SUPPORTING INFORMATION

For

Open Shell (4n+2)π and Closed Shell 4nπ Planar Core-Modified Decaphyrins

*Pragati Shukla, Madan D. Ambhore, Venkataramanarao G. Anand **

Department of Chemistry
Indian Institute of Science Education and Research,
Dr. Homi Bhabha Road, Pune – 411045
Maharashtra, India

Email: vg.anand@iiserpune.ac.in

Table of Contents

Experimental Section

1 a. General Information

All the moisture and air sensitive reactions were performed under inert atmosphere in a flame dried round bottom flask. Freshly distilled and dried solvents like dichloromethane and tetrahydrofuran were used to perform the reactions. All the chemicals were commercially available. For purification, column chromatography was done either with silica gel 100-200 mesh or basic aluminum oxide. Size exclusion chromatography with Bio-Beads S-X1 (BIO-RAD) was employed for purifying the synthesized macrocycles. The MALDI-TOF/TOF mass spectra were recorded with AB SCIEX TOF/TOF 5800 spectrometer and High-Resolution Mass spectrum (HRMS) of the molecules were recorded using WATERS G2 Synapt Mass Spectrometer. Nuclear Magnetic Resonance (NMR) spectra were recorded either with Bruker 400 MHz or 600 MHz spectrometer. The chemical shift values are reported as the delta scale in ppm relative to tetramethylsilane, using the deuterated solvent peak as the reference standard. A Perkin-Elmer λ-35 UV−vis Spectro-photometer was used to record the Ultraviolet-Visible absorption spectrum using optical quart cuvette of 10 mm path length. Cyclic voltammetry (CV) and Differential pulse voltammetry (DPV) experiments were performed in CH instruments Electrochemical Analyser using three electrode (glassy carbon as working electrode, Pt wire as counter and calomel or Ag/AgCl as reference electrode) system in presence of supporting electrolyte (0.1M tetrabutylammonium perchlorate solution prepared in dichloromethane). Scanning along the potential starting from zero to positive direction, then towards negative potential and finally end to the zero. Single crystal X-ray diffraction data was collected from a BRUKER KAPPA APEX II CCD Duo diffractometer using graphite monochromatic Mo Kα radiation (λ = 0.71073 Å). Further, the analysis of crystal structure was done with APEX2 and refinement was done in SHELXL-97,[1a,b] and WINGX[1c]. In case of disordered solvent molecules, the contributions to the scattering arising from the disordered solvents in the crystal were removed by use of the utility SQUEEZE in the PLATON software package[2]. Detailed information of crystals including the coordinates can be obtained from the following CCDC (Cambridge Crystallographic Data Centre) deposition numbers. **10** = 2294107, **12** = 2293502, **15** = 2294108, **[15]$^{2+}$**= 2294163.

The Quantum chemical calculation was performed using Gaussian09 rev D programme 2[3] suite utilizing a High Performance Computing Cluster facility of IISER PUNE. The Density Functional Theory (DFT) using Becke's three-parameter hybrid exchange functionals and Lee-Yang-Parr functional (B3LYP) and the basis set 6-31G(d, p) was employed for all the atoms in the investigating molecule. The geometry optimization for **10**, **12**, **15** and **[15]$^{2+}$** were carried out based on the structure obtained from crystal data. Singlet-triplet energies and NOON (natural orbital occupation number) calculations were performed using DFT unrestricted UCAM-B3LYP/631G(d,p) method. The diradical character were determined by Yamaguchi's scheme[4a]. AICD plot was calculated by using the method developed by Herges[4b].

1 b. Synthetic Procedures and Data Characterization

Decaphyrin 10

In two necked 100 mL RB, terthiophene diol **6**[5a, 5b] (202.26 mg, 315.78 µmol) and bithiophene **7**[6] (50 mg, 300.74 µmol) were dissolved in 60 mL of dried and distilled dichloromethane and degassed with nitrogen for the five minutes. Then boron trifluoride diethyl etherate (371.16 µmL, 300.74 µmol) was added under dark and resulting solution was stirred for 2 h. It was followed by addition of 2,3-dichloro-5,6-dicyano-1,4-benzoquinone DDQ (238 mg, 1.05 mmol) and the solution was exposed to the open air with additional stirring of 2 h. MALDI-TOF/TOF mass spectrum confirmed the formation of desired macrocycle. Then, the reaction mixture was passed through a short bed of basic alumina column and further eluted with 10% MeOH/DCM. The obtained mixture was purified with basic alumina column in 25% DCM/PE followed by size exclusion column chromatography in THF. Decaphyrin **10** was isolated as metallic green compound in 7.2 % yield (16.8 mg).

HR-MS (ESI-TOF): *m/z* = 1535.8490 (Calcd. for $C_{68}H_{20}F_{20}S_{10}$; $[M]^+$ 1535.8453)

UV-vis: (CH_2Cl_2): λ_{max} nm (ε, $M^{-1}cm^{-1}$): 507 nm (136500), 559 nm (80500) and 602 nm (185000).

^{1}H NMR (400 MHz, chloroform-*d*, 298 K) δ: 8.69 (s, 4H), 6.58 (d, *J* = 4 Hz, 4H), 6.55 (d, *J* = 5.6 Hz, 4H), 6.09 (d, *J* = 4 Hz, 4H), 5.87 (d, *J* = 5.6 Hz, 4H).

Crystal data: 2($C_{68}H_{20}F_{20}S_{10}$), Triclinic, space group P -1, a = 12.453 (3) b = 21.757 (6), c = 23.660 (6) Å, α = 66.193 (8), β = 79.426 (9), γ = 86.247 (8); V = 5765 (3) $Å^3$, Z = 3, T = 150 K, D_{calcd} = 1.329 g cm^{-3}, R_1 = 0.0893 (9371), R_w (all data) = 0.2642 (26532), GOF = 0.943.

Decaphyrin 11

Synthetic procedure for decaphyrin **11** is similar to as described above for **10**. Terthiophene diol **6** (200.97 mg, 313.75 µmol) was condensed with biselenophene **8** (80 mg, 307.60 µmol) using boron trifluoride diethyl etherate (379.62 µmL, 307.60 µmol) in 60 mL dry dichloromethane. Further, the reaction mixture was oxidized with DDQ (244.39 mg, 1.08 mmol). After passing the reaction mixture through a small bed of basic alumina oxide with 1:1 MeOH/DCM, the obtained reaction mixture was further purified on basic alumina column with 30% DCM/PE. Decaphyrin **11** was obtained as purple color compound in 4.5 % yield (11.9 mg).

HR-MS (ESI-TOF): m/z = 1727.6244 (Calcd. for $C_{68}H_{20}F_{20}S_6Se_4$; $[M]^+$ 1727.6231).

UV-vis: (CH_2Cl_2): λmax nm (ε, $M^{-1}cm^{-1}$): 589 nm (124700), 547 nm (63700) and 505 nm (94900).

^{1}H NMR (400 MHz, chloroform-d, 298 K) δ: 8.41 (s, 4H), 6.68 (d, J = 4.4 Hz, 4H), 6.66 (s, 4H) 6.21 (d, J = 4Hz, 4H) and 6.05 (d, J = 5.6 Hz, 4H).

Decaphyrin 12

A synthetic protocol similar to **10** was employed with terthiophene diol **6** (200.68 mg, 313.31 µmol) and bifuran **9** (41 mg, 305.66 µmol) in 60 mL of dichloromethane using boron trifluoride diethyl etherate (377.24 µmL, 305.66 µmol) and DDQ (242.84 mg, 1.07 mmol). The desired molecule, **12**, was isolated from basic alumina column in 30% DCM/PE and size exclusion column chromatography in THF as metallic brownish-green compound in 3.1 % yield (6.9 mg).

HR-MS (ESI-TOF): m/z = 1471.9408 and 735.9665 (Calcd. for $C_{68}F_{20}H_{20}S_6O_4$; $[M]^+$ 1471.9366 and $[M]^{2+}$ 735.9683).

UV-vis: (CH_2Cl_2): λmax nm (ε, $M^{-1}cm^{-1}$): 384 nm (112400), 494 nm (187000), 583 nm (41200) and 624 nm (52900).

^{1}H NMR (400 MHz, acetone-d6, 298 K) δ: 7.53 (d, J = 5.2 Hz, 4H), 7.22 (d, J = 4 Hz, 4H), 7.00 (s, 4H), 6.83 (d, J = 4 Hz, 4H), 6.81 (d, J = 5.6 Hz, 4H).

Crystal Data: ($C_{68}F_{20}H_{20}O_4S_6$), Monoclinic, space group P 21/c, a = 18.288 (4) b = 24.723 (5), c = 6.9501 (15) Å, α = 90, β = 92.813 (6), γ = 90; V = 3138.6 (12) $Å^3$, Z = 2, T = 100 K, D_{calcd} = 1.559 g cm^{-3}, R_1 = 0.0649 (4773) , R_w (all data) = 0.1754 (6679), GOF = 0.915.

Decaphyrin $[12]^{2+}$

The dicationic species was synthesized by addition of excess of Meerwein salt $[Et_3O]^+[SbCl_6]^-$ to a solution of **12** in dichloromethane at -20 °C. Subsequently, the solution was stirred for 25 minutes at the same temperature. A subtle color change indicated the formation of dicationic specie $[\mathbf{12}]^{2+}$ which crystallized as a purple colored solid. It further washed with pentane and obtained in quantitative yield (96%).

HR-MS (ESI-TOF): *m/z* = 735.9675 (Calcd. for $(C_{68}F_{20}H_{20}S_6O_4)^{2+}$; $[M]^{2+}$ 735.9683)

UV-vis: (CH_2Cl_2): λ_{max} nm (ε, $M^{-1}cm^{-1}$): 457 nm (129400) and 768 nm (296000).

^{1}H NMR (600 MHz, acetonitrile-d_3, 298 K) δ: 8.50 (d, *J* = 4.8 Hz, 2H), 8.48 (d, *J* = 4.8 Hz, 2H), 7.84 (d, *J* = 4.8 Hz, 2H), 7.74 (d, *J* = 4.8 Hz, 2H), 7.65 (d, *J* = 4.8 Hz, 2H), 7.57(d, *J* = 4.8 Hz, 2H), 6.96 (d, *J* = 4.2 Hz, 2H), 6.39 (d, *J* = 4.8 Hz, 2H), 6.10 (d, *J* = 4.2 Hz, 2H), 4.69 (d, *J* = 4.8 Hz, 2H).

Decaphyrin 15

A two necked 250 mL round-bottomed flask was charged with ((phenylmethylene)bis(thiophene-5,2-diyl) bis((mesityl)methanol[7] **14** (567.53 mg, 1.03 mmol) and terthiophene **13** (250.00 mg, 1.01 mmol) in 100 mL of dry dichloromethane. Condensation was initiated by the addition of boron trifluoride diethyl etherate (124.22 mmL, 1.01 mmol) under dark and inert atmosphere and stirred for 2 hours. Then DDQ (802.45 mg, 3.50 mmol) was

added and was stirred for additional 2 hours open to air. The reaction mixture was evaporated under vacuum and further purified by column chromatography (packed in basic alumina and eluted with 40-50% DCM/PE). After multiple column purifications in basic alumina and further size exclusion chromatographic purification in toluene, desired macrocycle **15** was isolated as intense brownish color compound in 2.2% yield (17mg).

HR-MS (ESI-TOF): *m/z* = 761.1470 (Calcd. for $C_{94}H_{74}S_{10}$; $[M]^+$ 1522.2998 and $[M]^{2+}$ 761.1499)

UV-vis: (CH_2Cl_2): λ_{max} nm (ε, $M^{-1}cm^{-1}$): 432 nm (117800), 546 nm (sh), 605 nm (153800), 664 nm (sh), 725 nm (128700) and 966 nm (112900).

^{1}H NMR (400 MHz, toluene-d_8, 218 K) δ: 8.35 (s, 4H) 7.84 (br s, 8H), 7.49 (s, 8H), 7.25 (s, 10 H), 7.04 (s, 4H) 6.20 (br s, 4H). 2.39 (s, 12H, CH_3), 2.28 (s, 12H, CH_3), 2.12 (s, 12H, CH_3).

Crystal data: ($C_{94}H_{74}S_{10}$), Monoclinic, space group P 21/c, a = 18.258 (4) b = 13.448 (3), c = 21.934 (5) Å, α = 90, β = 104.115 (7), γ = 90; V = 5223 (2) $Å^3$, Z = 2, T = 273 K, Dcalcd = 0.969 g cm^{-3}, R1 = 0.0754 (5509) , Rw (all data) = 0.2407 (13031), GOF = 1.051.

Decaphyrin $[15]^{2+}$

Dissolving **15** in deuterated trifluoroacetic acid (TFA) and CD_2Cl_2 resulting in a green colored solution to yield the dicationic species. Its absorption and NMR spectra was similar to the species obtained when **15** was oxidized with $[Et_3O]^+[SbCl_6]^-$.

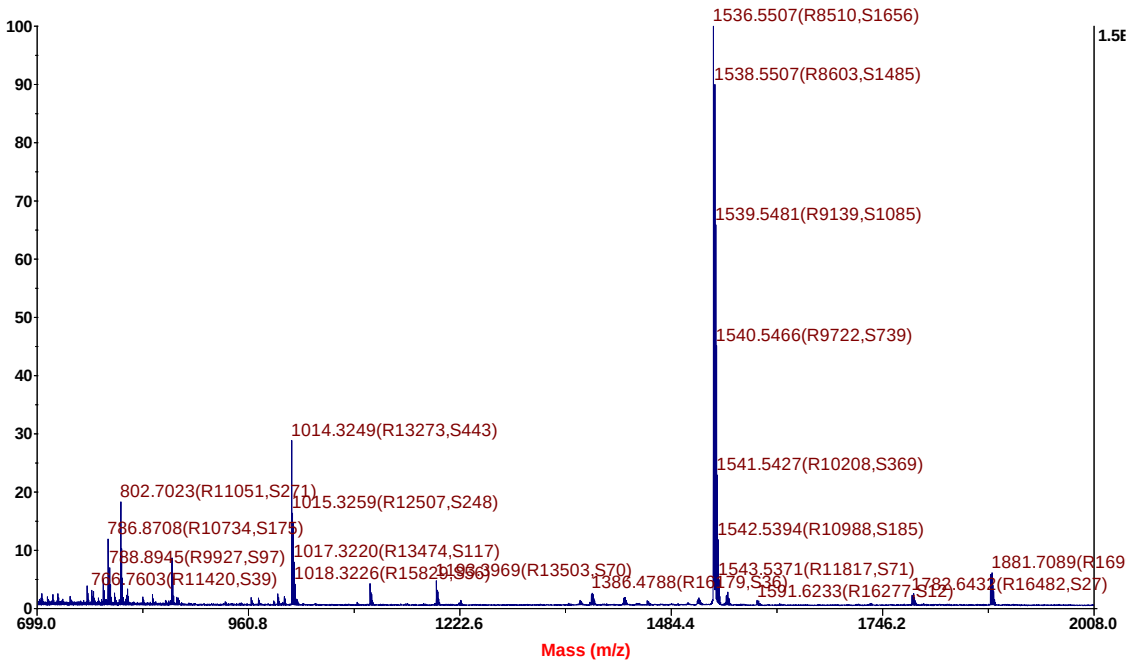
HR-MS (ESI-TOF): *m/z* = 761.1487 (Calcd. for $[C_{94}H_{74}S_{10}]^{2+}$; $[M]^{2+}$ 761.1499)

UV-vis: (CH_2Cl_2): λ_{max} nm (ε, $M^{-1}cm^{-1}$): 470 nm (125200), 698 nm (190100), 1008 (54000).

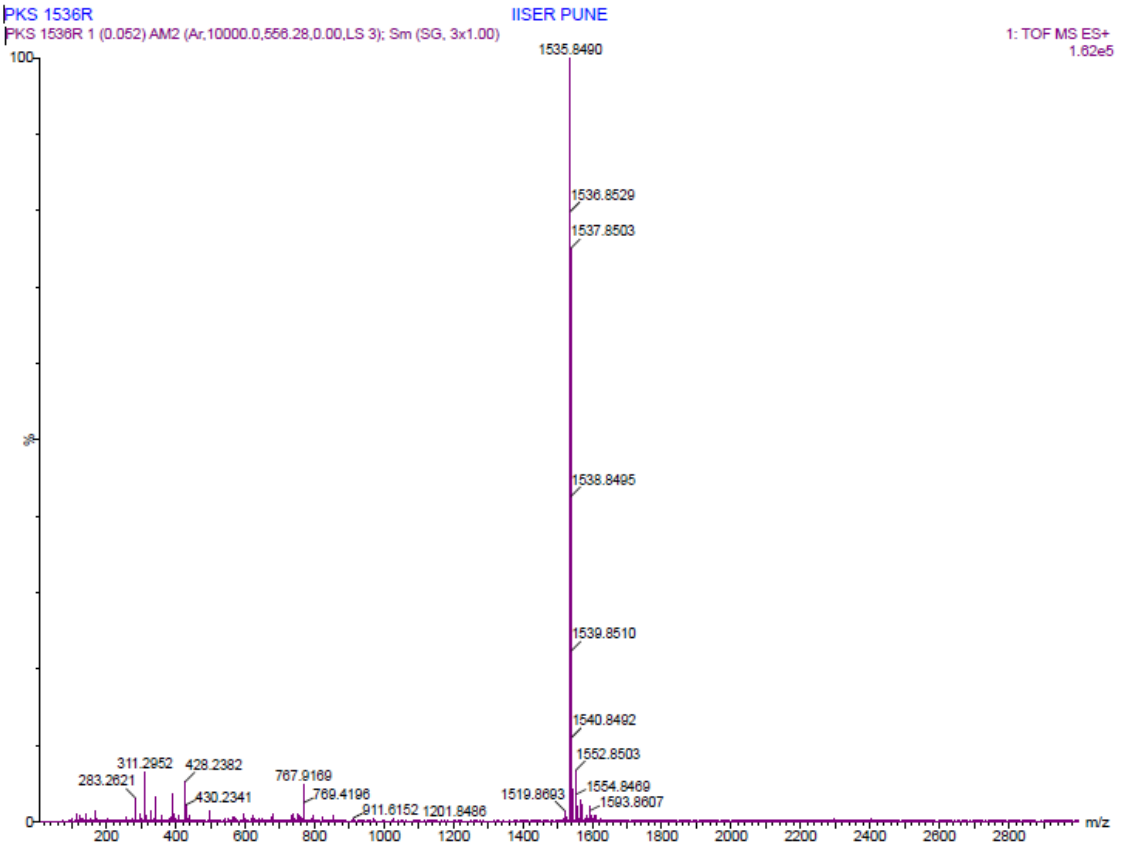
^{1}H NMR (400 MHz, dichloromethane-d_2, 203 K) δ: 8.12 (s, 2H), 7.97 (br s, 2H), 7.78 (br s, 2H), 7.65 (d, J= 4.12 Hz, 2H), 7.51(m, 3H), 7.44(m, 4H), 7.30 (d, J= 4.08 Hz, 2H), 7.26 (s, 2H), 7.20 (s, 2H), 7.13 (d, J= 7.04 Hz, 2H), 7.07 (d, J= 5.16 Hz, 2H), 7.04 (s, 1H), 6.98 (br s, 2H), 6.96 (d, J= 5.16 Hz, 2H), 6.93 (s, 2H), 6.89 (s, 2H), 6.83 (d, J=5.16, 2H), 6.77 (d, J= 5.12, 2H), 2.99 (s, 6H), 2.82 (s, 6H), 2.414 (d, 12H), 1.49 (d, 12H).

Crystal data: $(C_{94}H_{74}S_{10})^{2+}2(CF3COO)^-$, Monoclinic, space group P 21/c, a = 23.966 (8) b = 12.143 (4), c = 32.204 (12) Å, α = 90, β = 99.057 (11), γ = 90; V = 9255 (6) $Å^3$, Z = 4, T = 150 K, D_{calcd} = 1.317 g cm^{-3}, R_1 = 0.0994 (10088) , R_w (all data) = 0.3101 (16342), GOF = 1.002.

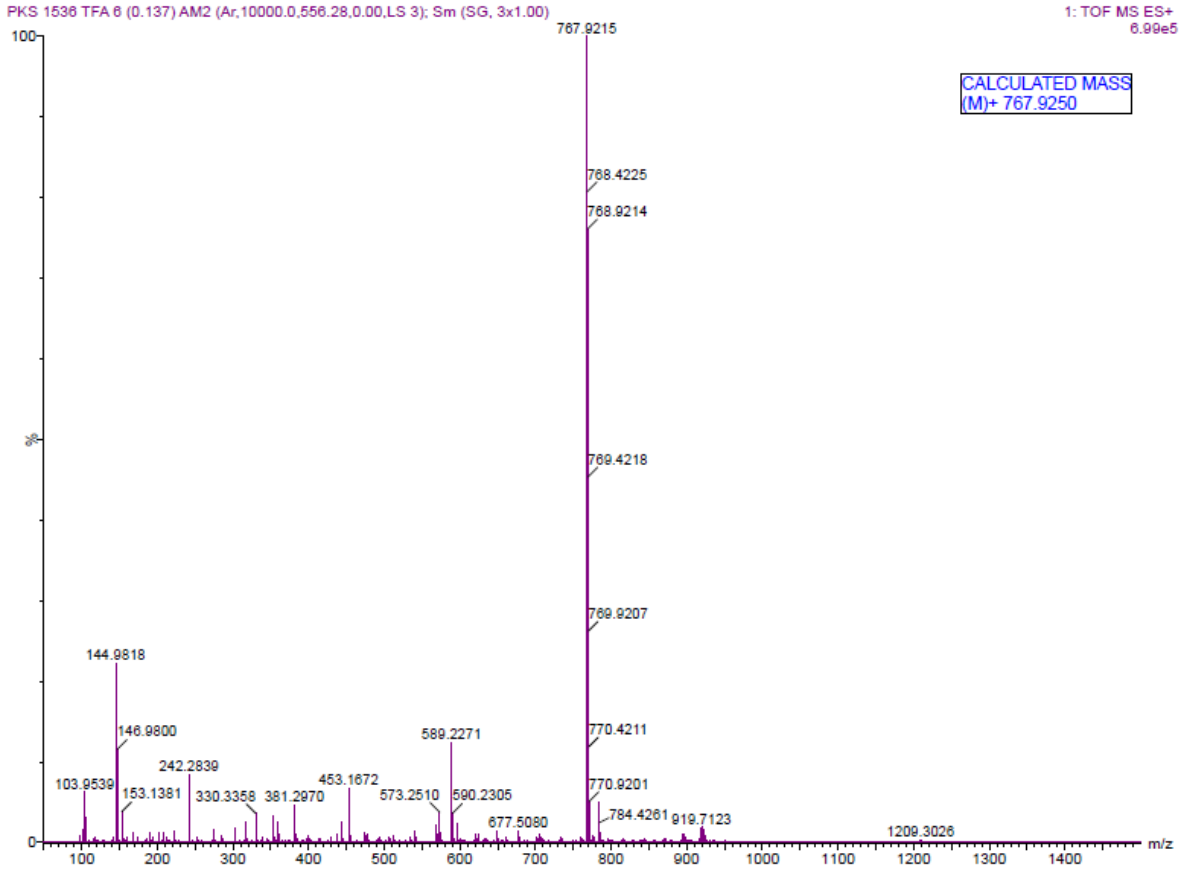
2. Mass Spectra of Macrocycles



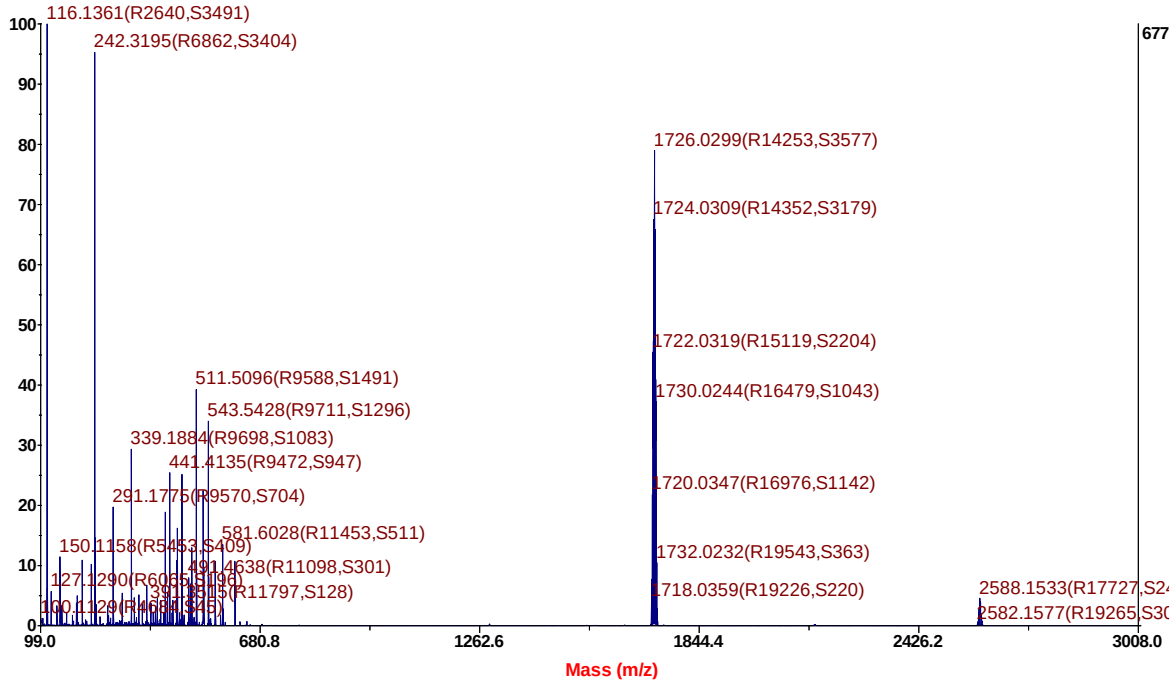
S1: MALDI-TOF/TOF mass spectrum of **10**.



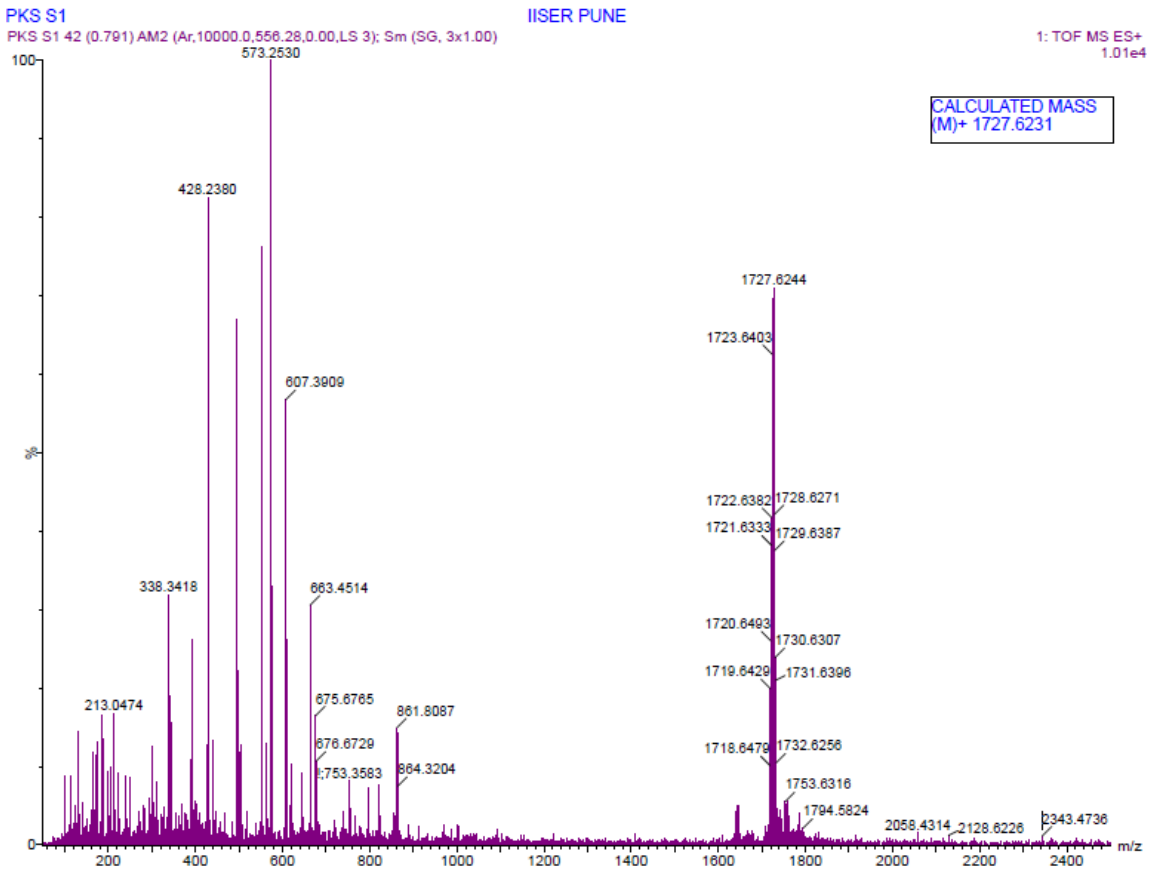
S2a: High resolution mass spectrum (ESI-TOF) of **10**.



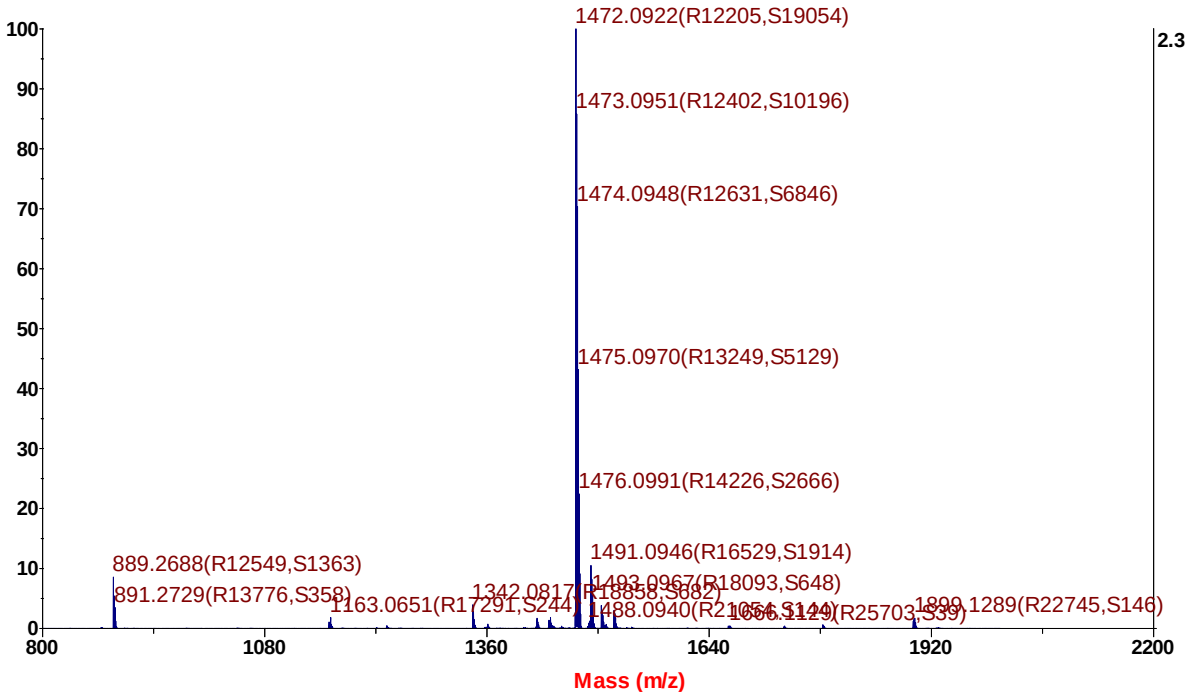
S2b: High resolution mass spectrum (ESI-TOF) of **[10]**$^{2+}$



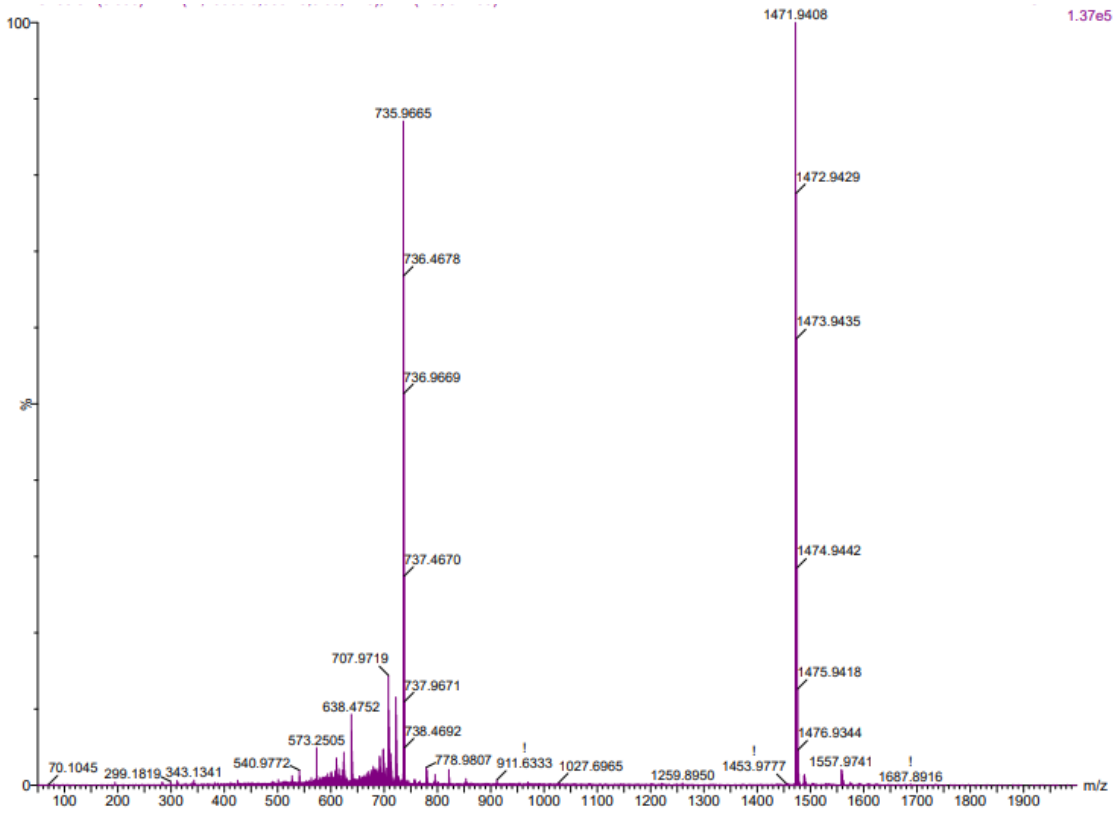
S3: MALDI-TOF/TOF mass spectrum of **11**.



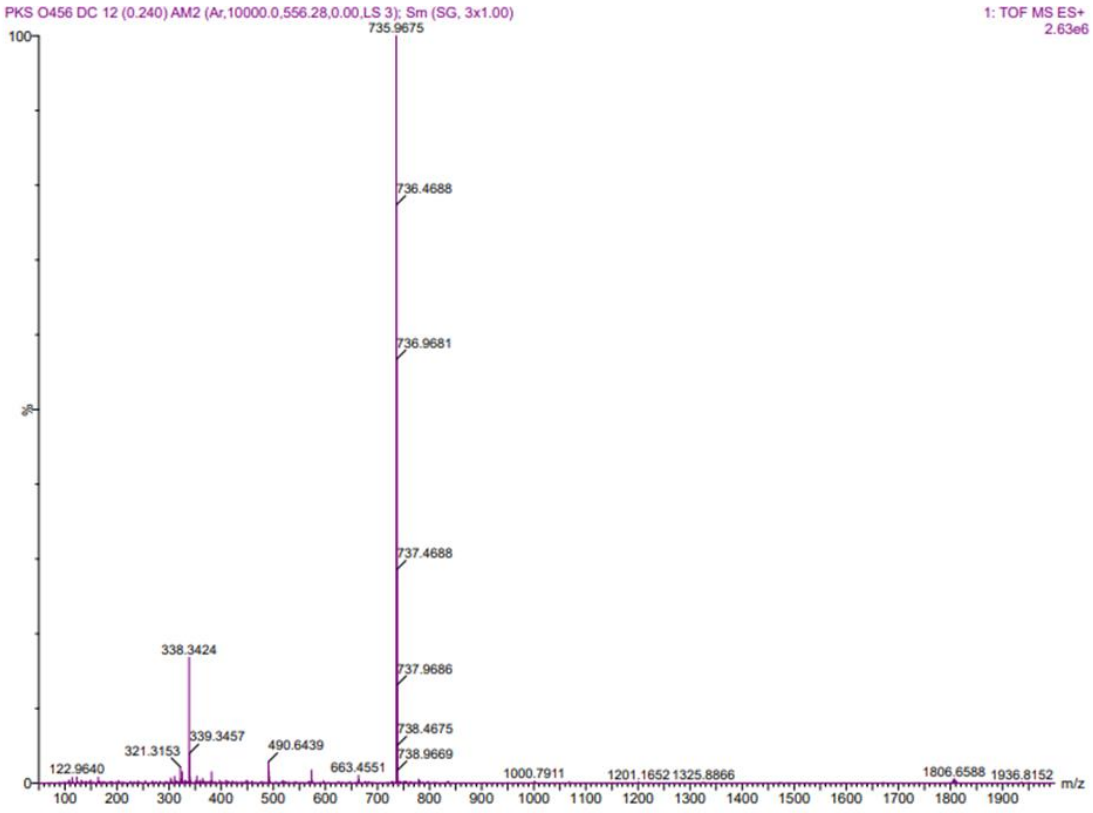
S4: High resolution mass spectrum (ESI-TOF) of **11**.



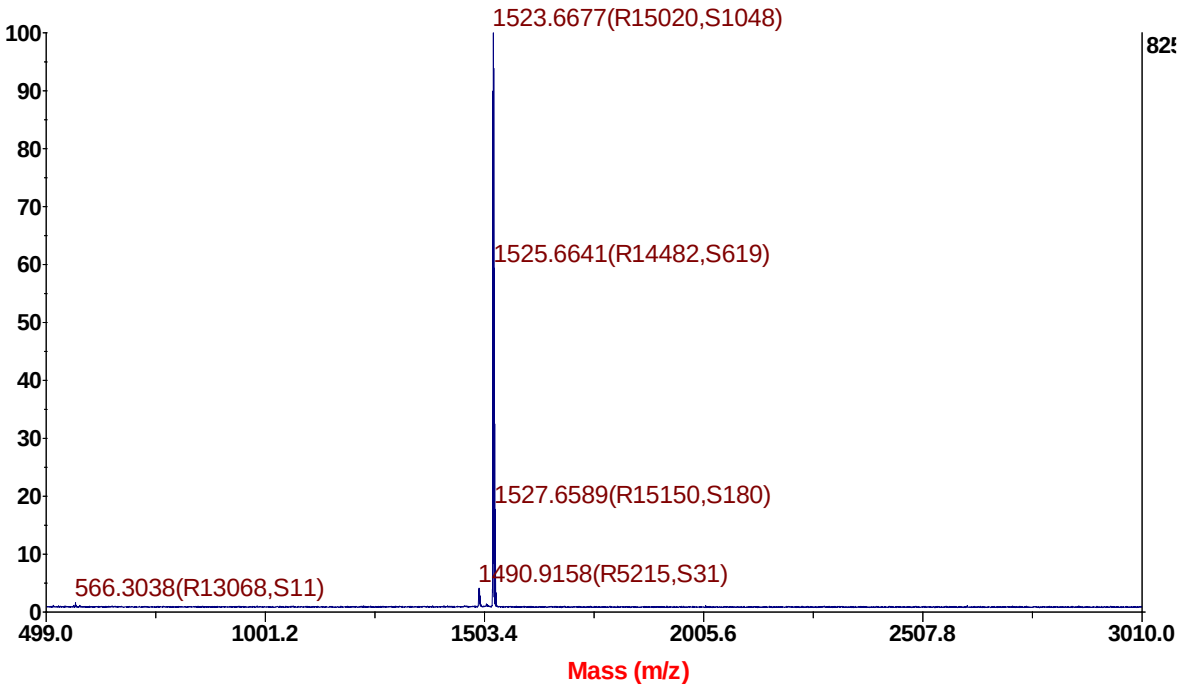
S5: MALDI-TOF/TOF mass spectrum of **12**.



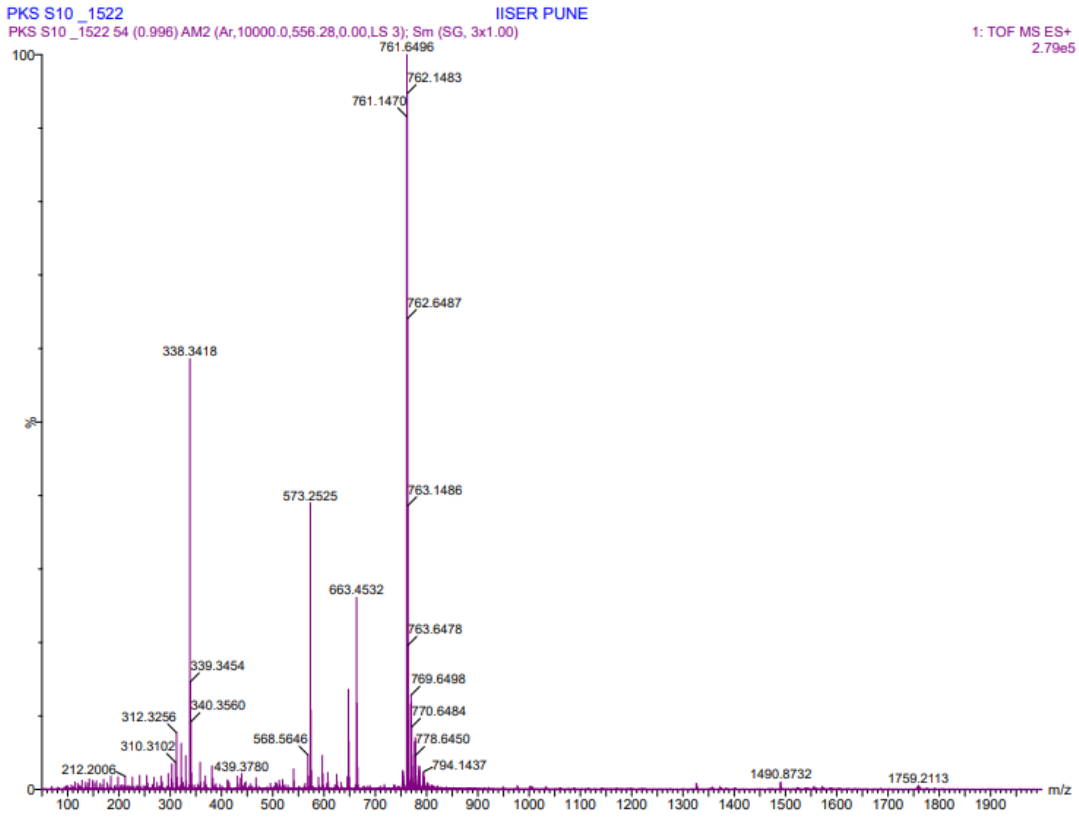
S6: High resolution mass spectrum (ESI-TOF) of **12**.



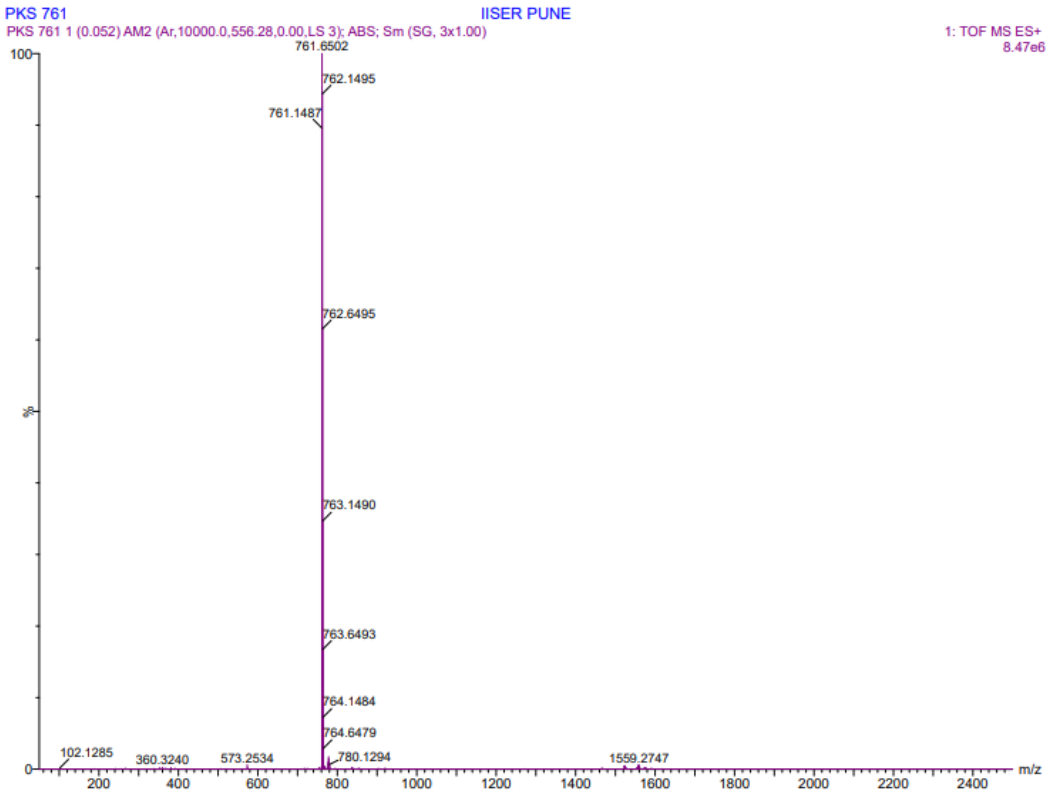
S7: High resolution mass spectrum (ESI-TOF) of **[12]**$^{2+}$.



S8: MALDI-TOF/TOF mass spectrum of **15**.

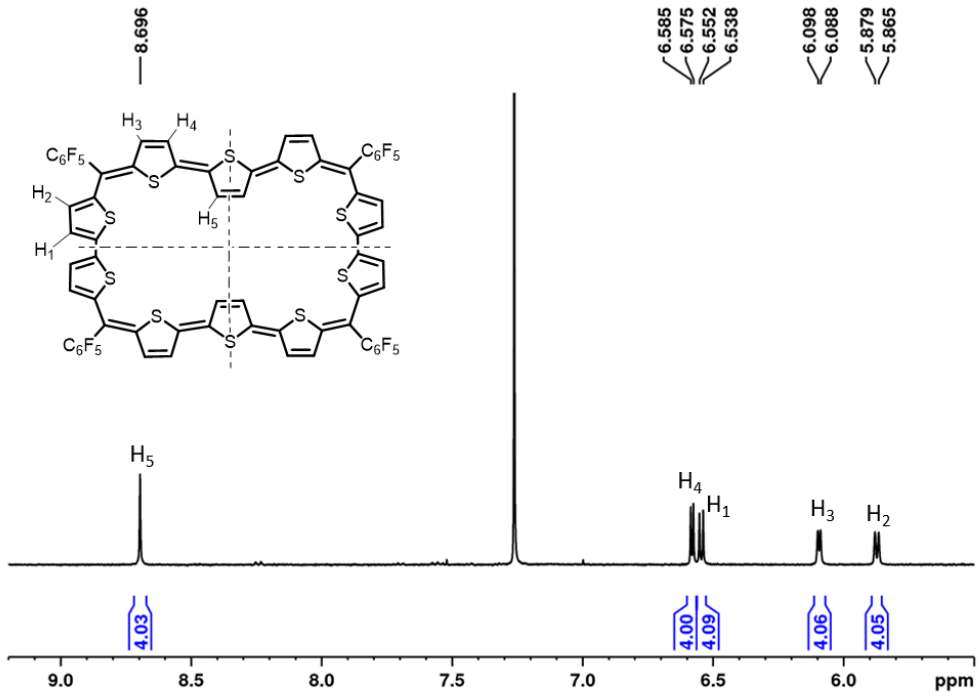


S9: High resolution mass spectrum (ESI-TOF) of **15.**

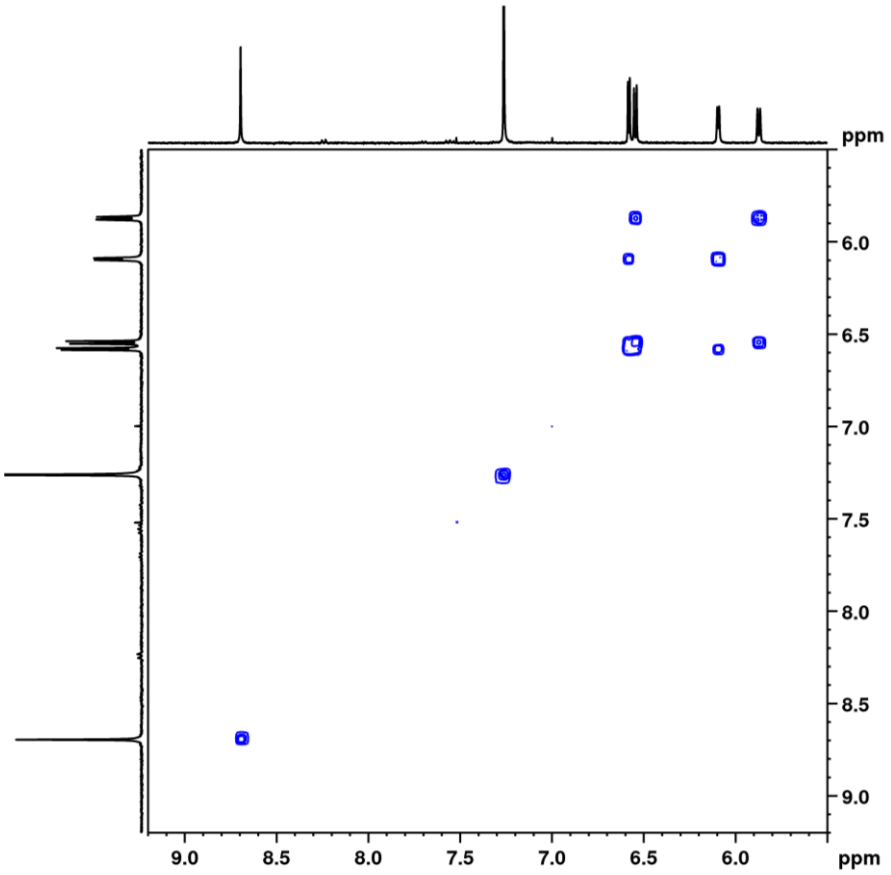


S10: High resolution mass spectrum (ESI-TOF) of **[15]$^{2+}$**.

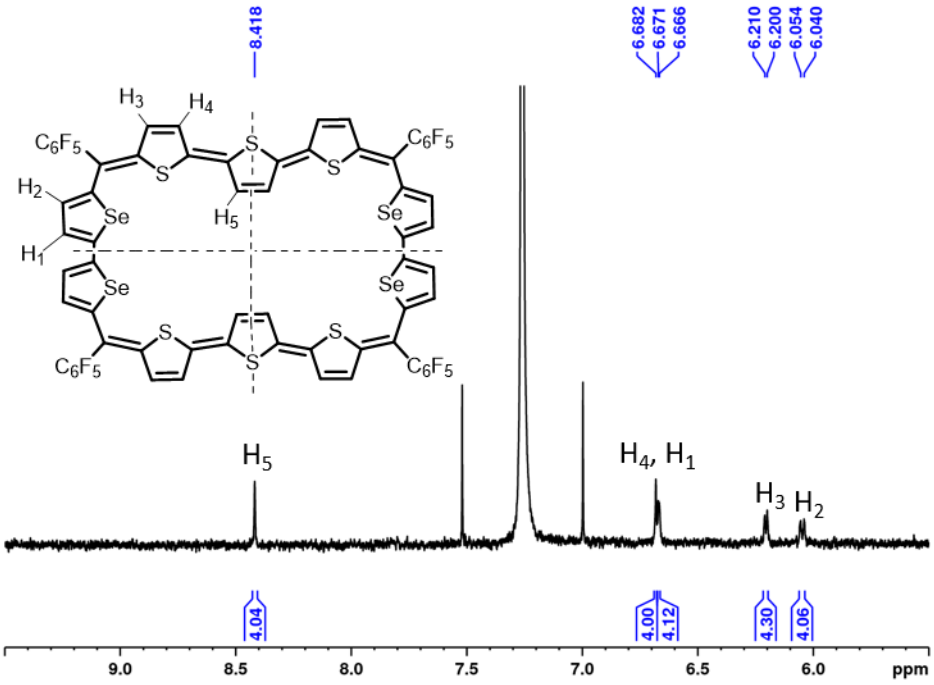
3. NMR Spectra of Macrocycles



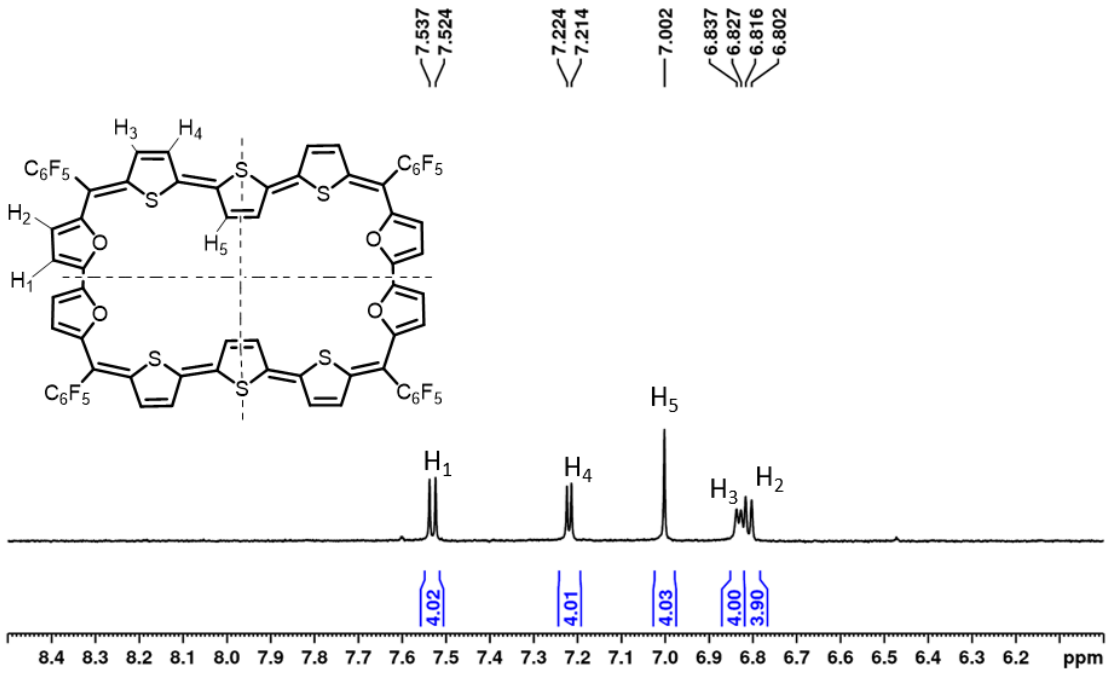
S11: 400 MHz ^{1}H NMR of spectrum of **10** in chloroform-*d* at 298 K.



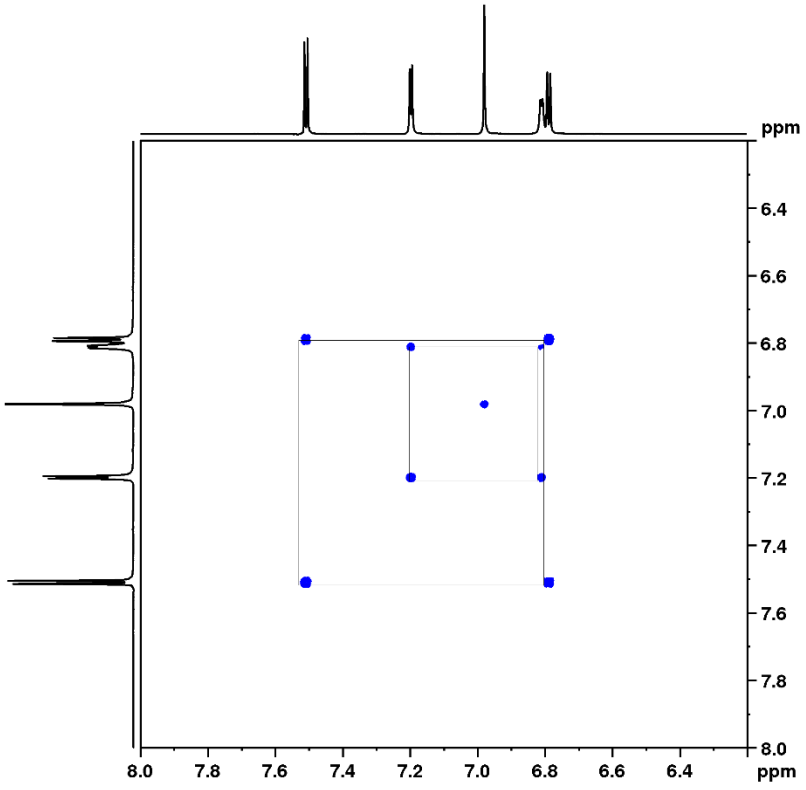
S12: ^{1}H-^{1}H COSY spectrum of **10** in chloroform-*d* at 298 K.



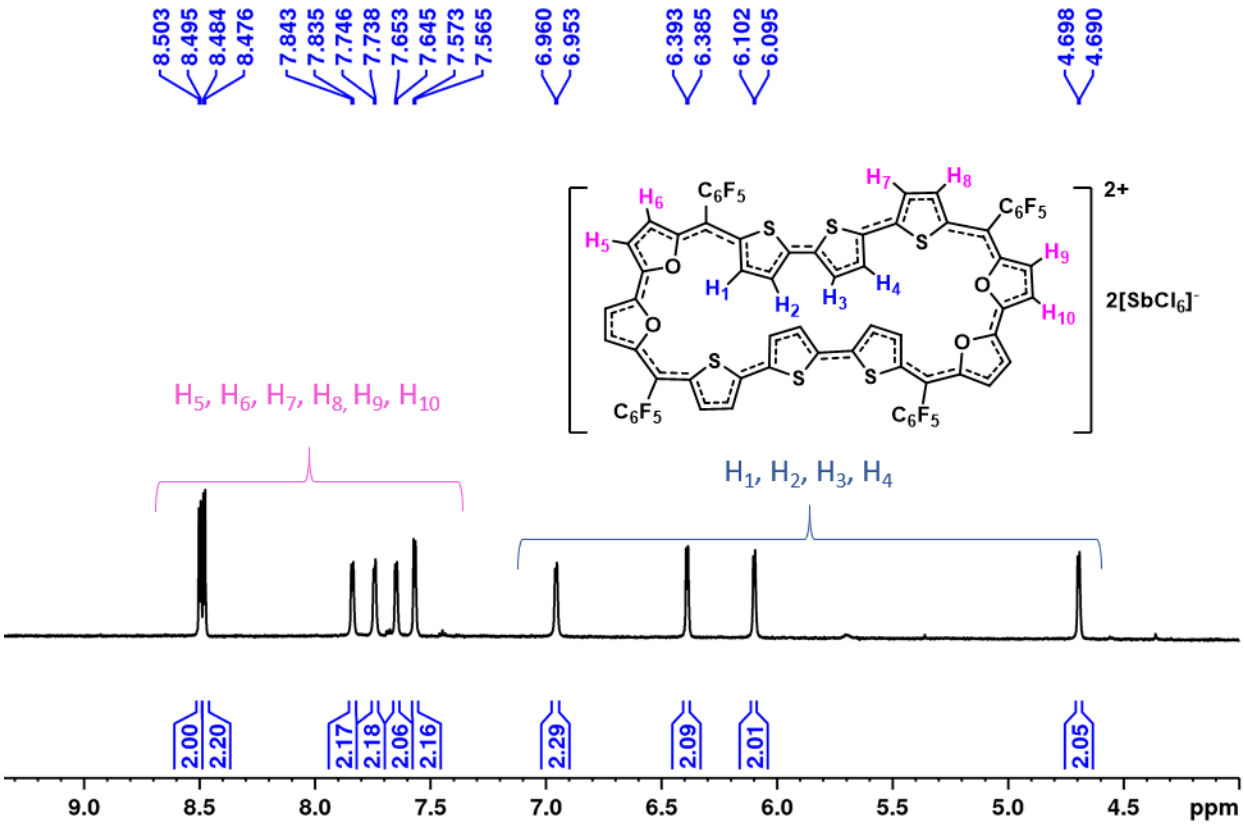
S13: 400 MHz ^{1}H NMR of spectrum of **11** in chloroform-*d* at 298 K.



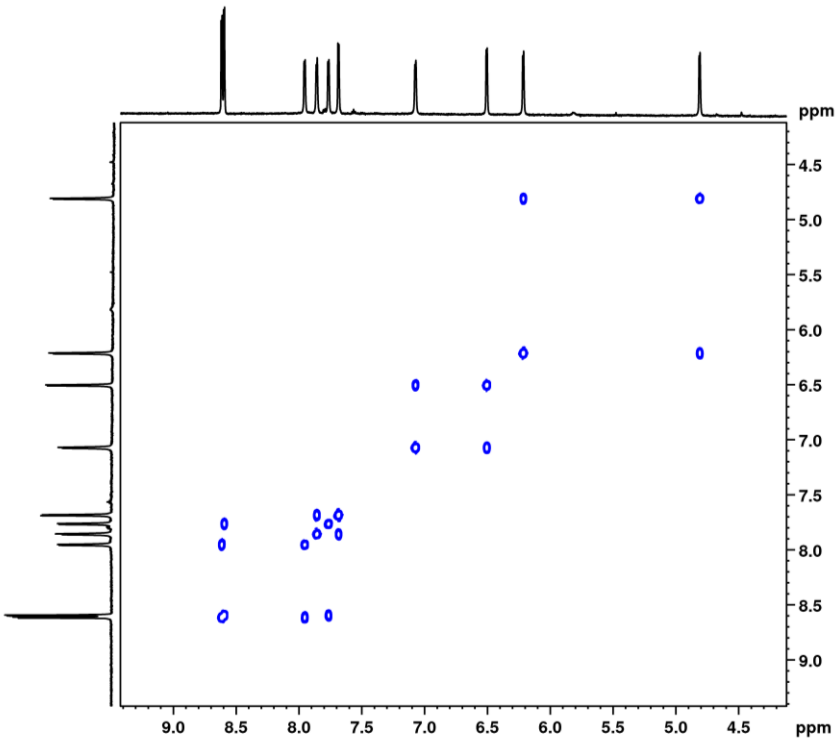
S14: 600 MHz ^{1}H NMR of spectrum of **12** in acetone-d_6 at 298 K.



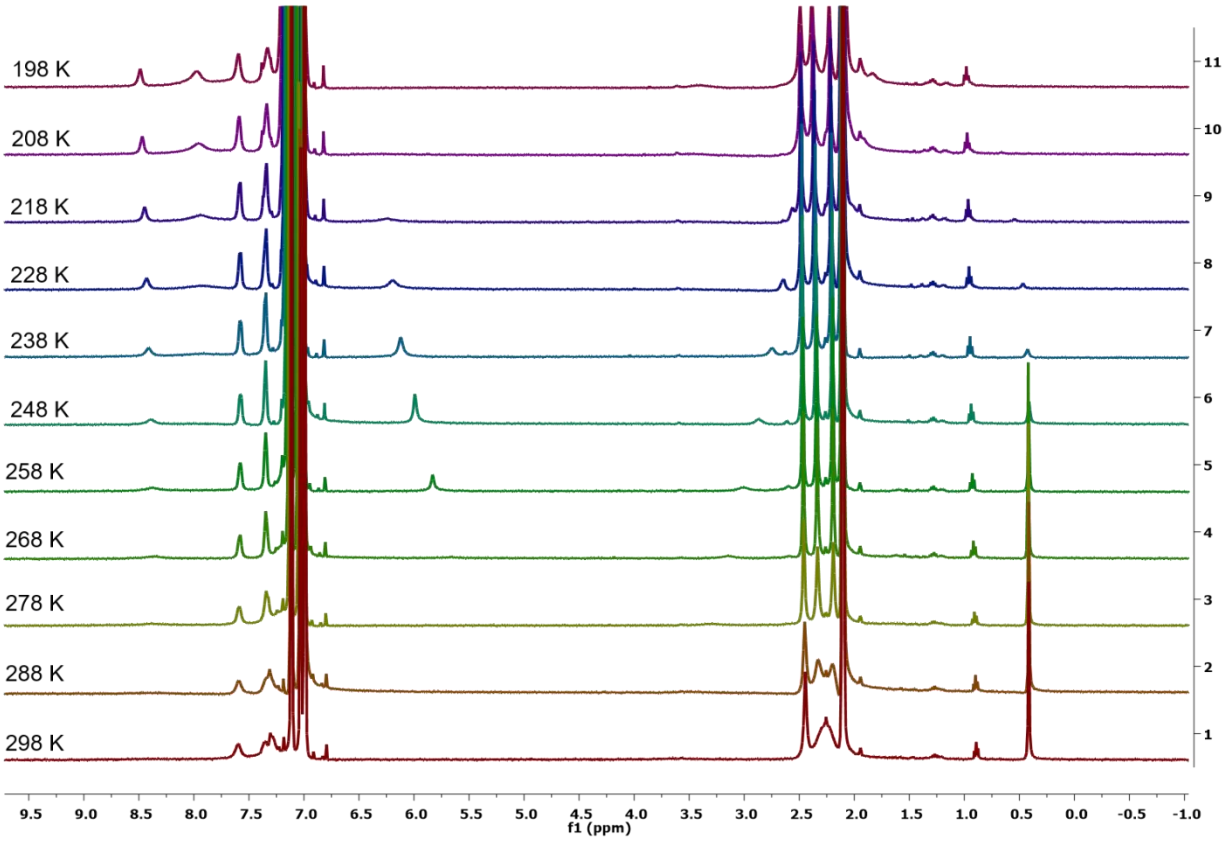
S15: ^{1}H-^{1}H COSY spectrum of **12** in acetone-d_6 at 298 K.



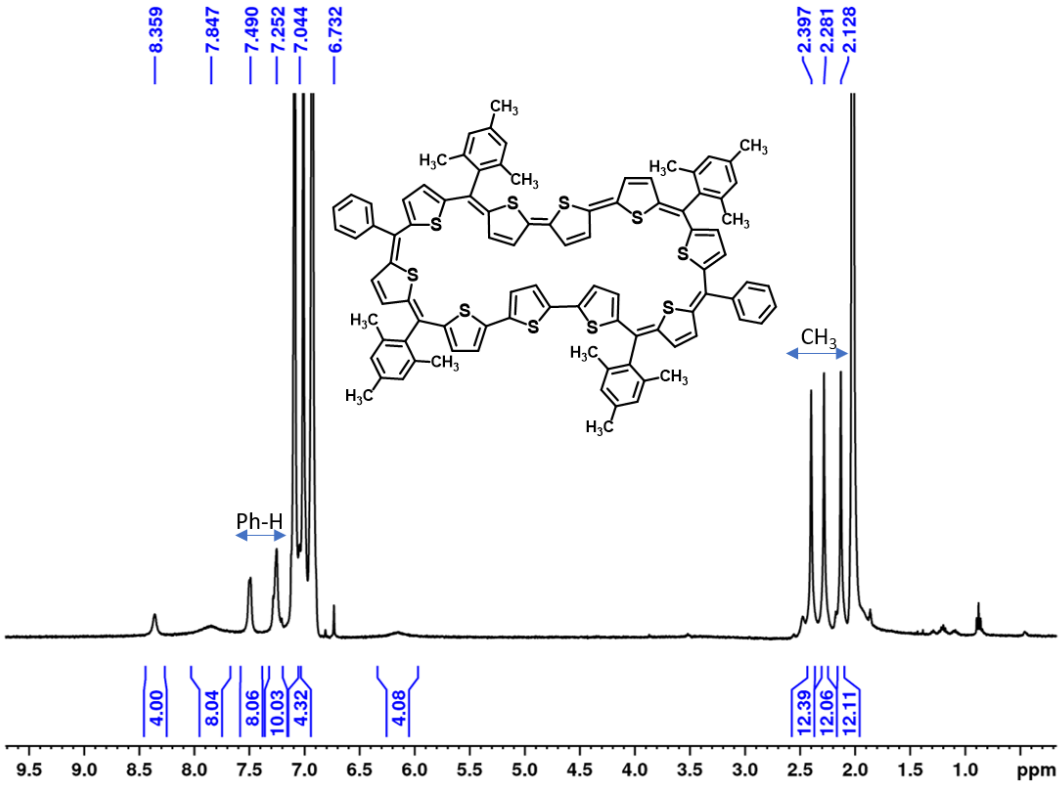
S16: 600 MHz ^{1}H NMR of spectrum of **[12]$^{2+}$** in acetonitrile-d_3 at 298 K.



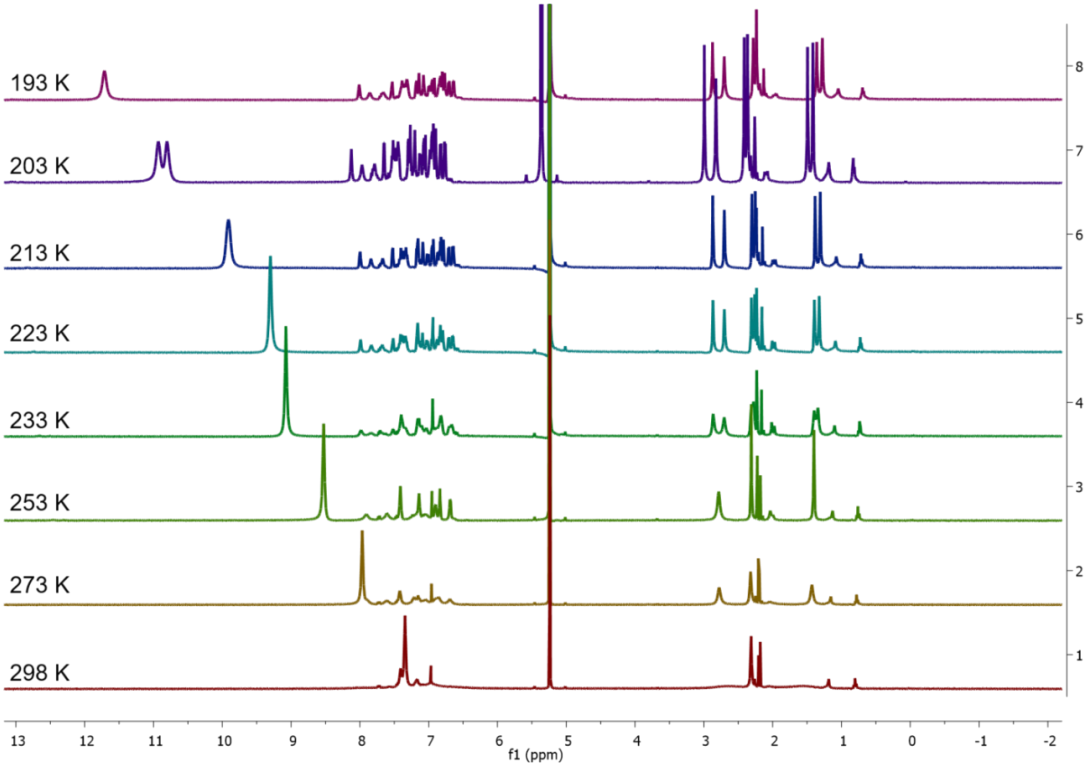
S17: ^{1}H-^{1}H COSY spectrum of **[12]$^{2+}$** acetonitrile-d_3 at 298 K.



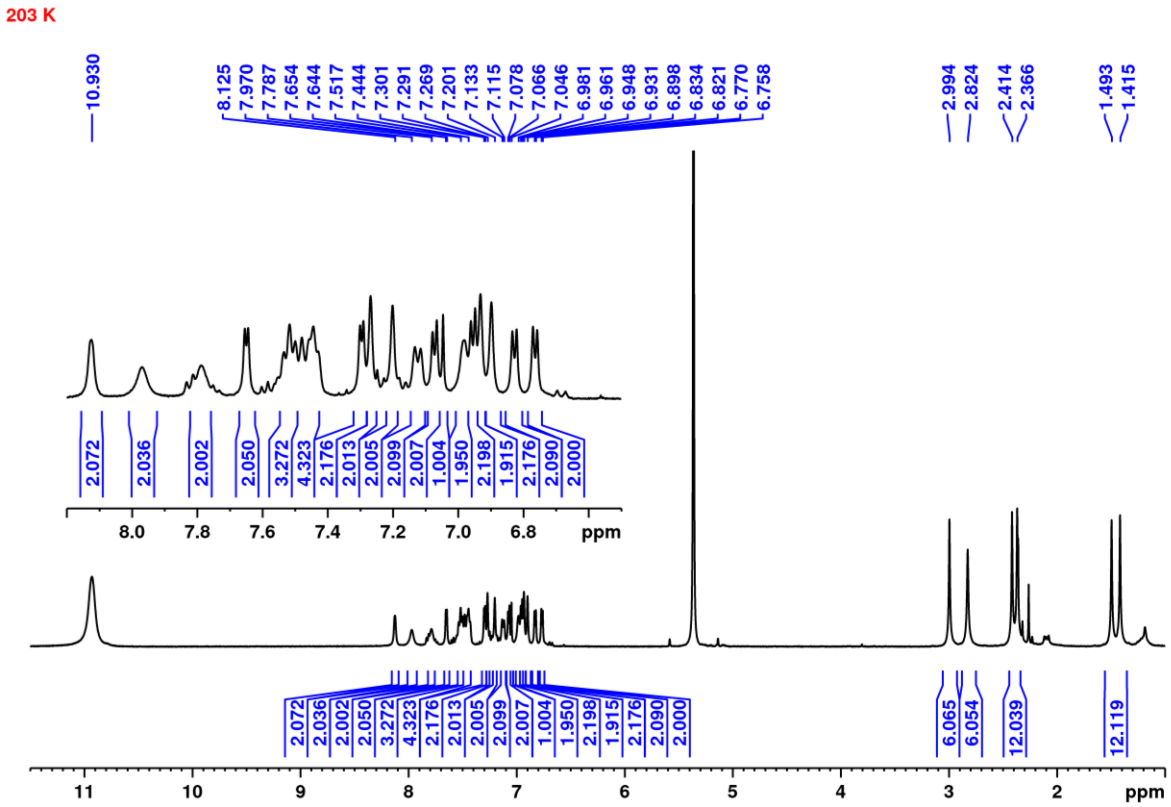
S18: Variable temperature 400 MHz ^{1}H NMR spectra of **15** in toluene-d_8.



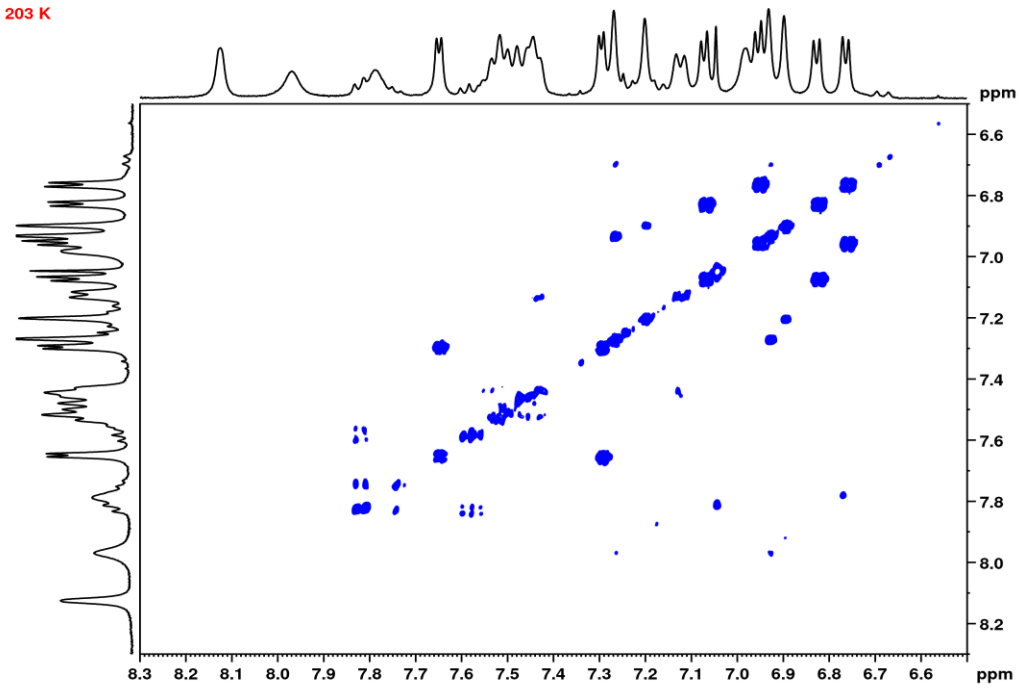
S19: 400 MHz ^{1}H NMR of spectrum of **15** in toluene-d_8 at 218 K.



S20: Variable Temperature 400 MHz ^{1}H NMR of spectra of **[15]$^{2+}$** in dichloromethane-d_2.

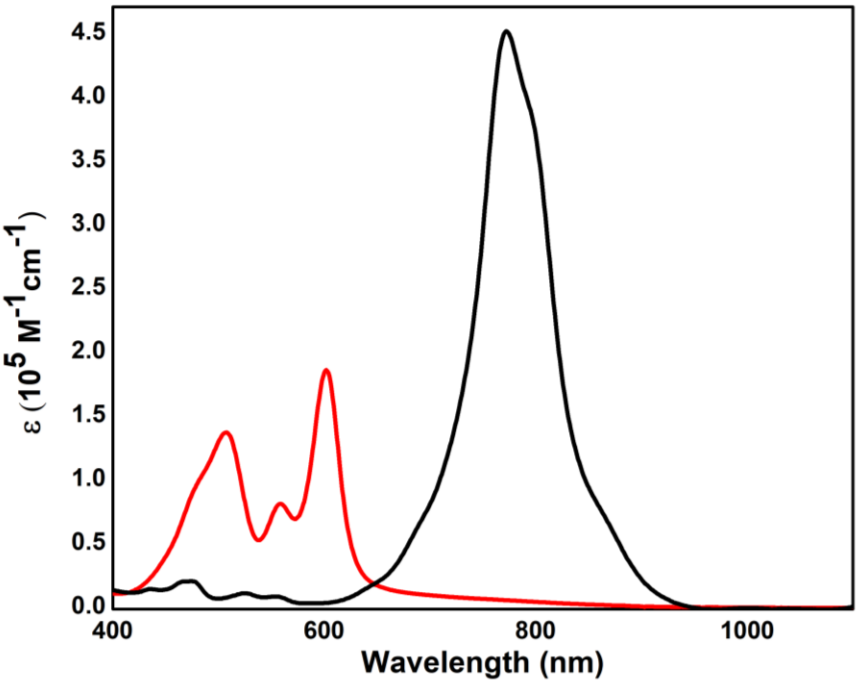


S21: 400 MHz ^{1}H NMR of spectrum of **[15]$^{2+}$** in dichloromethane-d_2 at 203 K (signal at δ ≈ 11.5 ppm is for deuterated trifluoroacetic acid (CF_3COOD) added in excess to oxidize the macrocycle).

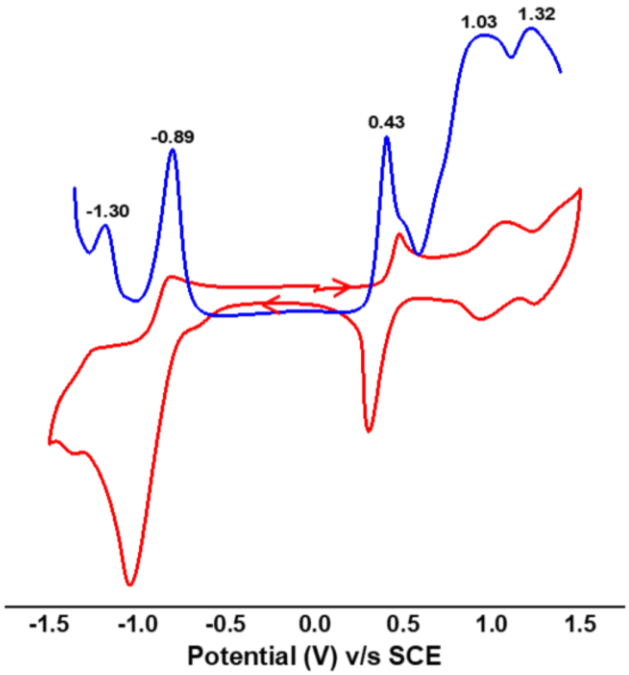


S22: ^{1}H-^{1}H COSY spectrum of [**15**]$^{2+}$ in dichloromethane-d_2 at 203K.

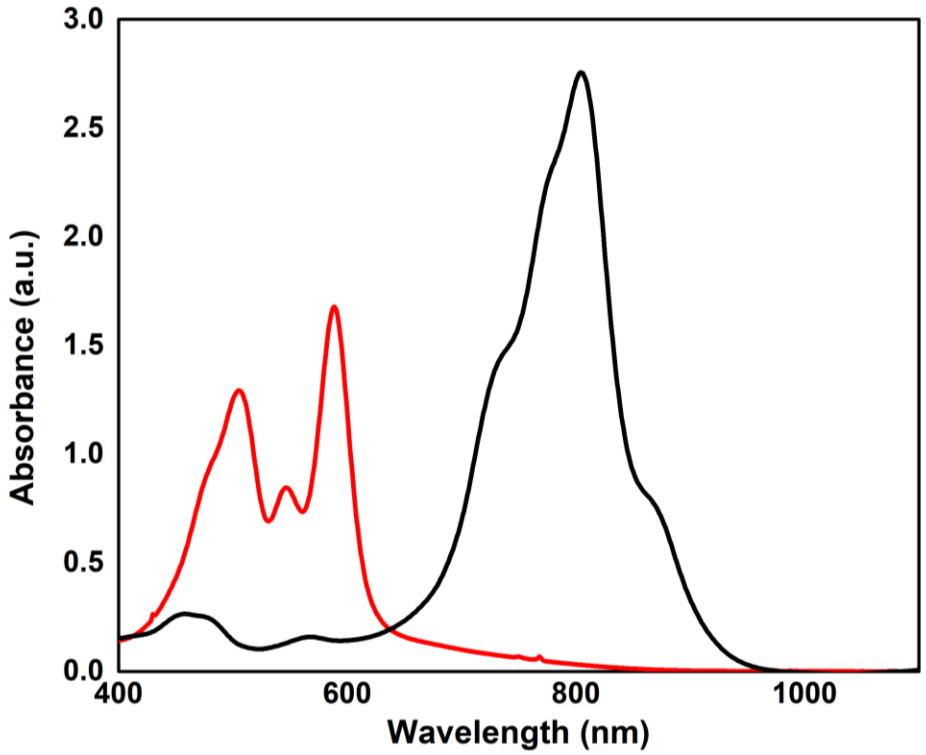
4. UV-vis Absorption Spectra and Cyclic Voltammetry & DPV



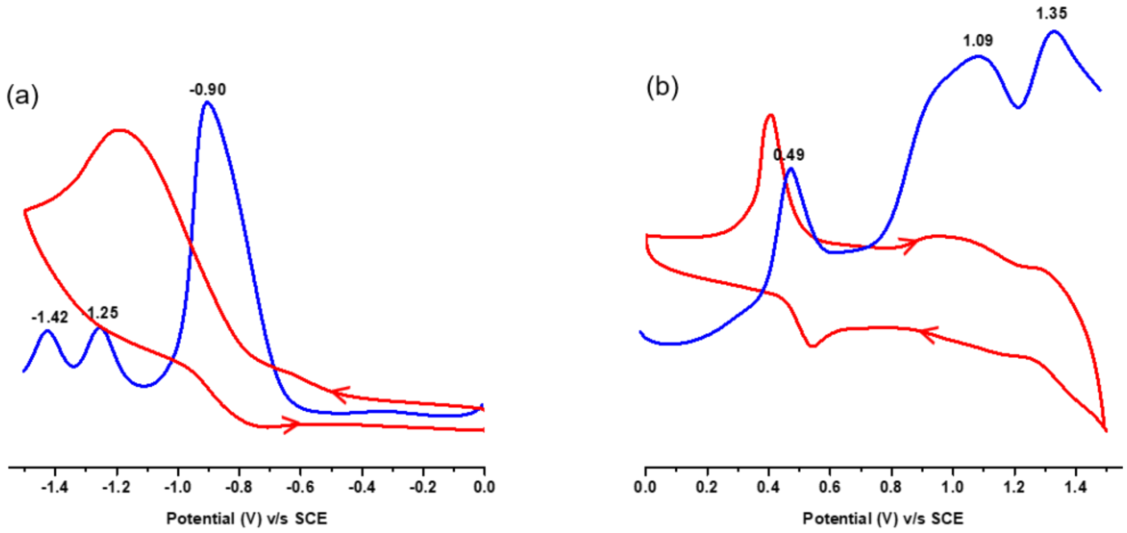
S23: UV-visible absorption spectra of **10** (red line) and **[10]**$^{2+}$ (black line).



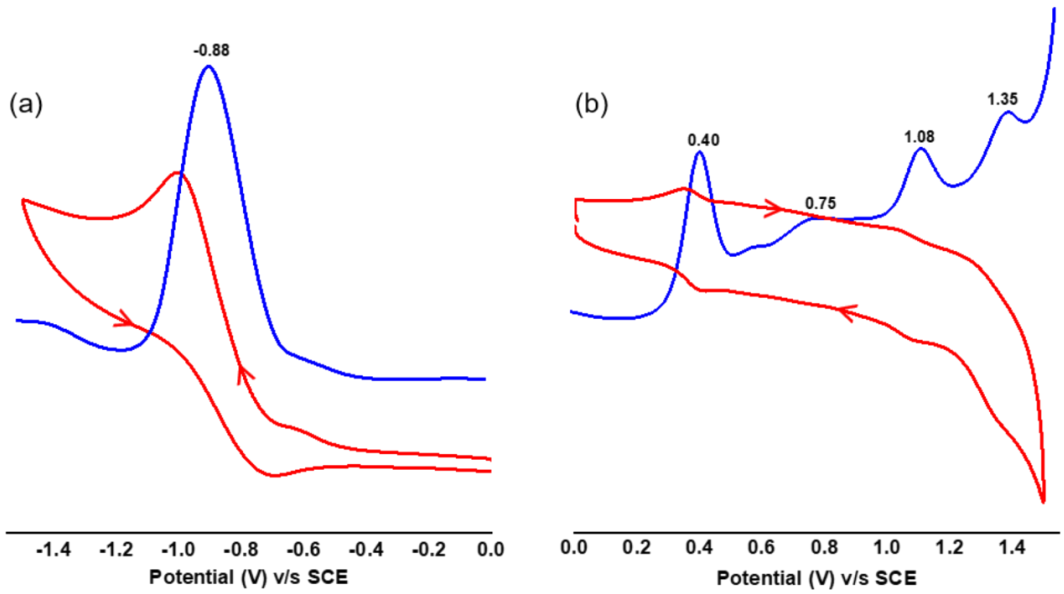
S24: Cyclic voltammetry of **10** (red line) and Differential Pulse Voltammetry (blue line) recorded with standard calomel as reference electrode, Pt wire as counter electrode and glassy carbon as working electrode with scan rate 50 mV/s.



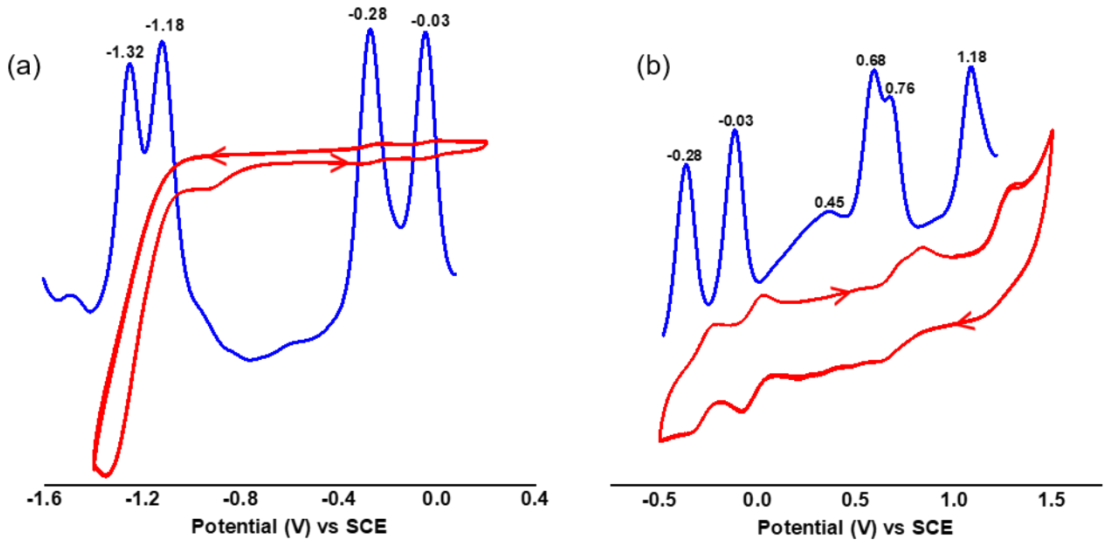
S25: UV-visible absorption Spectra of **11** (red line) and **[11]**$^{2+}$(black line).



S26: Cyclic voltammetry of **11** (red lines) and Differential Pulse Voltammetry (blue lines). (a) represent reduction potentials (b) oxidation potentials. Experiment performed with calomel as reference electrode, Pt wire as counter electrode and glassy carbon as working electrode with scan rate 100 mV/s.



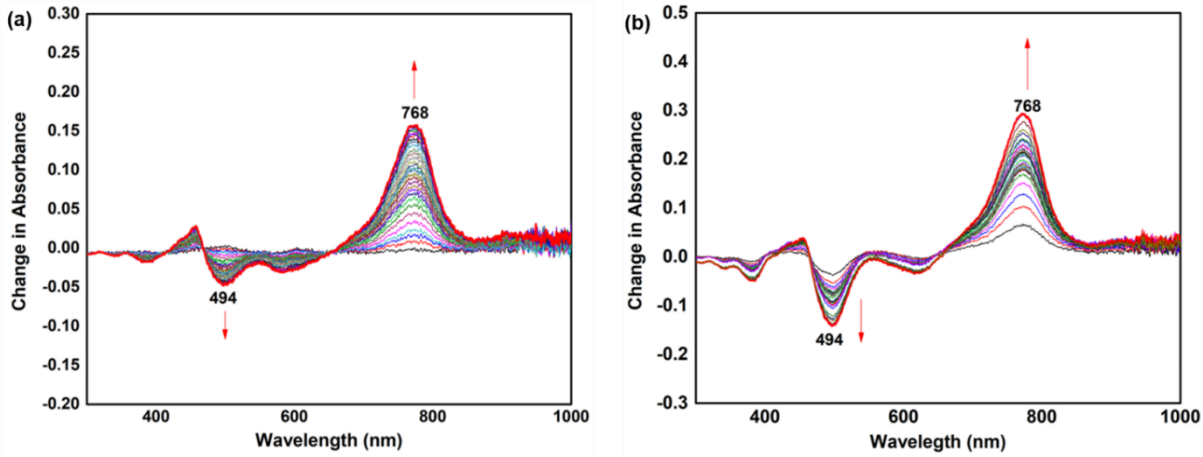
S27: Cyclic voltammetry of **12** (red line) and Differential Pulse Voltammetry (blue line). (a) reduction potentials (b) oxidation potential recorded with standard calomel as reference electrode, Pt wire as counter electrode and glassy carbon as working electrode with scan rate 100 mV/s.



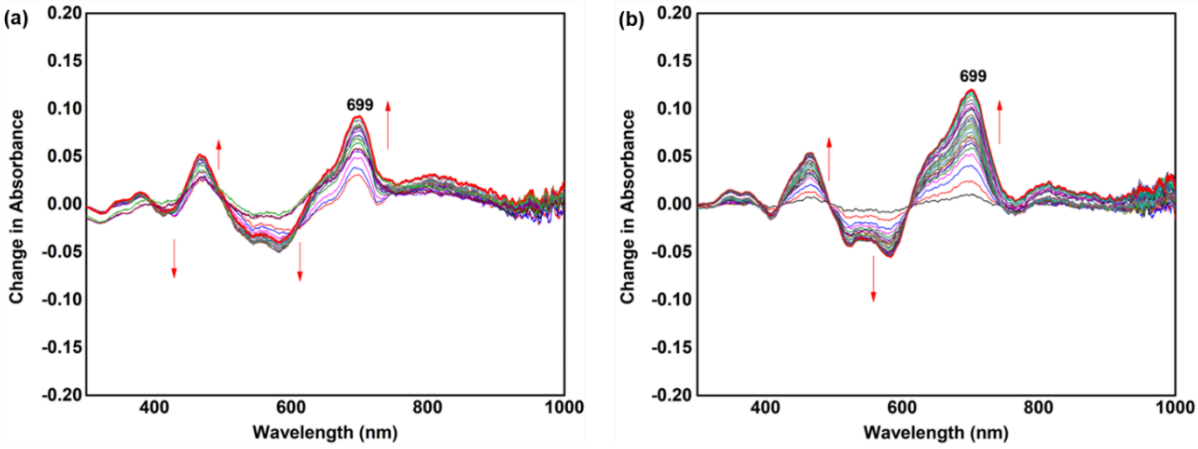
S28: Cyclic voltammetry of **15** (red) and Differential Pulse Voltammetry (blue). (a) reduction potential and (b) oxidation potential recorded with Ag/AgCl as reference electrode, Pt wire as counter electrode and glassy carbon as working electrode with scan rate 50 mV/s.

5. Spectro-electrochemical Studies of the Macrocycles

The Spectro-electrochemical measurements were performed in Ocean Insight FLAME Miniature Spectrometer by incorporation of CH Instrument Electrochemical Analyzer in 0.1 M tetrabutylammonium perchlorate (supporting electrolyte) solution prepared in freshly distilled dichloromethane. The assembly consisted of a thin layer quartz glass cell (optical path length of 1 mm), and a three electrode setup (Pt gauze, Pt wire and Calomel as reference electrode). The UV-vis spectra was taken after every 10 s, while adjusting the potential corresponding to first and second oxidation waves.

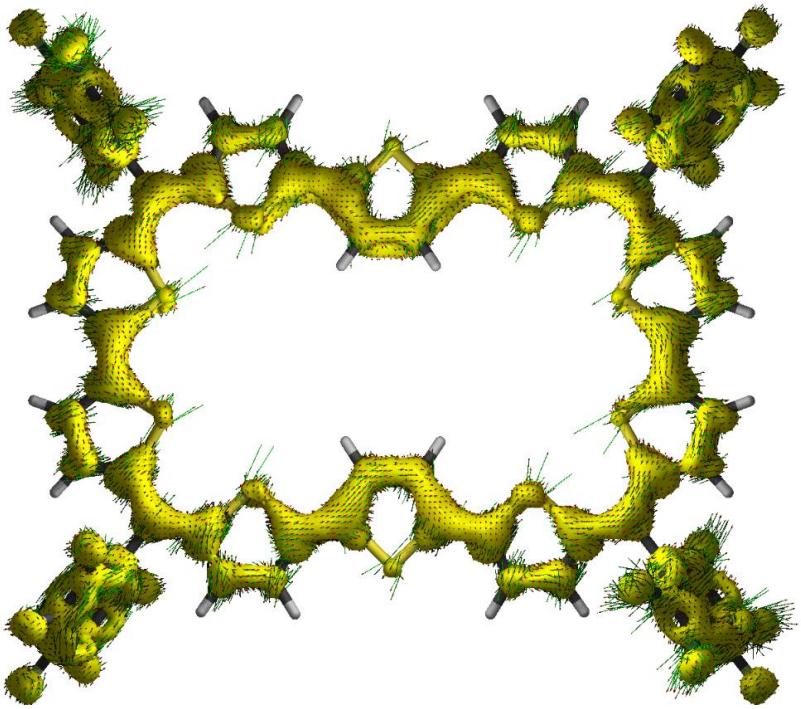


S29: Spectroelectrochemistry experiment of **12**, (a) for first oxidation potential at 0.47 V (b) for second oxidation potential at 0.87 V.

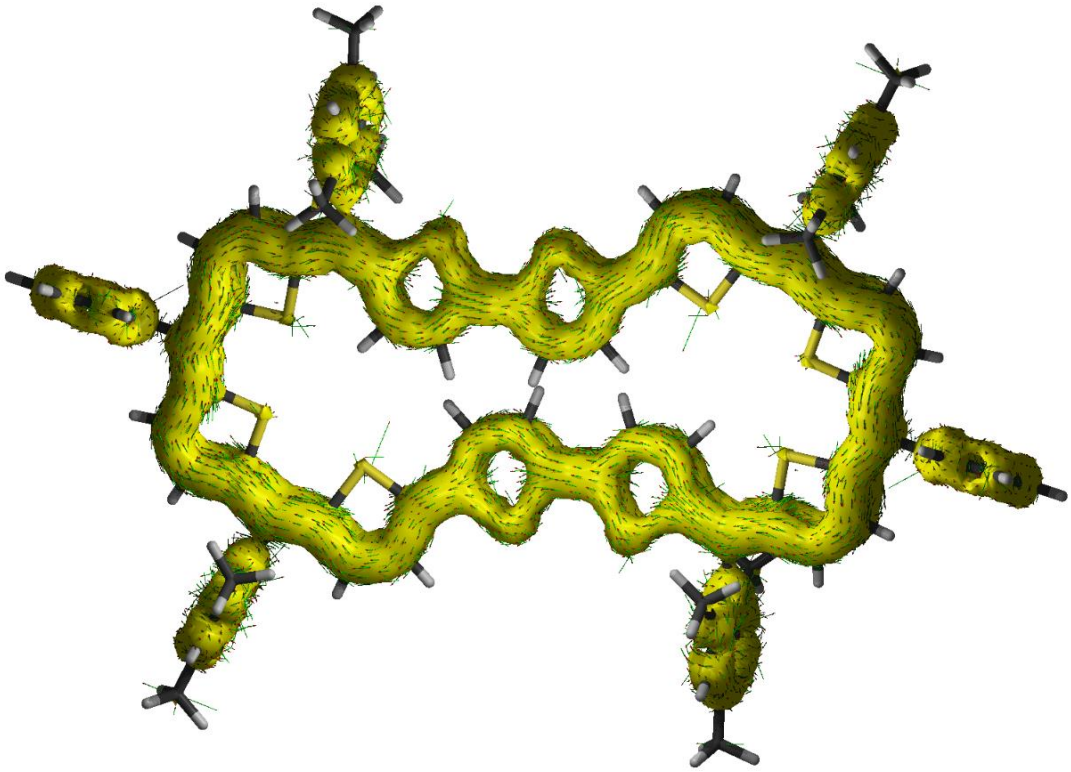


S30: Spectroelectrochemistry experiment of **15**, (a) for first oxidation potential at 0.54 V (b) for second oxidation potential 0.71V**.**

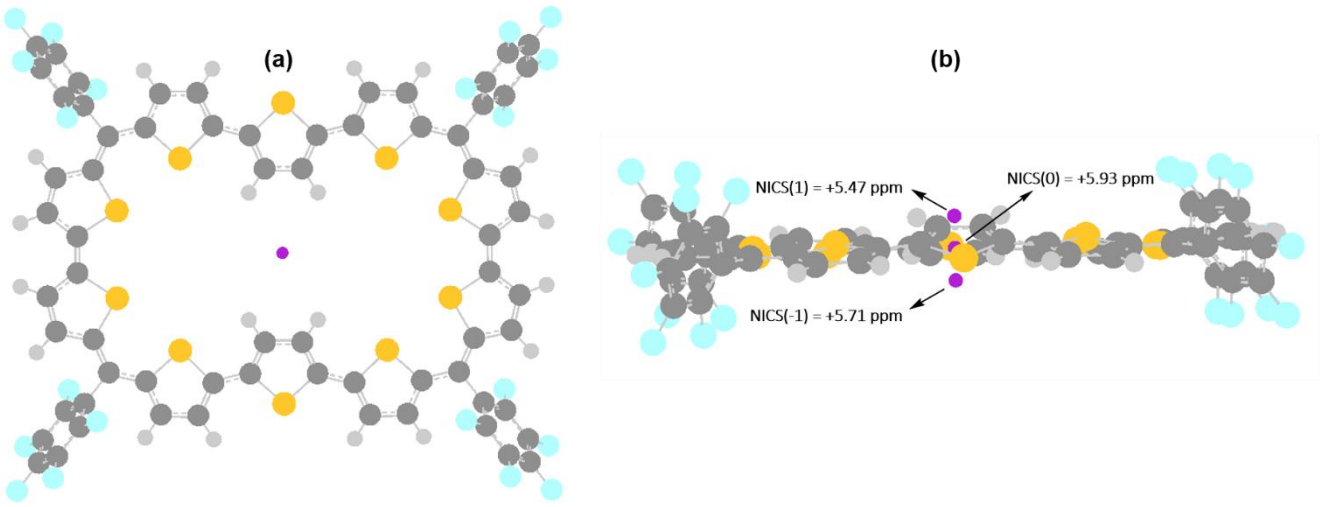
6. Quantum Chemical Calculations



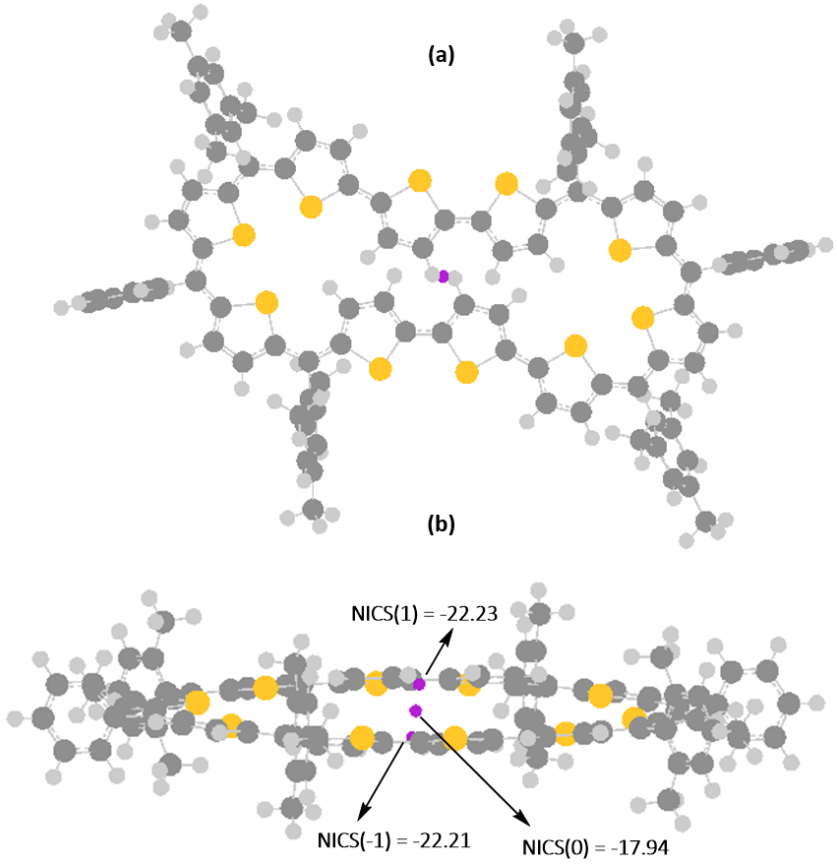
S31: Anisotropy of Induced Current Density (AICD) plot of **10** at isovalue 0.07, (π electrons only) calculated with B3LYP/6-31G(d,p) level of theory.



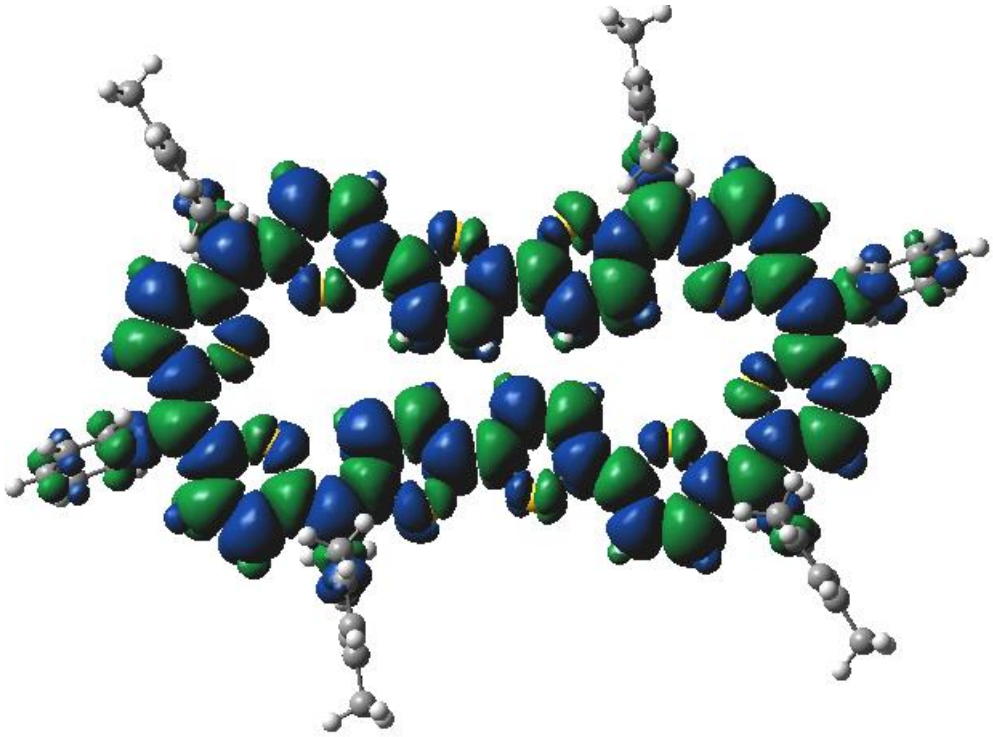
S32: Anisotropy of Induced Current Density (AICD) plot of **15** at isovalue 0.06, (π electrons only) calculated with B3LYP/6-31G(d,p) level of theory.



S33a. NICS values for **10** calculated using the standard GIAO (NMR=GIAO) at centre of the macrocycle and 1Å above & below the macrocyclic plane along z-axis (a) top view, (b) side view.



S33b. NICS values for **15** calculated using the standard GIAO (NMR=GIAO) at centre of the macrocycle and 1Å above & below the macrocyclic plane along z-axis (a) top view, (b) side view.



S33c. Spin-density distribution map, calculated using UCAM-B3LYP /6-31G(d, p) level for the singlet state of 15. Green and blue surfaces represent positive and negative spin densities respectively.

Diradical Calculations of 10, $[10]^{2+}$ and 15.

HOMO	LUMO	HOMO-LUMO ($2T_1$)	T_1	$1+ T_1^* T_1$	$2 T_1/1+ T_1^* T_1$	$1-2T1/1+ T_1^* T_1$
1.15774	0.84226	0.3155	0.1577	1.0245	0.3078	0.6921

Table S1a. Calucation of y_0 for **15**

HOMO-1	LUMO+1	HOMO-LUMO ($2T_2$)	T_2	$1+ T_2^* T_2$	$2 T_2/1+ T_2^* T_2$	$1-2T2/1+ T_2^* T_2$
1.8164	0.1836	1.6328	0.8164	1.6665	0.97977	0.02022

Table S1b. Calucation of y_1 for **15**

Molecule	$\Delta E_{S\text{-}T}$ (kcal/mol)	Occupation Number of HOMO	Occupation Number of LUMO	y_0	y_1	y_2	NICS (ppm)
10	-6.06	1.89	0.10	0.005	0.003	0	+5.93
$[10]^{2+}$	-2.61	1.26	0.74	0.507	0.007	0.002	-13.95
[15]	-2.19	1.16	0.84	0.692	0.020	0.009	-17.94

Table S2. Calculated singlet triplet energy gap $\Delta E_{S\text{-}T}$, occupation number of HOMO and LUMO, y_0, y_1. y_2 and NICS value of molecule **10**, **$[10]^{2+}$ and 15**.

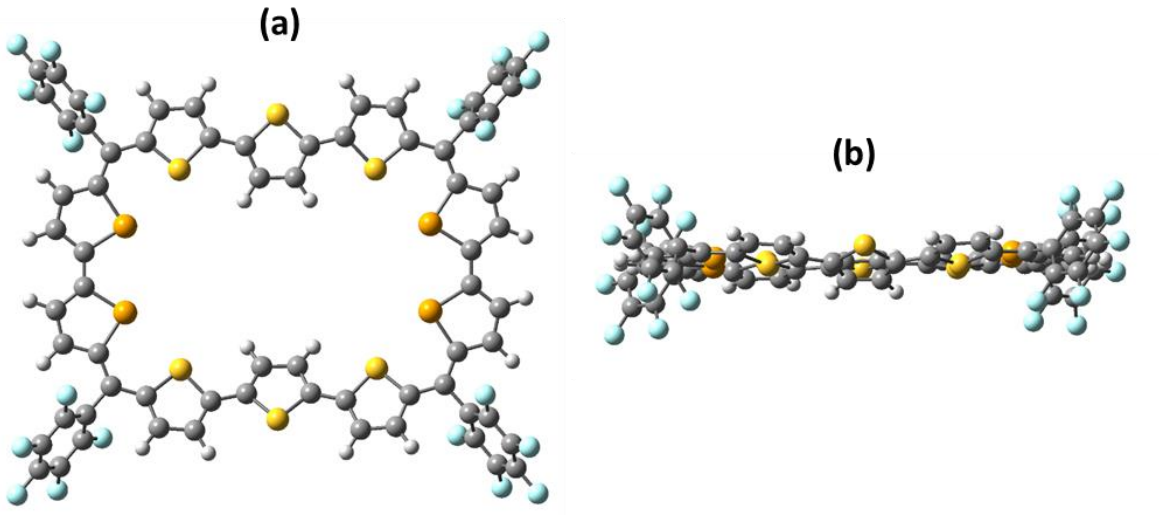


Figure. S34: Energy optimised structure of **11** obtained using B3LYP /6-31G(d, p) level of theory in DFT calucaltion. (a) top view and (b) side view.

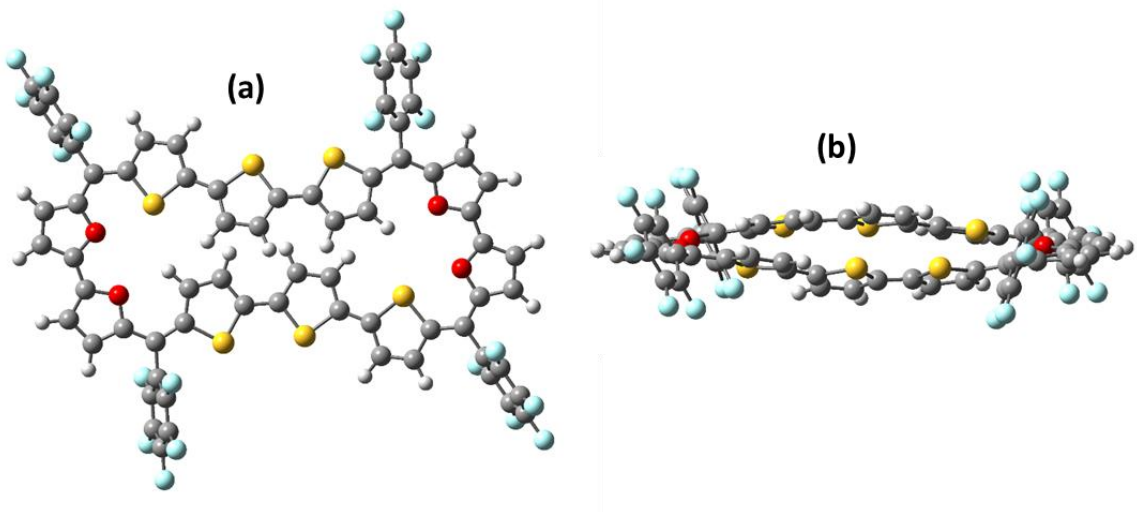


Figure. S35: Energy optimised structure of **[12]**$^{2+}$obtained using B3LYP /6-31G(d, p) level of theory in DFT calucaltion. (a) top view and (b) side view

7. Additional Figures

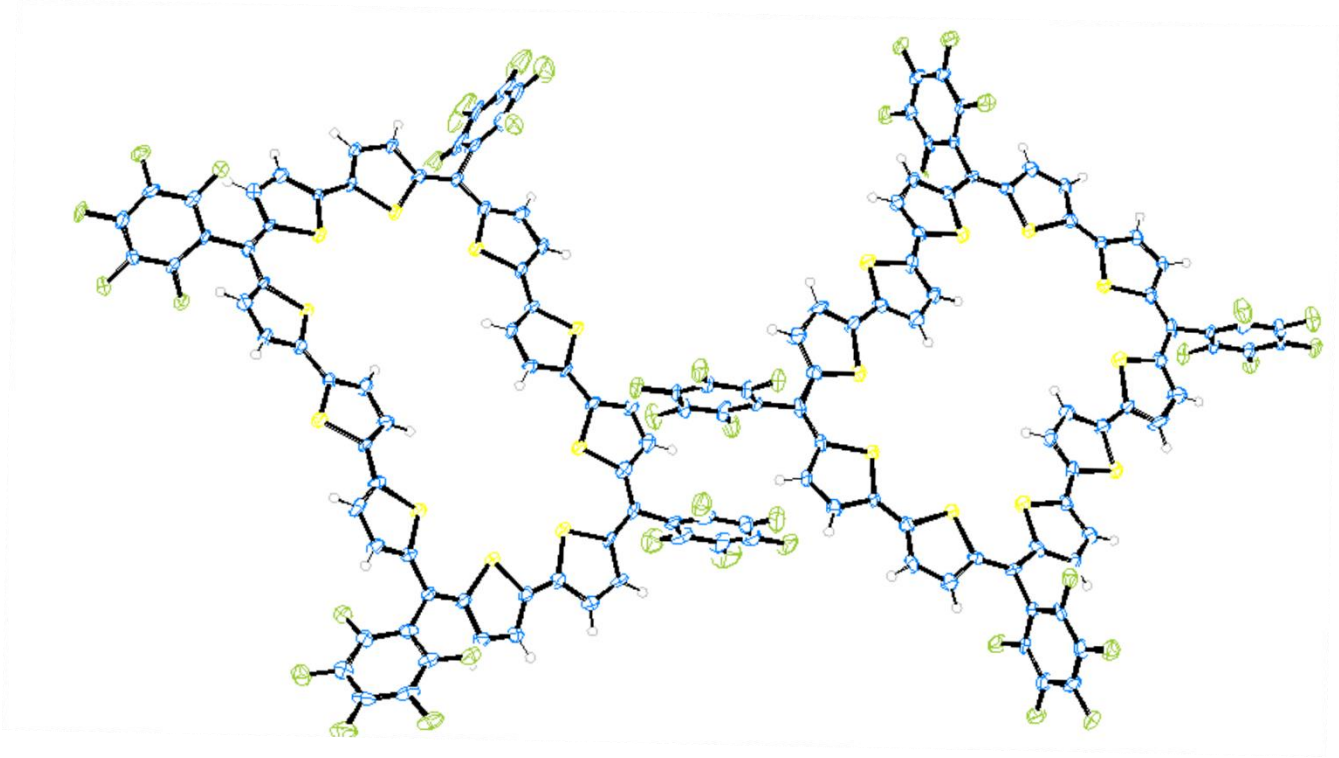


Figure S36. Thermal ellipsoidal plot of **10** with 50% ellipsoid probability using ORTEP.

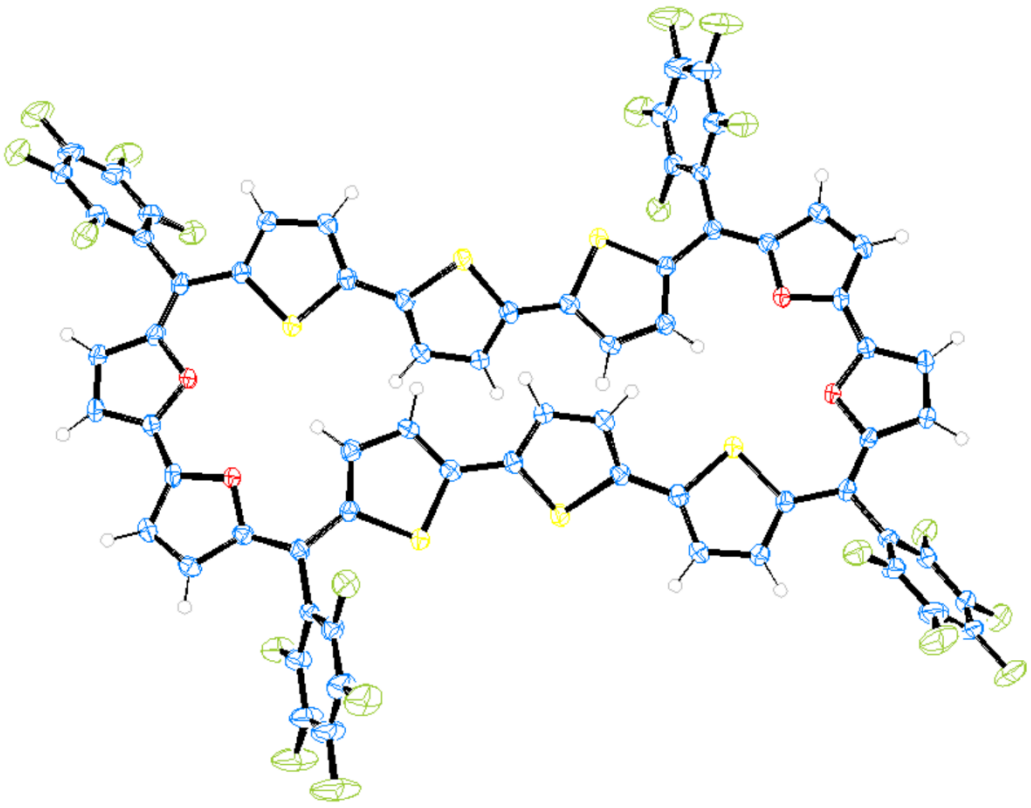


Figure S37. Thermal ellipsoidal plot of **12** with 50% ellipsoid probability using ORTEP.

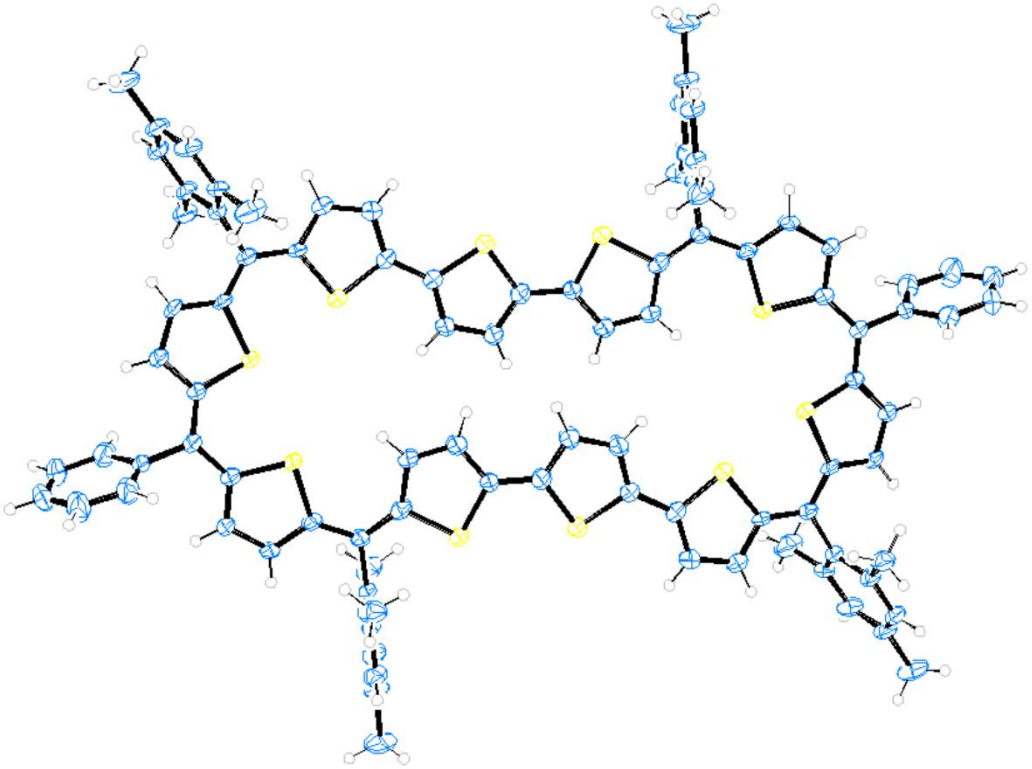


Figure S38. Thermal ellipsoidal plot of **15** with 50% ellipsoid probability using ORTEP.

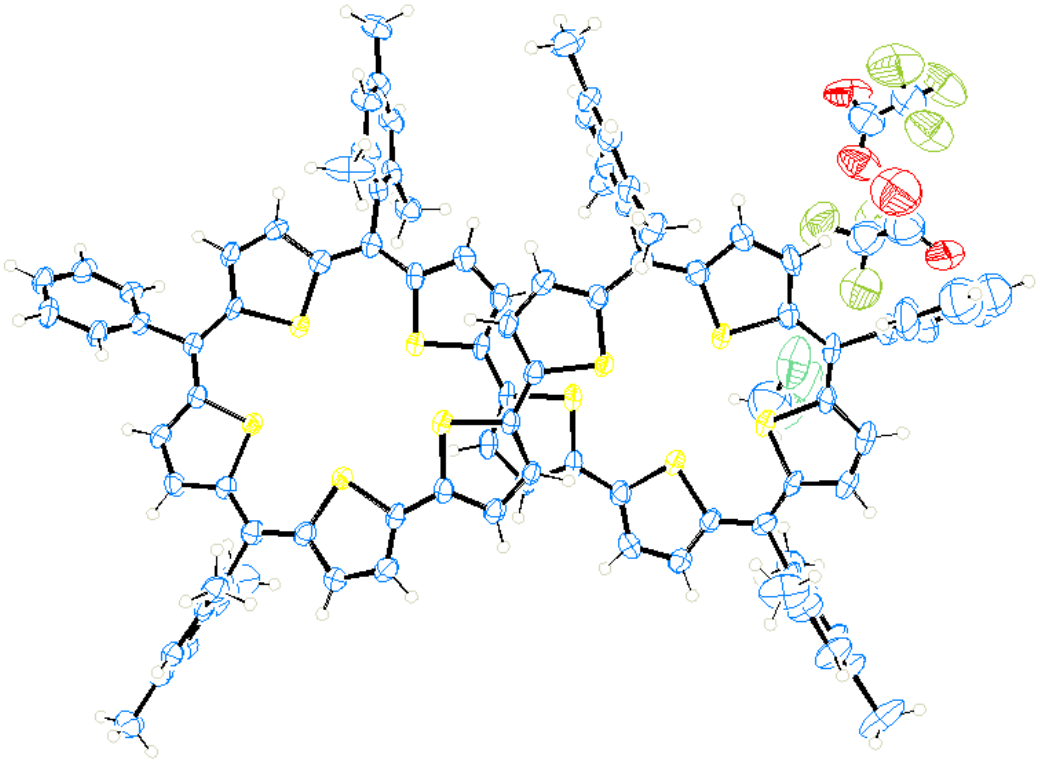


Figure S39. Thermal ellipsoidal plot of **[15]**$^{2+}$ with 50% ellipsoid probability using ORTEP.

Coordinates for optimized structure 11

Atom	X	Y	Z
S	-3.85868400	3.91165600	0.44201500
S	0.01309500	5.92025200	-0.16745600
S	-3.86756700	-3.88776800	-0.25576300
S	3.83825600	-3.89496200	0.11431300
S	-0.01032300	-6.03617500	-0.04373700
S	3.86594300	3.89528300	0.51345100
F	-7.07032000	6.47048000	1.99482300
F	-8.13943500	5.10121400	-2.41715700
F	-9.88243500	7.14922400	-2.62259500
F	-10.22922800	8.87017300	-0.53267700
F	-8.81243900	8.52049200	1.77265900
F	8.33845800	5.13608200	-2.11968500
F	6.92847300	6.40577500	2.22705700
F	8.68025300	8.45816900	2.18673900
F	8.34603700	-5.21420600	-2.21636300
F	10.08952600	7.18572000	-2.14185800
F	10.27120300	8.85899800	0.00671700
F	6.90532100	-6.37561300	2.14878100
F	-7.04573700	-6.38359600	-2.11376200
F	-8.25135400	-5.16396300	2.30612700
F	10.10873300	-7.25598700	-2.17025100
F	10.28016200	-8.87017700	0.02352700
F	8.66937500	-8.41935000	2.17919600
C	0.69299600	-3.55357800	-0.21357400
H	1.28893100	-2.65240100	-0.29901500
C	1.25367100	-4.81757200	-0.15274700
C	-7.63250000	0.69453300	-0.02769700
C	-7.54379100	5.71150600	-0.20181000
C	6.58524900	4.57117300	0.07356700
C	-5.17678000	4.98602000	-0.02490400
C	-1.25958500	4.86322100	0.42846300
C	-7.63857100	-0.67992400	-0.00042200
C	-6.56409600	4.58748900	-0.08072700
C	5.19571400	4.96914500	0.07887600
C	-0.71378600	-3.55126200	-0.17173600
H	-1.30879500	-2.64588600	-0.20196800
C	-8.28484100	5.92393200	-1.37035300
C	-2.65137300	5.16331700	0.21342300
C	-7.06325800	3.30084200	-0.05379800
C	8.74310800	1.56076600	0.13537700
H	9.75698300	1.18213200	0.20655700
C	-1.27501100	-4.81360800	-0.08190700
C	-8.47191800	-2.90591900	-0.02224700
H	-9.24934600	-3.65920300	-0.06220700
F	-10.01992400	-7.20014100	2.37822400
C	2.66706400	5.15077100	0.26068400
F	-8.81441700	-8.42186900	-2.02600500
C	2.65215100	-5.15597200	-0.16314100
F	-10.31156200	-8.84014500	0.21636000
C	7.57058600	5.69518200	0.05663200
C	-7.74544600	6.61622800	0.84828800
C	6.57428600	-4.59957400	-0.05628900
C	7.62990900	-0.70148900	-0.01060300

C	-9.18992600	6.97626000	-1.49125500
C	-2.67248300	-5.14774500	-0.01299400
C	3.28825800	-6.36765200	-0.37473700
H	2.74960500	-7.28766800	-0.57205100
C	7.56392000	-5.72167700	-0.03376700
C	-5.21036000	-4.98790600	0.04691200
C	7.68942400	6.57668000	1.13927700
C	-3.25785700	6.33993600	-0.19167900
H	-2.70259800	7.25125400	-0.38320700
C	-6.59491900	-4.58157800	0.04676400
C	-4.65655800	6.24246200	-0.32044400
H	-5.27975100	7.06874600	-0.63811600
C	-8.63975500	7.67847300	0.74797600
C	8.40129500	5.93344900	-1.04541900
C	-3.30207500	-6.35392600	0.24611100
H	-2.75824100	-7.27344800	0.43130900
C	-9.36580400	7.85763600	-0.42762000
C	1.27002100	4.85612900	0.44892000
C	8.45942200	2.89531800	0.16749500
H	9.23196000	3.64575300	0.28403200
C	4.68585900	6.22656100	-0.22581300
H	5.31886400	7.05229500	-0.52547300
C	-8.74467600	1.59194200	-0.05014800
H	-9.76415200	1.22174700	-0.05403700
C	7.62982600	0.67315800	0.01082800
C	8.73896800	-1.59578100	0.10343600
H	9.75285200	-1.22312700	0.20085600
C	3.28436300	6.32678600	-0.12902600
H	2.73546600	7.23983600	-0.33039100
C	0.70211800	3.75401400	1.06291000
H	1.29307000	2.97238300	1.52650500
C	-7.08546700	-3.29049200	0.02500200
C	-4.70691100	-6.26561700	0.27846600
H	-5.34658400	-7.11208900	0.49363300
C	-0.70778300	3.75788600	1.05145700
H	-1.31045600	2.97935800	1.50506700
C	7.07687400	3.28169600	0.06789600
C	8.58772200	7.64011400	1.13261000
C	8.40376300	-5.98452600	-1.12238400
C	5.18973100	-5.00185400	-0.11630700
C	-8.75593800	-1.57071700	-0.02939900
H	-9.77271400	-1.19488900	-0.06496400
C	7.06770500	-3.30982200	-0.03022200
C	-8.45302400	2.92518100	-0.05762100
H	-9.22665500	3.68340700	-0.05642400
C	-7.58739600	-5.70060400	0.09169300
C	7.67793800	-6.57141600	1.07334900
C	4.69361600	-6.28213900	-0.34911700
H	5.33999900	-7.13266900	-0.52475100
C	8.44979700	-2.92977300	0.09999000
H	9.21844600	-3.68525500	0.20895900
C	9.40314100	7.84512300	0.02153000
C	9.40688900	-7.86079100	0.00413500
C	-7.76164600	-6.56355900	-0.99717200
C	9.31165500	6.98772100	-1.07178500
C	8.58187000	-7.63012900	1.10287800
C	-8.36890900	-5.94753300	1.22635400

C	9.31994800	-7.03403400	-1.11302400
C	-9.28740900	-6.99379300	1.27817200
C	-9.43555200	-7.83374200	0.17737700
C	-8.66879600	-7.61946400	-0.96597000
Se	6.02420100	1.69283800	-0.09996000
Se	6.02520000	-1.71224100	-0.17620200
Se	-6.01535800	1.70141700	-0.03680700
Se	-6.03029300	-1.69605100	0.06996500

Coordinates for optimized structure [12]$^{2+}$

Atom	X	Y	Z
C	3.27779900	-3.85902900	0.36714000
C	3.39664200	-2.48128100	0.67547200
C	2.18878500	-1.85572700	0.91125300
C	1.06485000	-2.69998000	0.77760100
S	1.57445600	-4.32956000	0.39857800
C	-0.28956400	-2.30167000	0.87011700
C	-0.76220500	-1.01909500	1.20799600
C	-2.14066000	-0.89226900	1.13894800
C	-2.80403300	-2.06909000	0.75020500
S	-1.63678800	-3.36081200	0.48591400
C	-4.18922300	-2.25374300	0.54389300
C	-4.88247700	-3.45194400	0.29188400
C	-6.24390000	-3.28008500	0.12565800
C	-6.68099900	-1.93776300	0.22533200
S	-5.29541200	-0.88716700	0.53274100
C	4.27147700	-4.81678800	0.09187800
C	5.63845600	-4.52718200	-0.04770700
C	6.74314600	-5.38103700	-0.24402900
C	7.87708700	-4.58826400	-0.30840600
C	7.44986300	-3.25910500	-0.16786700
O	6.09340500	-3.23017500	-0.00709500
C	8.16525400	-2.05477700	-0.18739900
C	9.54634200	-1.80646600	-0.24422000
C	9.70796900	-0.43302300	-0.20254100
C	8.42349800	0.14469800	-0.13513800
O	7.49057800	-0.86848400	-0.12604300
C	8.01192400	1.48362700	-0.09225500
C	6.67338800	1.92377000	-0.20337400
C	6.22289100	3.24867700	-0.00838600
C	4.86476900	3.42692900	-0.20731500
C	4.19180400	2.25345600	-0.58735700
S	5.30722800	0.89644600	-0.64793100
C	2.81388700	2.08713800	-0.86903000
C	2.17338500	0.97797400	-1.44332800
C	0.79552400	1.11661900	-1.55481700
C	0.30485300	2.33938300	-1.06489800
S	1.63032800	3.32941100	-0.47524900
C	-1.05345700	2.73977900	-0.98619700
C	-2.17953200	1.95733200	-1.31703200
C	-3.39084600	2.58229200	-1.07844300
C	-3.26648300	3.89330800	-0.56472800
S	-1.55801300	4.30291100	-0.38847500
C	-8.01696500	-1.49682100	0.12018400
C	-8.41948000	-0.15303400	0.10563500

C	-9.69886600	0.43525800	0.15600200
C	-9.52652600	1.80848600	0.14367800
C	-8.14431500	2.04429800	0.07400200
O	-7.47919900	0.85114100	0.05191900
C	-4.26211100	4.83518700	-0.22787000
C	-7.42668600	3.24685800	0.02335000
C	-7.87026600	4.57561700	0.11204300
C	-6.74450200	5.37730700	0.04035500
C	-5.62756300	4.53017100	-0.10683200
O	-6.06769900	3.22526100	-0.11391600
C	3.88236300	-6.25163300	-0.06606000
C	-9.10212600	-2.51354200	0.02635700
C	-3.87542300	6.24946300	0.03365500
C	9.08575400	2.50135300	0.07892100
C	-9.34556700	-3.42293900	1.06594400
C	-10.36056400	-4.37207800	0.98916400
C	-11.16625800	-4.42702000	-0.14896400
C	-10.95084800	-3.53538900	-1.20046400
C	-9.92909600	-2.59519300	-1.10315700
C	-4.06592600	6.83710400	1.29331300
C	-3.70146500	8.15462600	1.55296200
C	-3.13337400	8.92266600	0.53570000
C	-2.93340700	8.36975600	-0.72979700
C	-3.30566900	7.05029000	-0.96808800
C	9.89987600	2.51882700	1.22106900
C	10.91078200	3.46052800	1.38981600
C	11.12837600	4.41972800	0.40000600
C	10.33569700	4.42996000	-0.74858200
C	9.33126200	3.47834400	-0.89756300
C	4.12288200	-7.18172600	0.95228900
C	3.76015900	-8.51976500	0.82333900
C	3.13960700	-8.95156600	-0.34952600
C	2.88769900	-8.04786500	-1.38215200
C	3.26382600	-6.71587400	-1.23301000
F	4.72097600	-6.78468300	2.08199800
F	3.01472400	-5.86267800	-2.23576400
F	2.29669200	-8.46088300	-2.50209100
F	2.78608700	-10.22398600	-0.48241400
F	3.99908600	-9.38195900	1.80885800
F	9.70716900	1.61518900	2.19063100
F	11.66098300	3.45346600	2.48916000
F	12.08871800	5.32175800	0.55027700
F	10.54732200	5.33993100	-1.69655700
F	8.59208300	3.50513800	-2.01320100
F	-4.60159700	6.11805700	2.28779200
F	-3.88524600	8.67960000	2.76241700
F	-2.78071000	10.17916500	0.77281500
F	-2.39902200	9.10557400	-1.70185900
F	-3.11555700	6.54737900	-2.19328900
F	-8.59208500	-3.38660100	2.17194200
F	-9.73941600	-1.75543000	-2.12927100
F	-11.71369700	-3.59093800	-2.28974600
F	-12.13668800	-5.32722500	-0.23091400
F	-10.56915300	-5.21786300	1.99546400
H	4.35207900	-1.98080900	0.73022000
H	2.10314000	-0.80520000	1.15853400
H	-0.10315300	-0.21192300	1.50122500

H	-2.66992200	0.02391800	1.37318600
H	-4.39196100	-4.41769900	0.25092700
H	-6.92837700	-4.09392700	-0.07350800
H	6.69661500	-6.45618400	-0.32650400
H	8.89637600	-4.91560000	-0.45342300
H	10.32306500	-2.55527000	-0.29965200
H	10.63862900	0.11264900	-0.23426200
H	6.89352700	4.04700200	0.28063800
H	4.36611500	4.38400500	-0.10599400
H	2.71587900	0.10461500	-1.78611100
H	0.15375500	0.36022400	-1.98886800
H	-2.09655600	0.95444600	-1.71691900
H	-4.35096700	2.12799300	-1.27772500
H	-10.63327100	-0.10170600	0.21340400
H	-10.29773700	2.56430000	0.17567900
H	-8.89577800	4.89639200	0.22367600
H	-6.71189200	6.45579200	0.06929400

Coordinates for optimized structure [15] with UCAM-B3LYP /6-31G(d, p)

Atom	X	Y	Z
S	-6.69830700	-2.26062000	-0.23113000
S	-7.76062600	0.55912300	0.13796000
S	-5.24031600	2.26285600	0.33736500
S	-2.14599400	-4.27698500	-0.22580000
S	1.17296000	-3.91856600	-0.30145400
C	-8.40484100	-2.63852600	-0.01283700
C	-9.44196800	-1.68914900	0.02832800
C	-9.92156400	1.97444600	-0.07038600
H	-10.58863500	2.82291100	-0.14864100
C	-8.95858600	5.12499300	-1.35787000
C	-8.54650700	-4.04303500	0.11133800
H	-9.51244000	-4.50398200	0.26704300
C	-9.12165200	5.25773600	1.06535000
C	-8.51402700	2.14629900	0.03226500
C	-8.65610400	4.60889100	-0.08849900
C	-7.37153300	-4.74887400	0.03526700
H	-7.30564100	-5.82599800	0.11648600
C	-10.33901900	0.66643200	-0.07269900
H	-11.37523800	0.36850000	-0.15820600
C	-6.21145200	-3.94958100	-0.15339100
C	-9.72344000	6.28539800	-1.45056800
H	-9.95866200	6.68161100	-2.43506000
C	-10.84098700	-2.21983400	0.07624800
C	-10.19331900	6.94709800	-0.31996400
C	-9.88434400	6.41506100	0.92845300
H	-10.24714900	6.91352300	1.82369800
C	-9.29763100	-0.28848200	0.02616500
C	-7.83224400	3.36031200	0.03529700
C	-4.89987500	-4.41138700	-0.22296100
C	-3.90546400	3.38003400	0.36256900
C	-8.81231100	4.71434900	2.43623200
H	-9.23417000	5.35461300	3.21348900
H	-7.73352100	4.64403200	2.60151100
H	-9.21995300	3.70773900	2.56678300
C	-6.41760600	3.54863600	0.13644000

C	-4.56152700	-6.73384100	-1.12428000
C	-4.67339300	-5.87970900	-0.01469000
C	-11.62927800	-2.04365500	1.21561800
H	-11.21425100	-1.51976000	2.07055800
C	-4.33849600	-7.76080900	1.45320100
H	-4.24584900	-8.15736800	2.46088300
C	-4.22576900	-8.62463300	0.36880700
C	-8.47403600	4.43783600	-2.60833500
H	-7.38561500	4.33219100	-2.60761100
H	-8.76062100	5.00150100	-3.49839500
H	-8.89118800	3.43040400	-2.69590200
C	-4.33979500	-8.09119400	-0.91210000
H	-4.25130700	-8.74952900	-1.77250400
C	-12.92808100	-2.53564500	1.26103800
H	-13.52615500	-2.39456900	2.15556100
C	-5.75196500	4.77177000	0.09147600
H	-6.28249200	5.70735500	-0.02548000
C	-4.56391100	-6.39624200	1.28596900
C	2.56362500	-2.88836200	-0.52222500
C	-11.38282900	-2.89891400	-1.01730700
H	-10.77762800	-3.03689800	-1.90743300
C	-4.35842400	4.67515300	0.21422700
H	-3.69600200	5.53275500	0.20728300
C	-13.45805900	-3.20960300	0.16658900
H	-14.47251200	-3.59326300	0.20157000
C	-3.74863500	-3.59239600	-0.45720000
C	-1.36330000	-2.78178100	-0.64842400
C	-10.99099800	8.21854100	-0.44300300
H	-11.56636300	8.24048800	-1.37167800
H	-10.33510100	9.09585400	-0.44496000
H	-11.68728400	8.33492900	0.39103100
C	-4.68237800	-6.19837600	-2.52724100
H	-4.61566400	-7.00590900	-3.25894600
H	-3.89048800	-5.47656000	-2.74749300
H	-5.63487500	-5.68165400	-2.67504400
C	-4.68716600	-5.50025200	2.49142100
H	-4.49106100	-6.05696400	3.40990200
H	-5.68930900	-5.06780800	2.56488700
H	-3.98186600	-4.66618600	2.44348500
C	0.06771800	-2.61560500	-0.65484300
C	-3.62766500	-2.26545900	-0.85678700
H	-4.46854100	-1.63609400	-1.10821300
C	-12.68216500	-3.38970000	-0.97291700
H	-13.09010900	-3.91140200	-1.83267000
C	-2.30332500	-1.81881300	-0.95998900
H	-2.04104700	-0.81356000	-1.26552600
C	2.16349200	-1.61040700	-0.84667400
H	2.86176700	-0.80426800	-1.03785700
C	-4.01135600	-10.10117900	0.57291200
H	-4.96308100	-10.64333500	0.55741200
H	-3.53435500	-10.30559700	1.53422300
H	-3.38358400	-10.52522300	-0.21478000
C	0.76633100	-1.45706200	-0.92148700
H	0.28356600	-0.51990300	-1.16751900
S	6.69830200	2.26062000	0.23112900
S	7.76061900	-0.55913400	-0.13795200
S	5.24032000	-2.26285300	-0.33735600

S	2.14599500	4.27699500	0.22580700
S	-1.17296100	3.91857700	0.30144800
C	8.40483600	2.63852100	0.01282700
C	9.44196100	1.68914100	-0.02833800
C	9.92156100	-1.97445200	0.07039200
H	10.58863300	-2.82291600	0.14864600
C	8.95860400	-5.12499700	1.35787000
C	8.54650500	4.04302900	-0.11135500
H	9.51243800	4.50397300	-0.26706900
C	9.12162600	-5.25775300	-1.06535300
C	8.51402400	-2.14630700	-0.03225600
C	8.65610000	-4.60890100	0.08850100
C	7.37153300	4.74887100	-0.03528000
H	7.30564300	5.82599600	-0.11650500
C	10.33901300	-0.66643700	0.07270000
H	11.37523100	-0.36850300	0.15820300
C	6.21145100	3.94958300	0.15339700
C	9.72345800	-6.28540300	1.45056000
H	9.95869800	-6.68161100	2.43505000
C	10.84098000	2.21982500	-0.07626300
C	10.19331400	-6.94711000	0.31995100
C	9.88431800	-6.41507900	-0.92846400
H	10.24710400	-6.91354800	-1.82371300
C	9.29762300	0.28847500	-0.02616700
C	7.83224100	-3.36032000	-0.03528700
C	4.89987700	4.41139300	0.22297600
C	3.90546200	-3.38002400	-0.36255800
C	8.81225800	-4.71437400	-2.43623100
H	9.23410300	-5.35464200	-3.21349300
H	7.73346500	-4.64405900	-2.60149000
H	9.21989600	-3.70776400	-2.56679500
C	6.41760300	-3.54863900	-0.13643000
C	4.56153300	6.73385500	1.12427900
C	4.67339900	5.87971400	0.01469500
C	11.62926900	2.04364100	-1.21563400
H	11.21423900	1.51974300	-2.07057100
C	4.33852400	7.76080600	-1.45321100
H	4.24588900	8.15735900	-2.46089600
C	4.22579300	8.62463800	-0.36882400
C	8.47408300	-4.43783000	2.60834100
H	7.38566300	-4.33217600	2.60763600
H	8.76068000	-5.00149300	3.49839800
H	8.89124400	-3.43040100	2.69589500
C	4.33980800	8.09120700	0.91208700
H	4.25131800	8.74954900	1.77248700
C	12.92807100	2.53562900	-1.26105800
H	13.52614400	2.39455000	-2.15558200
C	5.75195700	-4.77177100	-0.09147200
H	6.28247900	-5.70735900	0.02547900
C	4.56392900	6.39623900	-1.28596800
C	-2.56362600	2.88837500	0.52224000
C	11.38282500	2.89891000	1.01728800
H	10.77762600	3.03689800	1.90741400
C	4.35841700	-4.67514600	-0.21422300
H	3.69599100	-5.53274500	-0.20728400
C	13.45805200	3.20959100	-0.16661300
H	14.47250600	3.59325000	-0.20159800

C	3.74863400	3.59240700	0.45721900
C	1.36329800	2.78179700	0.64844600
C	10.99099200	-8.21855500	0.44298200
H	11.56638300	-8.24049300	1.37164200
H	10.33509300	-9.09586500	0.44496800
H	11.68725600	-8.33495400	-0.39107000
C	4.68237400	6.19839900	2.52724400
H	4.61565900	7.00593800	3.25894300
H	3.89048100	5.47658700	2.74749700
H	5.63486900	5.68167500	2.67505600
C	4.68719700	5.50024100	-2.49141300
H	4.49110400	6.05694700	-3.40990000
H	5.68933900	5.06779300	-2.56486300
H	3.98189400	4.66617700	-2.44347900
C	-0.06772000	2.61562200	0.65486400
C	3.62766100	2.26547000	0.85681000
H	4.46853500	1.63610400	1.10823700
C	12.68216100	3.38969400	0.97289300
H	13.09010700	3.91140000	1.83264400
C	2.30332000	1.81882900	0.96001400
H	2.04103900	0.81357700	1.26555500
C	-2.16349400	1.61042300	0.84669700
H	-2.86176800	0.80428500	1.03788500
C	4.01139100	10.10118400	-0.57294000
H	4.96311900	10.64333400	-0.55743500
H	3.53440000	10.30559800	-1.53425800
H	3.38361400	10.52523700	0.21474300
C	-0.76633200	1.45708100	0.92151600
H	-0.28356700	0.51992400	1.16755700

Coordinates for optimized structure $[15]^{2+}$

Atom	X	Y	Z
S	-3.09167500	-0.85238300	2.38990500
S	6.71596100	0.92633000	0.73259100
S	6.02452700	-1.24512400	-1.38466400
S	1.18269400	0.20127300	2.51309300
S	-6.05920300	-1.18313800	1.52828000
S	3.10264300	-0.84489100	-2.38715100
S	-4.06336700	1.81056400	-2.02634400
S	4.03799900	1.85714800	1.98218000
S	-1.19314900	0.17780900	-2.45646100
S	-6.70373100	0.98259500	-0.62664100
C	8.68065800	-0.69959500	-0.60074400
C	4.45374300	-5.11982300	-4.28232200
C	-1.35772300	-0.92330500	2.66673300
C	-0.98207000	1.58821900	2.83565000
C	0.56265400	0.25072900	-2.57011600
C	0.06620700	2.51780400	2.82893400
C	8.68616600	2.73543100	1.04377000
C	4.41320800	-4.77443900	-2.91289100
C	12.09465200	-1.57994800	-2.00850600
C	7.05164600	4.74645400	2.34083200

C	-6.39411700	3.43548400	-1.99171900
C	4.48146300	-3.32550800	-2.50603400
C	7.76065800	-1.57553600	-1.16578200
C	-4.50702800	-3.32878300	2.45708800
C	8.04132300	-2.89277500	-1.65629600
C	1.35474700	-0.91986500	-2.57364300
C	10.73821400	-1.27036800	-1.93094100
C	-4.21156000	-5.75770500	1.82109600
C	-4.44340300	-4.79094100	2.82257000
C	9.22128900	1.55504600	0.31930400
C	7.60791700	4.88420500	3.63054100
C	6.95787700	-3.56210000	-2.15347900
C	1.32634000	1.94539600	2.66038200
C	-7.02321400	4.73199400	-2.43204800
C	7.21446600	2.51953800	1.32309100
C	4.28587500	-7.48483700	-3.67688500
C	0.98281400	1.58764900	-2.67747100
C	2.58454700	2.62487900	2.59756500
C	-0.56615600	0.26775000	2.68224900
C	-8.71308300	-0.58133200	0.58846000
C	-0.95805600	-2.24192500	2.85928100
C	6.41039300	3.44211100	1.93733500
C	4.39227600	-6.47072500	-4.63476100
C	-4.61553000	-5.18566900	4.16682600
C	10.91426300	-1.12453400	0.48150100
C	-2.01135700	-3.16417900	2.80944400
C	-0.05732000	2.50634400	-2.69219800
C	8.34922800	0.54170800	0.07797900
C	-8.63900300	2.64730800	-1.18562800
C	-4.56456400	-6.54732900	4.48047100
C	-7.43709500	4.88642400	-3.77336000
C	10.12916700	-1.03833100	-0.68394200
C	1.98430600	-3.16606800	-2.74095700
C	-3.26290900	-2.59752900	2.55666800
C	-4.16597700	-7.10790100	2.18380600
C	-8.01885000	6.09741100	-4.16005500
C	8.27410200	7.17563400	3.08922600
C	8.20963900	6.09792700	3.97797300
C	4.19414600	4.31187000	2.77945900
C	-6.98923600	-3.66605400	2.00769300
C	-4.34620200	-7.52612200	3.50565100
C	-7.22922800	2.49638300	-1.36825100
C	5.73030300	-2.83098600	-2.10347500
C	2.85939000	3.93814500	2.97223500
C	-8.35499600	0.57154100	-0.10105000
C	-9.23979400	1.62277300	-0.50832700
C	7.54929100	3.75900300	4.63955000
C	-2.57400500	2.60271300	-2.51319000
C	3.26419500	-2.59646000	-2.54843000
C	7.09261400	5.82249800	1.42864200
C	5.00371800	3.30871900	2.23925400
C	12.86050600	-1.67444000	-0.84454100
C	-8.19764000	7.15564200	-3.26337900
C	4.23849300	-7.11433500	-2.32986300
C	-1.33291100	1.92562700	-2.56945800
C	0.94214400	-2.25353300	-2.73615600
C	-7.18984900	5.78416600	-1.50537000

C	4.30590700	-5.77713400	-1.92511700
C	-4.14622400	4.32630000	-2.67883900
C	-5.72248800	-2.83853700	2.06351800
C	-4.83565200	-4.16998800	5.26568800
C	-2.81974800	3.95468700	-2.81653600
C	-8.08712700	-2.83487300	1.45093400
C	-3.99779200	-5.36222600	0.37624300
C	-5.00360900	3.29314900	-2.23296200
C	12.26629800	-1.44909300	0.39948600
C	7.70335300	7.01742000	1.82242200
C	4.57076700	-4.06719800	-5.36188200
C	-7.77076100	6.97825500	-1.94354100
C	-7.78075600	-1.54776400	1.14577300
C	-7.26965400	3.77695100	-4.78729400
C	4.24853200	-8.93632600	-4.08823300
C	-4.32723200	-8.99105900	3.86869300
C	-10.15938400	-0.88051000	0.77937400
C	8.95682700	8.46408800	3.47874200
C	6.47788600	5.71304900	0.05035900
C	-11.02870700	-0.95956700	-0.32454000
C	-6.75331700	5.64777000	-0.06359000
C	4.25663500	-5.43736800	-0.45188500
C	-12.88805900	-1.43829100	1.14559700
C	-10.67996600	-1.09527700	2.06989900
C	-12.38075600	-1.24209900	-0.14065300
C	-8.85474900	8.44157600	-3.70126700
C	-12.03510400	-1.36177200	2.24928900
H	-2.02240100	1.85998700	2.97252200
H	-0.08062700	3.58605000	2.93208500
H	9.24245200	2.90023300	1.98012300
H	8.84633500	3.65870900	0.46763400
H	12.55490500	-1.74075500	-2.97825500
H	9.03474200	-3.31680700	-1.59775600
H	10.14901800	-1.18093800	-2.83820700
H	10.25201200	1.52123800	-0.01232600
H	6.99531300	-4.56899200	-2.54844200
H	2.02728700	1.86333800	-2.76553400
H	0.06928700	-2.51784200	3.06875700
H	4.42881600	-6.73787000	-5.68801300
H	10.45404300	-0.96122500	1.45083100
H	-1.88814200	-4.22846000	2.96233600
H	0.09000100	3.57645500	-2.77000600
H	-9.16159300	3.52124800	-1.55210200
H	-4.69590300	-6.85090400	5.51620200
H	1.85646800	-4.23236700	-2.87369400
H	-3.98236100	-7.85194300	1.41251000
H	-8.34076700	6.21627000	-5.19157600
H	8.63529700	6.20503000	4.97265100
H	4.58789900	5.28858400	3.02895300
H	-7.25591400	-4.03756200	3.01003900
H	-6.84026100	-4.57737700	1.41082500
H	2.11210200	4.59412900	3.40235500
H	-10.29316500	1.60074800	-0.26345700
H	8.02203800	2.84376400	4.26597200
H	8.05579900	4.04049400	5.56533800
H	6.51525800	3.49787700	4.89041500
H	13.91584800	-1.92022400	-0.90641300

H	4.14754000	-7.88653400	-1.57011200
H	-0.09641400	-2.52916100	-2.88012900
H	-4.52122600	5.32103400	-2.88091000
H	-5.01837200	-4.66526100	6.22185100
H	-5.68991200	-3.51628800	5.05845000
H	-3.96417500	-3.51741100	5.38929900
H	-2.04221100	4.62851800	-3.15527800
H	-9.07287200	-3.24988100	1.27861300
H	-3.78042000	-6.23977500	-0.23710300
H	-4.87838900	-4.87016900	-0.05276000
H	-3.16373800	-4.66023700	0.26933400
H	12.85598500	-1.52980600	1.30716400
H	7.73024000	7.84781500	1.12101700
H	4.67510600	-4.53135000	-6.34496600
H	3.68862500	-3.41805200	-5.39353300
H	5.43864500	-3.41788100	-5.20477300
H	-7.89188400	7.79216500	-1.23300900
H	-7.73349300	2.84383700	-4.45019700
H	-7.72728600	4.05142500	-5.74015300
H	-6.21331700	3.55687700	-4.97856800
H	3.79361600	-9.56129200	-3.31534800
H	3.68568500	-9.07512300	-5.01580400
H	5.26111400	-9.31860300	-4.26458500
H	-3.91202100	-9.15068700	4.86780300
H	-5.34168800	-9.40784400	3.86943900
H	-3.73682000	-9.57371600	3.15640200
H	8.88792500	8.64467000	4.55494200
H	10.02260900	8.43596900	3.22135400
H	8.52029600	9.32189900	2.95986900
H	5.40856500	5.48093600	0.10370600
H	6.94150100	4.92016000	-0.54787900
H	6.59059500	6.65012200	-0.49952100
H	-10.63399900	-0.82483100	-1.32667000
H	-5.71931300	5.29695700	0.01866800
H	-7.37764500	4.93164400	0.48304800
H	-6.82449700	6.60688200	0.45423300
H	4.03686200	-6.32686900	0.14286600
H	3.49035400	-4.68676600	-0.23122600
H	5.21088700	-5.03162400	-0.09726000
H	-13.94246300	-1.65310900	1.28728000
H	-10.02267600	-1.02602900	2.93081200
H	-13.03675700	-1.31562400	-1.00225100
H	-8.48995500	9.29527200	-3.12365700
H	-9.94113800	8.39284200	-3.55926800
H	-8.67491000	8.64327800	-4.76071800
H	-12.42685800	-1.50648900	3.25113100

Coordinates for optimized structure $[10]^{2+}$

Atom	X	Y	Z
S	6.24808900	1.64958100	-0.07221400
F	6.96549000	6.18026100	2.25723200
C	7.50024200	5.61990400	0.01828100
S	3.86673400	3.59536200	0.17132400
F	8.68000100	8.27273700	2.23261700
C	7.66588300	6.43488000	1.14486000
S	6.24814200	-1.65237600	-0.00239200
F	10.11976200	8.83126200	-0.01396300
C	8.54232100	7.51689300	1.14516200
S	0.00105000	5.74549200	0.14755000
F	9.83852300	7.28291100	-2.23994700
C	9.28069500	7.80304400	-0.00364800
S	3.87196000	-3.62366700	-0.35813100
F	8.13216200	5.18366200	-2.22284200
C	9.13718600	7.00885000	-1.14184400
S	-3.85978200	3.60132100	-0.04280100
F	6.83936200	-6.41702300	-2.07541600
C	8.25321400	5.93329400	-1.11998100
S	-0.00109100	-5.71114800	0.08855900
F	8.53583500	-8.51433700	-1.91114200
C	6.55479200	4.45853500	0.03009600
S	-6.25743000	1.65331900	0.06698500
F	10.08807800	-8.84498400	0.30497800
C	7.13772100	3.17463400	0.00264900
S	-3.87475400	-3.62145000	-0.34783000
F	9.93536800	-7.06240600	2.36161500
C	7.72565200	0.70228900	-0.06956200
S	-6.25466900	-1.64825200	0.03981200
F	8.24806600	-4.95741500	2.20696900
C	8.84947200	1.55481900	-0.02502800
H	9.86646400	1.18335200	-0.00904100
F	-6.73618600	6.29701600	-2.20130600
C	8.52899300	2.89558600	0.02013600
H	9.26981000	3.68134500	0.07956300
F	-8.44700700	8.39052400	-2.24554300
C	5.17719000	4.77270400	0.06331600
F	-10.11150400	8.83841000	-0.13374200
C	2.63816100	4.85159900	0.13023200
F	-10.05970900	7.17677400	2.02661100
C	3.24290000	6.11875100	0.05463800
H	2.67224400	7.03946700	0.01585600
F	-8.35801400	5.07557200	2.07842100
C	4.62451200	6.07576100	0.01392600
H	5.24438200	6.95827700	-0.06837300
F	-8.33755400	-4.90593900	2.15331500
C	7.72393400	-0.70687300	-0.09281500
F	-10.02989900	-7.00688500	2.28650800
C	8.84485800	-1.56042600	-0.18169500
H	9.85950600	-1.18936100	-0.25421600
F	-10.10207400	-8.83384200	0.26483800
C	8.52332400	-2.90144000	-0.18461900
H	9.25996900	-3.68914400	-0.26798200
F	-8.46460000	-8.55031500	-1.89555800

C	7.13512400	-3.17932600	-0.08995300
F	-6.76353900	-6.45691600	-2.03987100
C	1.26439200	4.52118200	0.14887900
C	0.69395600	3.23635400	0.14747200
H	1.29381900	2.33392700	0.15027000
C	-0.69152200	3.23630400	0.13576600
H	-1.29158800	2.33400500	0.13698400
C	-1.26197800	4.52101300	0.13551000
C	6.55334800	-4.46172400	-0.03108000
C	5.17247700	-4.77252700	-0.03552400
C	2.63564900	-4.85035700	-0.12578200
C	3.23008000	-6.08785000	0.17278400
H	2.65334900	-6.98772300	0.35297600
C	4.61278200	-6.04639200	0.21746700
H	5.22592200	-6.90639500	0.45116100
C	-2.63594100	4.85124100	0.12404500
C	-3.24398500	6.11433300	0.23420500
H	-2.67618800	7.03021200	0.35091400
C	-4.62587800	6.07242400	0.20216900
H	-5.24913800	6.95111900	0.29978100
C	-5.17466100	4.77529500	0.05351600
C	7.49277800	-5.62159900	0.05989200
C	7.59227300	-6.55842900	-0.97782800
C	8.46065100	-7.64412900	-0.90641000
C	9.25717200	-7.81358100	0.22666700
C	9.18019900	-6.89861600	1.27737900
C	8.30512600	-5.81985100	1.18453200
C	1.26149800	-4.52886300	-0.22836800
C	0.69171400	-3.28818500	-0.55754900
H	1.29093500	-2.41803700	-0.79875800
C	-0.69552900	-3.28661600	-0.54972400
H	-1.29533300	-2.41482200	-0.78344100
C	-1.26454800	-4.52569400	-0.21321200
C	-6.55060600	4.46425500	-0.03015400
C	-7.13171100	3.18022000	-0.09636000
C	-7.71966000	0.70811800	-0.15425600
C	-8.82857500	1.56231700	-0.33105900
H	-9.83452600	1.19284800	-0.48599700
C	-8.50771200	2.90385900	-0.30078700
H	-9.23481700	3.69206700	-0.44208300
C	-2.63829100	-4.84392100	-0.09668000
C	-5.17477800	-4.76552700	-0.00445300
C	-4.61446900	-6.03405600	0.27241400
H	-5.22723600	-6.88963900	0.52302500
C	-3.23193900	-6.07608200	0.22589500
H	-2.65459400	-6.97225500	0.42187800
C	-7.49512800	5.62472300	-0.05910600
C	-7.54562200	6.49730000	-1.15367200
C	-8.41998300	7.58017800	-1.18926100
C	-9.27392800	7.80939400	-0.10983200
C	-9.24793300	6.95697400	0.99454000
C	-8.36483900	5.88064400	1.00886600
C	-7.71933600	-0.70188900	-0.15766500
C	-7.13512500	-3.17429200	-0.10699600
C	-8.51331400	-2.89639600	-0.29141300
H	-9.24348000	-3.68412500	-0.42033000
C	-8.83215300	-1.55448800	-0.32041400

H	-9.83991300	-1.18325800	-0.45845000
C	-6.55574300	-4.45739400	-0.02458900
C	-7.49714500	-5.61531100	0.05227400
C	-8.35475000	-5.78909200	1.14763500
C	-9.23284900	-6.86616300	1.22949200
C	-9.26855900	-7.80400300	0.19686400
C	-8.42782100	-7.65897000	-0.90733600
C	-7.55669300	-6.57500500	-0.96815000

Coordinates for optimized structure [10] with B3LYP /6-31G(d, p)

Atom	X	Y	Z
S	6.27826200	-1.64761200	0.03650400
F	7.05049400	-6.20311700	-2.15075100
C	7.52971200	-5.61684500	0.09618000
S	3.89679600	-3.60682500	-0.18249600
F	8.71235900	-8.33037400	-2.05568800
C	7.70856500	-6.45280500	-1.01221300
S	6.27581900	1.64599600	-0.03739300
F	10.08815900	-8.89124000	0.23294000
C	8.56056200	-7.55387700	-0.97736500
S	-0.00099000	-5.69618000	-0.05609200
F	9.78465400	-7.30473400	2.43233000
C	9.26518300	-7.84111800	0.18972300
S	3.89815300	3.61887000	0.26797600
F	8.12232500	-5.17934700	2.35139100
C	9.11078100	-7.02876400	1.31025500
S	-3.88628100	-3.61132900	0.04593800
F	7.03829700	6.26960300	2.06083400
C	8.24770400	-5.93645600	1.25390400
S	-0.00332900	5.63870400	-0.18177800
F	8.69159800	8.39878100	1.90123000
C	6.59764800	-4.44561500	0.04706600
S	-6.27847500	-1.65092700	-0.07744100
F	10.06800000	8.89368300	-0.40224400
C	7.17243400	-3.18688800	0.02732100
S	-3.89439000	3.61680500	0.35619900
F	9.77280700	7.23846000	-2.55172300
C	7.76884300	-0.69058900	0.00456500
S	-6.27740800	1.64568100	-0.01442000
F	8.11933300	5.11046000	-2.40682400
C	8.89792900	-1.56755800	-0.00483100
H	9.91518400	-1.19528700	-0.02400000
F	-6.89264000	-6.22948800	2.15387700
C	8.58107700	-2.89427000	0.00350600
H	9.32110500	-3.68361900	-0.01686900
F	-8.55565300	-8.35782000	2.15338000
C	5.19621800	-4.77781900	0.03966600
F	-10.08659900	-8.89820200	-0.03924700
C	2.65643700	-4.83755400	-0.03261200
F	-9.93899700	-7.28906100	-2.23837700
C	3.23940300	-6.08016400	0.15901300
H	2.66086100	-6.98887300	0.28133700
F	-8.27711800	-5.16229500	-2.25236900

C	4.64368000	-6.04768900	0.19882200
H	5.25032200	-6.92946700	0.35943000
F	-8.28732000	5.12499900	-2.12728500
C	7.76770000	0.69011400	-0.01474800
F	-9.94038300	7.25669000	-2.14010300
C	8.89618400	1.56786500	-0.01936300
H	9.91378800	1.19621600	-0.00749600
F	-10.07434000	8.90117400	0.03387300
C	8.57853500	2.89422500	-0.03334600
H	9.31813300	3.68417300	-0.02394400
F	-8.53709800	8.38982300	2.22904000
C	7.16949000	3.18565500	-0.04827200
F	-6.88315400	6.25621800	2.25814300
C	1.26608400	-4.47708500	-0.10143300
C	0.70731100	-3.21385600	-0.19654100
H	1.30429100	-2.30994300	-0.23643000
C	-0.70136000	-3.21407700	-0.23669100
H	-1.29630200	-2.31230100	-0.32487700
C	-1.26335300	-4.47746700	-0.17225700
C	6.59347900	4.44321500	-0.08032700
C	5.19090000	4.77366300	-0.05716600
C	2.65550900	4.84508300	0.09887800
C	3.23208100	6.07100700	-0.19165900
H	2.65090300	6.97529100	-0.33266700
C	4.63433600	6.03218300	-0.27645800
H	5.23662200	6.90202400	-0.50459300
C	-2.65553400	-4.83891400	-0.18332600
C	-3.24618700	-6.08021100	-0.35665800
H	-2.67344800	-6.98538500	-0.52393800
C	-4.65106400	-6.04800000	-0.32621200
H	-5.26494000	-6.92809400	-0.46783800
C	-5.19497500	-4.78014800	-0.12716500
C	7.52168800	5.61477000	-0.16645500
C	7.69604900	6.48622800	0.91542500
C	8.54385900	7.58878500	0.84726700
C	9.24896500	7.84229600	-0.32736000
C	9.09907700	6.99470800	-1.42208400
C	8.24029600	5.90117500	-1.33273500
C	1.26675200	4.50126200	0.24896700
C	0.71130600	3.31622600	0.69966200
H	1.31133100	2.47580000	1.02948600
C	-0.69870500	3.31492100	0.71138300
H	-1.29150300	2.47328300	1.05104800
C	-1.26387000	4.49882300	0.26991500
C	-6.59522200	-4.44949400	-0.05348200
C	-7.16808800	-3.19109300	0.00323400
C	-7.76343200	-0.69532600	0.06690700
C	-8.88803700	-1.57327800	0.15944400
H	-9.90146300	-1.20189300	0.25324000
C	-8.57144800	-2.89964700	0.12936500
H	-9.30667200	-3.68975100	0.20872500
C	-2.65576500	4.84088000	0.14611200
C	-5.19372400	4.76957100	0.05052800
C	-4.64264200	6.02534500	-0.19321100
H	-5.25034000	6.89335700	-0.41435900
C	-3.23846700	6.06431300	-0.14221300
H	-2.66063000	6.96699700	-0.30545400

C	-7.52766000	-5.62110700	-0.04833200
C	-7.62824600	-6.46848600	1.06139400
C	-8.47955000	-7.57049200	1.07480900
C	-9.26350300	-7.84727300	-0.04319700
C	-9.18855400	-7.02343700	-1.16343700
C	-8.32475600	-5.93026800	-1.15631400
C	-7.76307300	0.68531500	0.08899700
C	-7.17021900	3.18202300	0.10089600
C	-8.57413000	2.88630800	0.20691200
H	-9.31071100	3.67334600	0.30256200
C	-8.88920200	1.55932600	0.19875800
H	-9.90301900	1.18445500	0.27239700
C	-6.59744000	4.44125200	0.07843100
C	-7.52683400	5.61392300	0.06747700
C	-8.32792600	5.90890600	-1.04214500
C	-9.18761400	7.00510800	-1.06335200
C	-9.25508500	7.84733200	0.04350300
C	-8.46751100	7.58549300	1.16265000
C	-7.62035700	6.48050900	1.16376900

References

[1] (a) Sheldrick, G. M. Acta Crystallogr., *Sect. A: Found. Crystallogr*. 2008, **64**, 112-122. . (b) Sheldrick, G. M. SHELXL-97, Program for Crystal Structure Solution and Refinement; University of Göttingen: Göttingen, Germany, 1997, (c) L. J. Farrugia, *J. Appl. Cryst.* 1999**, 32**, 837-838.

[2] (a) Spek, A. L.; PLATON, A Multipurpose Crystallographic Tool, Utrecht, The Netherlands, 2005; b) V. Sluis, and A. L. Spek. *Acta Crystallogr., Sect. A: Found. Crystallogr.* 1990, **46**, 194-201.

[3] Frisch, M. J.; et al. Gaussian 09, revision B.01; Gaussian, Inc.: Wallingford, CT, 2009.

[4] (a) S. Yamanaka, M. Okumura, M. Nakano and K. Yamaguchi, *J. Mol. Struct.* 1994, **310**, 205-218. (b) D. Geuenich, K. Hess, F. Kohler and R. Herges, *Chem. Rev.,* 2005, **105**, 3758-3772.

[5] (a) B. J. J. Smeets, R. H. Meijer, J. Meuldijk, J. A. J. M. Vekemans, and L. A. Hulshof, *Organic Process Research & Development*, 2003, **7**, 10-16. (b) D. Wu, A. B. Descalzo, F. Weik, F. Emmerling, Z. Shen, X. Z. You, and K. Rurack *Angew.Chem.Int.Ed.,* 2008, **47**, 193-197.

[6] R. Satapathy, Y.H. Wu and H. C. Lin, *Chem. Commun.,* 2012, **48**, 5668-5670.

[7] M. D. Ambhore, A. K. Basavarajappa, V. G. Anand, *Chem. Commun.,* 2019**, 55**, 6763-6766.