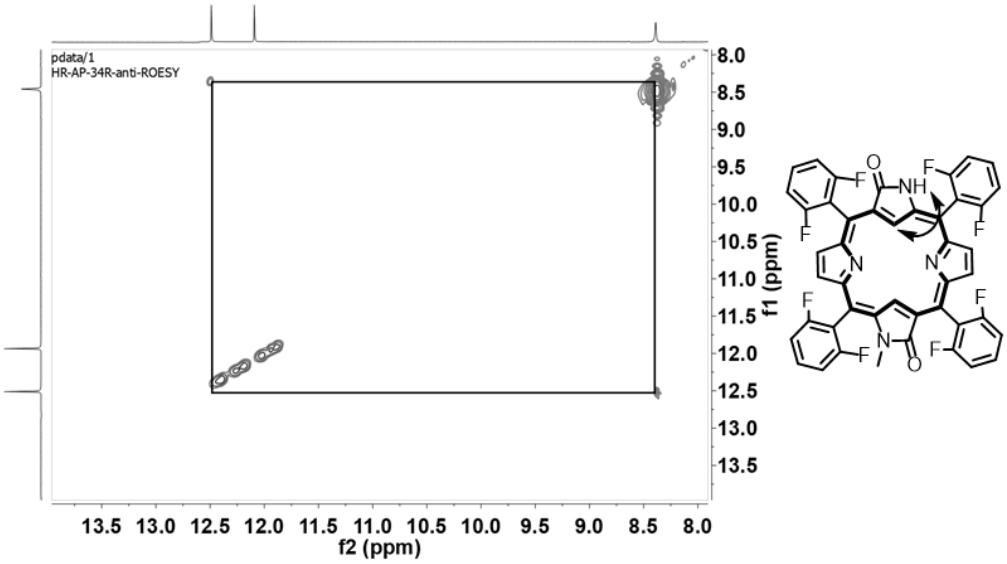


Fig. S32 ^{1}H -^{1}H 2D ROESY NMR spectra of **9** in CD_2Cl_2 at 298 K

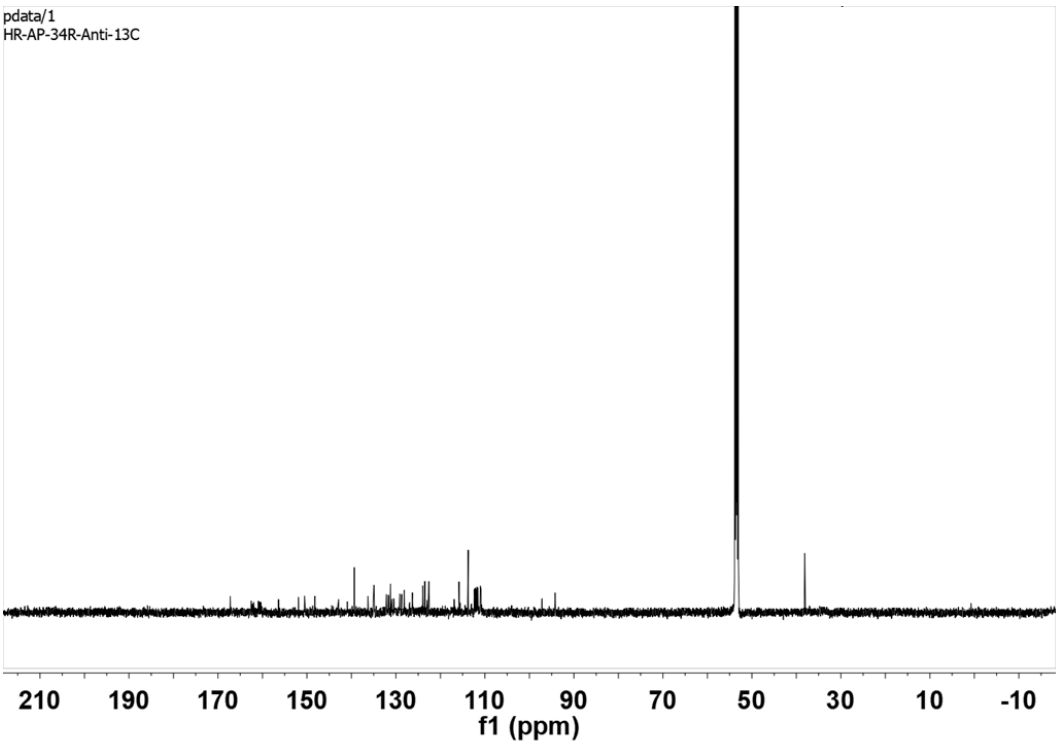
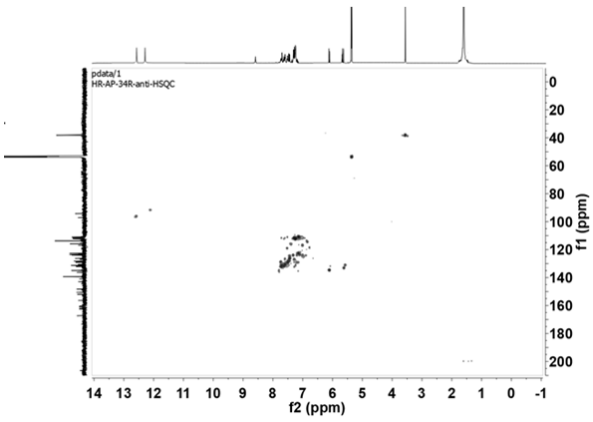


Fig. S33 ^{13}C NMR spectra of **9** in CD_2Cl_2 at 298 K



^{1}H ppm(Positions)	^{13}C ppm (Positions)
5.98 (c)	131.64 (17)
5.92 (a)	131.10 (8)
5.55 (d)	133.52 (18)
5.53 (b)	131.77 (7)
12.45 (g)	97.17 (13)
12.14 (h)	94.22 (3)
3.51 (e)	38.00 (21)
8.44 (f)	

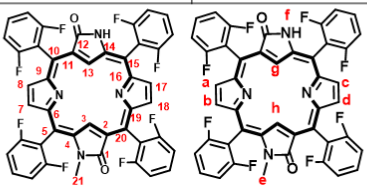
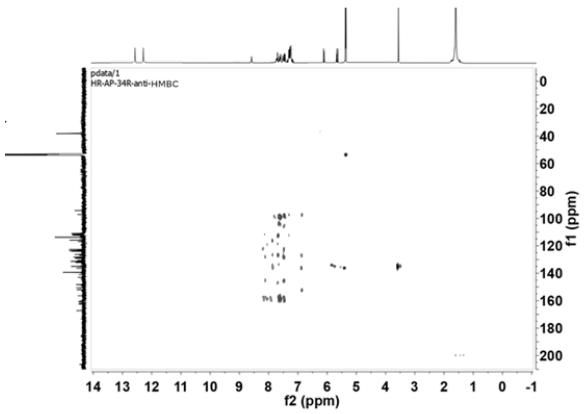


Fig. S34 ^{1}H -^{13}C 2D HSQC NMR spectra of **9** in CD_2Cl_2 at 298 K



^{1}H ppm(Positions)	^{13}C ppm (Positions)
5.98 (c)	133.52 (18), 150.54 (16)
5.92 (a)	131.77 (7), 142.88 (9)
5.55 (d)	131.64 (17), 151.91 (19)
5.53 (b)	131.10 (8), 134.92 (6)
3.51 (e)	139.36 (4)

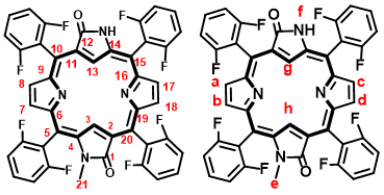


Fig. S35 ^{1}H -^{13}C 2D HMBC NMR spectra of **9** in CD_2Cl_2 at 298 K

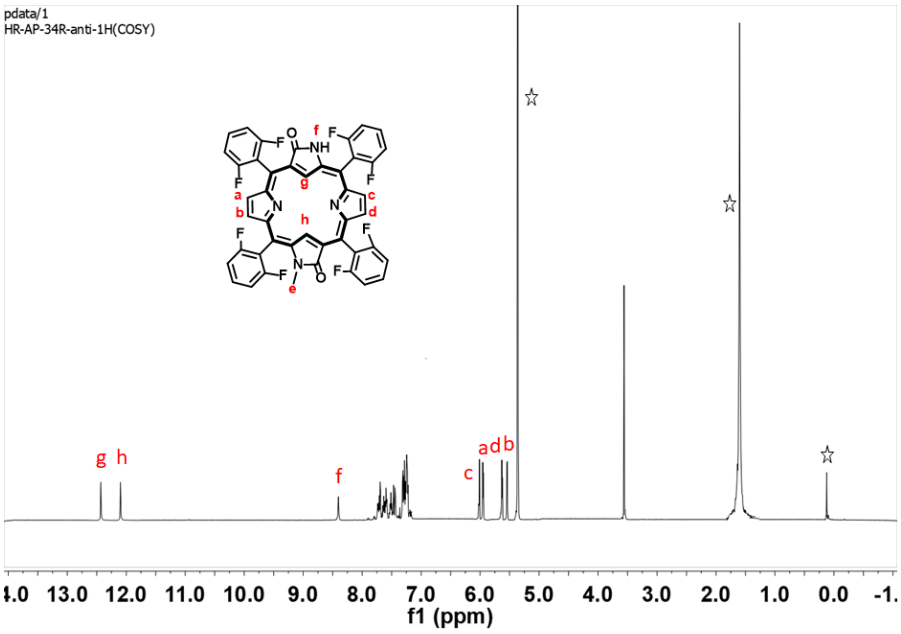


Fig. S36 Complete ^{1}H NMR spectral assignment of **9** in CD_2Cl_2 at 298 K

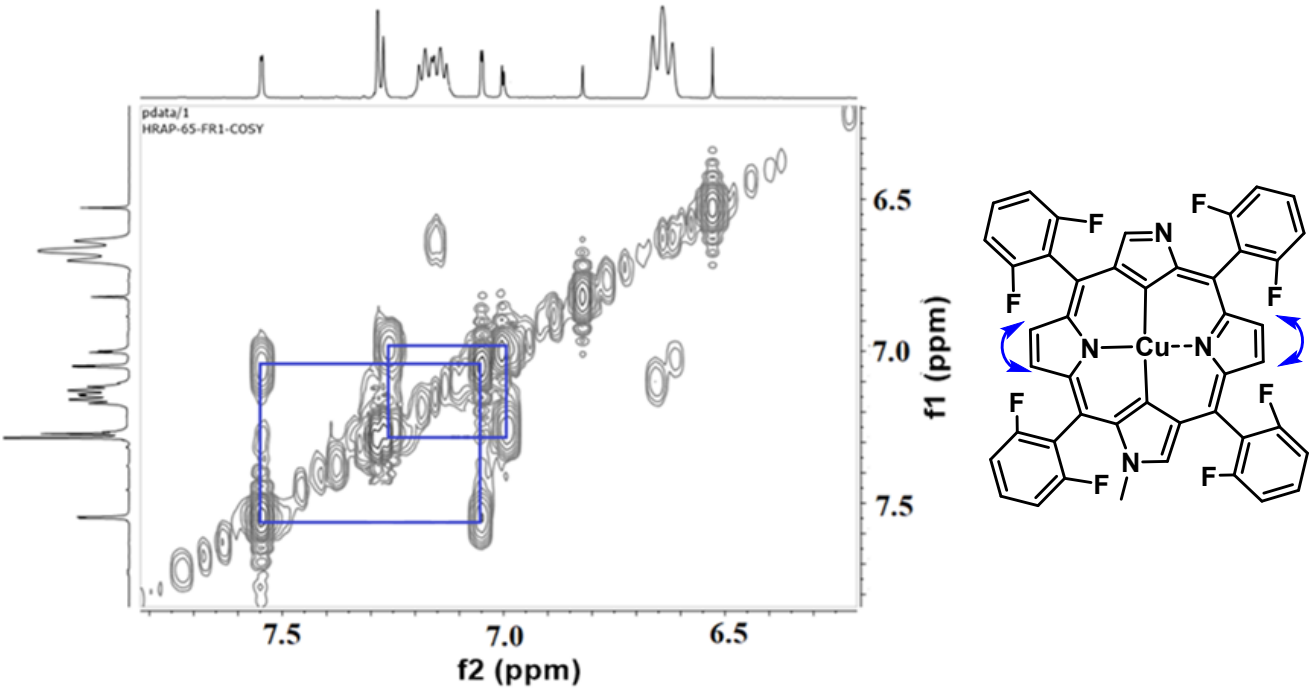


Fig. S37 ^{1}H -^{1}H 2D COSY NMR spectra of **10** in $CDCl_3$ at 298 K

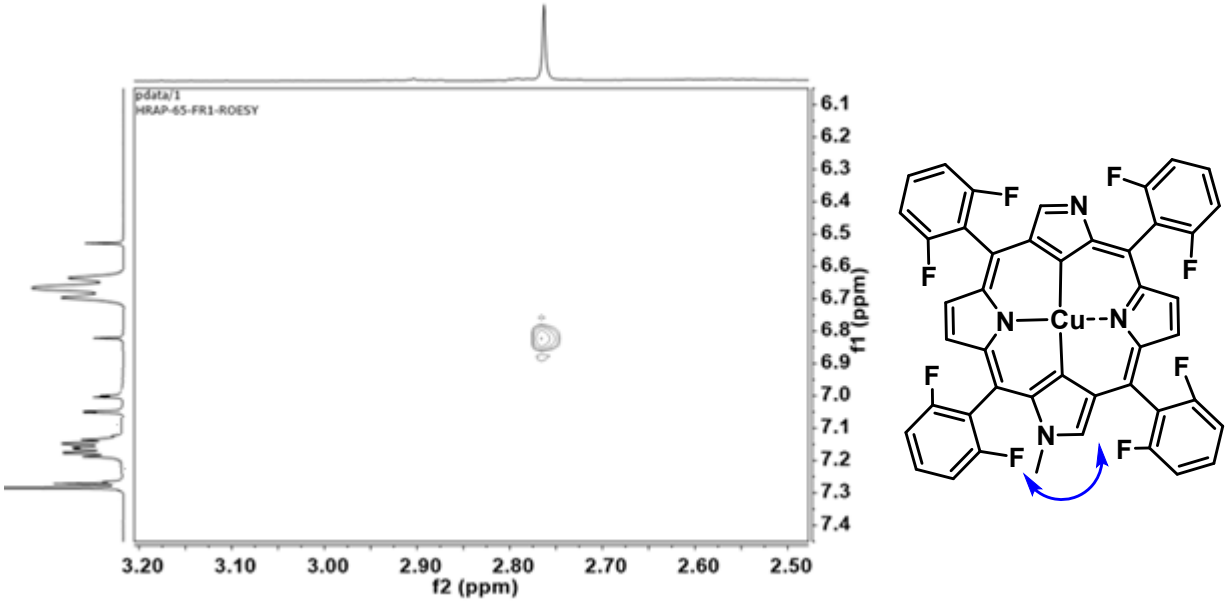


Fig. S38 ^{1}H -^{1}H 2D ROESY NMR spectra of **10** in $CDCl_3$ at 298 K

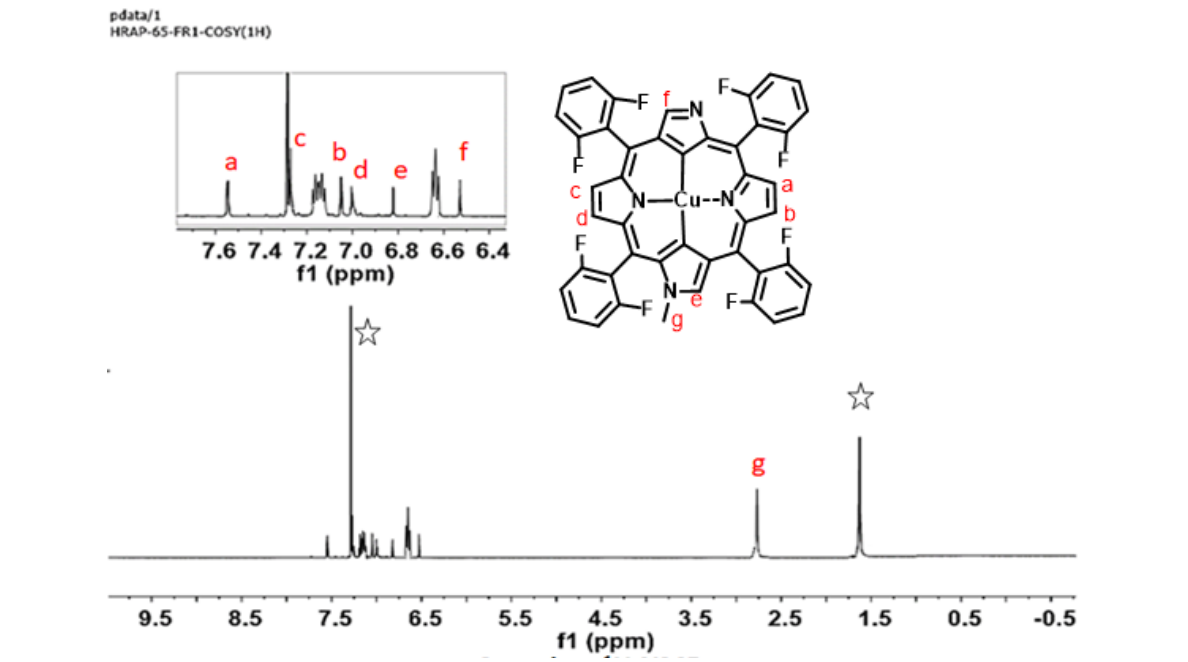


Fig. S39 Complete ^{1}H NMR spectral assignment of **10** in $CDCl_3$ at 298 K

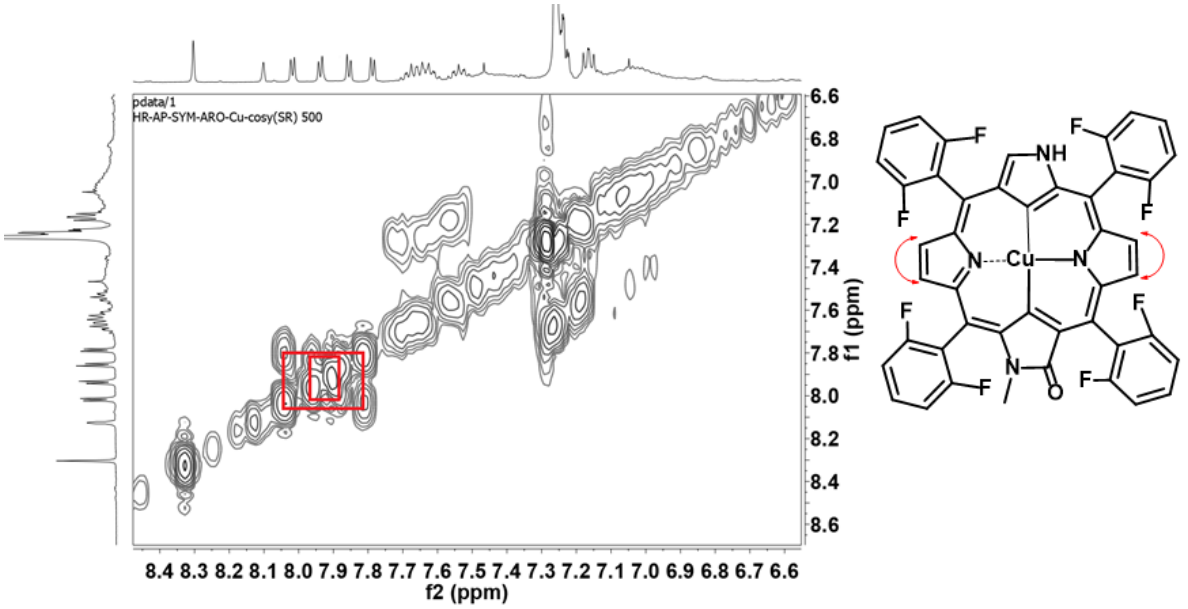


Fig. S40 ^{1}H -^{1}H 2D COSY NMR spectra of **11** in $CDCl_3$ at 298 K

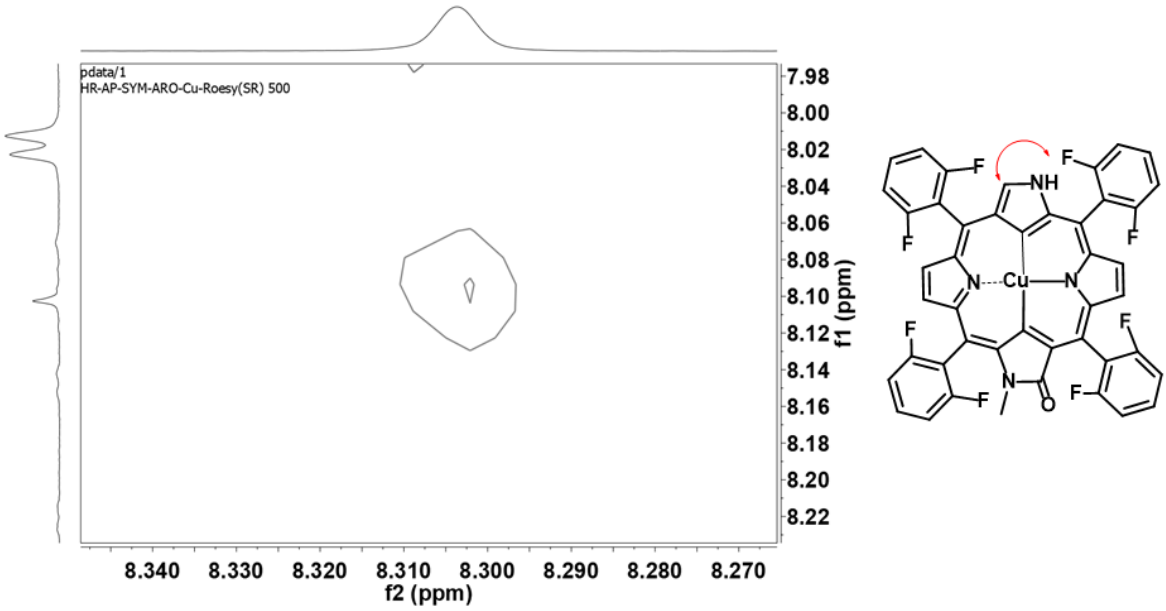


Fig. S41 ^{1}H -^{1}H 2D ROESY NMR spectra of **11** in $CDCl_3$ at 298 K

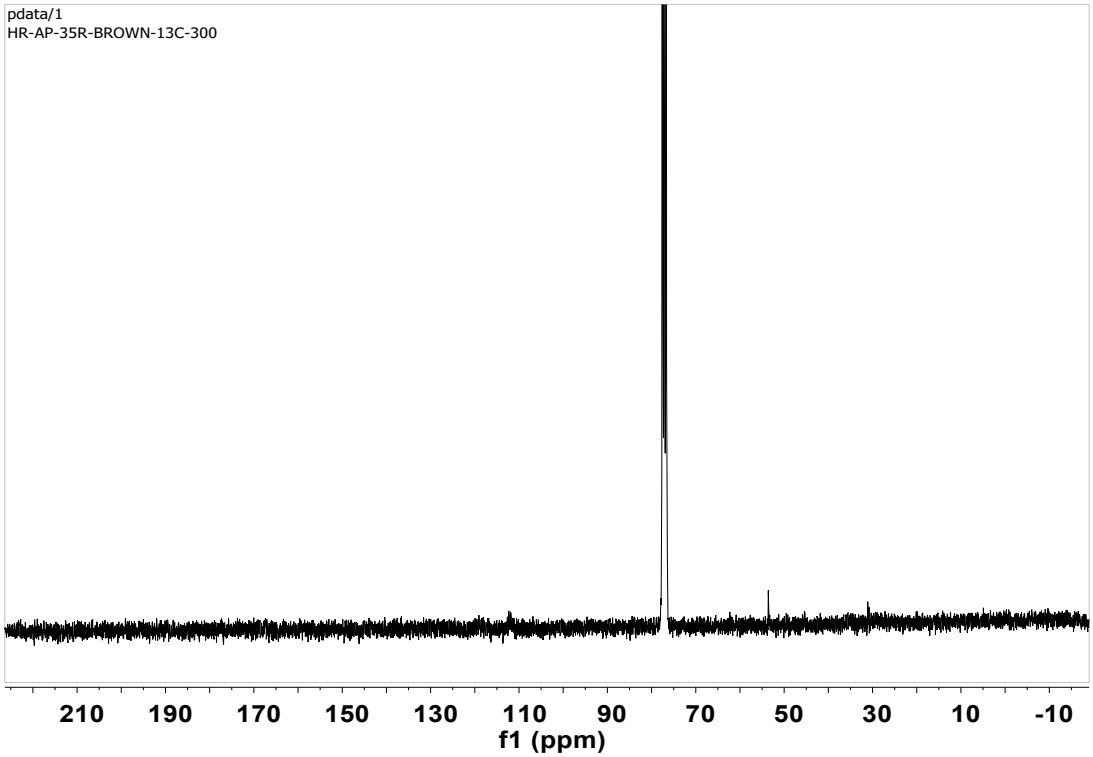


Fig. S42 ^{13}C NMR spectra of **11** in $CDCl_3$ at 298 K

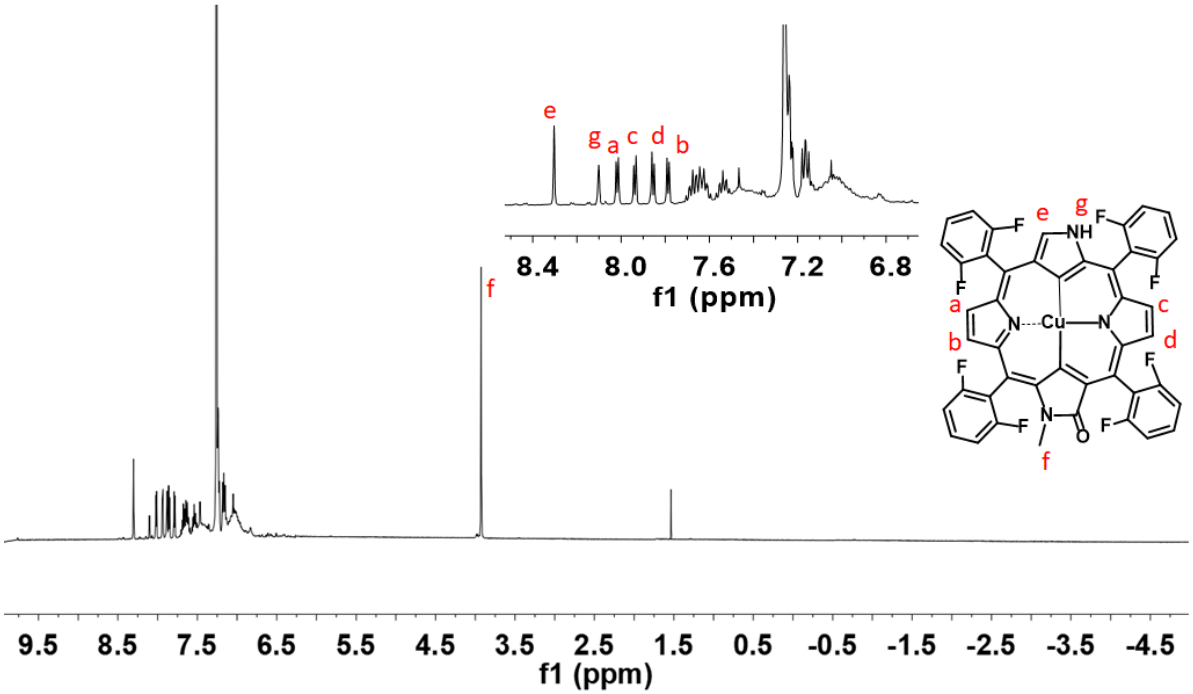


Fig. S43 Complete ^{1}H NMR spectral assignment of **11** in $CDCl_3$ at 298 K

3. Electrochemistry

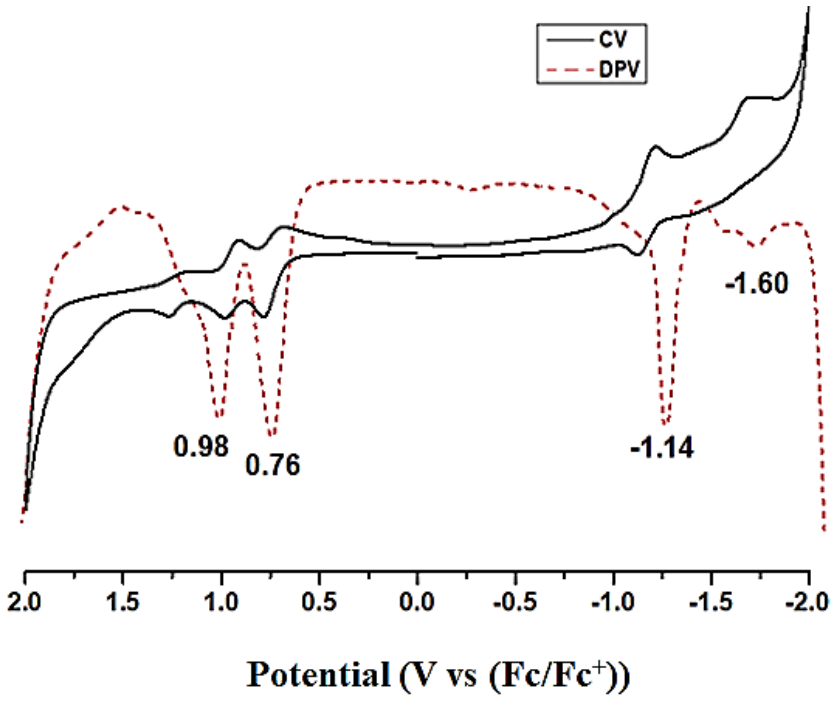


Fig. S44 Cyclic voltammogram of **7** (~10^{-4}M) in dichloromethane containing tetrabutylammonium hexafluorophosphate (0.01M) recorded at 100 mVs^{-1}.

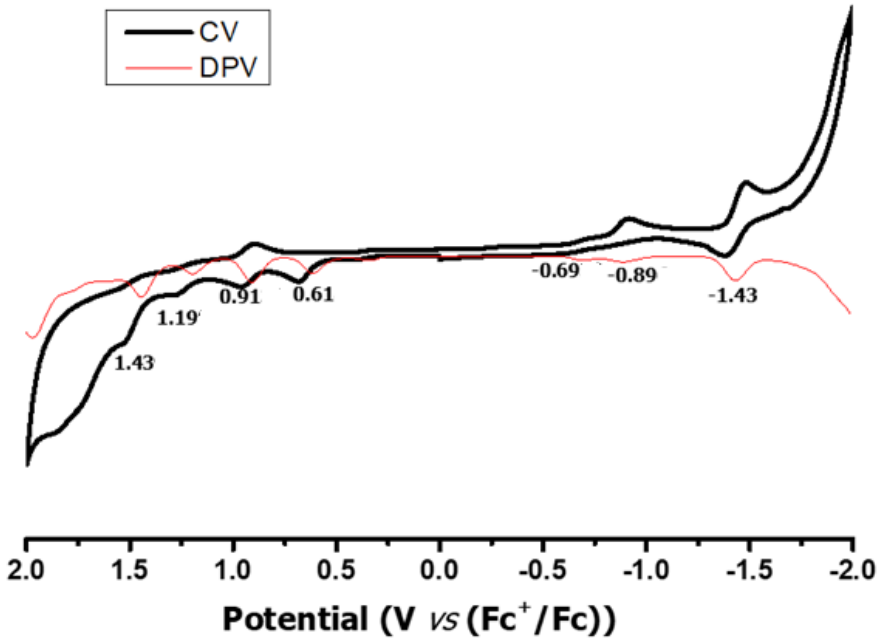


Fig. S45 Cyclic voltammogram of **8** (~10^{-4} M) in dichloromethane containing tetrabutylammonium hexafluorophosphate (0.01M) recorded at 100 mVs^{-1}.

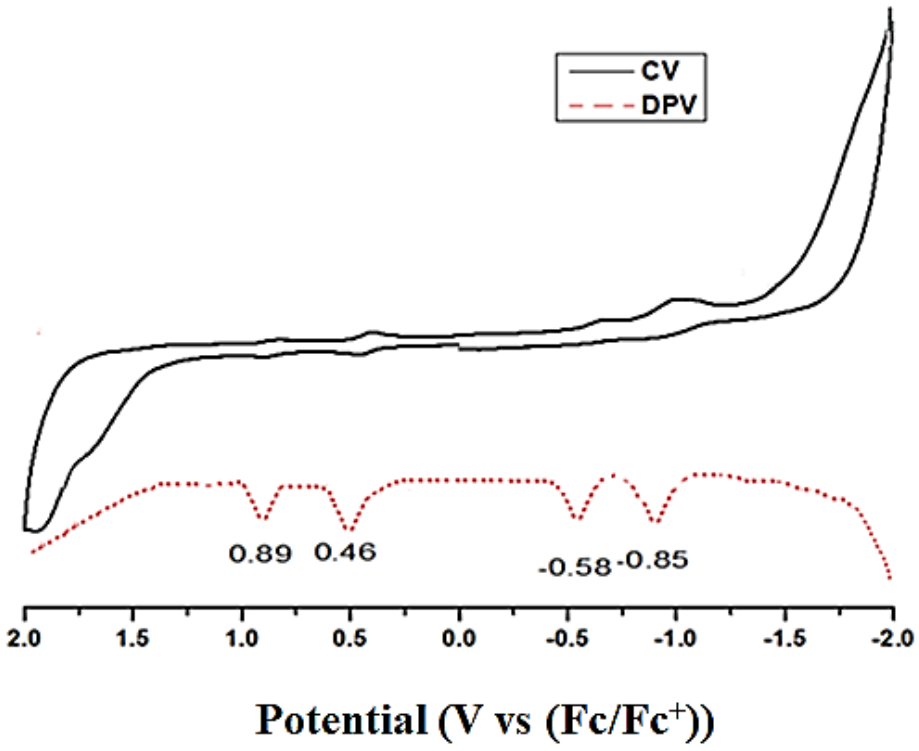


Fig. S46 Cyclic voltammogram of **9** (~10^{-4}M) in dichloromethane containing tetrabutylammonium hexafluorophosphate (0.01M) recorded at 100 mVs^{-1}.

4.0 Theoretical Calculation

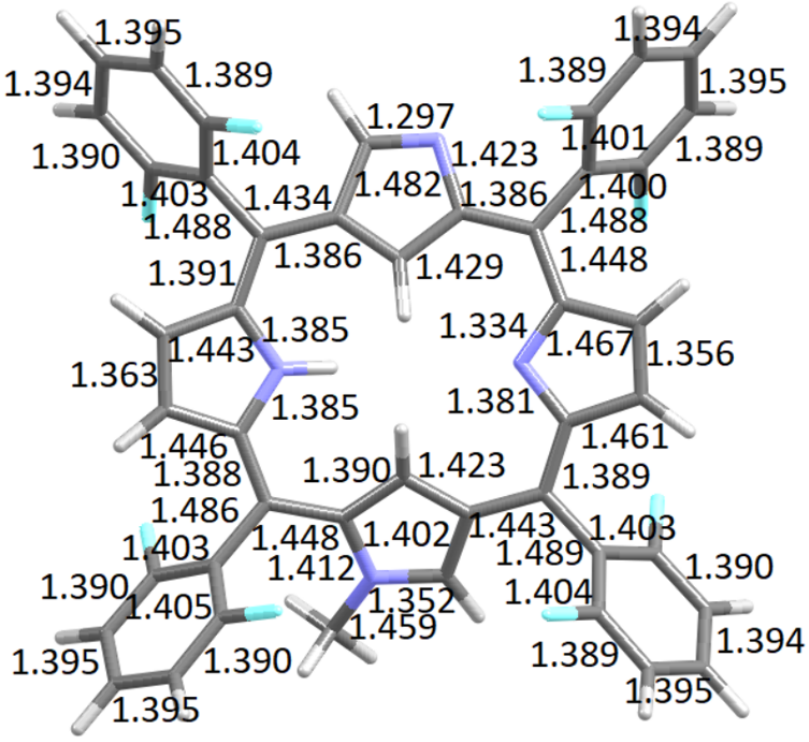


Fig. S47 Optimized geometry of **7** with selected bond length (Å).

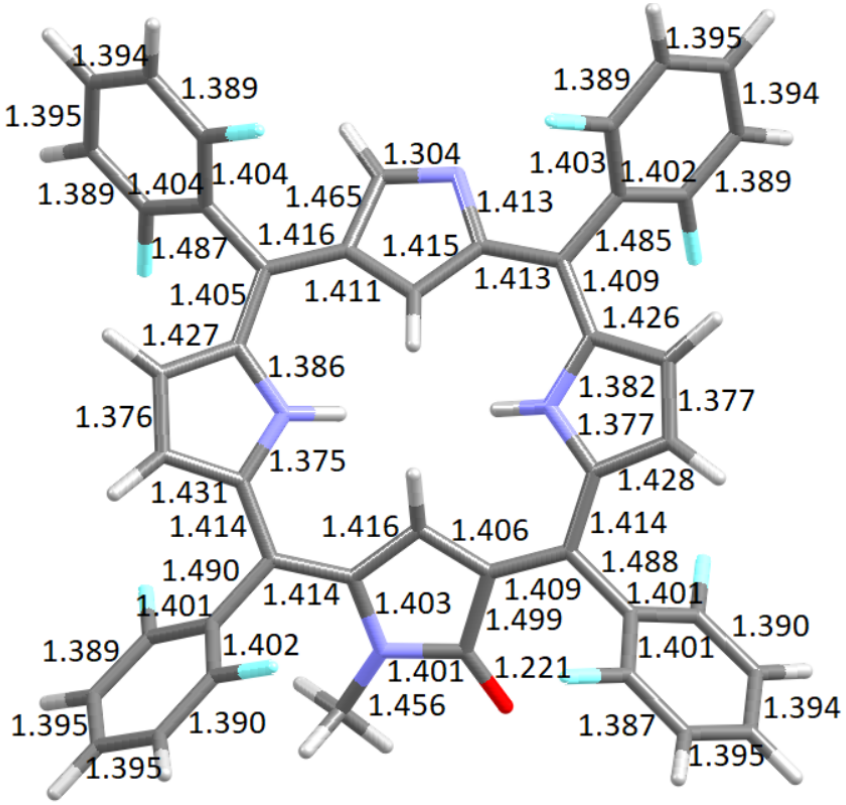


Fig. S48 Optimized geometry of **8** with selected bond length (Å).

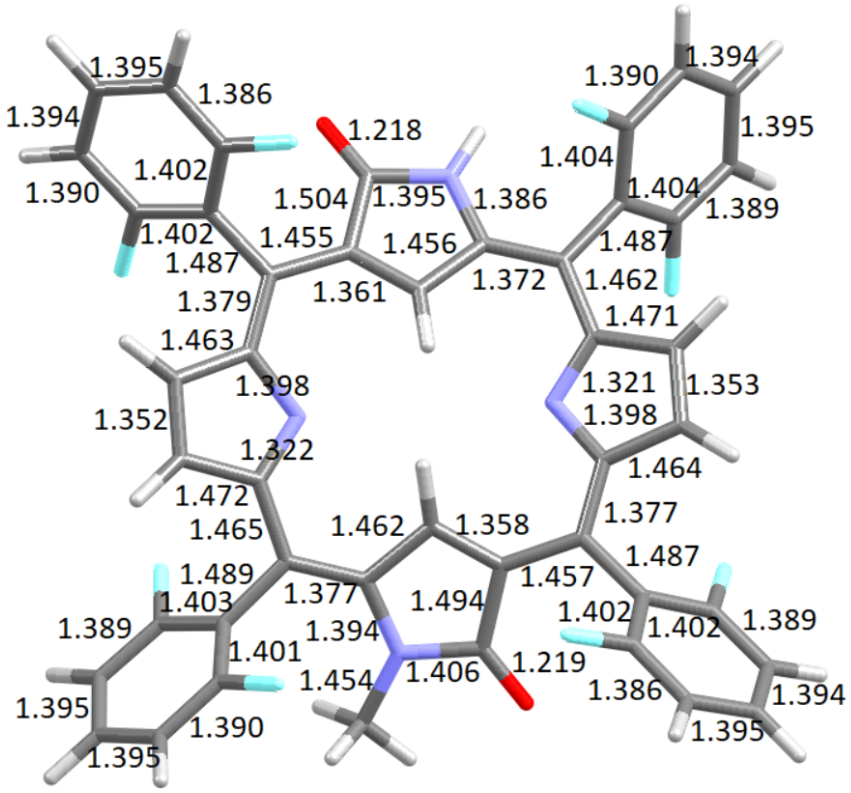


Fig. S49 Optimized geometry of **9** with selected bond length (Å).

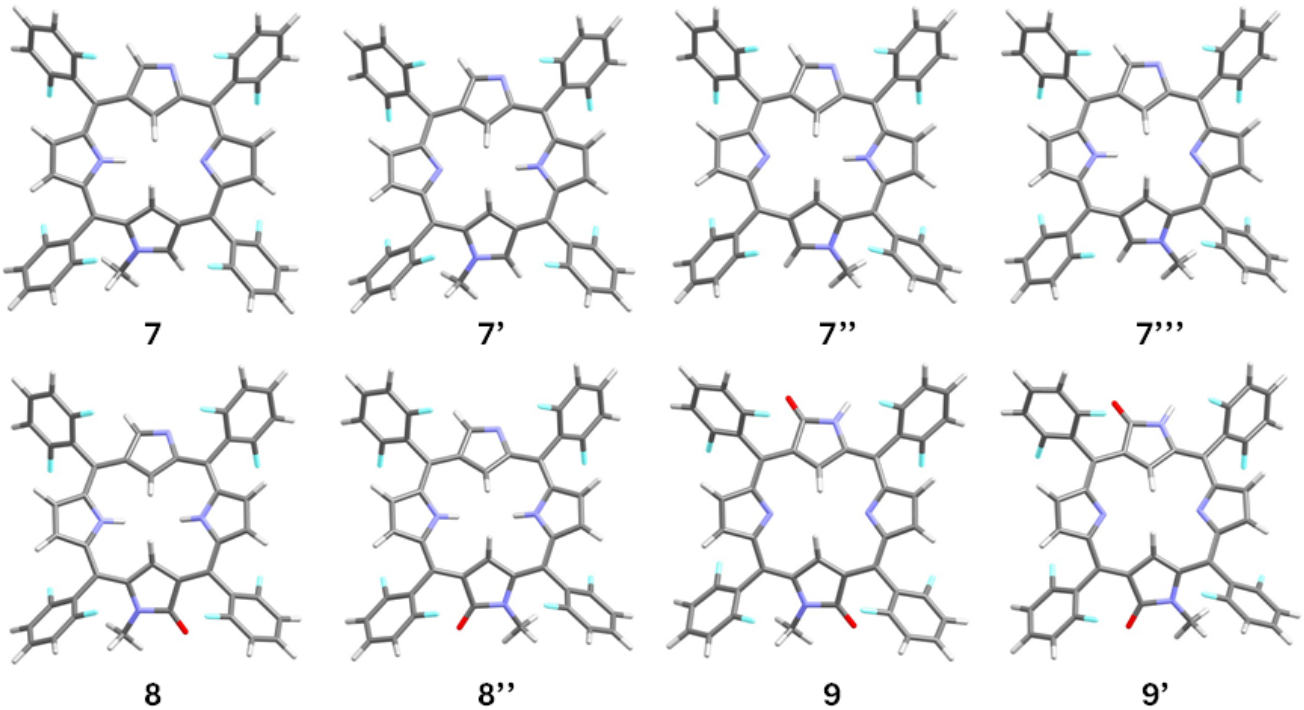


Fig. S50 Optimized geometry of plausible isomers and tautomers of macrocycles **7**, **8** and **9**.

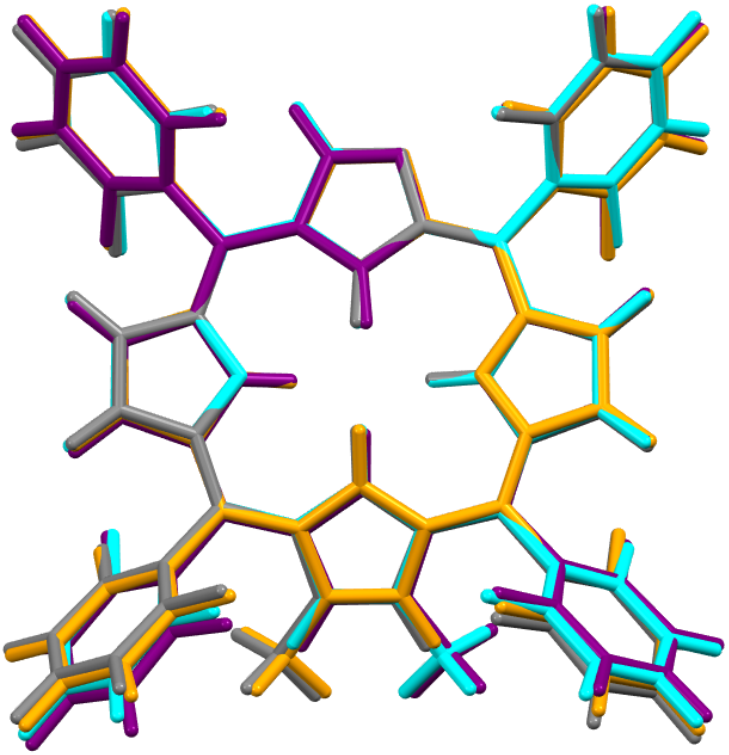


Fig. S51 Overlay plot of macrocycles **7** (Orange), **7′** (Grey), **7″** (Cyan) and **7‴**(Purple).

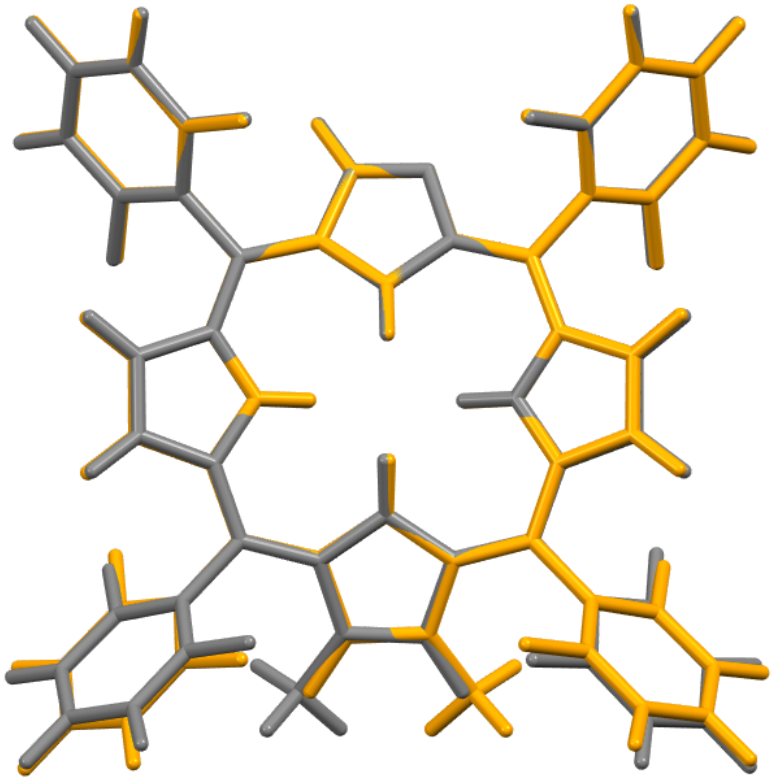


Fig. S52 Overlay plot of macrocycles **8** (Grey) and **8′** (Orange).

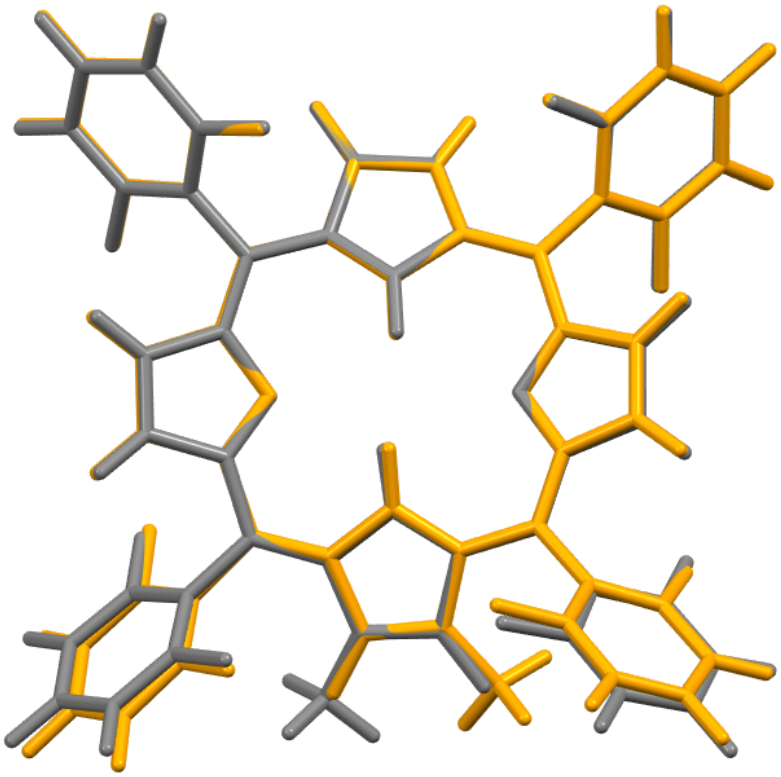


Fig. S53 Overlay plot of macrocycles **9** (Grey) and **9′** (Orange).

Table S1 Calculated energies of the optimized structures and relative energies (ΔE) for plausible isomers and tautomers of macrocycles **7**, **8** and **9**.

	Energy (hartree)	**ΔE (kJ/mol)**
7	-2746.898636	-8.14
7'	-2746.895537	0.00
7''	-2746.896960	-3.74
7'''	-2746.897227	-4.44
8	-2822.166334	0.00
8'	-2822.166551	-0.57
9	-2896.156102	0.00
9'	-2896.147399	22.85

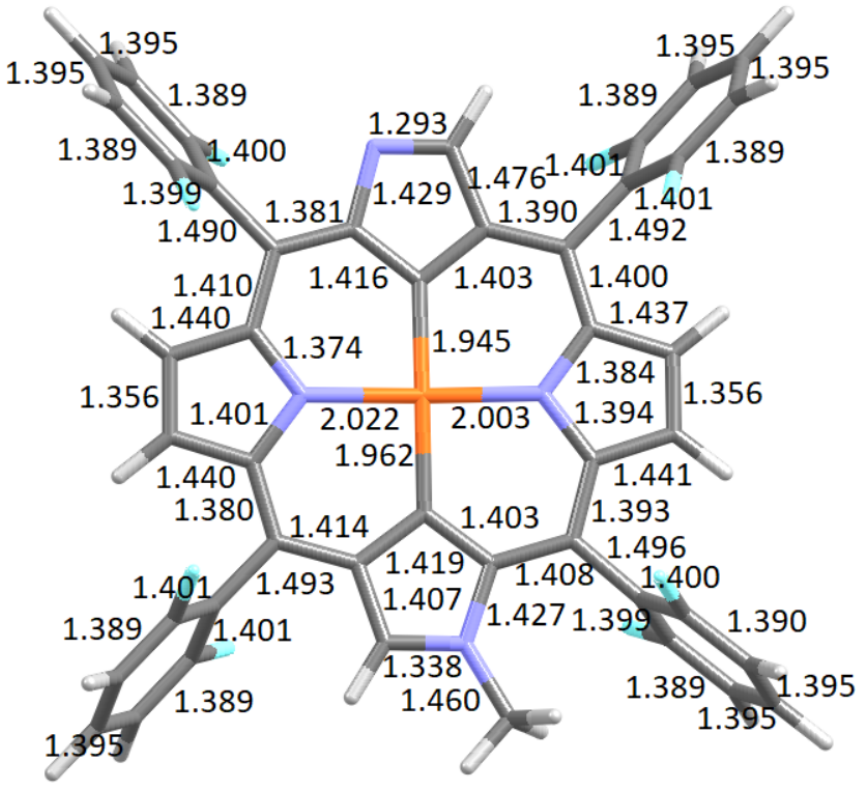


Fig. S54 Optimized geometry of **10** (singlet) with selected bond length (Å).

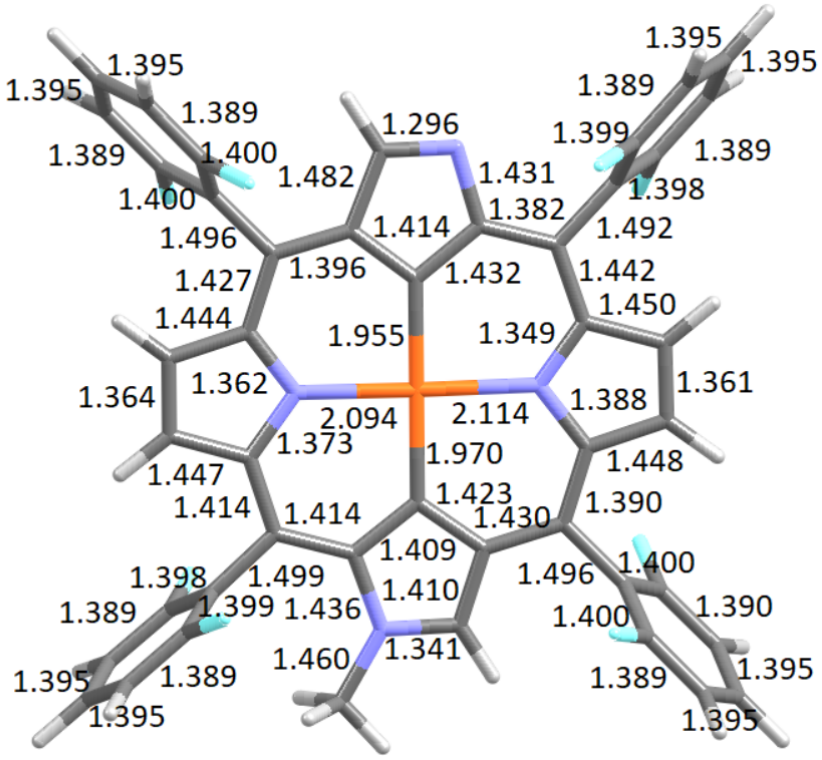


Fig. S55 Optimized geometry of **10** (triplet) with selected bond length (Å).

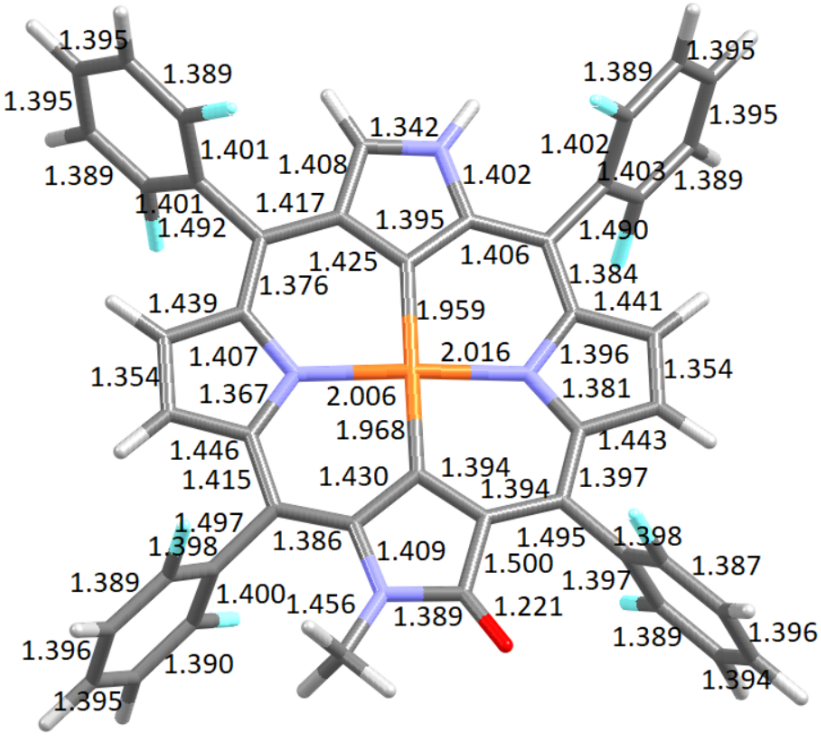


Fig. S56 Optimized geometry of **11** (singlet) with selected bond length (Å).

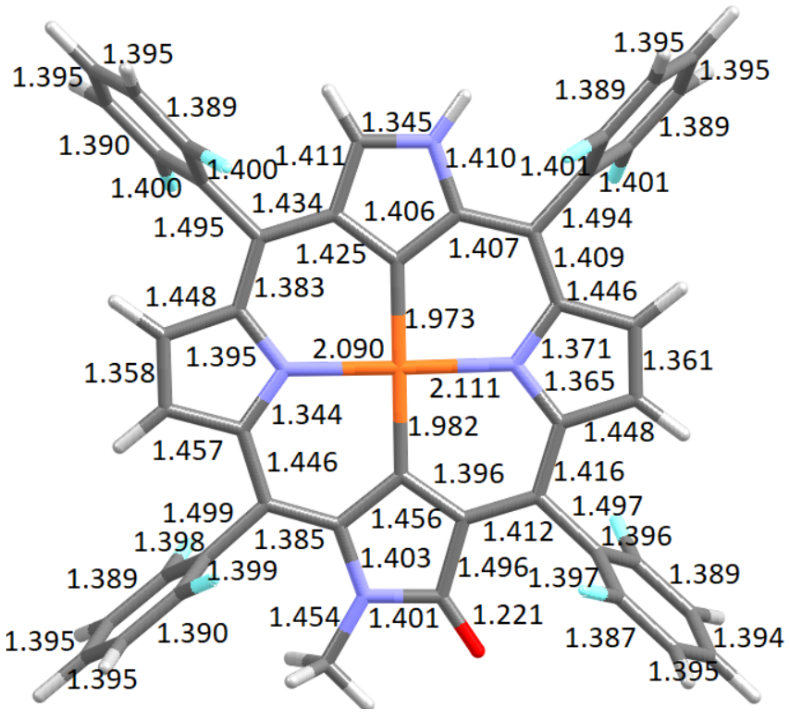


Fig. S57 Optimized geometry of **11** (triplet) with selected bond length (Å).

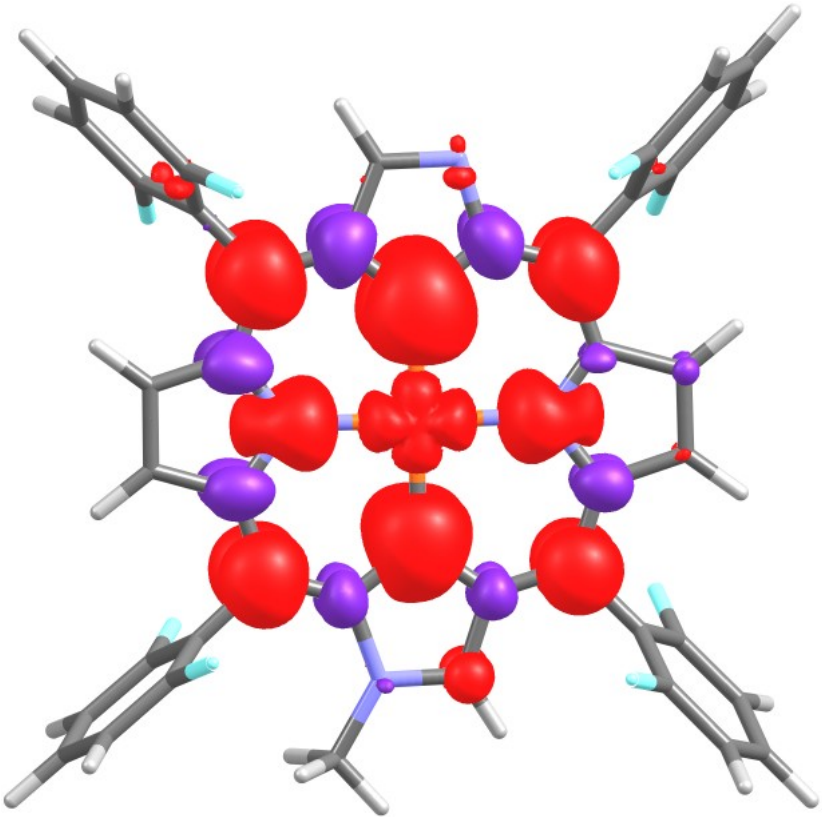


Fig. S58 Spin density plot of **10** at the triplet state.

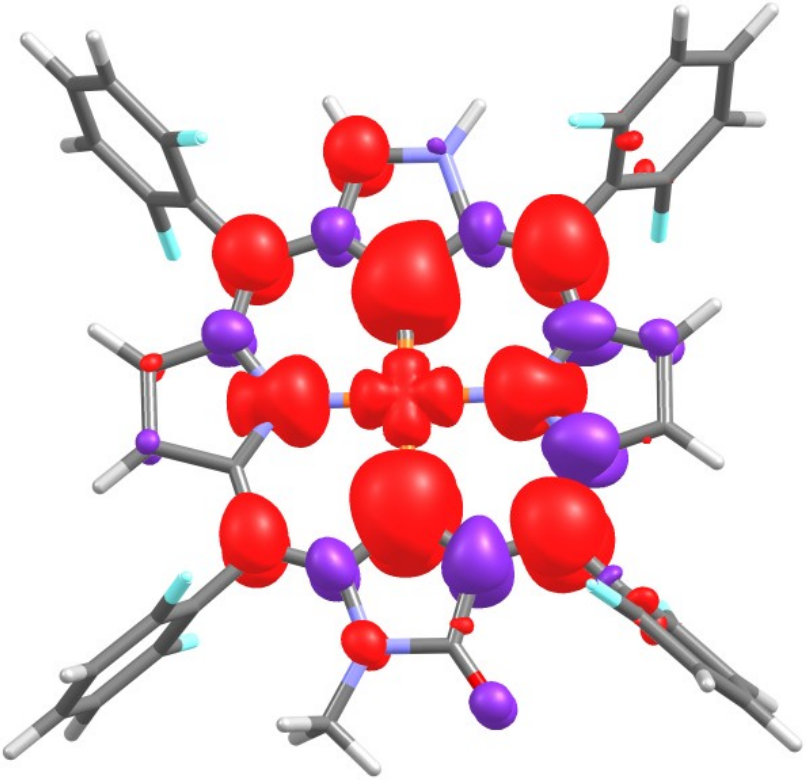


Fig. S59 Spin density plot of **11** at the triplet state.

Table S2 Important dihedral between the macrocyclic mean plane (M) and the rings of **7**, **8** and **9**.

Plane	Dihedral Angle (°)		
	7	**8**	**9**
Ar1-M	53.93	49.06	49.11
Ar2-M	55.37	49.16	48.93
Ar3-M	55.52	50.12	50.17
Ar4-M	52.71	53.62	48.14
Py1-M	11.73	15.44	21.33
Py2-M	13.41	21.35	19.27
Py3-M	9.24	16.60	19.66
Py4-M	29.73	24.47	24.29

Table S3 Frontier Molecular Orbital compositions (%) in the ground state for **7**. Ar1, Ar2, Ar3, Ar4 = *meso*-aryl, Py1 = imine type pyrrole, Py2 = N-confused pyrrole, Py3 = amino type pyrrole and Py4 = N-methyl N-confused pyrrole.

	Energy (eV)	Ar1	Ar2	Ar3	Ar4	Py1	Py2	Py3	Py4
HOMO-3	-6.181	2.80	0.69	5.87	3.74	10.35	17.40	34.02	25.12
HOMO-2	-6.031	1.22	0.70	3.03	1.20	8.83	33.07	39.72	12.23
HOMO-1	-5.342	1.58	1.43	3.51	10.24	8.85	22.37	26.35	25.66
HOMO	-4.597	20.12	18.45	8.55	4.90	17.93	13.60	4.42	12.02
LUMO	-2.648	9.39	1.47	12.58	18.79	9.27	18.34	12.84	17.31
LUMO+1	-1.991	12.94	19.16	3.28	11.35	22.80	8.33	13.23	8.90
LUMO+2	-1.13	4.99	9.34	20.56	13.66	7.43	18.48	16.93	8.61
LUMO+3	-0.656	74.36	3.37	0.07	2.62	9.61	0.50	0.45	9.02

Table S4 Frontier Molecular Orbital compositions (%) in the ground state for **8**. Ar1, Ar2, Ar3, Ar4 = *meso*-aryl, Py1, Py3 = amino type pyrrole, Py2 = N-confused pyrrole and Py4 = N-methyl N-confused pyrrole.

	Energy (eV)	Ar1	Ar2	Ar3	Ar4	Py1	Py2	Py3	Py4
HOMO-3	-6.526	0.21	0.08	3.22	86.68	0.29	3.21	0.50	5.81
HOMO-2	-6.171	1.99	2.85	2.33	12.65	2.60	34.61	14.5	28.47
HOMO-1	-5.234	10.51	3.79	3.10	0.77	21.27	19.34	13.48	27.74
HOMO	-4.897	7.71	11.08	10.57	16.76	10.49	12.11	12.88	18.40
LUMO	-2.526	15.20	3.85	18.46	2.75	13.55	12.38	16.47	17.34
LUMO+1	-2.519	1.47	20.00	2.07	12.51	17.13	17.69	11.31	17.84
LUMO+2	-1.288	15.17	11.79	10.83	14.73	10	9.29	11.99	16.19
LUMO+3	-0.682	60.85	16.98	0.04	1.65	11.46	1.58	0.87	6.56

Table S5 Frontier Molecular Orbital compositions (%) in the ground state for **9**. Ar1, Ar2, Ar3, Ar4 = *meso*-aryl, Py1, Py3 = imine type pyrrole, Py2 = N-confused pyrrole and Py4 = N-methyl N-confused pyrrole.

	Energy (eV)	Ar1	Ar2	Ar3	Ar4	Py1	Py2	Py3	Py4
HOMO-3	-6.495	2.58	8.77	3.27	4.78	21.95	12.62	31.82	14.21
HOMO-2	-6.431	5.56	7.64	5.24	6.53	29.38	11.25	23.51	10.89
HOMO-1	-5.869	7.23	9.57	6.27	10.18	8.00	22.1	9.44	27.21
HOMO	-5.239	11.76	8.11	11.40	7.67	13.5	16.69	12.41	18.46
LUMO	-3.314	6.27	10.62	6.84	10.11	13.42	19.48	12.88	20.38
LUMO+1	-2.132	6.02	15.55	6.54	17.00	18.17	8.09	19.98	8.66
LUMO+2	-1.947	15.02	4.23	13.81	4.37	6.31	24.02	6.09	26.16
LUMO+3	-1.195	17.64	11.66	19.19	10.49	8.49	12.45	8.08	12.00

Table S6 Frontier Molecular Orbital compositions (%) in the ground state for **10**. Ar1, Ar2, Ar3, Ar4 = *meso*-aryl, Py1, Py3 = pyrrole, Py2 = N-confused pyrrole and Py4 = N-methyl N-confused pyrrole.

	Energy (eV)	Cu	Ar1	Ar2	Ar3	Ar4	Py1	Py2	Py3	Py4
HOMO-3	-6.435	1.53	0.56	5.01	23.99	0.39	1.43	49.63	4.69	12.78
HOMO-2	-5.874	4.36	1.67	0.46	1.04	4.66	12.82	41.19	10.33	23.48
HOMO-1	-5.401	0.11	0.69	0.85	3.75	4.32	20.61	20.29	19.29	30.08
HOMO	-4.756	6.04	13.25	14.43	10.49	10.15	9.92	15.84	8.84	11.04
LUMO	-2.852	31.08	1.46	1.01	0.68	0.73	17.29	15.90	16.66	15.20
LUMO+1	-2.699	0.59	10.71	3.46	4.77	14.39	9.22	17.84	13.06	25.96
LUMO+2	-1.859	1.31	12.12	14.83	9.72	11.70	18.66	8.39	14.91	8.36
LUMO+3	-1.079	0.21	15.32	11.87	13.26	8.99	8.95	17.84	12.2	11.36

Table S7 Frontier Molecular Orbital compositions (%) in the ground state for **11**. Ar1, Ar2, Ar3, Ar4 = *meso*-aryl, Py1, Py3 = pyrrole, Py2 = N-confused pyrrole and Py4 = N-methyl N-confused pyrrole.

	Energy (eV)	Cu	Ar1	Ar2	Ar3	Ar4	Py1	Py2	Py3	Py4
HOMO-3	-6.288	1.66	0.37	0.24	0.98	26.53	1.13	9.70	3.44	55.93
HOMO-2	-5.948	3.25	0.93	2.53	1.08	4.13	2.44	26.18	21.88	37.57
HOMO-1	-5.252	0.46	13.02	10.20	1.14	0.49	19.17	22.27	9.99	23.26
HOMO	-4.83	6.64	4.91	5.65	14.64	15.89	8.07	14.21	11.84	18.16
LUMO	-2.928	30.08	0.72	0.70	1.86	1.47	16.59	16.59	16.33	15.67
LUMO+1	-2.560	0.50	1.91	14.90	12.09	1.11	15.33	23.75	10.20	20.22
LUMO+2	-1.897	1.20	10.54	12.54	13.43	10.99	16.32	7.79	17.72	9.47
LUMO+3	-0.959	0.12	3.22	4.13	73.09	1.16	2.33	5.10	5.67	5.17

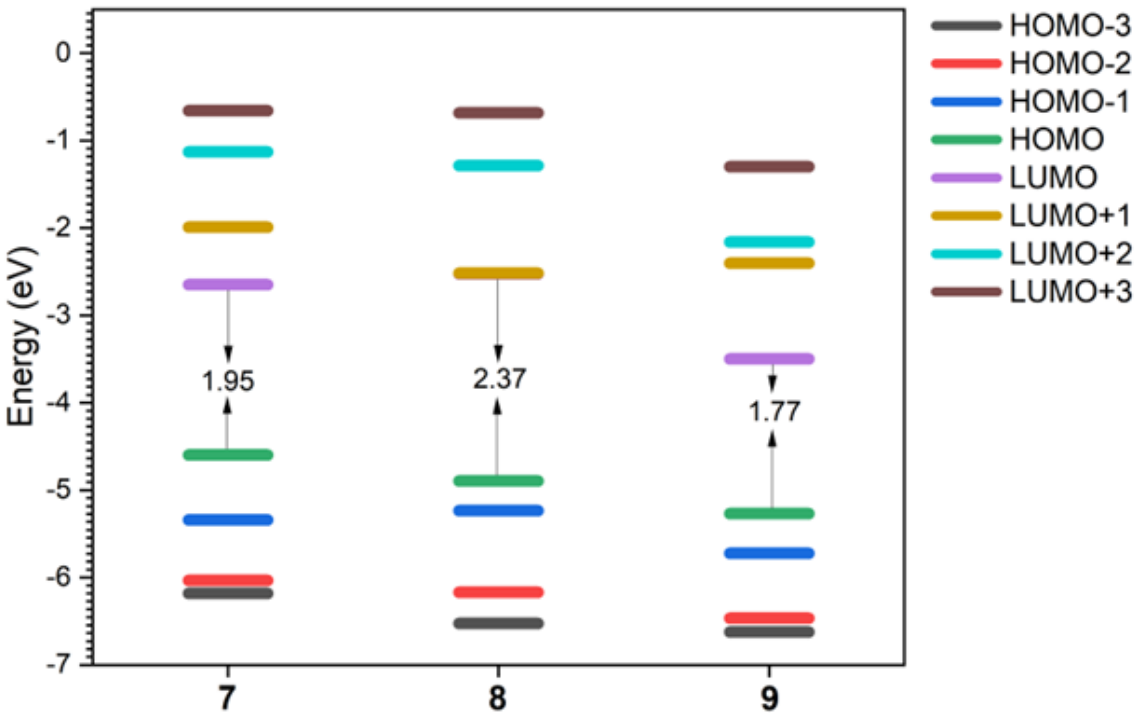


Fig. S60 FMO energy levels of **7-9**.

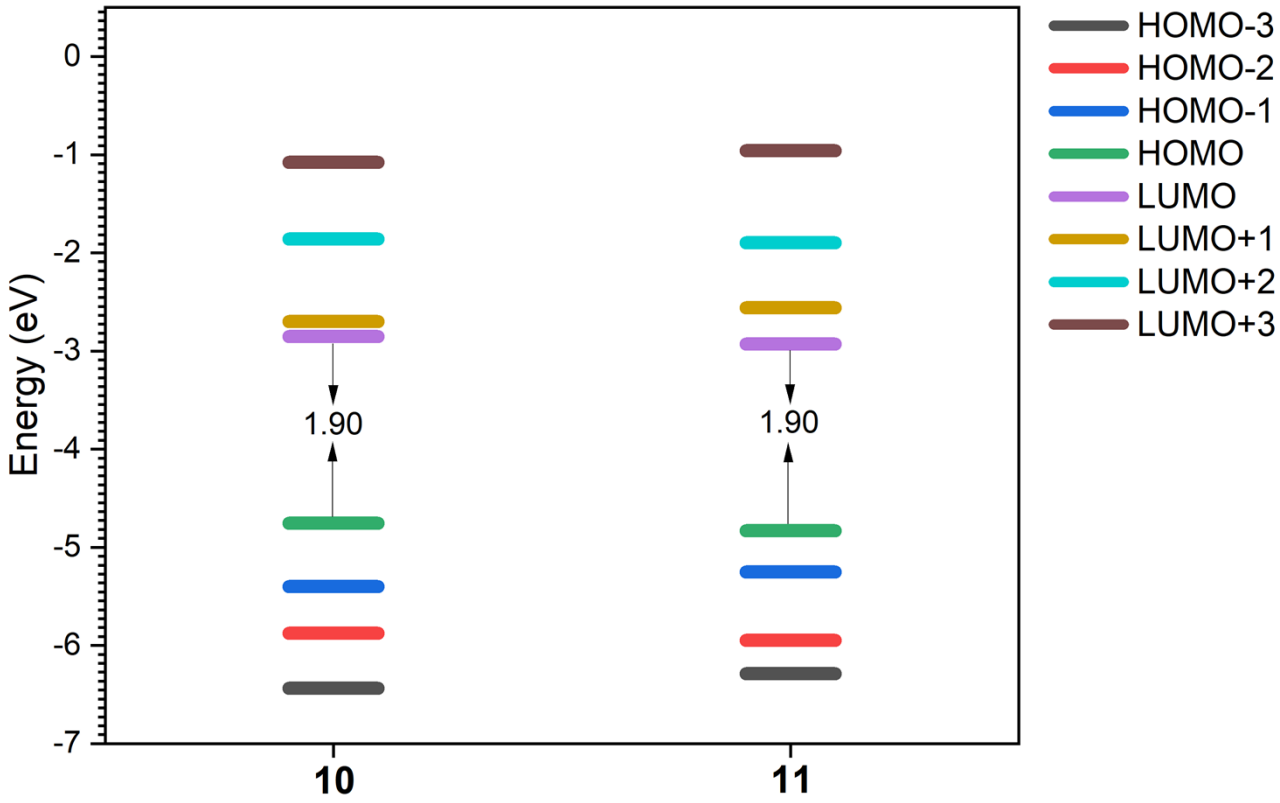


Fig. S61 FMO energy levels of **10**-**11**.

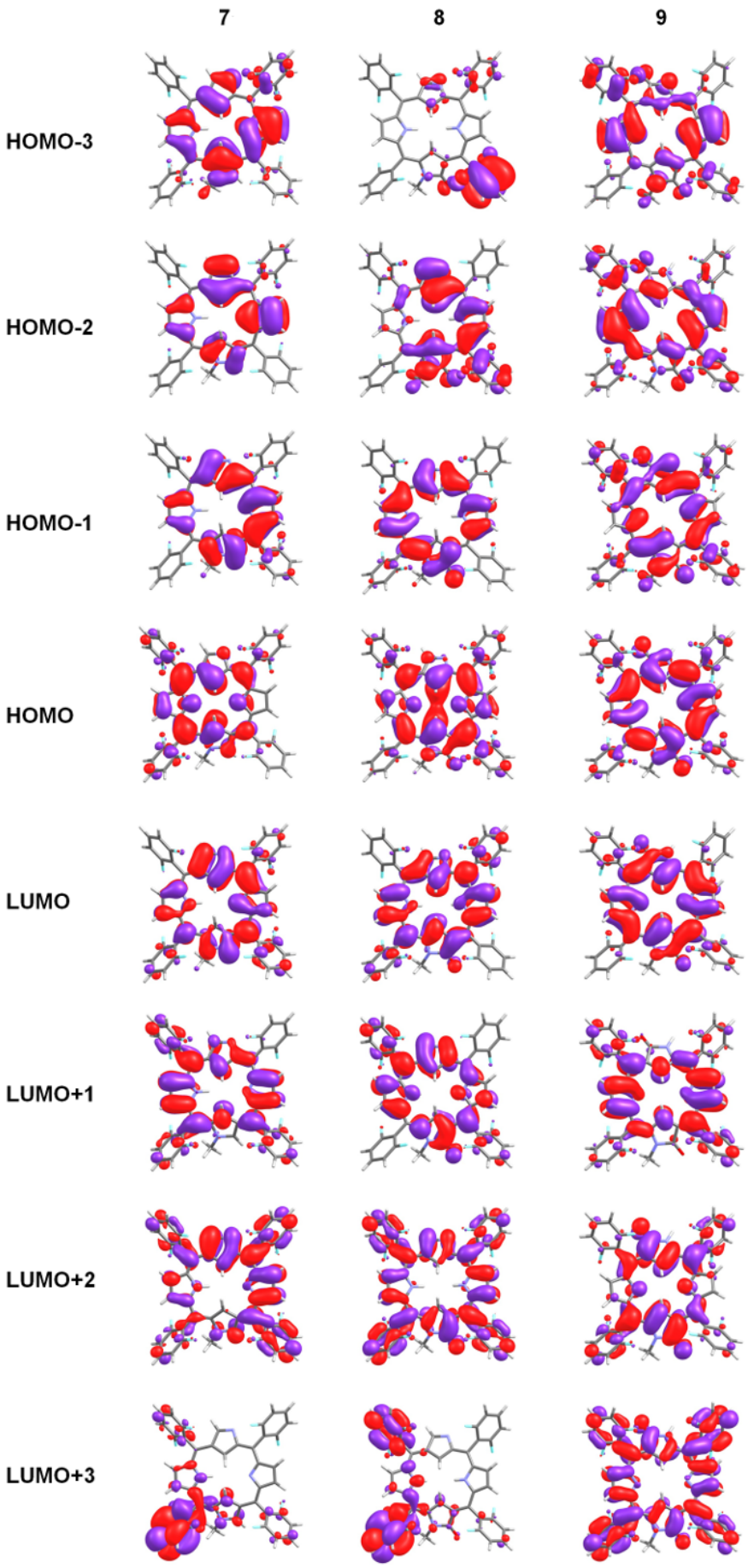


Fig. S62 Highest occupied molecular orbital and lowest unoccupied molecular orbitals of **7-9**.

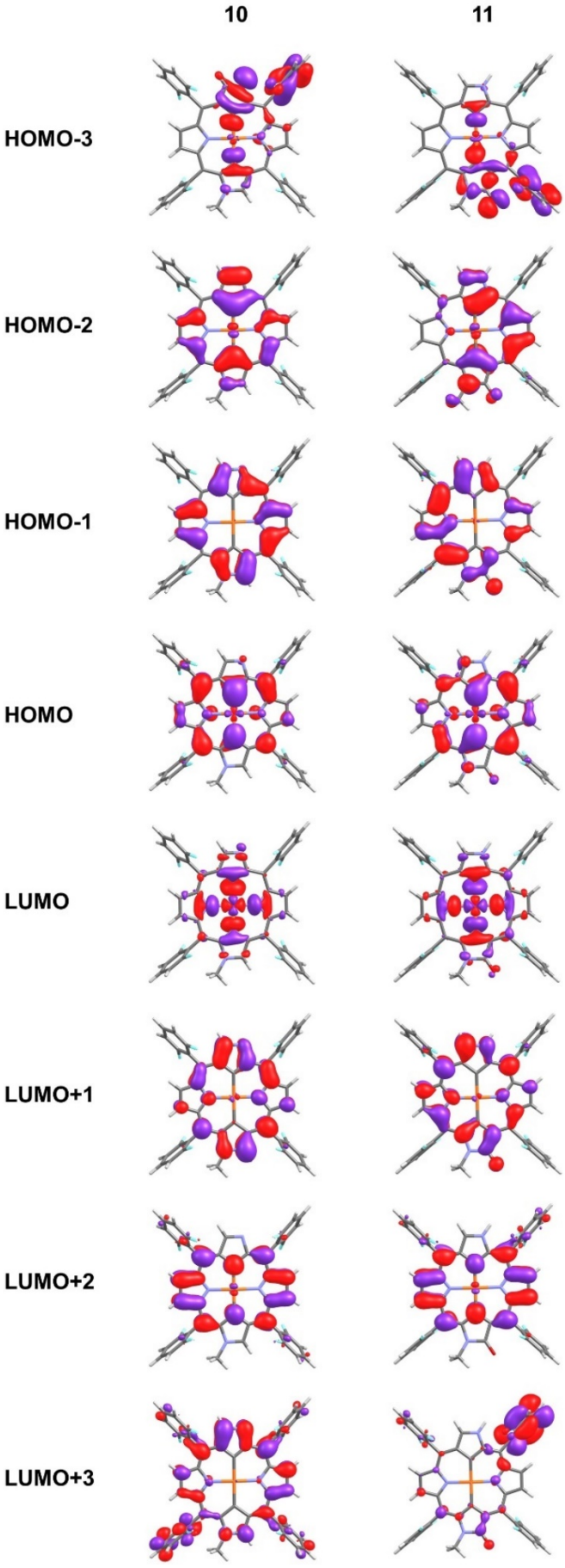


Fig. S63 Highest occupied molecular orbital and lowest unoccupied molecular orbitals of **10**-**11**.

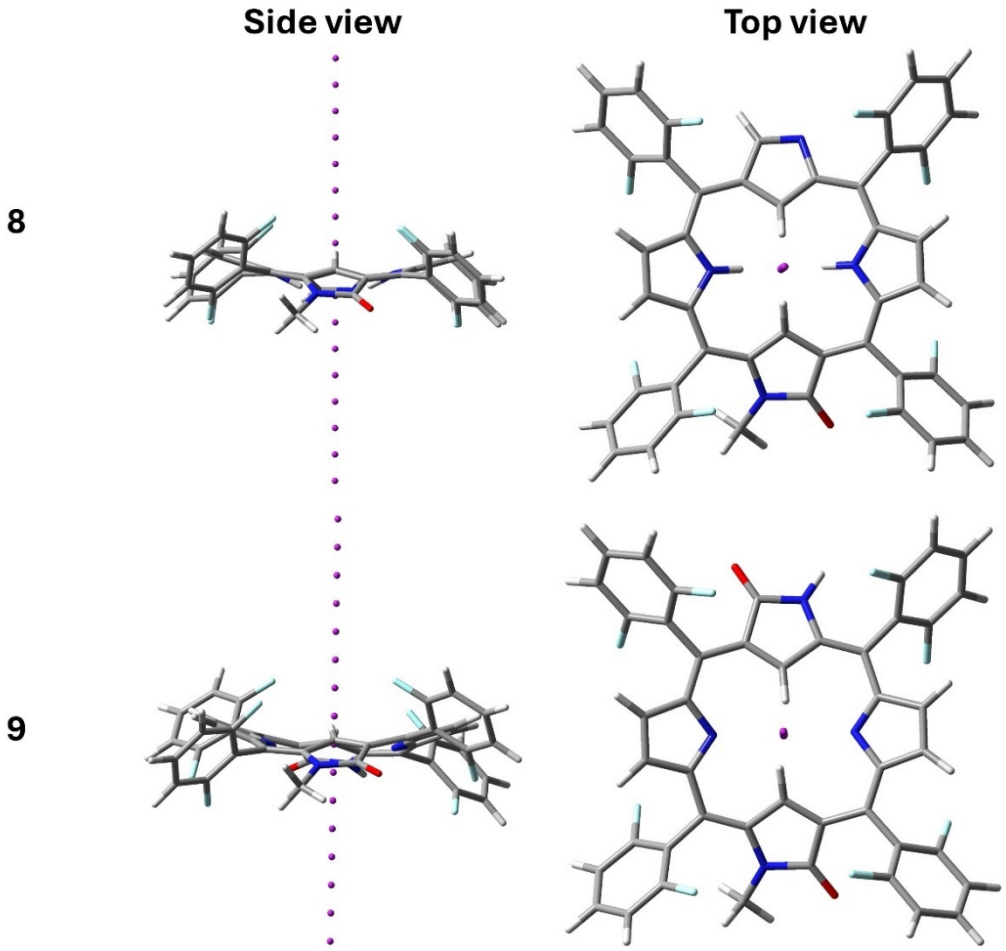


Fig. S64 The centers of macrocycles **8** and **9** for the NICS values were designated at the non-weighted mass of π conjugation pathway of the macrocycles.

Table S8 The calculated nucleus-independent chemical shifts (NICS) values for **8** and **9**.

Distance (Å)	**8**	**9**
-8	-0.8166	0.1540
-7	-1.1270	0.2411
-6	-1.6026	0.3937
-5	-2.3532	0.6721
-4	-3.5569	1.1981
-3	-5.4441	2.2078
-2	-8.1722	4.0580
-1	-11.3595	6.6857
0	-11.2394	7.9270
1	-9.7127	6.2062
2	-7.0111	3.8590
3	-4.8038	2.0480
4	-3.2010	1.0811
5	-2.1469	0.5908
6	-1.4758	0.3366
7	-1.0443	0.1999
8	-0.7600	0.1234

Table S9 Harmonic oscillator model of aromaticity (HOMA), multi-center indices (MCI), approximate multi-center bond order for large rings (AV1245 index) and Avmin index values for **7-9**.

	HOMA	MCI	AV1245	AVmin
7	0.648	0.555	1.819	0.712
8	0.804	0.576	2.778	2.010
9	0.421	0.532	0.778	0.104

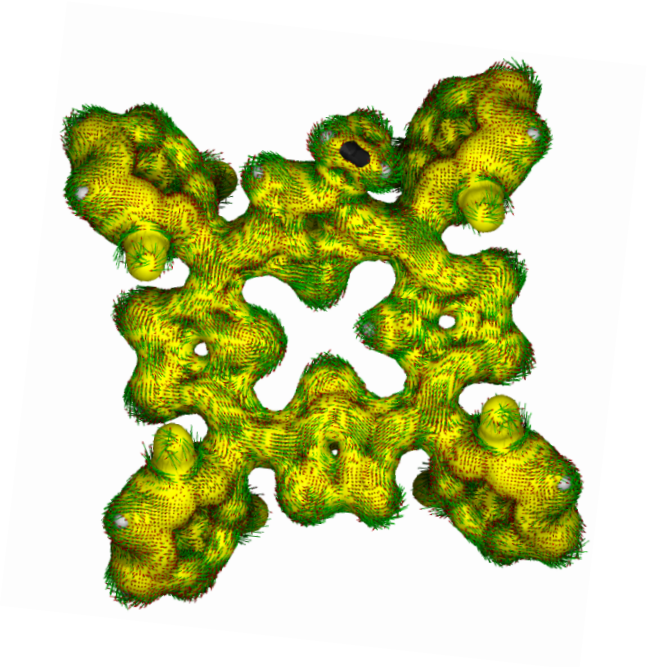


Fig. S65 The Anisotropy of Induced Current Density (AICD) plot of **7**. A clockwise interrupted ring current indicating the non-aromatic nature of macrocycle.

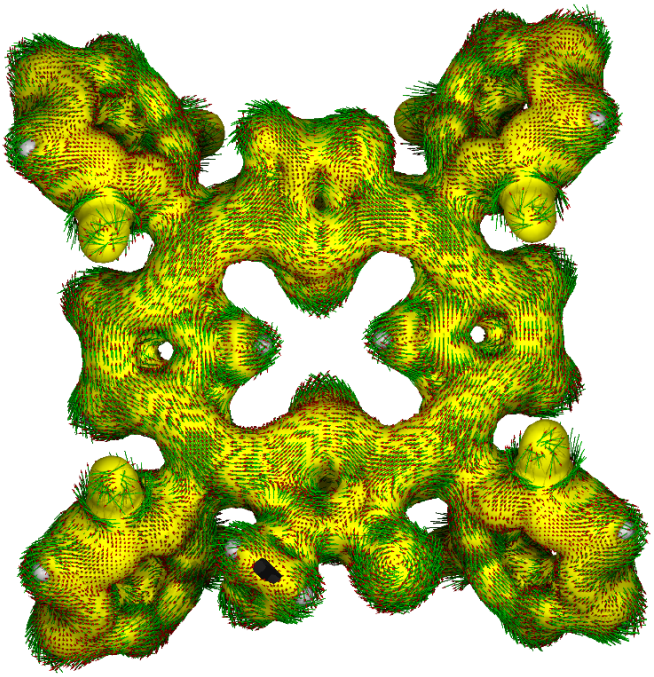


Fig. S66 The Anisotropy of Induced Current Density (AICD) plot of **8**. A continuous clockwise ring current along the macrocycle indicating the aromatic nature of macrocycle.

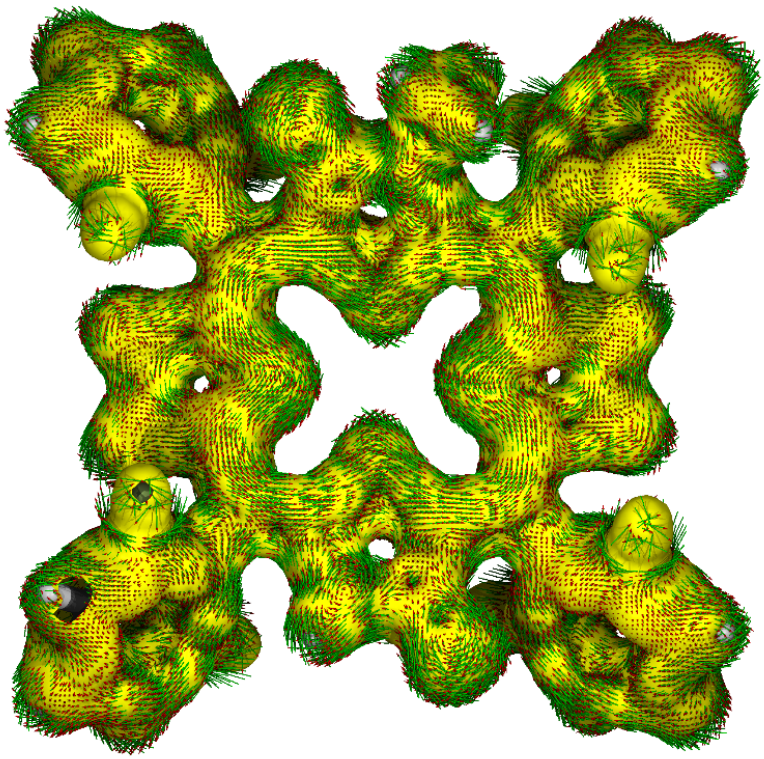


Fig. S67 The Anisotropy of Induced Current Density (AICD) plot of **9**. A continuous anti-clockwise ring current along the macrocycle indicating the anti-aromatic nature of macrocycle.

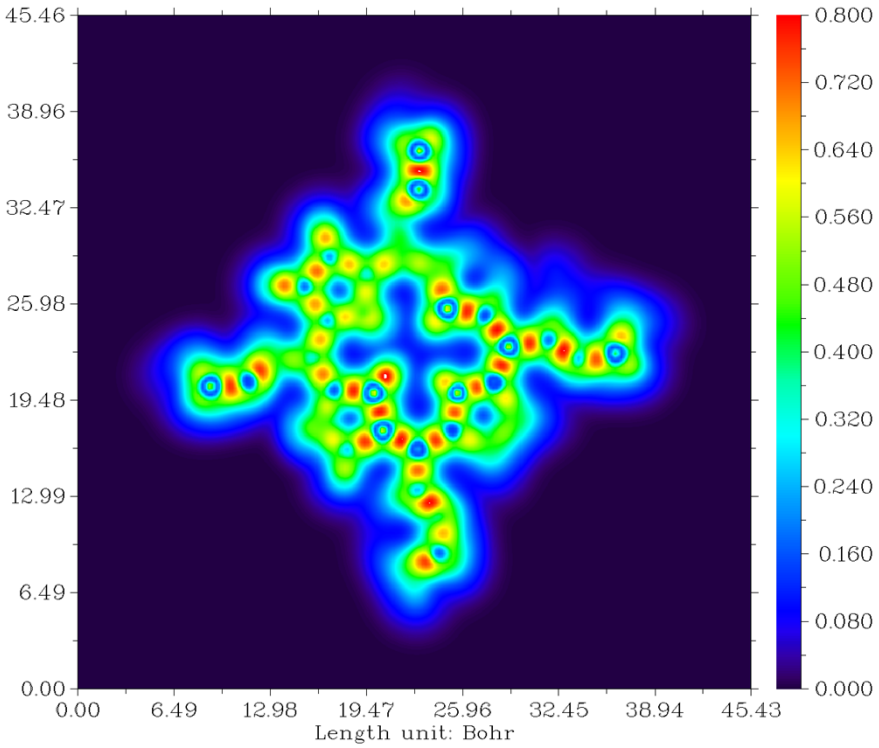


Fig. S68 Color-filled map of the electron localization function of **7**.

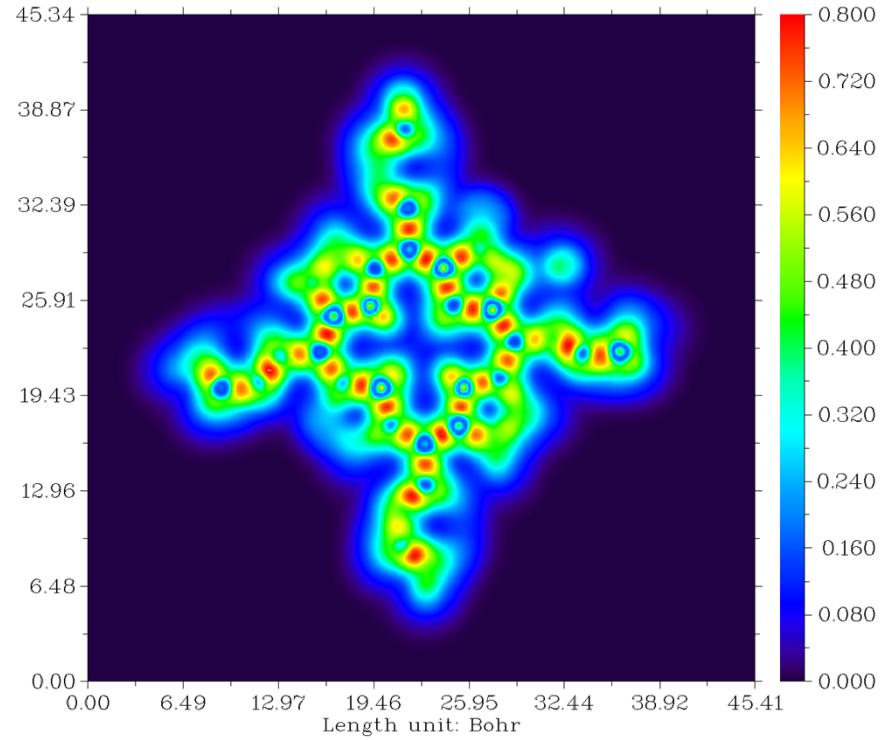


Fig. S69 Color-filled map of the electron localization function of **8**.

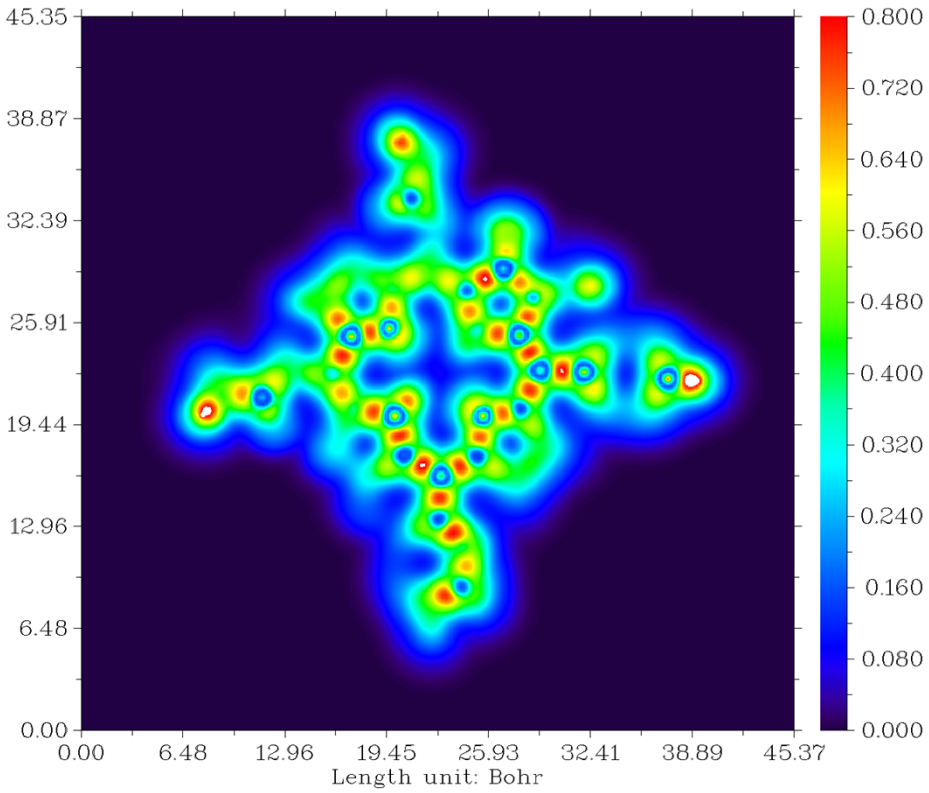


Fig. S70 Color-filled map of the electron localization function of **9**.

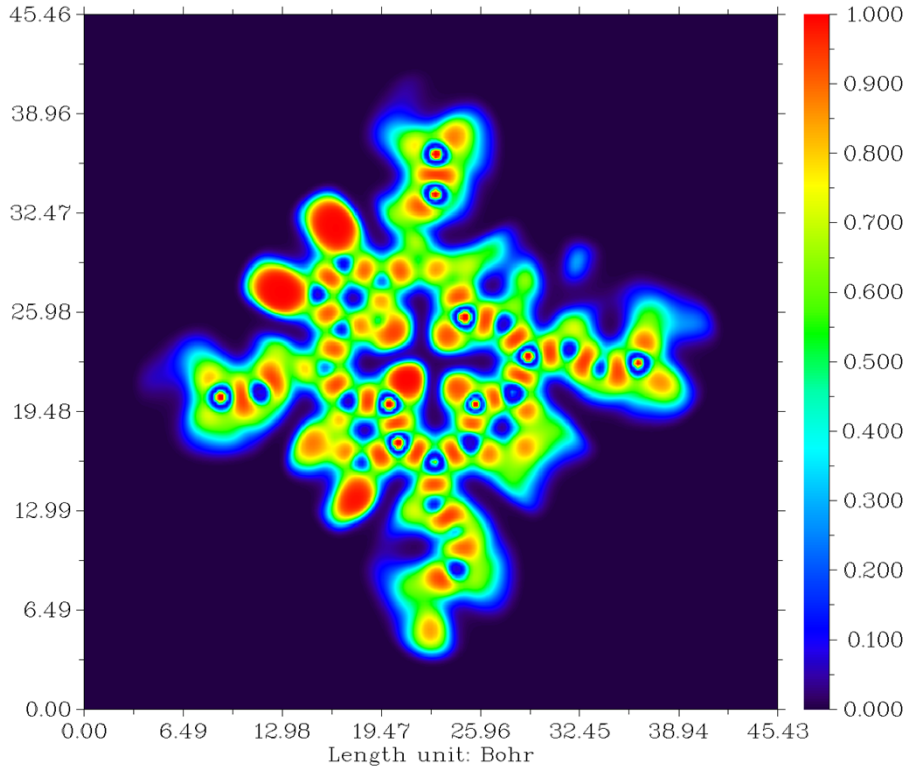


Fig. S71 Color-filled map of the electron localization function of **7**.

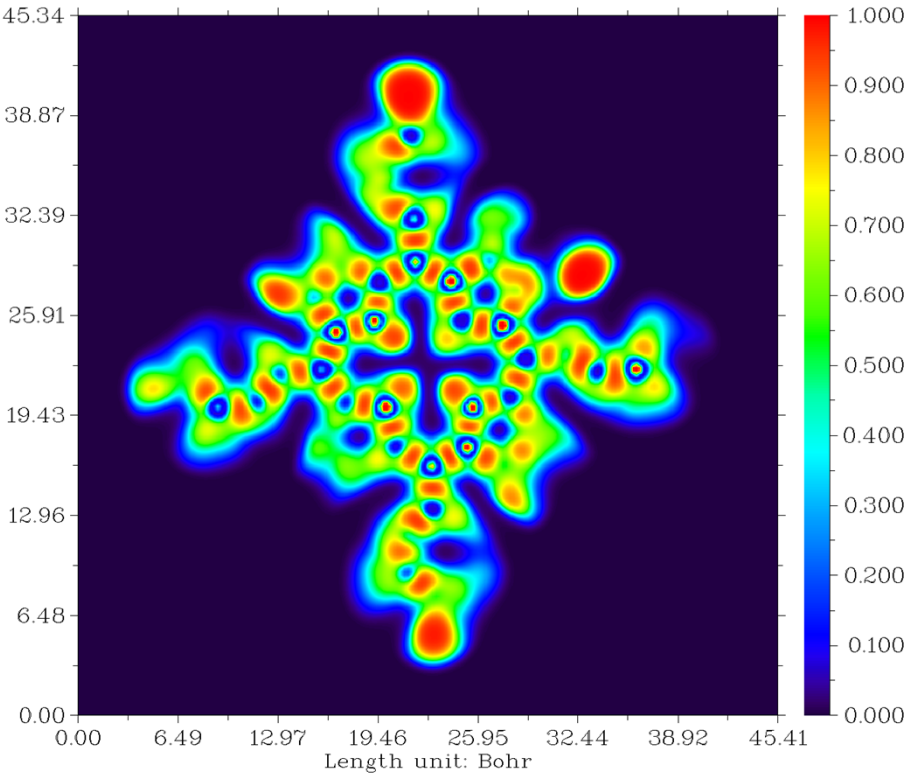


Fig. S72 Color-filled map of the electron localization function of **8**.

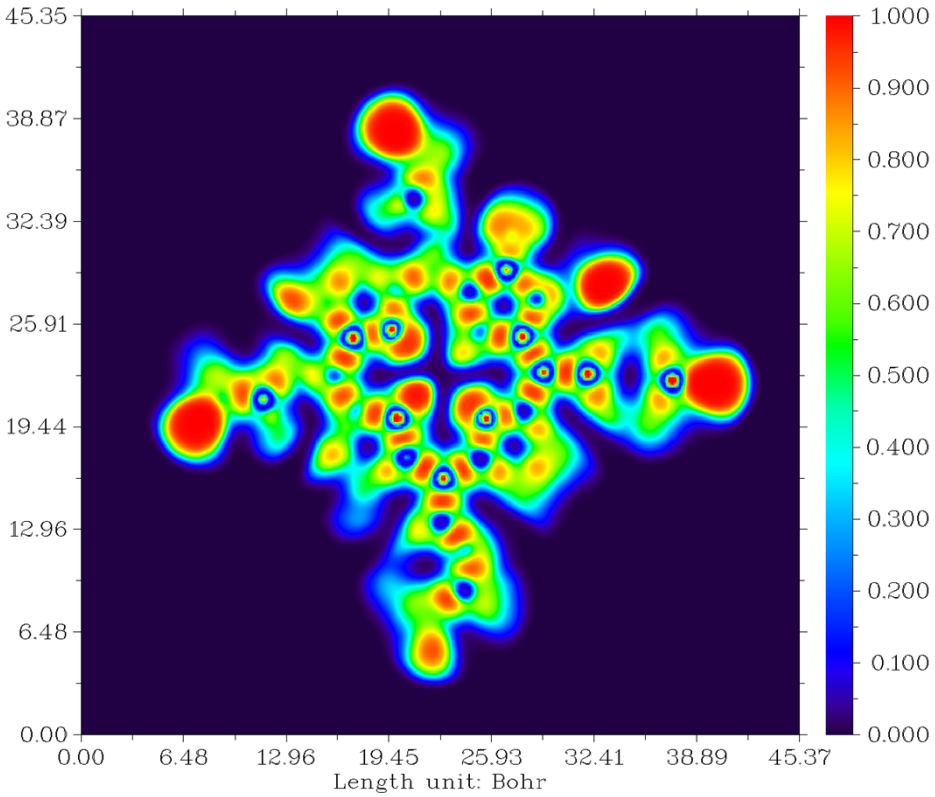


Fig. S73 Color-filled map of the electron localization function of **9**.

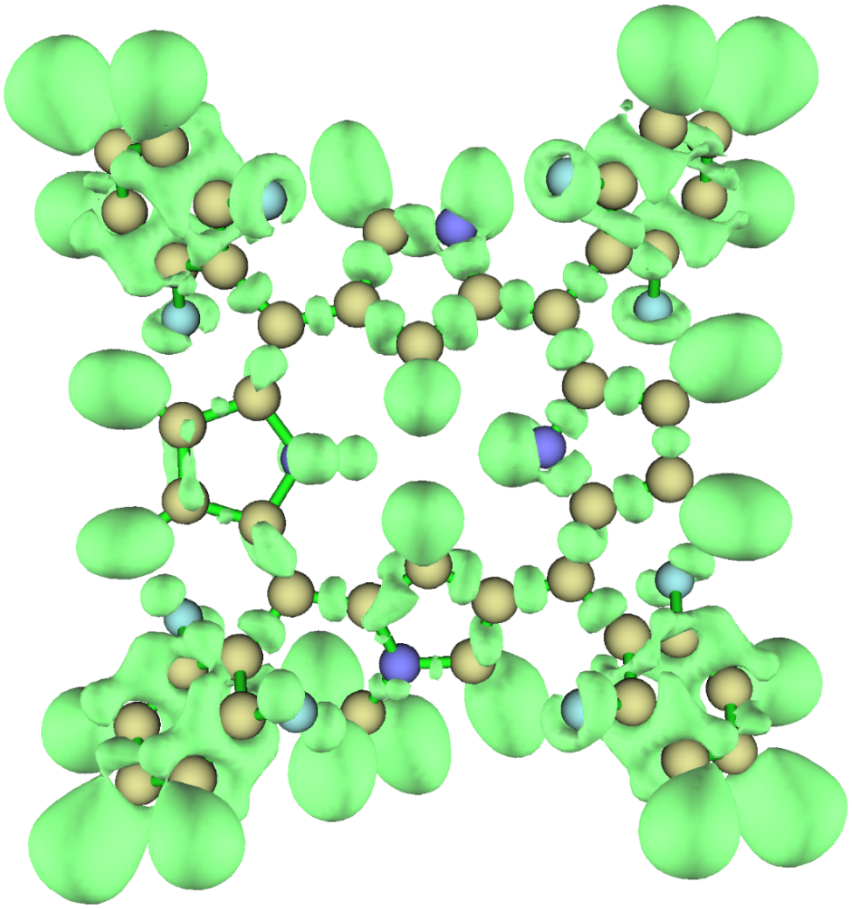


Fig. S74 Computed ELF index of **7**.

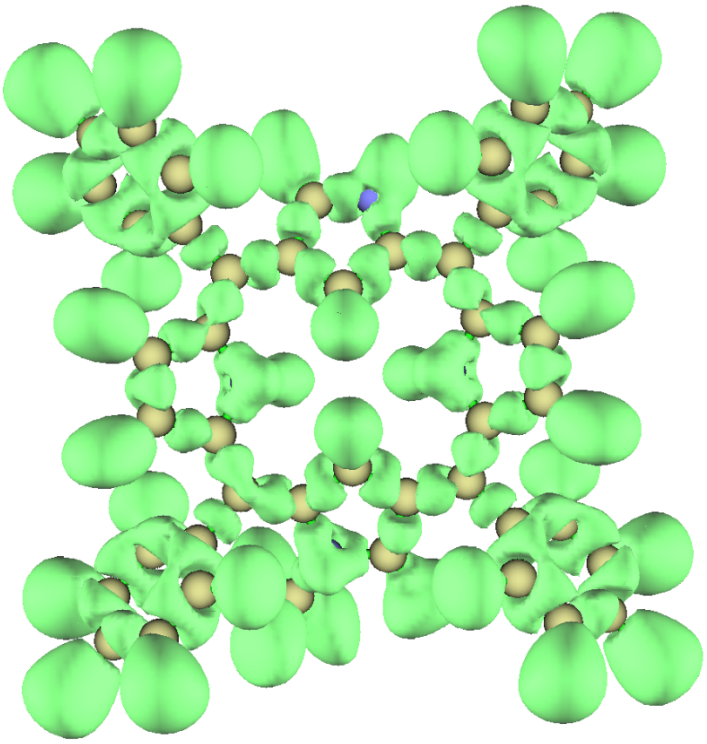


Fig. S75 Computed ELF index of **8**.

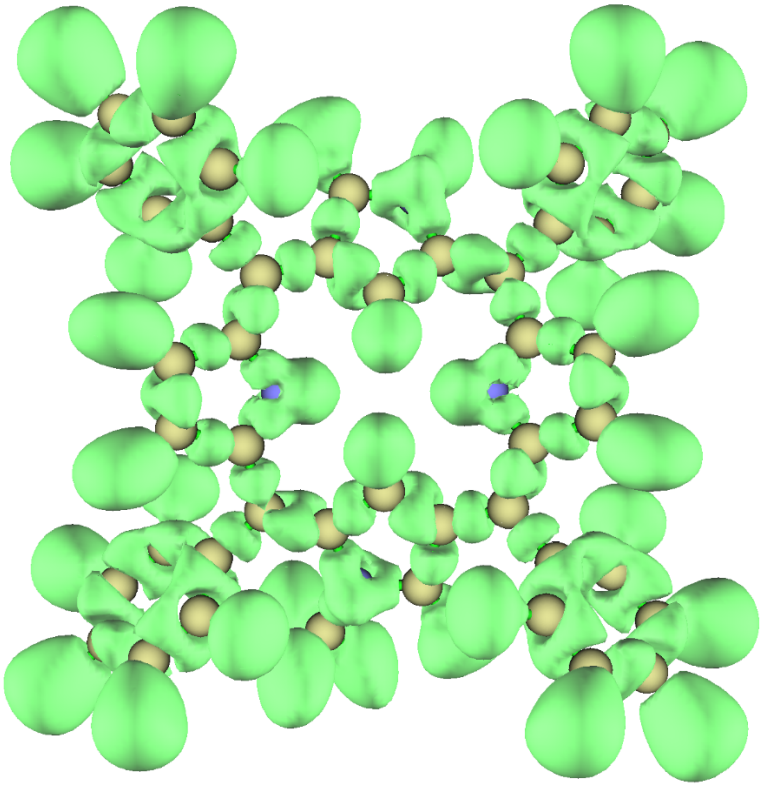


Fig. S76 Computed ELF index of **9**.

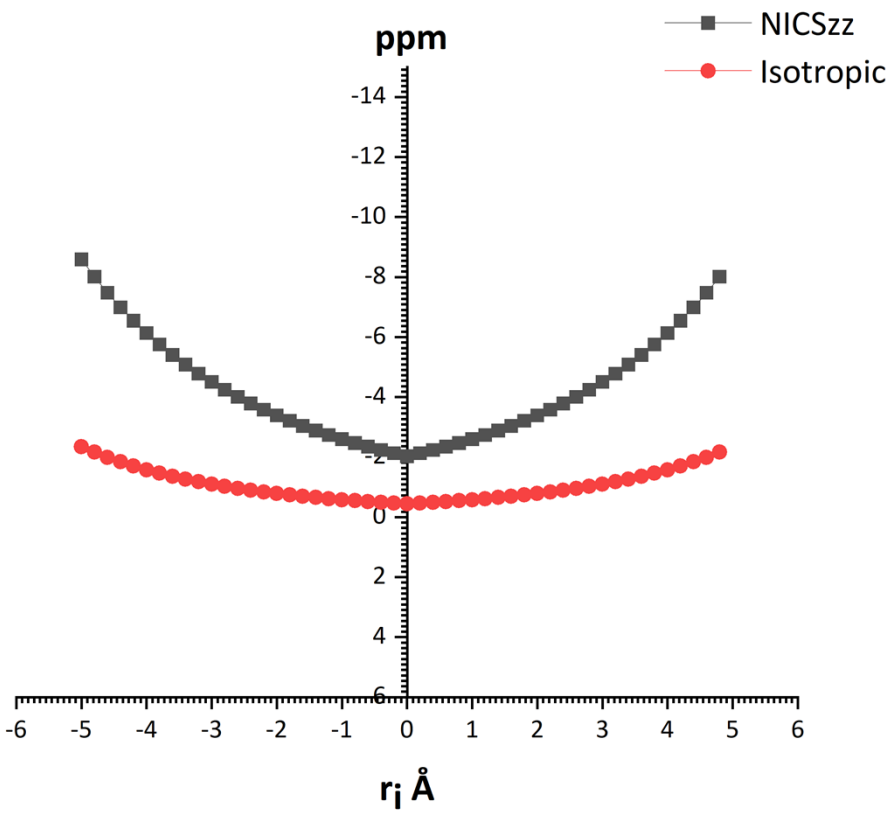


Fig. S77 Isotropic NICS and NICSzz scan plot of **8** where NICSzz is the out of plane contribution.

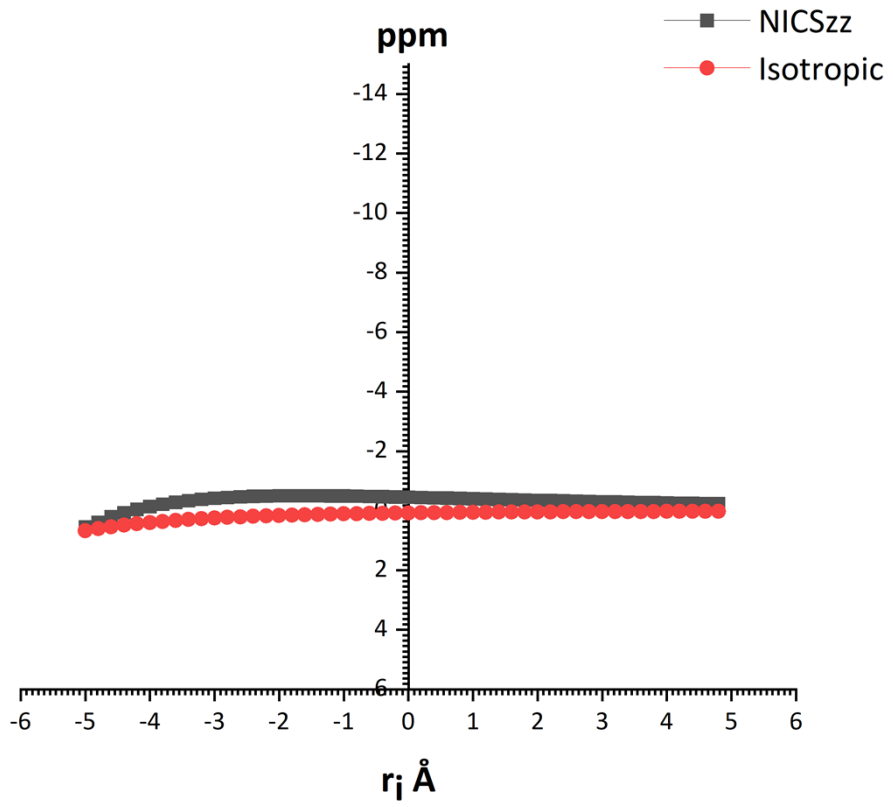


Fig. S78 Isotropic NICS and NICSzz scan plot of **9** where NICSzz is the out of plane contribution.

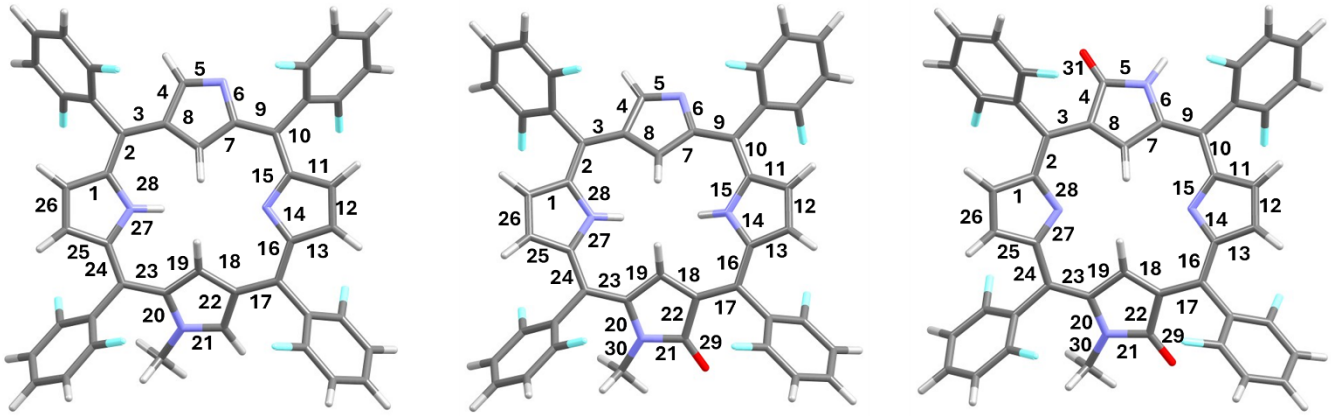


Fig. S79 Label used to show the computed Weiberg Bond Index and π-character of each bond.

Table S10 Computed Weiberg Bond Index and π-character of each bond.

Number of Bond	7		8		9	
	Wieberg Bond Index	π-character of the bond	Wieberg Bond Index	π-character of the bond	Wieberg Bond Index	π-character of the bond
1	1.1776	0.5784	1.2447	0.6849	1.1087	0.5708
2	1.4057	0.6324	1.3264	0.7289	1.5062	0.8956
3	1.2008	0.7920	1.2819	0.6923	1.1157	0.5458
4	1.0758	0.5429	1.1167	0.5794	1.0024	0.4744
5	1.7304	1.1255	1.6829	1.0650	1.0746	0.5716
6	1.0939	0.5787	1.1257	0.6127	1.1048	0.5811
7	1.2136	0.8267	1.3218	0.7433	1.1146	0.5789
8	1.4784	0.7207	1.3386	0.7714	1.6199	1.0172
9	1.4466	0.6667	1.2982	0.7097	1.5178	0.8977
10	1.1673	0.7555	1.3081	0.7127	1.1021	0.5420
11	1.1214	0.6440	1.2487	0.6886	1.1049	0.5668
12	1.7078	1.0196	1.5640	0.9562	1.7245	1.1069
13	1.1189	0.6344	1.2473	0.6889	1.1068	0.5687
14	1.2111	0.6003	1.1571	0.6331	1.1531	0.6217
15	1.4613	0.6241	1.1380	0.6189	1.5438	0.9443
16	1.4374	0.8146	1.2897	0.6967	1.5161	0.9044
17	1.1579	0.5707	1.3274	0.7289	1.1037	0.5366
18	1.2663	0.7418	1.3550	0.7755	1.6261	1.0213
19	1.4704	0.8307	1.3117	0.7397	1.1070	0.5766
20	1.0738	0.5824	1.0743	0.5675	1.0980	0.5821
21	1.2669	0.7580	1.0664	0.5832	1.0482	0.5686
22	1.3645	0.7667	1.0104	0.4825	1.0114	0.4793
23	1.1414	0.6054	1.3063	0.7096	1.5154	0.8938
24	1.4312	0.8036	1.2928	0.6986	1.1050	0.5476
25	1.1688	0.5762	1.2393	0.6836	1.1054	0.5681
26	1.6556	1.0952	1.5689	0.9602	1.7227	1.1050
27	1.1295	0.6913	1.1652	0.6382	1.5371	0.9377
28	1.1298	0.8370	1.1257	0.6083	1.1574	0.6250
29	1.1776	0.4741	1.6766	1.0332	1.6867	1.0430
30	-	-	0.9500	0.4732	0.9491	0.4715
31	-	-	-	-	1.6994	1.0520

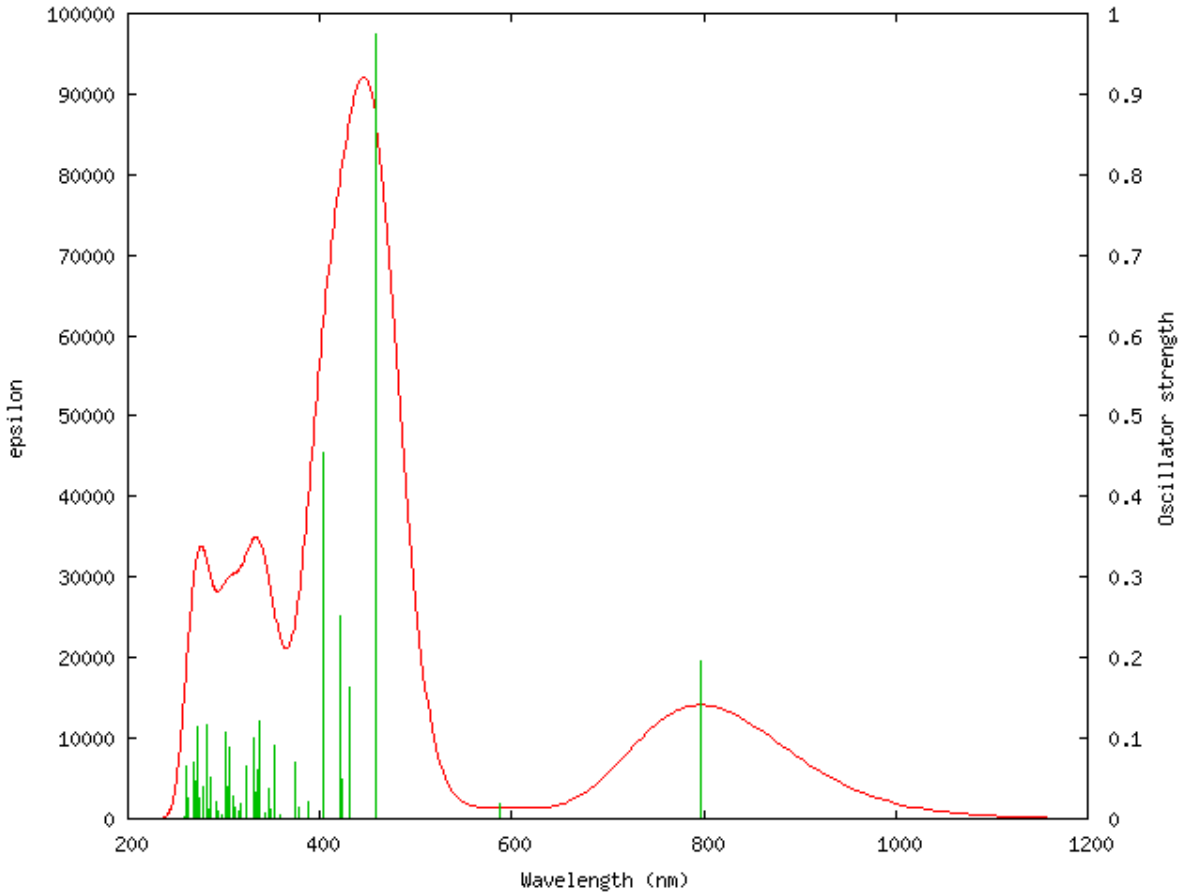


Fig. S80 Computed absorption spectrum of **7** in solvent phase (CH_2Cl_2).

Table S11 Computed absorption maxima (λ_{max} nm), Electronic excitation energies (E, eV), and Oscillator strength (f) of **7** in solvent phase (CH_2Cl_2).

No.	E (cm^{-1})	Cal. λ_{max} (nm)	Oscillator Strength *f*	Main Contributing Configurations
1	12539.59	797.47	0.195	HOMO→LUMO (97%)
2	17000.67	588.21	0.018	HOMO-1→LUMO (41%), HOMO→LUMO+1 (58%)
3	21822.29	458.25	0.974	HOMO-1→LUMO (45%), HOMO→LUMO+1 (34%)
4	23183.76	431.34	0.164	HOMO-2→LUMO (83%)
5	23589.46	423.92	0.050	HOMO-3→LUMO (71%), HOMO-1→LUMO+1 (17%)
6	23733.83	421.34	0.251	HOMO→LUMO+2 (80%)
7	24784.78	403.47	0.454	HOMO-3→LUMO (17%), HOMO-1→LUMO+1 (58%), HOMO→LUMO+2 (10%)
8	25812.34	387.41	0.021	HOMO-5→LUMO (27%), HOMO-4→LUMO (62%)
9	26489.85	377.50	0.015	HOMO-10→LUMO (12%), HOMO-9→LUMO (25%), HOMO-5→LUMO (17%), HOMO-4→LUMO (18%)
10	26697.14	374.57	0.070	HOMO-9→LUMO (15%), HOMO-5→LUMO (45%), HOMO-4→LUMO (17%)
11	27919.07	358.18	0.003	HOMO-7→LUMO (85%), HOMO-6→LUMO (10%)
12	27931.98	358.01	0.004	HOMO-6→LUMO (87%)
13	28388.49	352.26	0.090	HOMO-13→LUMO (17%), HOMO-10→LUMO (27%), HOMO-9→LUMO (23%), HOMO-8→LUMO (13%)
14	28721.60	348.17	0.012	HOMO-9→LUMO (20%), HOMO-8→LUMO (60%), HOMO-2→LUMO+1 (10%)
15	28789.35	347.35	0.038	HOMO-8→LUMO (13%), HOMO-3→LUMO+1 (15%), HOMO-2→LUMO+1 (56%)
16	29210.38	342.34	0.006	HOMO-13→LUMO (32%), HOMO-12→LUMO (14%), HOMO-11→LUMO (25%)
17	29674.96	336.98	0.122	HOMO-12→LUMO (29%), HOMO-11→LUMO (27%), HOMO→LUMO+3 (31%)
18	29799.97	335.57	0.060	HOMO-13→LUMO (16%), HOMO-12→LUMO (25%), HOMO-

				10→LUMO (28%), HOMO→LUMO+3 (21%)
19	29952.41	333.86	0.033	HOMO-3→LUMO+1 (45%), HOMO-2→LUMO+1 (16%), HOMO-1→LUMO+2 (12%)
20	30283.91	330.21	0.100	HOMO-11→LUMO (26%), HOMO-10→LUMO (13%), HOMO→LUMO+3 (33%)
21	30944.48	323.16	0.066	HOMO-3→LUMO+1 (10%), HOMO-1→LUMO+2 (57%)
22	31549.40	316.96	0.019	HOMO→LUMO+4 (53%), HOMO→LUMO+5 (36%)
23	31626.02	316.20	0.010	HOMO→LUMO+4 (39%), HOMO→LUMO+5 (50%)
24	32172.87	310.82	0.013	HOMO-5→LUMO+1 (31%), HOMO-4→LUMO+1 (58%)
25	32366.45	308.96	0.029	HOMO-15→LUMO (18%), HOMO-14→LUMO (69%)
26	32614.06	306.62	0.090	HOMO-9→LUMO+1 (32%), HOMO-5→LUMO+1 (11%), HOMO-4→LUMO+1 (22%)
27	32688.26	305.92	0.005	HOMO-6→LUMO+1 (81%)
28	32863.29	304.29	0.039	HOMO-9→LUMO+1 (15%), HOMO-5→LUMO+1 (44%), HOMO-4→LUMO+1 (13%)
29	32936.68	303.61	0.009	HOMO→LUMO+6 (50%), HOMO→LUMO+7 (42%)
30	33077.03	302.32	0.108	HOMO-15→LUMO (44%), HOMO-14→LUMO (15%)
31	33623.07	297.41	0.005	HOMO→LUMO+6 (33%), HOMO→LUMO+7 (44%)
32	33986.02	294.24	0.003	HOMO-9→LUMO+1 (10%), HOMO-8→LUMO+1 (67%)
33	34022.31	293.92	0.009	HOMO-7→LUMO+1 (16%), HOMO→LUMO+8 (55%), HOMO→LUMO+9 (21%)
34	34081.19	293.42	0.004	HOMO-7→LUMO+1 (17%), HOMO→LUMO+9 (44%)
35	34256.22	291.92	0.022	HOMO-10→LUMO+1 (26%), HOMO-9→LUMO+1 (14%), HOMO→LUMO+9 (19%)
36	34274.77	291.76	0.002	HOMO-7→LUMO+1 (54%), HOMO→LUMO+8 (29%)
37	34853.07	286.92	0.051	HOMO-11→LUMO+1 (62%), HOMO-10→LUMO+1 (27%)
38	35099.88	284.90	0.011	HOMO-16→LUMO (31%), HOMO-2→LUMO+2 (50%)
39	35482.19	281.83	0.116	HOMO-16→LUMO (52%), HOMO-2→LUMO+2 (34%)
40	35839.49	279.02	0.013	HOMO→LUMO+10 (91%)
41	35908.05	278.49	0.041	HOMO-13→LUMO+1 (27%), HOMO-12→LUMO+1 (35%), HOMO-10→LUMO+1 (10%)
42	36025.00	277.58	0.008	HOMO-13→LUMO+1 (62%), HOMO-12→LUMO+1 (22%)
43	36358.11	275.04	0.026	HOMO-3→LUMO+2 (52%), HOMO-1→LUMO+3 (23%), HOMO-1→LUMO+4 (14%)
44	36646.05	272.88	0.113	HOMO-3→LUMO+2 (23%), HOMO-1→LUMO+3 (54%)
45	37079.18	269.69	0.047	HOMO-14→LUMO+1 (75%)
46	37132.41	269.31	0.070	HOMO-1→LUMO+3 (17%), HOMO-1→LUMO+4 (67%)
47	38029.30	262.96	0.025	HOMO-5→LUMO+2 (15%), HOMO-4→LUMO+2 (69%)
48	38350.31	260.75	0.019	HOMO-1→LUMO+5 (70%), HOMO→LUMO+11 (18%)
49	38418.87	260.29	0.065	HOMO-15→LUMO+1 (42%), HOMO-5→LUMO+2 (15%), HOMO-4→LUMO+2 (18%)
50	38746.34	258.09	0.003	HOMO-17→LUMO (17%), HOMO-5→LUMO+2 (51%)

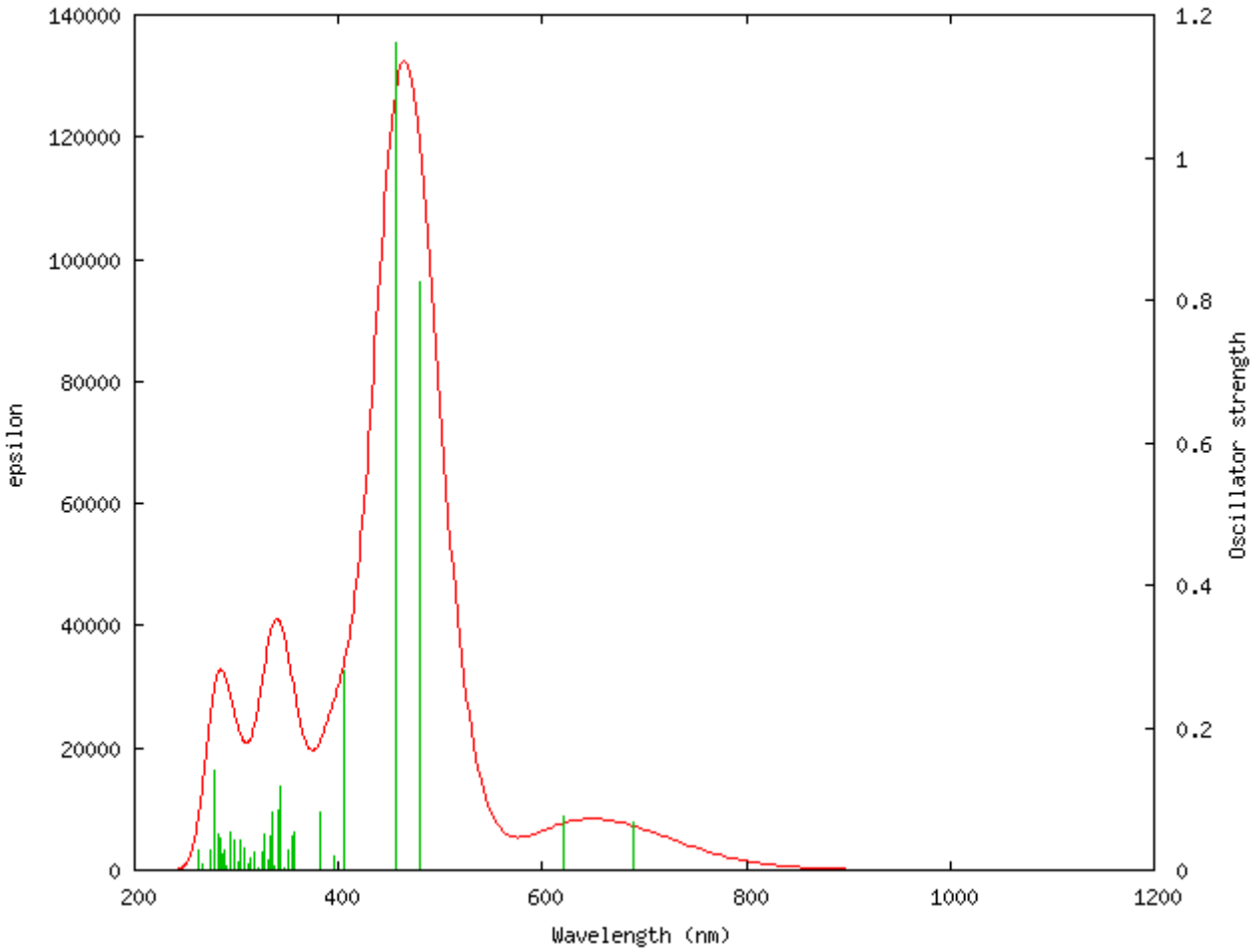


Fig. S81 Computed absorption spectrum of **8** in solvent phase (CH_2Cl_2).

Table S12 Computed absorption maxima (λ_{max} nm), Electronic excitation energies (E, eV), and Oscillator strength (f) of **8** in solvent phase (CH_2Cl_2).

No.	E (cm^{-1})	Cal. λ_{max} (nm)	Oscillator Strength *f*	Main Contributing Configurations
1	14494.69	689.91	0.068	HOMO-1→LUMO+1 (21%), HOMO→LUMO (78%)
2	16129.59	619.98	0.075	HOMO-1→LUMO (27%), HOMO→LUMO+1 (72%)
3	20835.06	479.96	0.824	HOMO-1→LUMO (12%), HOMO-1→LUMO+1 (65%), HOMO→LUMO (15%)
4	21935.21	455.89	1.162	HOMO-1→LUMO (55%), HOMO-1→LUMO+1 (11%), HOMO→LUMO+1 (22%)
5	24655.73	405.59	0.281	HOMO-2→LUMO (76%)
6	25288.88	395.43	0.019	HOMO→LUMO+2 (90%)
7	26122.06	382.82	0.081	HOMO-2→LUMO+1 (91%)
8	27981.18	357.38	0.052	HOMO-5→LUMO (27%), HOMO-4→LUMO (24%), HOMO-3→LUMO (28%)
9	28255.41	353.91	0.047	HOMO-9→LUMO (12%), HOMO-6→LUMO (11%), HOMO-4→LUMO (31%), HOMO-3→LUMO (23%)
10	28594.97	349.71	0.027	HOMO-5→LUMO (19%), HOMO-4→LUMO (22%), HOMO-1→LUMO+2 (44%)
11	28856.30	346.54	0.004	HOMO-6→LUMO (15%), HOMO-5→LUMO (22%), HOMO-3→LUMO (39%)
12	29116.01	343.45	0.057	HOMO-9→LUMO (40%), HOMO-8→LUMO (14%), HOMO-4→LUMO+1 (14%)
13	29203.12	342.43	0.024	HOMO-3→LUMO+1 (82%)
14	29222.48	342.20	0.119	HOMO-6→LUMO (38%), HOMO-5→LUMO+1 (15%), HOMO-1→LUMO+2 (16%)

15	29383.79	340.32	0.083	HOMO-5→LUMO+1 (18%), HOMO-4→LUMO+1 (46%)
16	29677.38	336.96	0.005	HOMO-7→LUMO (60%), HOMO-7→LUMO+1 (32%)
17	29869.34	334.79	0.080	HOMO-5→LUMO+1 (53%), HOMO-4→LUMO+1 (21%)
18	29973.38	333.63	0.049	HOMO-6→LUMO+1 (92%)
19	30286.33	330.18	0.013	HOMO-9→LUMO (14%), HOMO-8→LUMO (45%), HOMO-8→LUMO+1 (32%)
20	30486.35	328.02	0.050	HOMO-9→LUMO+1 (22%), HOMO-8→LUMO (27%), HOMO-8→LUMO+1 (31%)
21	30565.40	327.17	0.001	HOMO-7→LUMO (34%), HOMO-7→LUMO+1 (58%)
22	30781.56	324.87	0.026	HOMO-9→LUMO+1 (61%), HOMO-8→LUMO+1 (29%)
23	31126.76	321.27	0.003	HOMO-11→LUMO (11%), HOMO-10→LUMO (65%)
24	31508.27	317.38	0.026	HOMO-10→LUMO+1 (48%), HOMO→LUMO+3 (35%)
25	31930.10	313.18	0.018	HOMO-11→LUMO (17%), HOMO-10→LUMO+1 (13%), HOMO→LUMO+3 (49%)
26	32105.12	311.48	0.009	HOMO-11→LUMO (36%), HOMO-10→LUMO (15%), HOMO-10→LUMO+1 (28%)
27	32586.64	306.87	0.030	HOMO-13→LUMO (62%)
28	32939.10	303.59	0.041	HOMO-11→LUMO+1 (40%), HOMO→LUMO+4 (36%), HOMO→LUMO+5 (15%)
29	33143.16	301.72	0.011	HOMO-11→LUMO+1 (47%), HOMO→LUMO+4 (24%), HOMO→LUMO+5 (13%)
30	33198.01	301.22	0.007	HOMO→LUMO+4 (28%), HOMO→LUMO+5 (51%)
31	33514.99	298.37	0.042	HOMO-12→LUMO (25%), HOMO-12→LUMO+1 (52%)
32	33925.53	294.76	0.055	HOMO-15→LUMO+1 (16%), HOMO-12→LUMO (29%), HOMO-12→LUMO+1 (34%)
33	34122.33	293.06	0.032	HOMO-1→LUMO+3 (79%)
34	34192.50	292.46	0.001	HOMO-15→LUMO+1 (12%), HOMO-13→LUMO+1 (58%), HOMO-12→LUMO (22%)
35	34483.67	289.99	0.005	HOMO-15→LUMO (66%)
36	34658.69	288.53	0.008	HOMO-15→LUMO+1 (29%), HOMO-14→LUMO (20%), HOMO-14→LUMO+1 (20%), HOMO-13→LUMO+1 (12%)
37	34740.96	287.84	0.027	HOMO-14→LUMO (37%), HOMO-1→LUMO+3 (12%), HOMO→LUMO+6 (11%)
38	34863.56	286.83	0.022	HOMO-15→LUMO+1 (11%), HOMO-14→LUMO (13%), HOMO→LUMO+6 (26%), HOMO→LUMO+7 (26%)
39	35121.66	284.72	0.046	HOMO-14→LUMO+1 (27%), HOMO→LUMO+6 (22%), HOMO→LUMO+7 (27%)
40	35214.41	283.97	0.039	HOMO-14→LUMO+1 (26%), HOMO→LUMO+6 (30%), HOMO→LUMO+7 (17%)
41	35411.21	282.40	0.010	HOMO→LUMO+7 (12%), HOMO→LUMO+8 (78%)
42	35487.83	281.79	0.050	HOMO-2→LUMO+2 (69%), HOMO-1→LUMO+4 (10%)
43	35962.09	278.07	0.139	HOMO-1→LUMO+4 (75%)
44	36325.85	275.29	0.015	HOMO-1→LUMO+5 (34%), HOMO→LUMO+9 (10%), HOMO→LUMO+10 (50%)
45	36357.31	275.05	0.014	HOMO-1→LUMO+5 (30%), HOMO→LUMO+9 (21%), HOMO→LUMO+10 (42%)
46	36453.29	274.32	0.029	HOMO-1→LUMO+5 (27%), HOMO→LUMO+9 (65%)
47	37473.58	266.85	0.006	HOMO-16→LUMO (60%), HOMO-1→LUMO+6 (11%), HOMO-1→LUMO+7 (12%)
48	37600.21	265.96	0.007	HOMO-1→LUMO+6 (71%), HOMO-1→LUMO+7 (22%)
49	37939.78	263.58	0.028	HOMO-16→LUMO+1 (67%), HOMO-1→LUMO+7 (13%)
50	38218.85	261.65	0.003	HOMO-1→LUMO+7 (34%), HOMO-1→LUMO+8 (44%)

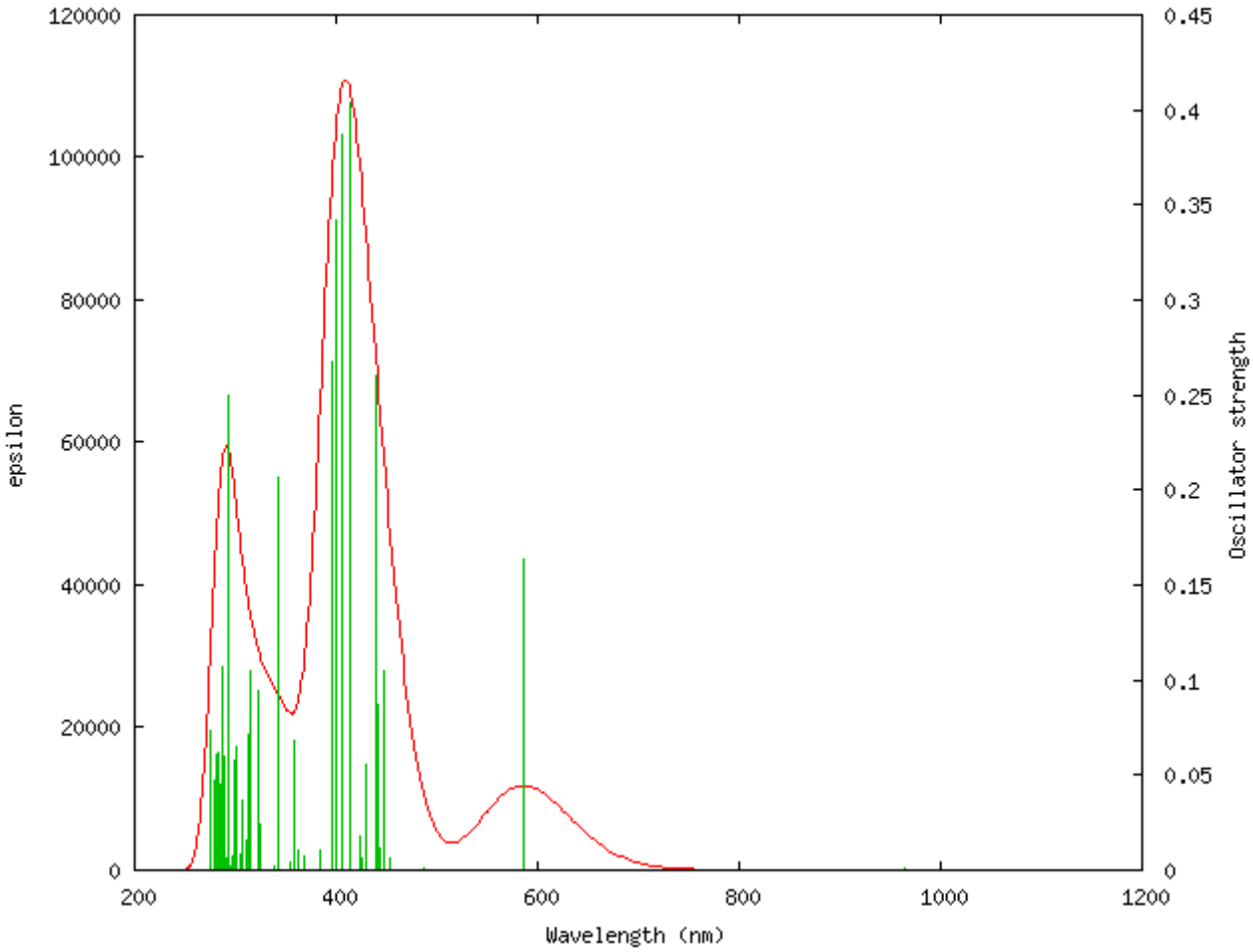


Fig. S82 Computed absorption spectrum of **9** in solvent phase (CH_2Cl_2).

Table S13 Computed absorption maxima (λ_{max} nm), Electronic excitation energies (E, eV), and Oscillator strength (f) of **9** in solvent phase (CH_2Cl_2).

No.	E (cm^{-1})	Cal. λ_{max} (nm)	Oscillator Strength *f*	Main Contributing Configurations
1	10373.97	963.95	0.001	HOMO→LUMO (100%)
2	17059.55	586.18	0.164	HOMO-1→LUMO (89%)
3	20210.78	494.79	0.001	HOMO-2→LUMO (72%), HOMO→LUMO+1 (21%)
4	20561.63	486.34	0.001	HOMO-3→LUMO (84%)
5	22077.16	452.96	0.006	HOMO-7→LUMO (19%), HOMO-6→LUMO (26%), HOMO-5→LUMO (15%), HOMO-4→LUMO (23%)
6	22296.54	448.50	0.105	HOMO-9→LUMO (14%), HOMO-6→LUMO (12%), HOMO-4→LUMO (32%), HOMO→LUMO+1 (17%)
7	22577.23	442.92	0.012	HOMO-6→LUMO (18%), HOMO-5→LUMO (61%)
8	22696.60	440.59	0.087	HOMO-9→LUMO (12%), HOMO-7→LUMO (20%), HOMO-4→LUMO (40%), HOMO→LUMO+1 (10%)
9	22736.12	439.83	0.261	HOMO-9→LUMO (14%), HOMO-7→LUMO (23%), HOMO-5→LUMO (11%), HOMO-2→LUMO (10%), HOMO→LUMO+1 (22%)
10	23228.93	430.50	0.056	HOMO-11→LUMO (20%), HOMO-10→LUMO (19%), HOMO-8→LUMO (14%), HOMO-7→LUMO (10%)
11	23478.96	425.91	0.006	HOMO-12→LUMO (11%), HOMO-11→LUMO (13%), HOMO-10→LUMO (12%), HOMO-9→LUMO (16%), HOMO-6→LUMO (27%)
12	23602.37	423.69	0.018	HOMO-9→LUMO (13%), HOMO-8→LUMO (69%), HOMO-7→LUMO (15%)
13	24169.38	413.75	0.404	HOMO-13→LUMO (24%), HOMO-11→LUMO (11%), HOMO-10→LUMO (13%), HOMO→LUMO+1 (10%), HOMO→LUMO+2 (24%)
14	24638.79	405.86	0.387	HOMO-13→LUMO (26%), HOMO-9→LUMO (11%), HOMO→LUMO+2 (31%)

15	25051.75	399.17	0.342	HOMO-12→LUMO (41%), HOMO-10→LUMO (25%), HOMO→LUMO+2 (14%)
16	25291.30	395.39	0.267	HOMO-13→LUMO (24%), HOMO-12→LUMO (14%), HOMO-11→LUMO (33%)
17	26020.43	384.31	0.010	HOMO-1→LUMO+1 (92%)
18	27214.95	367.45	0.007	HOMO-1→LUMO+2 (87%)
19	27649.68	361.67	0.010	HOMO-15→LUMO (32%), HOMO-14→LUMO (43%)
20	27853.74	359.02	0.069	HOMO-16→LUMO (15%), HOMO-15→LUMO (33%), HOMO-14→LUMO (41%)
21	28260.25	353.85	0.004	HOMO-17→LUMO (82%)
22	29207.96	342.37	0.207	HOMO-16→LUMO (48%), HOMO-15→LUMO (21%), HOMO-3→LUMO+1 (14%)
23	29605.59	337.77	0.002	HOMO-2→LUMO+1 (24%), HOMO→LUMO+3 (69%)
24	30732.36	325.39	0.024	HOMO-3→LUMO+1 (17%), HOMO-2→LUMO+1 (39%), HOMO→LUMO+3 (12%)
25	30888.83	323.74	0.094	HOMO-3→LUMO+1 (43%), HOMO-2→LUMO+1 (16%)
26	31723.62	315.22	0.105	HOMO-3→LUMO+2 (35%), HOMO-2→LUMO+2 (33%)
27	31865.57	313.82	0.072	HOMO-3→LUMO+2 (30%), HOMO-2→LUMO+2 (44%)
28	32200.29	310.56	0.016	HOMO-4→LUMO+1 (68%), HOMO-3→LUMO+2 (11%)
29	32219.65	310.37	0.003	HOMO-5→LUMO+1 (74%), HOMO-4→LUMO+1 (15%)
30	32567.28	307.06	0.037	HOMO-7→LUMO+1 (12%), HOMO-6→LUMO+1 (56%)
31	32756.01	305.29	0.008	HOMO-9→LUMO+1 (23%), HOMO-7→LUMO+1 (48%)
32	33161.71	301.55	0.065	HOMO-11→LUMO+1 (24%), HOMO-10→LUMO+1 (20%), HOMO-9→LUMO+1 (12%), HOMO-8→LUMO+1 (16%)
33	33333.51	300.00	0.058	HOMO-10→LUMO+1 (10%), HOMO-6→LUMO+2 (30%), HOMO-4→LUMO+2 (12%)
34	33405.30	299.35	0.022	HOMO-9→LUMO+1 (16%), HOMO-8→LUMO+1 (20%), HOMO-7→LUMO+1 (10%), HOMO-6→LUMO+1 (23%)
35	33502.08	298.49	0.003	HOMO-9→LUMO+1 (19%), HOMO-8→LUMO+1 (44%), HOMO-7→LUMO+1 (13%)
36	33609.36	297.54	0.008	HOMO-9→LUMO+1 (11%), HOMO-9→LUMO+2 (16%), HOMO-7→LUMO+2 (15%), HOMO-5→LUMO+2 (10%)
37	33892.46	295.05	0.002	HOMO-5→LUMO+2 (26%), HOMO-4→LUMO+2 (62%)
38	34027.96	293.88	0.026	HOMO-7→LUMO+2 (13%), HOMO-6→LUMO+2 (11%), HOMO-5→LUMO+2 (43%), HOMO-4→LUMO+2 (10%)
39	34170.72	292.65	0.250	HOMO-1→LUMO+3 (60%)
40	34390.11	290.78	0.006	HOMO-11→LUMO+1 (11%), HOMO-10→LUMO+1 (20%), HOMO-7→LUMO+2 (13%), HOMO-6→LUMO+2 (23%)
41	34597.39	289.04	0.059	HOMO-18→LUMO (14%), HOMO-9→LUMO+2 (23%), HOMO-8→LUMO+2 (24%)
42	34729.67	287.94	0.107	HOMO-18→LUMO (28%), HOMO-13→LUMO+1 (19%), HOMO-11→LUMO+1 (14%)
43	34734.51	287.90	0.010	HOMO-9→LUMO+2 (24%), HOMO-8→LUMO+2 (43%), HOMO-7→LUMO+2 (17%)
44	34901.46	286.52	0.006	HOMO-13→LUMO+1 (38%), HOMO-10→LUMO+2 (16%)
45	34959.54	286.04	0.046	HOMO-10→LUMO+2 (42%)
46	35207.15	284.03	0.062	HOMO-11→LUMO+2 (48%)
47	35445.89	282.12	0.043	HOMO-12→LUMO+1 (11%), HOMO→LUMO+4 (61%)
48	35503.96	281.66	0.060	HOMO-12→LUMO+1 (24%), HOMO-12→LUMO+2 (11%), HOMO→LUMO+4 (19%)
49	35804.81	279.29	0.047	HOMO-12→LUMO+2 (34%), HOMO→LUMO+5 (41%)
50	36316.17	275.36	0.073	HOMO-12→LUMO+1 (19%), HOMO-12→LUMO+2 (21%), HOMO→LUMO+5 (27%)

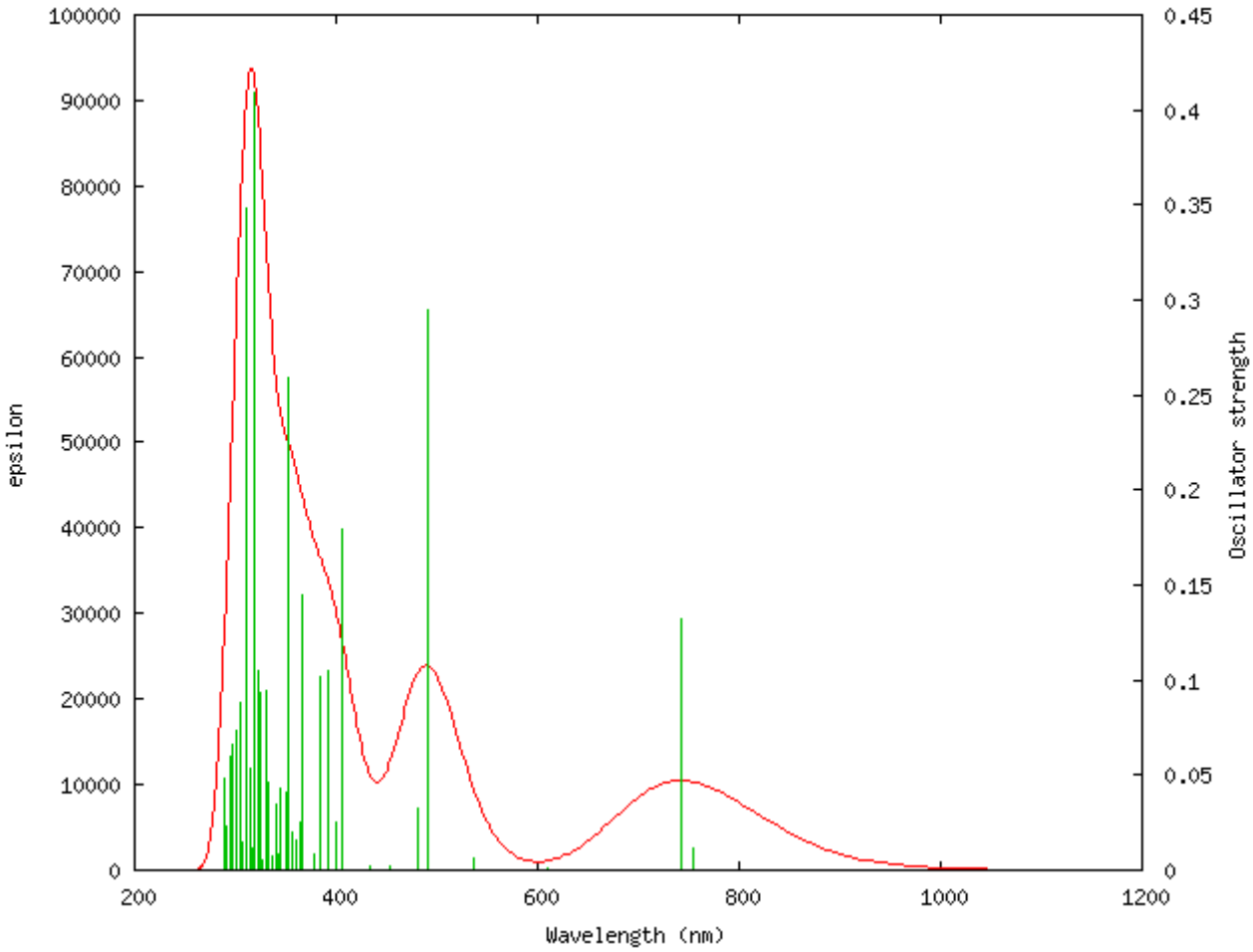


Fig. S83 Computed absorption spectrum of **10** in solvent phase (CH_2Cl_2).

Table S14 Computed absorption maxima (λ_{max} nm), Electronic excitation energies (E, eV), and Oscillator strength (f) of **10** in solvent phase (CH_2Cl_2).

No.	E (cm^{-1})	Cal. λ_{max} (nm)	Oscillator Strength *f*	Main Contributing Configurations
1	8276.92	1208.18	0.000	HOMO→LUMO (100%)
2	13259.85	754.16	0.012	HOMO-1→LUMO (89%), HOMO→LUMO+1 (10%)
3	13472.78	742.24	0.133	HOMO-1→LUMO (10%), HOMO→LUMO+1 (86%)
4	16382.04	610.42	0.001	HOMO-2→LUMO (96%)
5	18658.15	535.96	0.007	HOMO-1→LUMO+1 (48%), HOMO→LUMO+2 (51%)
6	20381.77	490.63	0.295	HOMO-3→LUMO (12%), HOMO-1→LUMO+1 (35%), HOMO→LUMO+2 (28%)
7	20821.35	480.28	0.032	HOMO-2→LUMO+1 (93%)
8	22008.60	454.37	0.002	HOMO-6→LUMO (22%), HOMO-5→LUMO (51%), HOMO-4→LUMO (10%)
9	23060.36	433.64	0.002	HOMO-6→LUMO (39%), HOMO-5→LUMO (40%), HOMO-3→LUMO (12%)
10	24672.67	405.31	0.179	HOMO-1→LUMO+2 (67%), HOMO→LUMO+3 (23%)
11	25023.52	399.62	0.025	HOMO-6→LUMO+1 (16%), HOMO-3→LUMO+1 (60%)
12	25542.95	391.50	0.105	HOMO-8→LUMO (16%), HOMO-3→LUMO (51%)
13	26010.75	384.46	0.102	HOMO-1→LUMO+2 (15%), HOMO→LUMO+3 (65%)
14	26405.97	378.70	0.008	HOMO-4→LUMO (79%)
15	27227.05	367.28	0.002	HOMO-7→LUMO (94%)
16	27335.12	365.83	0.145	HOMO-6→LUMO+1 (56%), HOMO-3→LUMO+1 (20%)
17	27471.43	364.01	0.026	HOMO-14→LUMO (14%), HOMO-11→LUMO (20%), HOMO-5→LUMO+1 (44%)
18	27786.80	359.88	0.016	HOMO-14→LUMO (10%), HOMO-11→LUMO (20%), HOMO-

				10→LUMO (11%), HOMO-5→LUMO+1 (35%)
19	28078.77	356.14	0.002	HOMO-4→LUMO+1 (63%), HOMO-3→LUMO+1 (11%)
20	28133.62	355.45	0.020	HOMO-9→LUMO (45%), HOMO-8→LUMO (43%)
21	28329.61	352.99	0.259	HOMO-9→LUMO (23%), HOMO-2→LUMO+2 (13%)
22	28451.40	351.48	0.041	HOMO-9→LUMO+1 (11%), HOMO-8→LUMO+1 (19%), HOMO-4→LUMO+1 (17%)
23	28582.87	349.86	0.005	HOMO-11→LUMO (24%), HOMO-10→LUMO (56%)
24	28983.73	345.02	0.043	HOMO-8→LUMO+1 (12%), HOMO-2→LUMO+2 (61%)
25	29192.63	342.55	0.009	HOMO-14→LUMO (10%), HOMO-13→LUMO (37%), HOMO-12→LUMO (12%), HOMO-11→LUMO (12%)
26	29234.57	342.06	0.000	HOMO-7→LUMO+1 (88%)
27	29389.43	340.26	0.001	HOMO-9→LUMO+1 (66%), HOMO-8→LUMO+1 (30%)
28	29436.21	339.72	0.035	HOMO-12→LUMO (76%)
29	29790.29	335.68	0.007	HOMO→LUMO+4 (97%)
30	30119.37	332.01	0.046	HOMO-10→LUMO+1 (88%)
31	30302.46	330.01	0.094	HOMO-15→LUMO (10%), HOMO-14→LUMO (28%), HOMO-13→LUMO (21%), HOMO-12→LUMO+1 (16%)
32	30530.72	327.54	0.006	HOMO-13→LUMO+1 (10%), HOMO-11→LUMO+1 (62%)
33	30848.50	324.16	0.093	HOMO-12→LUMO+1 (30%), HOMO→LUMO+5 (50%)
34	30963.84	322.96	0.105	HOMO-15→LUMO (11%), HOMO-12→LUMO+1 (35%), HOMO→LUMO+5 (29%)
35	31009.81	322.48	0.023	HOMO-15→LUMO+1 (25%), HOMO-13→LUMO+1 (33%), HOMO-1→LUMO+3 (10%)
36	31324.37	319.24	0.410	HOMO-15→LUMO (13%), HOMO→LUMO+5 (15%), HOMO→LUMO+6 (27%)
37	31543.76	317.02	0.012	HOMO-16→LUMO (61%), HOMO-13→LUMO+1 (10%)
38	31713.13	315.33	0.053	HOMO-16→LUMO (28%), HOMO-13→LUMO+1 (21%), HOMO-1→LUMO+3 (13%)
39	31799.43	314.47	0.037	HOMO-20→LUMO (13%), HOMO-15→LUMO+1 (16%), HOMO-1→LUMO+3 (27%), HOMO→LUMO+6 (16%)
40	32093.83	311.59	0.006	HOMO-6→LUMO+2 (13%), HOMO-3→LUMO+2 (62%)
41	32208.36	310.48	0.349	HOMO→LUMO+6 (40%)
42	32500.34	307.69	0.014	HOMO-20→LUMO (51%), HOMO-1→LUMO+3 (16%)
43	32877.00	304.16	0.088	HOMO-15→LUMO+1 (10%), HOMO-14→LUMO+1 (24%), HOMO-6→LUMO+2 (10%), HOMO-5→LUMO+2 (39%)
44	33127.03	301.87	0.061	HOMO-15→LUMO+1 (10%), HOMO-14→LUMO+1 (34%), HOMO-6→LUMO+2 (10%), HOMO-5→LUMO+2 (25%)
45	33256.08	300.70	0.074	HOMO-6→LUMO+2 (19%), HOMO→LUMO+7 (34%), HOMO→LUMO+8 (26%)
46	33275.44	300.52	0.018	HOMO→LUMO+7 (36%), HOMO→LUMO+8 (57%)
47	33691.62	296.81	0.066	HOMO-6→LUMO+2 (28%), HOMO-5→LUMO+2 (15%), HOMO→LUMO+9 (14%)
48	33916.65	294.84	0.060	HOMO→LUMO+9 (78%)
49	34431.24	290.43	0.023	HOMO→LUMO+10 (80%)
50	34475.60	290.06	0.049	HOMO-4→LUMO+2 (22%), HOMO-2→LUMO+3 (52%)

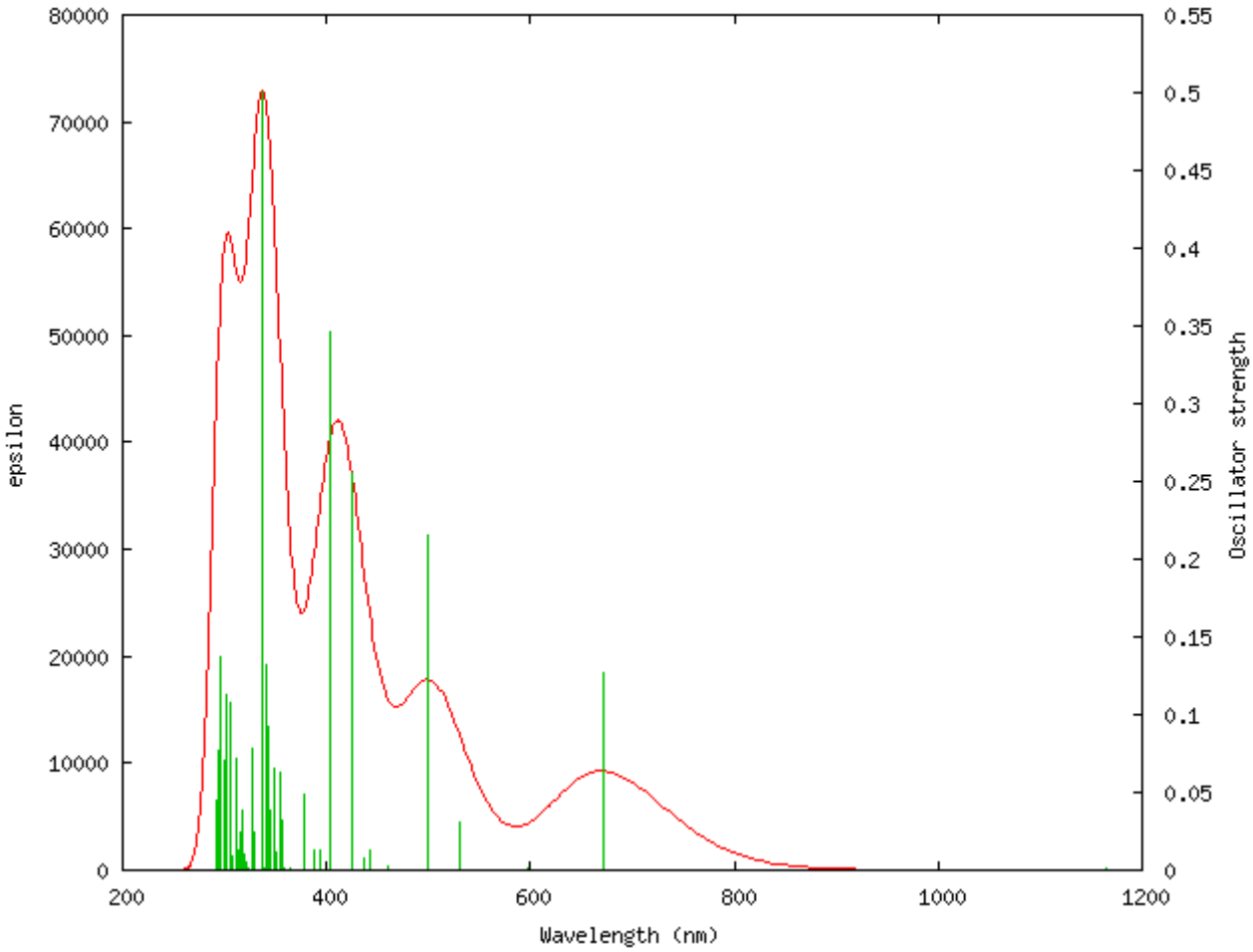


Fig. S84 Computed absorption spectrum of **11** in solvent phase (CH_2Cl_2).

Table S15 Computed absorption maxima (λ_{max} nm), Electronic excitation energies (E, eV), and Oscillator strength (f) of **11** in solvent phase (CH_2Cl_2).

No.	E (cm^{-1})	Cal. λ_{max} (nm)	Oscillator Strength *f*	Main Contributing Configurations
1	8578.57	1165.70	0.001	HOMO→LUMO (100%)
2	11783.84	848.62	0.000	HOMO-1→LUMO (100%)
3	14889.90	671.60	0.127	HOMO→LUMO+1 (92%)
4	16723.22	597.97	0.001	HOMO-2→LUMO (92%)
5	18874.31	529.82	0.031	HOMO-1→LUMO+1 (52%), HOMO→LUMO+2 (44%)
6	20021.24	499.47	0.216	HOMO-3→LUMO (27%), HOMO-1→LUMO+1 (26%), HOMO→LUMO+2 (31%)
7	21715.01	460.51	0.003	HOMO-6→LUMO (32%), HOMO-5→LUMO (31%), HOMO-4→LUMO (30%)
8	22601.42	442.45	0.012	HOMO-2→LUMO+1 (63%), HOMO-1→LUMO+2 (23%)
9	22907.92	436.53	0.008	HOMO-6→LUMO (51%), HOMO-5→LUMO (34%)
10	23559.62	424.46	0.255	HOMO-2→LUMO+1 (29%), HOMO-1→LUMO+2 (54%)
11	24746.07	404.10	0.346	HOMO-10→LUMO (17%), HOMO-3→LUMO (51%)
12	25409.06	393.56	0.012	HOMO-3→LUMO+1 (88%)
13	25758.30	388.22	0.013	HOMO-5→LUMO (21%), HOMO-4→LUMO (59%)
14	26420.49	378.49	0.049	HOMO-12→LUMO (60%)
15	27481.11	363.89	0.001	HOMO-7→LUMO (89%)
16	27850.52	359.06	0.001	HOMO-8→LUMO (94%)
17	27979.57	357.40	0.032	HOMO-2→LUMO+2 (18%), HOMO→LUMO+3 (70%)
18	28197.34	354.64	0.063	HOMO-5→LUMO+1 (46%), HOMO-4→LUMO+1 (21%)
19	28229.60	354.24	0.004	HOMO-10→LUMO (15%), HOMO-9→LUMO (71%)
20	28499.80	350.88	0.011	HOMO-13→LUMO (12%), HOMO-11→LUMO (46%)

21	28621.59	349.39	0.065	HOMO-11→LUMO (14%), HOMO-6→LUMO+1 (28%), HOMO-4→LUMO+1 (14%), HOMO-2→LUMO+2 (20%)
22	28991.80	344.93	0.039	HOMO-14→LUMO (11%), HOMO-13→LUMO (42%), HOMO-11→LUMO (10%), HOMO-6→LUMO+1 (10%)
23	29158.76	342.95	0.092	HOMO-13→LUMO (16%), HOMO-6→LUMO+1 (12%), HOMO-4→LUMO+1 (15%), HOMO-2→LUMO+2 (38%)
24	29406.37	340.06	0.132	HOMO-14→LUMO (29%), HOMO-13→LUMO (18%)
25	29437.83	339.70	0.001	HOMO-14→LUMO (22%), HOMO-6→LUMO+1 (16%), HOMO-5→LUMO+1 (20%), HOMO-4→LUMO+1 (28%)
26	29691.89	336.79	0.500	HOMO-10→LUMO (20%), HOMO→LUMO+4 (14%)
27	30333.11	329.67	0.025	HOMO-10→LUMO+1 (67%), HOMO→LUMO+4 (11%)
28	30571.85	327.10	0.078	HOMO-8→LUMO+1 (10%), HOMO→LUMO+4 (61%)
29	30610.57	326.68	0.017	HOMO-8→LUMO+1 (86%)
30	31003.36	322.55	0.001	HOMO-7→LUMO+1 (19%), HOMO-3→LUMO+2 (70%)
31	31038.04	322.19	0.006	HOMO-7→LUMO+1 (76%), HOMO-3→LUMO+2 (18%)
32	31353.41	318.94	0.010	HOMO→LUMO+5 (93%)
33	31496.97	317.49	0.003	HOMO-10→LUMO+1 (11%), HOMO-9→LUMO+1 (82%)
34	31589.73	316.56	0.039	HOMO-16→LUMO (29%), HOMO-15→LUMO (22%), HOMO-1→LUMO+3 (13%)
35	31681.68	315.64	0.006	HOMO→LUMO+6 (66%)
36	31785.72	314.61	0.025	HOMO-16→LUMO (11%), HOMO-12→LUMO+1 (30%), HOMO-1→LUMO+3 (16%), HOMO→LUMO+6 (20%)
37	31937.36	313.11	0.013	HOMO-13→LUMO+1 (48%), HOMO-11→LUMO+1 (26%)
38	32165.61	310.89	0.071	HOMO-20→LUMO (57%), HOMO-12→LUMO+1 (13%)
39	32407.58	308.57	0.009	HOMO-13→LUMO+1 (31%), HOMO-11→LUMO+1 (52%)
40	32723.75	305.59	0.108	HOMO-14→LUMO+1 (18%), HOMO-6→LUMO+2 (14%), HOMO-5→LUMO+2 (10%), HOMO-4→LUMO+2 (13%), HOMO-1→LUMO+3 (24%)
41	33092.35	302.18	0.061	HOMO-14→LUMO+1 (11%), HOMO→LUMO+7 (14%), HOMO→LUMO+8 (39%)
42	33130.26	301.84	0.094	HOMO-14→LUMO+1 (53%), HOMO→LUMO+8 (15%)
43	33189.94	301.30	0.113	HOMO-5→LUMO+2 (16%), HOMO→LUMO+7 (49%)
44	33369.00	299.68	0.005	HOMO-6→LUMO+2 (36%), HOMO→LUMO+7 (17%), HOMO→LUMO+8 (26%)
45	33419.81	299.22	0.070	HOMO-12→LUMO+1 (12%), HOMO-4→LUMO+2 (13%), HOMO-1→LUMO+5 (17%), HOMO→LUMO+7 (15%)
46	33754.54	296.26	0.137	HOMO-1→LUMO+5 (55%)
47	33935.21	294.68	0.076	HOMO-1→LUMO+6 (57%)
48	34158.62	292.75	0.019	HOMO-5→LUMO+2 (14%), HOMO-4→LUMO+2 (13%), HOMO-1→LUMO+4 (46%), HOMO-1→LUMO+6 (12%)
49	34207.02	292.34	0.010	HOMO-6→LUMO+2 (14%), HOMO-5→LUMO+2 (12%), HOMO-4→LUMO+2 (39%), HOMO-1→LUMO+4 (20%)
50	34355.42	291.07	0.045	HOMO-1→LUMO+4 (20%), HOMO-1→LUMO+5 (11%), HOMO-1→LUMO+6 (13%), HOMO→LUMO+9 (37%)

5. X, Y, Z Coordinates

7

C	4.12880000	-2.66740000	0.12430000
C	5.01310000	-2.37070000	1.17460000
C	6.22750000	-3.01940000	1.36260000
H	6.85130000	-2.73920000	2.20360000
C	6.59670000	-4.02520000	0.46880000
H	7.53880000	-4.54660000	0.60250000
C	5.76210000	-4.36270000	-0.59660000
H	6.02650000	-5.13040000	-1.31460000
C	4.56130000	-3.67960000	-0.74550000
C	2.83690000	-1.95010000	-0.03380000
C	1.66420000	-2.68900000	0.03780000
C	0.30600000	3.16220000	0.28960000
C	1.67510000	3.00450000	0.11880000
C	3.53380000	1.54710000	-0.73970000
C	2.81910000	-0.50710000	-0.15530000
C	1.88160000	0.41820000	0.28790000
C	-1.72930000	4.09550000	0.53460000
C	2.55020000	4.20900000	0.08380000
C	2.40860000	5.22660000	-0.87210000
C	3.23110000	6.34640000	-0.92240000
H	3.06420000	7.08850000	-1.69450000
C	4.25060000	6.47410000	0.02000000
H	4.89900000	7.34400000	-0.00230000
C	4.44290000	5.49170000	0.99130000
H	5.22190000	5.56710000	1.74100000
C	3.59930000	4.38790000	0.99910000
C	-4.31010000	2.66460000	0.00880000
C	-4.54420000	3.60400000	-1.00280000
C	-5.72720000	4.32250000	-1.12360000
H	-5.83790000	5.02670000	-1.94000000
C	-6.74030000	4.10030000	-0.19140000
C	-6.56290000	3.17700000	0.83820000
H	-7.33080000	2.98630000	1.57890000
C	-5.36310000	2.48050000	0.91480000
C	-3.03410000	1.90430000	0.10570000
C	-1.80680000	2.65490000	0.26860000
C	-0.57470000	-3.17740000	0.02320000
C	-1.95120000	-2.98060000	-0.02240000
C	-2.55910000	-1.68160000	-0.05430000
C	-3.08030000	0.52200000	0.00900000
C	1.49390000	-4.10110000	0.29930000
C	-2.82880000	-4.18270000	-0.02550000
C	-3.81600000	-4.38860000	0.95100000
C	-4.66340000	-5.48940000	0.96740000
H	-5.39770000	-5.57840000	1.75960000
C	-4.53410000	-6.44980000	-0.03550000
C	-3.57190000	-6.30120000	-1.03380000
H	-3.45300000	-7.02530000	-1.83160000
C	-2.75080000	-5.18030000	-1.00930000
N	-0.59000000	2.11980000	0.15210000
C	-0.41030000	4.40940000	0.54840000
C	0.16280000	-4.39230000	0.27480000
N	0.38260000	-2.18550000	-0.10810000
H	2.30380000	-4.78560000	0.50230000
H	-0.29490000	-5.35330000	0.45710000
H	-2.56810000	4.75840000	0.69420000
H	0.03690000	5.37750000	0.72510000
C	-3.98170000	-1.40720000	-0.36550000
H	-4.71780000	-2.16040000	-0.63080000
C	2.31430000	1.72510000	-0.07210000
N	3.83400000	0.23010000	-0.80420000
F	3.78310000	-3.98520000	-1.80460000
F	4.66420000	-1.40630000	2.04640000
F	3.78500000	3.45200000	1.94830000
F	1.44490000	5.10760000	-1.80280000
C	4.94010000	-0.29600000	-1.59720000
H	5.75300000	-0.65960000	-0.96460000
H	4.59070000	-1.11330000	-2.23090000
H	5.31730000	0.50490000	-2.23490000
H	1.02280000	0.20450000	0.89960000
H	-7.67300000	4.64980000	-0.26800000
H	-5.18630000	-7.31700000	-0.03950000
C	-2.02370000	-0.42510000	0.18070000
H	-1.04000000	-0.13930000	0.50010000
N	-4.29020000	-0.14810000	-0.32540000
F	-5.19680000	1.61260000	1.92720000
F	-3.57370000	3.81480000	-1.91550000
F	-3.94350000	-3.47390000	1.93080000
F	-1.83510000	-5.04590000	-1.99020000
H	4.16430000	2.28130000	-1.21980000
H	0.18490000	-1.25830000	-0.45430000

7′

C	-4.13967900	2.58168800	0.21033900
C	-4.98114400	2.34485200	1.30714800
C	-6.18815600	3.00587200	1.50188700
H	-6.78071100	2.77811000	2.38038800
C	-6.59092200	3.95480300	0.56169700
H	-7.52879400	4.48325600	0.69785600
C	-5.79806400	4.22745900	-0.55309200
H	-6.09099800	4.95066200	-1.30535200
C	-4.59964000	3.53976400	-0.70229500
C	-2.83844700	1.86839100	0.06185800
C	-1.66470200	2.61950300	0.16360500
C	-0.27079500	-3.21783300	0.15495400
C	-1.64376200	-3.07466400	0.01449500
C	-3.54738200	-1.59673600	-0.72566200
C	-2.83027300	0.44230900	-0.10792100
C	-1.85965500	-0.49060400	0.25569600
C	1.82654900	-4.05605800	0.46733300
C	-2.49124200	-4.29274700	-0.02525100
C	-2.30549700	-5.32464400	-0.96081600
C	-3.10176600	-6.46226800	-1.01812800
H	-2.89566600	-7.21191500	-1.77334700
C	-4.14984400	-6.59592500	-0.10822900
H	-4.78128500	-7.47785200	-0.13791500
C	-4.39030000	-5.60173100	0.84011900
H	-5.19107400	-5.67995600	1.56639600
C	-3.56545200	-4.48424300	0.86089600
C	4.41786400	-2.54573200	0.11308100
C	4.77531300	-3.49837100	-0.84971700
C	6.00897300	-4.13798600	-0.87621000
H	6.21327700	-4.86022700	-1.65814000
C	6.95046500	-3.81443300	0.09969900
C	6.65245800	-2.87042400	1.08214000
H	7.36216500	-2.60047300	1.85551000
C	5.40503600	-2.26009100	1.06701000
C	3.09895100	-1.85932600	0.11535800

C	1.94401500	-2.64643200	0.19849300
C	0.44946200	3.12191100	0.10842900
C	1.87404200	2.98726300	-0.01936100
C	2.52575900	1.75329400	-0.04132100
C	3.06893100	-0.44051100	0.01699600
C	-1.58338200	4.06191800	0.40589700
C	2.68289400	4.23354700	-0.13513600
C	3.68959400	4.56705300	0.78290600
C	4.45582400	5.72339500	0.69341700
H	5.21202500	5.91471200	1.44589800
C	4.22054900	6.60386100	-0.36168200
C	3.23309700	6.32565100	-1.30665000
H	3.03276200	6.98590600	-2.14250400
C	2.49311100	5.15741400	-1.17349000
N	0.65143900	-2.18683200	0.04421500
C	0.50454600	-4.39830000	0.44441400
C	-0.26620700	4.37772300	0.35880800
N	-0.40547400	2.09350600	0.00643200
H	-2.41388100	4.72839000	0.59089700
H	0.18341800	5.35143900	0.49502100
H	2.66313300	-4.70345100	0.68408600
H	0.08200200	-5.37279100	0.63946600
C	3.95159400	1.51379700	-0.35568300
H	4.67500800	2.27770700	-0.62290400
C	-2.29213900	-1.78801300	-0.12017700
N	-3.87732400	-0.28920700	-0.71529500
F	-3.86169100	3.77362100	-1.80530500
F	-4.59667900	1.43303200	2.21907400
F	-3.80133900	-3.54063500	1.79246000
F	-1.31303800	-5.20428700	-1.86365100
C	-5.03362600	0.23158700	-1.44096000
H	-5.80053600	0.60407600	-0.75942200
H	-4.72668500	1.03762900	-2.10965300
H	-5.45342700	-0.57846300	-2.03905200
H	-0.98300600	-0.22700800	0.81920600
H	7.92084000	-4.30041500	0.09512600
H	4.81028300	7.51059600	-0.44897300
C	2.01387900	0.45518500	0.19332200
H	1.01156900	0.27331200	0.52761000
N	4.27194100	0.25948400	-0.33023100
F	5.12138600	-1.36969700	2.03334200
F	3.87884400	-3.81189900	-1.80944600
F	3.92051700	3.73231400	1.81404300
F	1.55079800	4.89238400	-2.09903300
H	0.43302600	-1.28800800	-0.36109800
H	-4.19166600	-2.32442700	-1.19758200

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C	-2.56400000	4.20560000	0.02660000
C	-3.61080000	4.40870000	0.93940000
C	-4.45540000	5.51150000	0.90460000
H	-5.23270000	5.60590000	1.65390000
C	-4.26580000	6.46840000	-0.09220000
H	-4.91470000	7.33710000	-0.13590000
C	-3.24840000	6.31620000	-1.03350000
H	-3.08370000	7.03770000	-1.82530000
C	-2.42590000	5.19800000	-0.95600000
C	-1.68700000	3.00350000	0.09200000
C	-0.31590000	3.16950000	0.26340000
C	-1.65300000	-2.69010000	0.06200000
C	-2.83160000	-1.95390000	-0.00390000
C	-2.32130000	1.72040000	-0.07160000
C	-1.87530000	0.41720000	0.28230000
C	-0.13930000	-4.38060000	0.29890000
C	-4.11660000	-2.68000000	0.16860000
C	-4.54860000	-3.69840000	-0.69430000
C	-5.74090000	-4.39280000	-0.53010000
H	-6.00620000	-5.16440000	-1.24350000
C	-6.56610000	-4.06160000	0.54460000
H	-7.50130000	-4.59210000	0.69030000
C	-6.19650000	-3.05070000	1.43250000
H	-6.81310000	-2.77560000	2.28050000
C	-4.99110000	-2.39010000	1.22890000
C	2.84650000	-4.16400000	-0.07900000
C	2.75050000	-5.14140000	-1.07810000
C	3.57550000	-6.25810000	-1.14180000
H	3.44370000	-6.96730000	-1.95070000
C	4.55820000	-6.41920000	-0.16620000
C	4.70210000	-5.47790000	0.85280000
H	5.45330000	-5.57820000	1.62750000
C	3.85240000	-4.37950000	0.87400000
C	1.96580000	-2.96700000	-0.04120000
C	0.58500000	-3.16720000	0.02400000
C	1.80030000	2.67350000	0.26530000
C	3.01930000	1.91880000	0.12850000
C	3.05710000	0.53010000	0.03090000
C	2.56790000	-1.67460000	-0.06590000
C	0.39420000	4.42970000	0.47720000
C	4.30200000	2.67710000	0.06420000
C	5.31950000	2.51020000	1.01430000
C	6.52360000	3.20390000	0.97630000
H	7.26020000	3.02530000	1.75100000
C	6.74140000	4.11230000	-0.05850000
C	5.76670000	4.31830000	-1.03480000
H	5.91100000	5.01040000	-1.85640000
C	4.57920000	3.60200000	-0.95260000
N	-0.37700000	-2.18280000	-0.10900000
C	-1.47400000	-4.09570000	0.33760000
C	1.71470000	4.12270000	0.47630000
N	0.58110000	2.12820000	0.17110000
H	-0.05750000	5.40210000	0.61520000
H	2.54800000	4.79780000	0.61220000
H	0.32810000	-5.33590000	0.48640000
H	-2.27750000	-4.78160000	0.56000000
C	4.23500000	-0.29600000	-0.30930000
H	5.22870000	0.08230000	-0.52730000
C	-2.82190000	-0.51490000	-0.13040000
F	-1.46400000	5.05490000	-1.88560000
F	-3.79500000	3.49740000	1.91290000
F	-4.64180000	-1.42020000	2.09460000
F	-3.77990000	-3.99790000	-1.76140000
H	-1.00000000	0.21160000	0.87230000
H	5.21450000	-7.28300000	-0.19930000
H	7.67630000	4.66130000	-0.10590000
C	2.01430000	-0.42040000	0.17830000
H	1.02610000	-0.15750000	0.50100000
N	3.96330000	-1.56070000	-0.37520000
F	3.98370000	-3.49410000	1.87660000
F	1.81150000	-4.99280000	-2.03690000
F	5.11830000	1.64210000	2.02370000
F	3.64920000	3.79760000	-1.90720000
H	-0.18610000	-1.25850000	-0.46700000
C	-3.55850000	1.53300000	-0.70780000
H	-4.20250000	2.26300000	-1.17620000
N	-3.85850000	0.21760000	-0.75540000

C	-4.98220000	-0.31300000	-1.52130000
H	-4.64510000	-1.12730000	-2.16510000
H	-5.77650000	-0.68120000	-0.86850000
H	-5.37920000	0.48740000	-2.14740000

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C	-2.51720000	4.27840000	-0.07980000
C	-3.60300000	4.46860000	0.79240000
C	-4.43900000	5.57710000	0.75080000
H	-5.24850000	5.65440000	1.46740000
C	-4.19840000	6.56390000	-0.20530000
H	-4.83830000	7.43900000	-0.25110000
C	-3.13910000	6.43120000	-1.10210000
H	-2.93220000	7.17490000	-1.86300000
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C	-0.29300000	3.21850000	0.13200000
C	-1.64530000	-2.62460000	0.19800000
C	-2.82100000	-1.88460000	0.09550000
C	-2.30140000	1.77260000	-0.15030000
C	-1.86780000	0.48700000	0.26230000
C	-0.22460000	-4.35710000	0.44250000
C	-4.11890000	-2.59680000	0.27390000
C	-4.57760000	-3.58730000	-0.60440000
C	-5.77450000	-4.27140000	-0.42920000
H	-6.06710000	-5.02110000	-1.15520000
C	-6.56610000	-3.96150000	0.67670000
H	-7.50250000	-4.48690000	0.83280000
C	-6.16430000	-2.97920000	1.58240000
H	-6.75620000	-2.72200000	2.45320000
C	-4.95940000	-2.32240000	1.36260000
C	2.70560000	-4.21550000	-0.19450000
C	2.46810000	-5.13070000	-1.22810000
C	3.20440000	-6.29510000	-1.40710000
H	2.96700000	-6.94920000	-2.23810000
C	4.23690000	-6.57490000	-0.51260000
C	4.51680000	-5.70260000	0.53850000
H	5.30860000	-5.89710000	1.25260000
C	3.75420000	-4.54890000	0.67430000
C	1.90190000	-2.97390000	-0.03970000
C	0.47180000	-3.10640000	0.12100000
C	1.92920000	2.66480000	0.20460000
C	3.08300000	1.88600000	0.14000000
C	3.05760000	0.45790000	0.03180000
C	2.55270000	-1.74830000	-0.06180000
C	0.47360000	4.41130000	0.40820000
C	4.40020000	2.57810000	0.17190000
C	5.36900000	2.28730000	1.14520000
C	6.61540000	2.89900000	1.19700000
H	7.30690000	2.62240000	1.98440000
C	6.93210000	3.85710000	0.23430000
C	6.01200000	4.18800000	-0.75990000
H	6.23230000	4.92050000	-1.52780000
C	4.78030000	3.54440000	-0.77190000
N	-0.38990000	-2.09480000	-0.01440000
C	-1.54430000	-4.05310000	0.50090000
C	1.79550000	4.08130000	0.44950000
N	0.63850000	2.19130000	0.05200000
H	0.04160000	5.38580000	0.58170000
H	2.62310000	4.74130000	0.66290000
H	0.24140000	-5.31780000	0.61170000
H	-2.36430000	-4.71730000	0.73410000
C	4.21340000	-0.39240000	-0.34330000
H	5.20520000	-0.02240000	-0.58570000
C	-2.82170000	-0.46030000	-0.10670000
F	-1.32820000	5.18320000	-1.91500000
F	-3.83950000	3.53200000	1.73090000
F	-4.57510000	-1.37900000	2.24160000
F	-3.84140000	-3.85750000	-1.69990000
H	-1.00170000	0.24520000	0.85210000
H	4.82580000	-7.47830000	-0.63470000
H	7.90020000	4.34670000	0.25820000
C	2.02360000	-0.44980000	0.20570000
H	1.01850000	-0.29300000	0.54670000
N	3.93450000	-1.65760000	-0.39420000
F	4.01630000	-3.73540000	1.71080000
F	1.47860000	-4.86160000	-2.10460000
F	5.07170000	1.37030000	2.08550000
F	3.90930000	3.86500000	-1.75030000
C	-3.53900000	1.55960000	-0.78010000
H	-4.18000000	2.27170000	-1.27920000
N	-3.85920000	0.24710000	-0.74900000
C	-4.99670000	-0.30180000	-1.48260000
H	-4.67260000	-1.12790000	-2.11810000
H	-5.77750000	-0.65560000	-0.80640000
H	-5.40660000	0.48600000	-2.11610000
H	0.43120000	1.28770000	-0.34840000

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C	-3.53744300	3.34328100	0.17514400
C	-4.47429100	3.23684600	1.21328700
C	-5.52662100	4.12789500	1.38764500
H	-6.21033800	3.98379200	2.21612000
C	-5.66268100	5.18690400	0.49007100
H	-6.47754500	5.89320400	0.61056900
C	-4.76161300	5.34298300	-0.56350800
H	-4.84977500	6.14933100	-1.28231600
C	-3.72873600	4.42342600	-0.69653800
C	-2.40604400	2.38235300	0.04917700
C	-1.10734100	2.91814900	0.20711800
C	-0.79288600	-3.03849000	0.32005300
C	-2.13142500	-2.63900000	0.10240000
C	-3.81688100	-0.90070700	-0.71917300
C	-2.65419200	1.00713400	-0.16397400
C	-1.83254100	-0.09613100	0.17329100
C	1.10219200	-4.23867800	0.70280400
C	-3.15728000	-3.71725600	0.08293500
C	-3.10485300	-4.79524000	-0.80961700
C	-4.04152600	-5.82173800	-0.82614700
H	-3.93678800	-6.62074100	-1.55087400
C	-5.09617900	-5.77927400	0.08392200
H	-5.83886000	-6.57048700	0.08559500
C	-5.20596800	-4.72417400	0.99034200
H	-6.01697700	-4.66176800	1.70644900
C	-4.24649900	-3.72301700	0.96475500
C	3.92261900	-3.30155600	0.04596400
C	3.99765500	-4.35968200	-0.87034900
C	5.07918000	-5.22835500	-0.94865800
H	5.06941300	-6.01857700	-1.69027600
C	6.15038000	-5.04256700	-0.07585700
C	6.13195000	-4.00517200	0.85601900
H	6.94831100	-3.83905300	1.54915600
C	5.03037200	-3.16059500	0.89486700
C	2.76499700	-2.37328700	0.10423100

C	1.48366400	-2.92277600	0.30571700
C	1.17046700	3.06010800	0.16231600
C	2.49956400	2.63631500	-0.00240400
C	2.86639700	1.27268000	-0.11238800
C	2.99291000	-0.98991100	-0.06981500
C	-0.72495600	4.24645900	0.57806300
C	3.55659600	3.68075600	-0.06488500
C	4.64965400	3.69074800	0.81629400
C	5.65647600	4.64732500	0.77495100
H	6.46543100	4.59306900	1.49407800
C	5.58810200	5.65182200	-0.18976200
C	4.52732700	5.69279800	-1.09417100
H	4.45289000	6.45518800	-1.86084900
C	3.54350700	4.71523800	-1.01375200
N	0.30288400	-2.22847600	0.11975900
C	-0.27296200	-4.30857100	0.71628500
C	0.64777900	4.33318300	0.53843300
N	0.06806000	2.23898700	-0.01155400
H	-1.41606300	5.02699600	0.85818100
H	1.25149900	5.19415800	0.78505300
H	1.79671800	-5.02052900	0.97238800
H	-0.87935300	-5.15824300	0.99179400
C	4.14887800	0.76402600	-0.60466300
H	4.95818400	1.37413600	-0.99313100
C	-2.50840300	-1.29724200	-0.10413500
N	-3.84400900	0.50044200	-0.70706400
F	-2.87998500	4.55961100	-1.73495800
F	-4.34664200	2.21923900	2.08390800
F	-4.36139000	-2.70422000	1.83939100
F	-2.09883300	-4.83865800	-1.70668600
C	-4.83685400	1.20465700	-1.50573700
H	-5.56345800	1.73625100	-0.88657700
H	-4.35159500	1.91599500	-2.17898000
H	-5.36197100	0.44505300	-2.08713200
H	-0.96170600	-0.00471500	0.80378500
H	7.00478300	-5.71006000	-0.12214200
H	6.36643000	6.40635000	-0.23791400
C	2.14217400	0.10539200	0.21013100
H	1.24049200	0.06550300	0.80030100
N	4.22878800	-0.53696000	-0.58478800
F	5.01320300	-2.18041200	1.81374100
F	2.97686200	-4.53886300	-1.73283300
F	4.71955100	2.73620100	1.76132800
F	2.53445400	4.75683700	-1.90536500
H	0.26080600	-1.34560400	-0.36745000
O	-4.69062400	-1.59647800	-1.21316000
H	0.12143800	1.33466500	-0.45581100

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C	3.12680000	-3.74730000	0.04670000
C	4.21050000	-3.76980000	0.93480000
C	5.16800000	-4.77310000	0.95060000
H	5.97480000	-4.72370000	1.67240000
C	5.06140000	-5.81360000	0.02710000
H	5.80230000	-6.60660000	0.02080000
C	4.01220000	-5.83920000	-0.88990000
H	3.91020000	-6.62650000	-1.62770000
C	3.07810000	-4.81060000	-0.86320000
C	2.10560000	-2.66420000	0.07680000
C	0.76860000	-3.05490000	0.28650000
C	1.12930000	2.89640000	0.24630000
C	2.42990000	2.35450000	0.07620000
C	2.49500000	-1.31860000	-0.11650000
C	1.83460000	-0.11780000	0.17330000
C	-0.62180000	4.30350000	0.61860000
C	3.56220000	3.31300000	0.20730000
C	3.73960000	4.41110000	-0.64510000
C	4.77070000	5.33160000	-0.50510000
H	4.84800000	6.15220000	-1.20890000
C	5.68330000	5.15880000	0.53580000
H	6.49670000	5.86600000	0.66150000
C	5.56080000	4.08210000	1.41410000
H	6.25360000	3.92490000	2.23260000
C	4.51040000	3.19020000	1.23340000
C	-3.52220000	3.70460000	-0.10620000
C	-3.45880000	4.74470000	-1.04450000
C	-4.42900000	5.73250000	-1.15820000
H	-4.31640000	6.49920000	-1.91590000
C	-5.52610000	5.69380000	-0.29870000
C	-5.64230000	4.68340000	0.65540000
H	-6.48100000	4.63120000	1.33970000
C	-4.64920000	3.71540000	0.72960000
C	-2.48190000	2.65020000	-0.01410000
C	-1.14480000	3.05530000	0.18170000
C	-1.50960000	-2.92270000	0.29420000
C	-2.78090000	-2.35640000	0.11880000
C	-2.99160000	-0.96350000	-0.05150000
C	-2.86500000	1.29810000	-0.13110000
C	0.23890000	-4.33850000	0.63900000
C	-3.95290000	-3.27250000	0.08800000
C	-5.02880000	-3.13310000	0.97880000
C	-6.14240000	-3.96380000	0.96970000
H	-6.93070000	-3.79790000	1.69470000
C	-6.20500000	-4.99050000	0.02810000
C	-5.16790000	-5.17640000	-0.88550000
H	-5.19360000	-5.95870000	-1.63510000
C	-4.07450000	-4.32040000	-0.83770000
N	-0.04700000	2.23610000	-0.01950000
C	0.75350000	4.20580000	0.67040000
C	-1.13230000	-4.25880000	0.63920000
N	-0.32330000	-2.22880000	0.13020000
H	0.84100000	-5.20220000	0.87740000
H	-1.82890000	-5.04700000	0.88370000
H	-1.22490000	5.15500000	0.89740000
H	1.44620000	4.96820000	0.99330000
C	-4.20920000	-0.34050000	-0.57830000
H	-5.08160000	-0.87640000	-0.93850000
C	2.66980000	0.98570000	-0.15100000
F	2.07660000	-4.83830000	-1.76660000
F	4.32220000	-2.76420000	1.82530000
F	4.39650000	2.15510000	2.08520000
F	2.87930000	4.56450000	-1.67090000
H	0.95980000	-0.02070000	0.79750000
H	-6.29510000	6.45600000	-0.37240000
H	-7.06740000	-5.64860000	0.00510000
C	-2.14210000	0.12880000	0.21240000
H	-1.24010000	0.10260000	0.80290000
N	-4.14320000	0.96060000	-0.62830000
F	-4.75890000	2.76510000	1.67240000
F	-2.41280000	4.78310000	-1.89450000
F	-4.97360000	-2.15410000	1.90000000
F	-3.08880000	-4.50000000	-1.73810000
H	-0.10180000	1.35220000	-0.50230000
H	-0.27990000	-1.33150000	-0.33010000
O	4.67280000	-1.63100000	-1.22960000

C	4.86170000	1.17210000	-1.47740000
H	4.38960000	1.89540000	-2.14720000
H	5.58830000	1.68980000	-0.84670000
H	5.38360000	0.41300000	-2.06230000
N	3.85530000	0.47020000	-0.69410000
C	3.80840000	-0.92970000	-0.72730000

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C	3.35707600	-3.53195400	-0.40114500
C	4.47310200	-3.69415000	0.43067300
C	5.35904200	-4.75976700	0.32652100
H	6.20029200	-4.81739600	1.00742600
C	5.13025500	-5.72606400	-0.65260000
H	5.81128800	-6.56506600	-0.75060000
C	4.03323400	-5.62096500	-1.50847700
H	3.83307200	-6.35379400	-2.28141600
C	3.17590900	-4.53819000	-1.36183100
C	2.37890600	-2.42463800	-0.21824400
C	1.01071700	-2.84537700	0.09459600
C	0.96708200	2.99879100	0.34903400
C	2.27371600	2.56432700	0.32316800
C	3.94770300	0.82919200	-0.63003800
C	2.74415600	-1.09900900	-0.29370600
C	1.94813200	0.03728300	0.16751000
C	-0.85563200	4.29774500	0.61438700
C	3.37437600	3.51679900	0.62537400
C	3.56571500	4.71715200	-0.07296000
C	4.60252000	5.60017800	0.20253500
H	4.69139700	6.50661300	-0.38478700
C	5.50598700	5.28234000	1.21508300
H	6.32033900	5.96217700	1.44330800
C	5.37440400	4.09343600	1.93291900
H	6.06397300	3.81545100	2.72125300
C	4.32792800	3.24132200	1.61529600
C	-3.56571100	3.56870300	-0.47860900
C	-3.38404000	4.52339800	-1.49219000
C	-4.30177300	5.52720900	-1.77284900
H	-4.09422400	6.22341400	-2.57704100
C	-5.46855900	5.59985600	-1.01158800
C	-5.70376100	4.68284400	0.01223000
H	-6.59622900	4.72033600	0.62597300
C	-4.75377000	3.69845000	0.25734700
C	-2.55000100	2.51890700	-0.20059200
C	-1.19007200	2.95789400	0.10641500
C	-1.15360000	-2.89964300	0.28554600
C	-2.46682600	-2.47876700	0.25165500
C	-2.84507600	-1.10251700	-0.02931300
C	-2.90487600	1.19403700	-0.23946800
C	0.67128000	-4.17784700	0.62130700
C	-3.55306800	-3.45677900	0.52471200
C	-4.51227300	-3.23090400	1.52166500
C	-5.54174900	-4.11283700	1.81097300
H	-6.23831000	-3.87248000	2.60545900
C	-5.64846500	-5.28198400	1.05720400
C	-4.73662300	-5.55222300	0.03848000
H	-4.80510500	-6.44335200	-0.57442900
C	-3.71682800	-4.64080500	-0.20748600
N	-0.11466000	2.20647400	-0.04526200
C	0.48868500	4.31827100	0.76467200
C	-0.67640400	-4.20959400	0.72853500
N	-0.06824900	-2.10511800	-0.09570000
H	1.37336900	-4.95895600	0.87706000
H	-1.29164000	-5.01288400	1.10687400
H	-1.56002800	5.08915000	0.83107400
H	1.09992700	5.12413700	1.14382600
C	-4.20031800	-0.69104500	-0.53650500
C	2.63945200	1.19299400	-0.00722700
N	3.94848000	-0.57106300	-0.75552100
F	2.12049700	-4.43828700	-2.19034100
F	4.70555400	-2.75970000	1.37406400
F	4.20785900	2.08725700	2.30258100
F	2.71933200	5.02850000	-1.07273500
C	5.00424500	-1.21812900	-1.51804200
H	5.67472300	-1.79222800	-0.87484500
H	4.58344900	-1.87499700	-2.28206800
H	5.57575100	-0.41931000	-1.99256900
H	0.98298100	-0.08405600	0.62213400
H	-6.19829700	6.37605900	-1.21715500
H	-6.44979700	-5.98414400	1.26289400
C	-2.11046700	0.03216600	0.13273700
H	-1.10233800	0.11215900	0.49207600
N	-4.14458600	0.70025700	-0.61392700
F	-4.98490500	2.82464000	1.25715000
F	-2.26404900	4.45350800	-2.23308500
F	-4.41323500	-2.09843900	2.24651000
F	-2.85894800	-4.90713600	-1.21070900
O	4.85659400	1.55033400	-1.00558200
O	-5.16652300	-1.36584900	-0.84296900
H	-4.91338300	1.24571700	-0.97029600

9′

C	2.85540000	-3.93280000	-0.46050000
C	4.04060000	-4.21680000	0.23380000
C	4.80820000	-5.34820000	-0.00140000
H	5.71030000	-5.50290000	0.57870000
C	4.39590000	-6.24800000	-0.98450000
H	4.98870000	-7.13440000	-1.18560000
C	3.22920000	-6.01630000	-1.71170000
H	2.88760000	-6.69170000	-2.48720000
C	2.49050000	-4.87380000	-1.43360000
C	2.01310000	-2.74500000	-0.17060000
C	0.60570000	-3.00780000	0.15020000
C	1.37270000	2.80750000	0.28900000
C	2.60920000	2.19500000	0.29430000
C	2.52920000	-1.47180000	-0.19480000
C	1.92030000	-0.23940000	0.21110000
C	-0.26430000	4.32880000	0.57950000
C	3.80720000	2.97620000	0.71080000
C	4.24970000	4.12230000	0.03720000
C	5.36470000	4.85380000	0.42760000
H	5.65280000	5.72600000	-0.14750000
C	6.08550000	4.43050000	1.54410000
H	6.95840000	4.98970000	1.86450000
C	5.69650000	3.29150000	2.24940000
H	6.23660000	2.94070000	3.12100000
C	4.57630000	2.59230000	1.81900000
C	-3.03510000	3.97640000	-0.57990000
C	-2.71100000	4.88900000	-1.59710000
C	-3.47840000	6.00670000	-1.89750000
H	-3.16710000	6.66030000	-2.70400000
C	-4.63340000	6.24600000	-1.15270000
C	-5.00470000	5.37960000	-0.12520000
H	-5.89060000	5.54530000	0.47680000
C	-4.20240000	4.27620000	0.13990000

C	-2.17320000	2.80280000	-0.28150000
C	-0.76650000	3.06150000	0.02770000
C	-1.54200000	-2.76130000	0.35630000
C	-2.77840000	-2.15310000	0.31320000
C	-2.95680000	-0.74090000	-0.00460000
C	-2.70170000	1.53710000	-0.28810000
C	0.08700000	-4.29090000	0.64920000
C	-3.99550000	-2.95540000	0.60620000
C	-4.90180000	-2.57300000	1.60470000
C	-6.04740000	-3.28810000	1.91620000
H	-6.69360000	-2.93470000	2.71090000
C	-6.33260000	-4.44040000	1.18300000
C	-5.48030000	-4.85880000	0.16270000
H	-5.68590000	-5.73920000	-0.43480000
C	-4.33890000	-4.11310000	-0.10530000
N	0.20260000	2.18380000	-0.15300000
C	1.07040000	4.16520000	0.74170000
C	-1.25060000	-4.13280000	0.77600000
N	-0.35600000	-2.11740000	-0.01040000
H	0.67660000	-5.16910000	0.87220000
H	-1.97010000	-4.85130000	1.14050000
H	-0.85960000	5.20100000	0.81340000
H	1.77780000	4.87100000	1.15260000
C	-4.24520000	-0.16180000	-0.52140000
C	2.78410000	0.79400000	-0.04670000
F	1.36740000	-4.64980000	-2.14390000
F	4.44180000	-3.36460000	1.19340000
F	4.20040000	1.49700000	2.50300000
F	3.58290000	4.51350000	-1.06600000
H	0.97850000	-0.14150000	0.71530000
H	-5.24700000	7.11310000	-1.37390000
H	-7.22710000	-5.01280000	1.40590000
C	-2.07020000	0.28480000	0.11640000
H	-1.05420000	0.23060000	0.45920000
N	-3.99790000	1.20480000	-0.64580000
F	-4.56340000	3.45320000	1.14450000
F	-1.60160000	4.66000000	-2.32190000
F	-4.62920000	-1.45530000	2.30770000
F	-3.53930000	-4.51820000	-1.10980000
O	-5.29840000	-0.70460000	-0.80240000
H	-4.69040000	1.83930000	-1.01110000
C	5.00020000	1.03090000	-1.33800000
H	4.55690000	1.84080000	-1.92430000
H	5.74720000	1.45050000	-0.65810000
H	5.49460000	0.32320000	-2.00570000
O	4.72450000	-1.79450000	-1.29500000
C	3.87930000	-1.09660000	-0.75640000
N	3.96790000	0.28970000	0.63190000

10 (singlet spin state)

C	4.54023700	1.79667100	0.07547200
C	5.29551200	2.06637800	-1.07069200
C	6.54475000	2.67361800	-1.04917300
H	7.06633700	2.85166500	-1.98252000
C	7.08443900	3.04010300	0.18431000
H	8.05800600	3.51743000	0.22584700
C	6.38004500	2.79965300	1.36440300
H	6.77241000	3.07577400	2.33633500
C	5.13339500	2.19137300	1.28041800
C	3.17133700	1.19617900	0.01780900
C	2.10729300	2.09478400	0.02269800
C	-0.31676500	-3.06893800	-0.03357700
C	1.04485300	-3.29217000	-0.06880400
C	3.36291300	-2.38595300	-0.03539700
C	2.93780000	-0.19052700	-0.04765600
C	1.69197800	-0.82898100	-0.13348500
C	-2.51869800	-3.53354300	-0.06687100
C	1.55781000	-4.69387800	-0.08109300
C	1.52555500	-5.52159400	1.04876800
C	2.00552400	-6.82536000	1.06416800
H	1.94429000	-7.40192200	1.97993100
C	2.55617800	-7.34783900	-0.10610100
H	2.93473100	-8.36471200	-0.11647800
C	2.62302400	-6.57170700	-1.26337000
H	3.03985000	-6.95114700	-2.18917900
C	2.12792600	-5.27439100	-1.22129700
C	-4.77226700	-1.66706400	0.07614400
C	-5.30359600	-2.23296400	1.23954800
C	-6.61690500	-2.66913400	1.35782400
H	-6.95394400	-3.09094100	2.29762600
C	-7.46222000	-2.53714600	0.25641600
C	-6.99042600	-1.98199000	-0.93312900
H	-7.62203700	-1.86927800	-1.80667300
C	-5.66805100	-1.56284000	-0.99409600
C	-3.36618800	-1.18228700	-0.00733100
C	-2.30604900	-2.11156400	0.00412800
C	0.10193400	3.03233400	-0.00644000
C	-1.28023800	3.24936600	-0.05406200
C	-2.15996400	2.17693300	-0.14061400
C	-3.11267000	0.17084100	-0.11176600
C	2.29722200	3.52267600	-0.02940200
C	-1.80136600	4.64703300	-0.01768200
C	-2.39712100	5.25642600	-1.12907000
C	-2.90938800	6.54771700	-1.12102600
H	-3.35238800	6.94814700	-2.02554900
C	-2.83061700	7.28867200	0.05803200
C	-2.24846800	6.73851600	1.20015300
H	-2.17797100	7.28655800	2.13260700
C	-1.75362800	5.44233100	1.13428400
N	-0.96261800	-1.82765000	0.03894500
C	-1.29760500	-4.12167100	-0.09179600
C	1.06821300	4.09473400	-0.04989700
N	0.74368500	1.80784400	0.05592700
H	3.25505200	4.01881100	-0.06933100
H	0.82454000	5.14508700	-0.10962300
H	-3.48878000	-4.00566200	-0.11186800
H	-1.06721000	-5.17421300	-0.16685200
C	-3.63298400	2.26309500	-0.12633400
H	-4.21458500	3.18056300	-0.12139800
C	1.96678400	-2.22017600	-0.08990800
N	3.95809700	-1.18817300	-0.01120700
F	4.45736100	1.95480800	2.43627900
F	4.78175500	1.69933300	-2.27692400
F	2.19483100	-4.52791600	-2.35778500
F	1.00371100	-5.02033000	2.19968900
C	5.41157600	-1.05377300	0.01768800
H	5.78042800	-0.57617800	-0.89182900
H	5.73871300	-0.47920900	0.88492000
H	5.83766400	-2.05633600	0.08225100
H	-8.49325600	-2.86879500	0.32516400
H	-3.22542100	8.29900600	0.08734400
C	-1.85178800	0.80901100	-0.19846100
N	-4.19824800	1.09984900	-0.10869500
F	-5.21598000	-1.04719900	-2.16689700
F	-4.48820400	-2.35787000	2.32509200

F	-2.47225400	4.54732400	-2.28806300
F	-1.19677100	4.91398900	2.25827200
H	3.94628700	-3.29587700	-0.01298000
Cu	-0.08982500	-0.00789000	-0.08558200

11 (singlet spin state)

C	-3.24934600	3.55761600	-0.28208500
C	-3.72172600	4.43000900	0.70333200
C	-4.59858800	5.47796200	0.45598800
H	-4.92252000	6.10692200	1.27715900
C	-5.03843600	5.68076200	-0.85282300
H	-5.72565500	6.49181300	-1.07060000
C	-4.60052300	4.84839800	-1.88280700
H	-4.92236100	4.98287800	-2.90902200
C	-3.71951700	3.81867700	-1.57427200
C	-2.27579100	2.45295500	-0.01479300
C	-0.90663700	2.81017500	-0.03587300
C	-0.96553300	-2.84829600	0.01698800
C	-2.29857900	-2.45927100	0.17163300
C	-4.06253200	-0.65419500	0.40962000
C	-2.67419400	1.14376600	0.20543400
C	-1.80973700	0.00702800	0.28828600
C	0.79708400	-4.24743700	-0.10522200
C	-3.34166500	-3.52944100	0.20040500
C	-3.81331600	-4.14589700	-0.96073500
C	-4.77045300	-5.15293700	-0.96663400
H	-5.08753200	-5.57960700	-1.91118500
C	-5.29591300	-5.57637400	0.25340600
H	-6.04569500	-6.36070700	0.27422100
C	-4.86499300	-4.99780500	1.44803100
H	-5.25772300	-5.30306700	2.41096700
C	-3.90914100	-3.99422000	1.39018000
C	3.63595100	-3.54555500	-0.25710000
C	3.86612200	-4.24505300	-1.45100900
C	4.85098800	-5.21339000	-1.60019500
H	4.96485300	-5.70957100	-2.55708100
C	5.66720900	-5.51130800	-0.50884500
C	5.49448100	-4.84603800	0.70505200
H	6.10741600	-5.06018500	1.57296600
C	4.49275300	-3.88799300	0.79892300
C	2.57382900	-2.50859100	-0.12507900
C	1.23958800	-2.87680100	-0.13178300
C	1.30470100	2.82996900	0.06389300
C	2.62478900	2.45030200	0.14087600
C	2.99100800	1.08115700	0.15595200
C	2.92826900	-1.15627200	0.02290600
C	-0.48329000	4.19269900	-0.03153500
C	3.69606600	3.48853700	0.17401800
C	4.43398100	3.76156200	1.33294800
C	5.45073500	4.70596900	1.39705000
H	5.96840600	4.86561200	2.33584300
C	5.76512200	5.42558600	0.24404800
C	5.07105900	5.19543600	-0.94382100
H	5.29595600	5.73477400	-1.85669500
C	4.06342600	4.23883300	-0.95019200
N	0.13642000	-2.02256600	-0.09132400
C	-0.55341000	-4.23091000	-0.00913500
C	0.86812900	4.20114100	0.04767300
N	0.18199200	1.98455700	-0.01112400
H	-1.14741000	5.04251500	-0.06025000
H	1.52454800	5.05683700	0.10677300
H	1.45225800	-5.10623300	-0.12140000
H	-1.22763400	-5.07077100	0.06448700
C	4.31310300	0.60501800	0.07462700
H	5.24969000	1.14350500	0.06833900
C	-2.63921000	-1.11313400	0.29475000
N	-4.01598900	0.73190300	0.32642900
F	-3.29434500	3.01659100	-2.58653200
F	-3.30860800	4.22956300	1.98674900
F	-3.49236300	-3.43391900	2.55875900
F	-3.30661200	-3.73563700	-2.15843400
C	-5.20860400	1.50612400	0.63745900
H	-5.04271800	2.15096000	1.50457800
H	-5.54100100	2.11104700	-0.20861400
H	-5.98502900	0.77724300	0.87567400
H	6.44127500	-6.26559400	-0.60463100
H	6.55468600	6.16941100	0.27147000
C	2.10862700	-0.03706500	0.17109000
N	4.26462100	-0.73375900	-0.00619600
F	4.33090100	-3.24765000	1.98998200
F	3.08904100	-3.95583800	-2.52667300
F	4.13233400	3.06886500	2.46451400
F	3.40311800	4.01561100	-2.11828900
O	-5.08209900	-1.30672300	0.56821200
Cu	0.15082000	-0.01749200	0.11488600
H	5.06339800	-1.34612800	-0.07937900

10 (triplet spin state)

C	-4.55572600	-1.79286400	-0.00270900
C	-5.21845100	-2.10270700	-1.19475500
C	-6.47311600	-2.69742600	-1.24674300
H	-6.92218300	-2.90786700	-2.21052000
C	-7.11136200	-3.01069000	-0.04613600
H	-8.09033500	-3.47831800	-0.06277800
C	-6.49876400	-2.72984400	1.17563200
H	-6.96840700	-2.96501000	2.12375900
C	-5.24388300	-2.13379500	1.16566600
C	-3.17470900	-1.20963000	0.01650200
C	-2.13393900	-2.16609300	0.01203200
C	0.34936200	3.13401600	-0.03928900
C	-1.03059800	3.30289300	-0.03070100
C	-3.37406300	2.39124800	0.03100300
C	-2.95048500	0.18693500	0.02551300
C	-1.69772000	0.83184500	0.00265400
C	2.55423000	3.60377500	-0.09551700
C	-1.56534300	4.70038700	-0.05364900
C	-1.55562000	5.52962600	1.07425300
C	-2.05200700	6.82745400	1.08011700
H	-2.00803200	7.40756400	1.99461300
C	-2.59421700	7.33990500	-0.09840700
H	-2.98456800	8.35218900	-0.11640200
C	-2.63759700	6.56007000	-1.25444400
H	-3.04784100	6.93190500	-2.18623800
C	-2.12828800	5.26873700	-1.20236700
C	4.78930900	1.66911600	0.00640700
C	5.35689500	2.29557800	1.12006800
C	6.67353300	2.73384900	1.17331800
H	7.04063000	3.20431800	2.07809400
C	7.48327400	2.54087300	0.05419900
C	6.97389100	1.92281600	-1.08778600
H	7.57758000	1.76079500	-1.97321500
C	5.65031300	1.50315600	-1.08376800
C	3.37741600	1.18587500	-0.00788600
C	2.32629400	2.17321900	-0.02645200

C	-0.13957900	-3.09490000	0.01865100
C	1.27775100	-3.26040400	0.02037400
C	2.18144100	-2.19588900	0.00293100
C	3.14283700	-0.17651100	-0.00611400
C	-2.33646200	-3.59910600	-0.00297900
C	1.80990900	-4.65807000	0.04180000
C	2.40877700	-5.24975400	-1.07633100
C	2.92732300	-6.53851100	-1.08209400
H	3.37253000	-6.92688300	-1.99074900
C	2.85323800	-7.29193700	0.08935800
C	2.26902100	-6.75731600	1.23784100
H	2.20217100	-7.31556300	2.16446300
C	1.76577600	-5.46383400	1.18546400
N	1.00359800	1.91095900	-0.00033900
C	1.33020700	4.19794500	-0.10296500
C	-1.09953800	-4.17328500	-0.00011000
N	-0.78742600	-1.89690200	0.02157900
H	-3.29080100	-4.10494500	-0.01484700
H	-0.86397600	-5.22764800	-0.01438300
H	3.52119300	4.08317700	-0.14009700
H	1.11055000	5.25483000	-0.15417800
C	3.66110900	-2.27588700	0.02805100
H	4.25201900	-3.18753000	0.05450300
C	-1.97381200	2.22807500	-0.00195200
N	-3.97530600	1.19218900	0.04516600
F	-4.65689500	-1.85040900	2.36027100
F	-4.60398100	-1.79421200	-2.36844200
F	-2.17269800	4.51583100	-2.33564600
F	-1.04046600	5.03643400	2.23161200
C	-5.42859500	1.06525100	0.10494800
H	-5.81606900	0.53303200	-0.76523400
H	-5.74028700	0.54420200	1.01209900
H	-5.85543100	2.06942700	0.11674900
H	8.51614900	2.87335100	0.07225800
H	3.25377700	-8.30024300	0.10787100
C	1.86246400	-0.81864000	-0.01591200
N	4.22695500	-1.11024600	0.02504000
F	5.16096500	0.92241200	-2.21053700
F	4.57499500	2.47910700	2.22192300
F	2.47942200	-4.52579500	-2.22608200
F	1.20582900	-4.94781400	2.31360200
H	-3.96563700	3.29672300	0.05067000
Cu	0.08981800	0.00473100	-0.00390300

11 (triplet spin state)

C	-3.68219100	3.17883200	0.03893900
C	-4.20956600	3.63315200	1.25231300
C	-5.19336700	4.60962100	1.35066300
H	-5.55514300	4.90370200	2.32916400
C	-5.68230300	5.18171900	0.17592500
H	-6.45093800	5.94591300	0.22809000
C	-5.18927600	4.77859100	-1.06556200
H	-5.54932200	5.20466600	-1.99489700
C	-4.20652200	3.79737200	-1.10012400
C	-2.58225600	2.16187500	-0.02080700
C	-1.25316100	2.73082600	-0.01224500
C	-0.58155900	-3.03953000	0.02754900
C	-1.96916100	-2.76005400	0.01156000
C	-3.97962300	-1.18999600	-0.08891600
C	-2.84061600	0.80122800	-0.05598300
C	-1.82353100	-0.24082900	-0.02669600
C	1.34572600	-4.21098300	0.08058800
C	-2.88554600	-3.94342000	0.03976400
C	-3.15026000	-4.71248300	-1.09501300
C	-3.98454900	-5.82277500	-1.09547100
H	-4.14436100	-6.36683600	-2.01914100
C	-4.59606800	-6.19493500	0.10119600
H	-5.25301700	-7.05835100	0.12489100
C	-4.37007300	-5.46412100	1.26822100
H	-4.83319300	-5.72691400	2.21218500
C	-3.52994300	-4.36224800	1.20626900
C	4.07656700	-3.08572600	0.00640500
C	4.47719300	-3.81357700	-1.12207600
C	5.58768900	-4.64795700	-1.14520200
H	5.83294300	-5.17847700	-2.05795800
C	6.35414500	-4.77200000	0.01383200
C	6.01041400	-4.06867900	1.16850400
H	6.58284900	-4.14932000	2.08532800
C	4.88976600	-3.24802900	1.13583000
C	2.87689200	-2.19457000	0.00415100
C	1.59928900	-2.78842900	0.01928800
C	0.93106900	3.02554300	-0.02675800
C	2.28923600	2.76356100	-0.03498200
C	2.84294500	1.44037100	-0.03265000
C	3.06795600	-0.80096700	-0.01299400
C	-1.01231700	4.16759400	0.01695700
C	3.23872900	3.91886700	-0.04809400
C	3.97322700	4.29733000	1.08216200
C	4.87408700	5.35454300	1.09931100
H	5.39692300	5.59167600	2.01867100
C	5.06842100	6.08289300	-0.07466100
C	4.37115200	5.75061000	-1.23601700
H	4.50375700	6.29499600	-2.16383500
C	3.48150300	4.68394400	-1.19516200
N	0.41139300	-2.10354700	-0.00615500
C	-0.00664400	-4.36764000	0.08686400
C	0.33361600	4.34426100	0.00693700
N	-0.08429200	2.06833700	-0.03433200
H	-1.77197400	4.93416100	0.04301100
H	0.87567300	5.27895100	0.02713800
H	2.09921600	-4.98460400	0.12169700
H	-0.56446200	-5.29135800	0.13172500
C	4.21890100	1.12768700	-0.06196400
H	5.08656600	1.77213000	-0.09257600
C	-2.50914000	-1.45633500	-0.02364000
N	-4.11002600	0.20448300	-0.09943300
F	-3.73581600	3.40411900	-2.31606400
F	-3.73649900	3.08270700	2.40350700
F	-3.31298600	-3.64962800	2.34659100
F	-2.55878000	-4.35038100	-2.26881500
C	-5.43518500	0.78391400	-0.24620600
H	-5.70719200	1.40459400	0.61025400
H	-5.51254600	1.37593100	-1.16163800
H	-6.12501800	-0.05951900	-0.30710600
H	7.22413500	-5.42039200	0.01727900
H	5.76628800	6.91375000	-0.08409300
C	2.10370800	0.22194200	-0.00653600
N	4.34772600	-0.21096600	-0.05036000
F	4.55991000	-2.56742300	2.26702600
F	3.74477800	-3.69018300	-2.25925900
F	3.78775400	3.59486500	2.23313800
F	2.81621600	4.36284900	-2.33698600
O	-4.92350300	-1.96316400	-0.14395100
Cu	0.14447900	-0.00922200	-0.01157500
H	5.22590700	-0.70838000	-0.06401700