Electronic Supplementary Information

Substituent Effects on Paratropicity and Diatropicity in π-Extended Hexapyrrolohexaazacoronene

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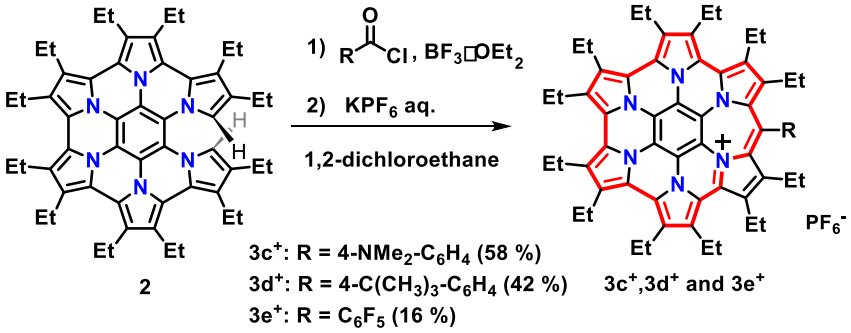
S1. Materials and methods

General: All reagents and solvents were of commercial reagent grade and were used without further purification except where noted. Unless otherwise noted, all reactions were performed with dry solvents under an atmosphere of nitrogen in dried glassware with standard vacuum-line techniques. All workup and purification procedures were carried out with reagent-grade solvents in air. TLC analyses were performed on commercial aluminum oxide 60 F_{254}, neutral (Merck). Alumina column chromatography was performed on activated alumina (about 200 mesh) purchased from FUJIFILM Wako Pure Chemical Corporation.

^{1}H,^{13}C, and ^{19}F NMR spectra were recorded on a BRUKER AV500 spectrometer (at 500, 125, and 471 MHz, respectively) with use of residual solvent for ^{1}H (2.09 and 5.32 ppm for acetone-d_6 and CD_2Cl_2, respectively) and ^{13}C (30.60 and 53.84 ppm for acetone-d_6 and CD_2Cl_2, respectively) and with use of hexafluorobenzene for ^{19}F (-162.0 ppm) as an internal standard. Cyclic voltammetry (CV) measurements were performed on CH Instruments-ALS612B electrochemical analyzer using a standard three-electrode cell under nitrogen atmosphere. The potentials were calibrated with ferrocene as an external standard. Fast-atom bombardment (FAB) mass spectra were measured on a JEOL JMS-700 instrument. LDI-TOF MS spectrum was measured on a JEOL JMS-S3000 at Ehime Institute of Industrial Technology. Melting points and decomposition points were determined on an SII Exstar 600 TG/DTA 6200 under nitrogen flow or a M-565 Büchi melting point apparatus. Absorption spectra were recorded on a JASCO V-570 spectrophotometer.

S2. Synthetic procedures



3c$^+$: R = 4-NMe_2-C_6H_4 (58 %)
3d$^+$: R = 4-$C(CH_3)_3$-C_6H_4 (42 %)
3e$^+$: R = C_6F_5 (16 %)

3c$^+$

To 4-(dimethlyamino)benzoyl chloride (102.7 mg, 0.56 mmol), was add BF_3·OEt_2 (0.1 mL, 0.79 mmol) and 1,2-dichloroethane (0.3 mL) at room temperature under Ar atmosphere. The reaction mixture was stirred for 3 h at 70 °C, and then a 1,2-dichloroethane (1.5 mL) solution of secoHPHAC **2** (61 mg, 0.077 mmol) was added. The reaction mixture was stirred for an additional 8 h at 100 °C. The reaction was quenched by addition of $NaHCO_3$ aq. and the aqueous phase was extracted with EtOAc. The combined organic layers were washed with $NaHCO_3$ aq. and KPF_6 aq., and the solvent was removed under reduced pressure. The residue was subjected to the alumina column chromatography (eluent: EtOAc) and then recrystallized from EtOAc and hexane to give **3c**$^+$ as green solid. (44.8 mg, 0.0484 mmol as PF_6 salt, 58%)

^{1}H NMR (500 MHz, acetone-d_6): δ 6.60 (d, 2H, J = 8.7 Hz), 6.54 (d, 2H, J = 8.7 Hz), 2.49 (s, 6H), 1.91–1.73 (m, 20H), 0.96–0.91 (m, 10H), 0.82–0.76 (m, 30H). **^{13}C NMR** (125 MHz, acetone-d_6): δ 156.82, 153.18, 146.21, 143.30, 133.39, 133.18, 132.28, 131.71, 127.42, 127.01, 125.98, 125.58, 123.44, 122.63, 120.88, 120.41, 120.21, 119.63, 119.29, 112.00, 40.05, 20.39, 18.20, 17.47, 17.38, 17.22, 17.06, 16.87, 15.93, 15.82, 15.64, 15.15, 13.69. **MS** (LDI-TOF): m/z: $[M]^+$ Calcd. for $C_{63}H_{70}N_7$: 924.5687; found: 924.5951, **mp**.: > 244°C (decomp.) This compound was further confirmed by X-ray crystallography.

3d$^+$

To 4-*tert*-butylbenzoyl chloride (0.1 mL, 0.55 mmol), was add BF_3·OEt_2 (0.1 mL, 0.79 mmol) at room temperature under Ar atmosphere. The reaction mixture was stirred for 4 h at 50 °C, and then a 1,2-dichloroethane (2.5 mL) solution of secoHPHAC **2** (87.2 mg, 0.11 mmol) was added. The reaction mixture was stirred for an additional 12 h at 90 °C. The reaction was quenched by addition of $NaHCO_3$ aq. and the aqueous phase was extracted with EtOAc. The combined organic layers were washed with $NaHCO_3$ aq. and $NaSbF_6$ aq., and the solvent was removed under reduced pressure. The residue was subjected to the alumina column chromatography (eluent: EtOAc) and then recrystallized from EtOAc and hexane to give **3d**$^+$ as blown solid. (50.2 mg, 0.046 mmol as PF_6 salt, 42%)

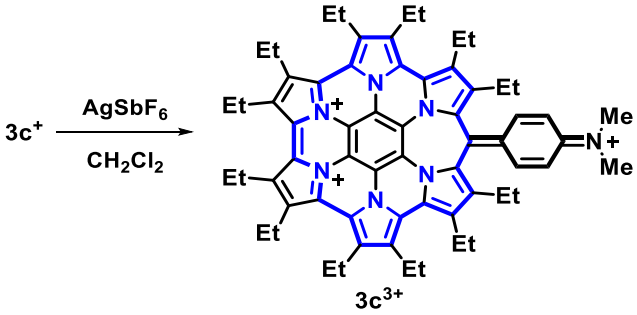
^{1}H NMR (500 MHz, acetone-d_6): δ 7.32 (d, 2H, J = 8.0 Hz), 6.85 (d, 2H, J = 8.0 Hz), 1.84–1.67 (m, 20H), 1.23 (s, 9H), 0.82–0.74 (m, 36H), 0.67–0.62 (m, 4H). **^{13}C NMR** (125 MHz, acetone-d_6): δ 156.25, 155.63, 144.06, 134.63, 133.71, 133.10, 132.32, 127.76, 127.63, 126.40, 126.20, 125.70, 123.86, 121.14, 121.00, 120.27, 119.93, 35.38, 19.94, 18.09, 17.28, 17.21, 17.05, 16.87, 16.56, 15.73, 15.68, 15.43, 15.01, 13.48. **MS** (LDI-TOF): m/z: $[M]^+$ Calcd. for $C_{65}H_{73}N_6^+$: 937.5891; found 937.6108, **mp**.: > 250 °C (decomp.) This compound was further confirmed by X-ray crystallography.

3e$^+$

To pentafluorobenzoyl chloride (0.1 mL, 0.72 mmol), was add $BF_3 \cdot OEt_2$ (0.1 mL, 0.79 mmol) at room temperature under Ar atmosphere. The reaction mixture was stirred for 1.5 h at 50 °C, and then a 1,2-dichloroethane (2.5 mL) solution of secoHPHAC **2** (123.9 mg, 0.16 mmol) was added. The reaction mixture was stirred for an additional 12 h at 90 °C. The reaction was quenched by addition of $NaHCO_3$ aq. and the aqueous phase was extracted with EtOAc. The combined organic layers were washed with $NaHCO_3$ aq. and KPF_6 aq., and the solvent was removed under reduced pressure. The residue was subjected to the alumina column chromatography (eluent: EtOAc) and then recrystallized from EtOAc and hexane to give **3e**$^+$ as red solid. (27.3 mg, 0.0244 mmol as PF_6 salt, 16%)

^{1}H NMR (500 MHz, acetone-d_6): δ 1.52–1.44 (m, 8H), 1.43–1.28 (m, 12H), 0.97–0.94 (m, 6H), 0.72–0.56 (m, 34H). **^{13}C NMR** (125 MHz, acetone-d_6): δ 153.90, 146.23, 135.76, 135.05, 133.62, 133.59, 129.89, 128.60, 128.56, 126.93, 126.89, 126.03, 126.01, 125.49, 124.37, 123.63, 123.17, 122.41, 121.39, 19.77, 17.76, 16.93, 16.77, 16.57, 16.37, 15.55, 15.20, 14.79, 14.32, 13.73, 12.57. **^{19}F NMR** (471 MHz, acetone-d_6): δ -137.70 (m, 2F), -146.39 (m, 1F), -157.87 (m, 2F). **MS** (FAB with 3-NBA matrix): *m*/*z*: $[M]^+$ Calcd. for $C_{61}H_{60}F_5N_6^+$: 971.4794; found 971.4819, **mp**.: > 250 °C (decomp.) This compound was further confirmed by X-ray crystallography.

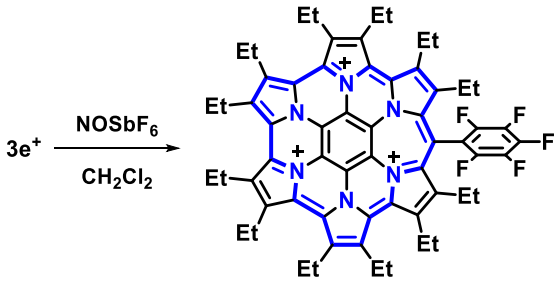
3c^{3+}



To a CH_2Cl_2 (1.0 mL) solution of **3c**$^+$[PF_6^-] (30 mg, 28.0 μmol), was added $AgSbF_6$ (30 mg, 87.3 μmol) at room temperature under air. The mixture was stirred for 10 min and then filtrated. Trication **3c**$^{3+}$ was obtained as indigo blue solid (43.4 mg, 26.6 μmol as SbF_6 salt, 95%) after removal of the solvent.

^{1}H NMR (500 MHz, acetone-d_6): δ 7.59 (d, 2H, J = 10.8 Hz), 7.37 (d, 2H, J = 10.8 Hz), 4.12–3.82 (m, 20H), 3.74 (s, 6H), 3.71–3.66 (m, 4H), 1.84–1.75 (m, 24H), 1.69–1.64 (m, 6H), 1.60–1.55 (m, 6H). **^{13}C NMR** (125 MHz, acetone-d_6): δ 158.45, 146.29, 145.58, 143.90, 143. 44, 141.94, 141.78, 141.59, 140.32, 140.02, 139.79, 139.41, 131.76, 130.32, 129.80, 128.47, 127.31, 125.09, 124.38, 122.23, 107.2, 103. 8, 92.58, 44.23, 22.80, 22.01, 21.91, 21.75, 21.71, 21.51, 21.33, 21.10, 21.05, 20.68, 19.61, 19.19, 18.98, 18.94, 18.59, 18.45, 18.07, 17.83. This compound was further confirmed by X-ray crystallography.

3e^{3+}



3e^{3+}

To a CH_2Cl_2 (1.0 mL) solution of **3e**$^{+}$[PF_6^-] (32 mg, 29.4 μmol), was added $NOSbF_6$ (30 mg, 112 μmol) at room temperature under air. The mixture was stirred for 10 min and then filtrated. Trication **3e**$^{3+}$ was obtained as indigo blue solid (49.4 mg, 29.4 μmol as SbF_6 salt, 100%) after removal of the solvent.

^{1}H NMR (500 MHz, CD_2Cl_2): δ 4.83–4.62 (m, 16H), 4.47–4.34 (m, 4H), 3.22–3.16 (m, 4H), 2.27–2.00 (m, 24H), 1.90–1.82 (m, 6H), 1.03–0.96 (m, 6H). **^{13}C NMR** (125 MHz, CD_2Cl_2): δ155.55, 149.96, 148.13, 148.04, 145.11, 143.58, 136.53, 132.14, 128.61, 127.62, 127.13, 123.30, 99.25, 98.05, 92.69, 29.69, 22.76, 22.55, 22.31, 21.91, 21.63, 21.11, 17.66, 17.56, 17.46, 17.31, 16.52, 15.69.

S3. ^{1}H-, ^{13}C- and ^{19}F-NMR spectra of $3c^{+}$, $3d^{+}$, $3e^{+}$, $3c^{3+}$ and $3e^{3+}$

$3c^{+}$

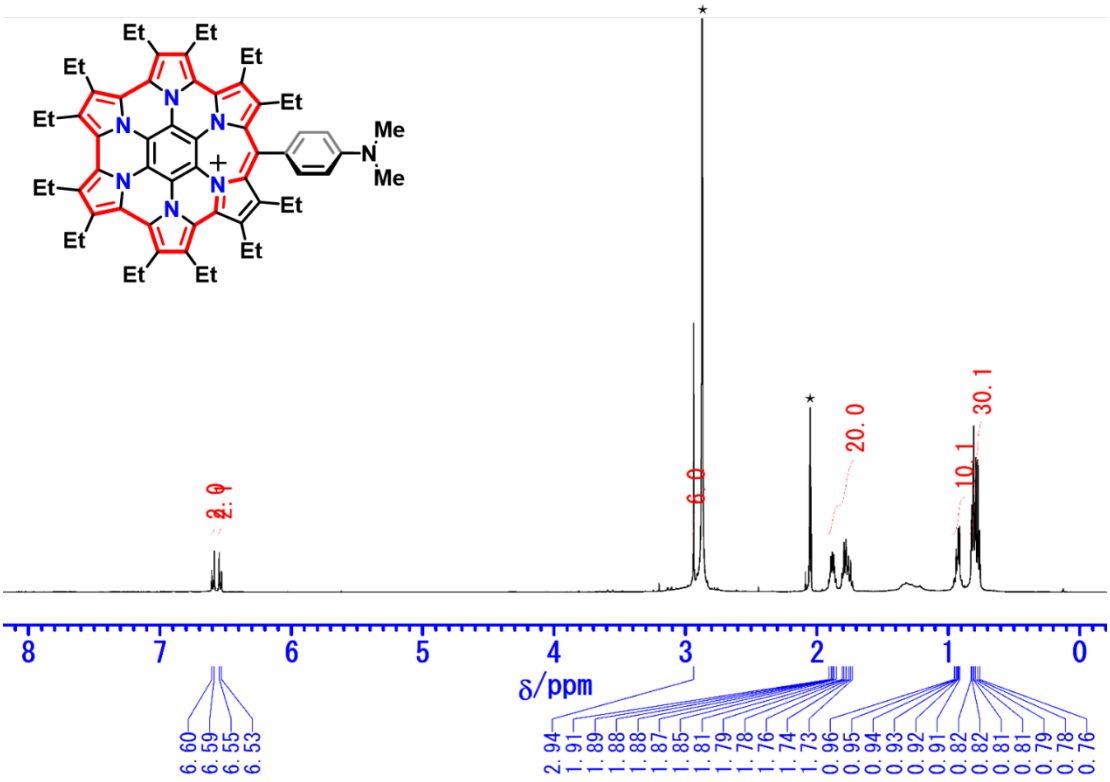


Figure S3a. ^{1}H-NMR spectrum of **$3c^{+}$** in acetone-d_6.

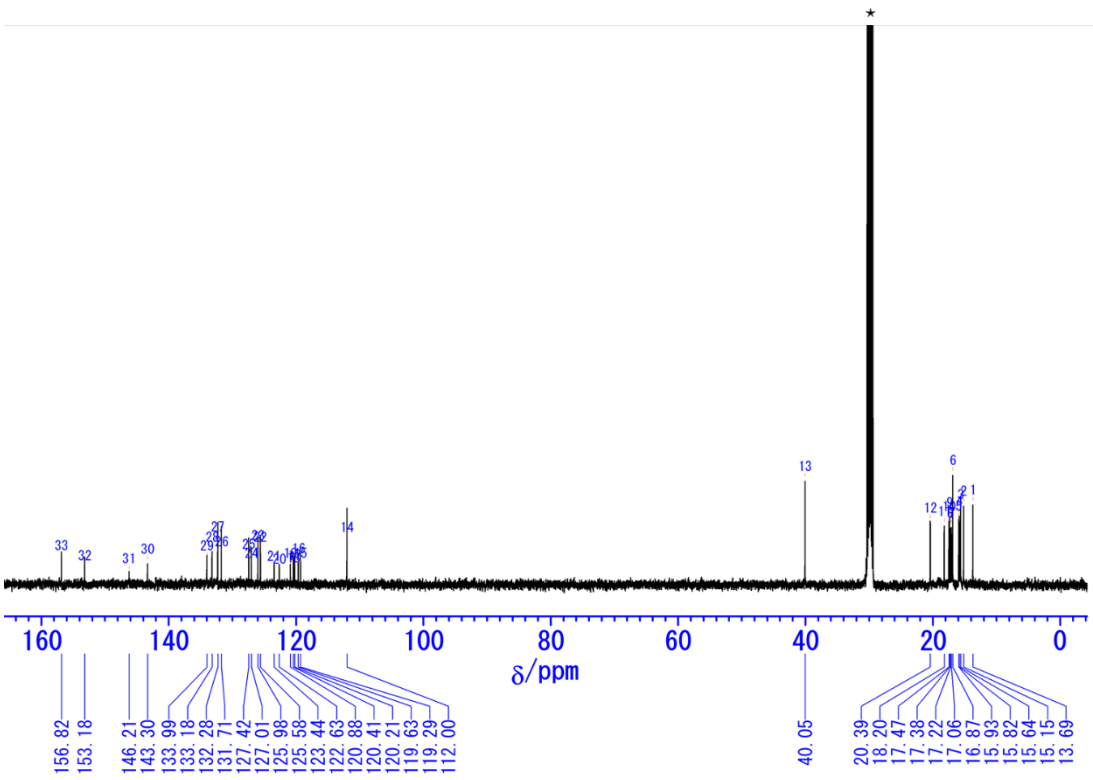


Figure S3b. ^{13}C-NMR spectrum of **$3c^{+}$** in acetone-d_6.

3d^{+}

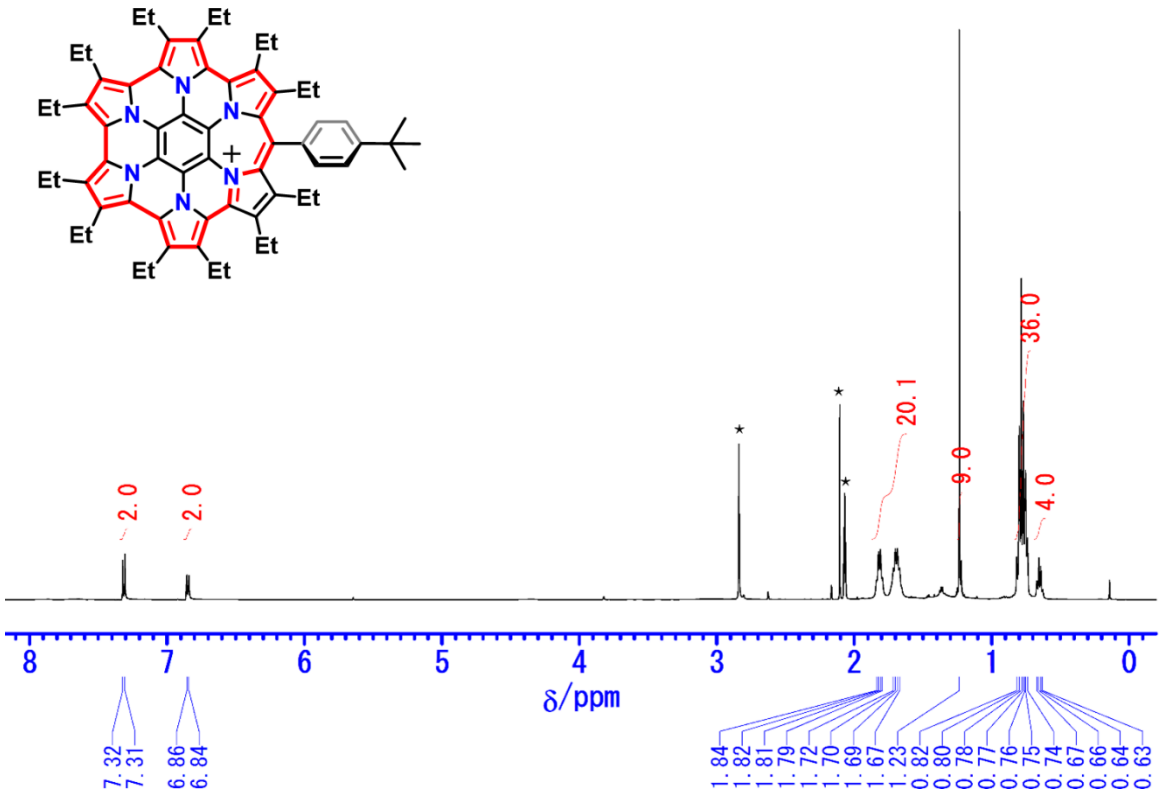


Figure S3c. ^{1}H-NMR spectrum of **3d**$^{+}$ in acetone-d_6.

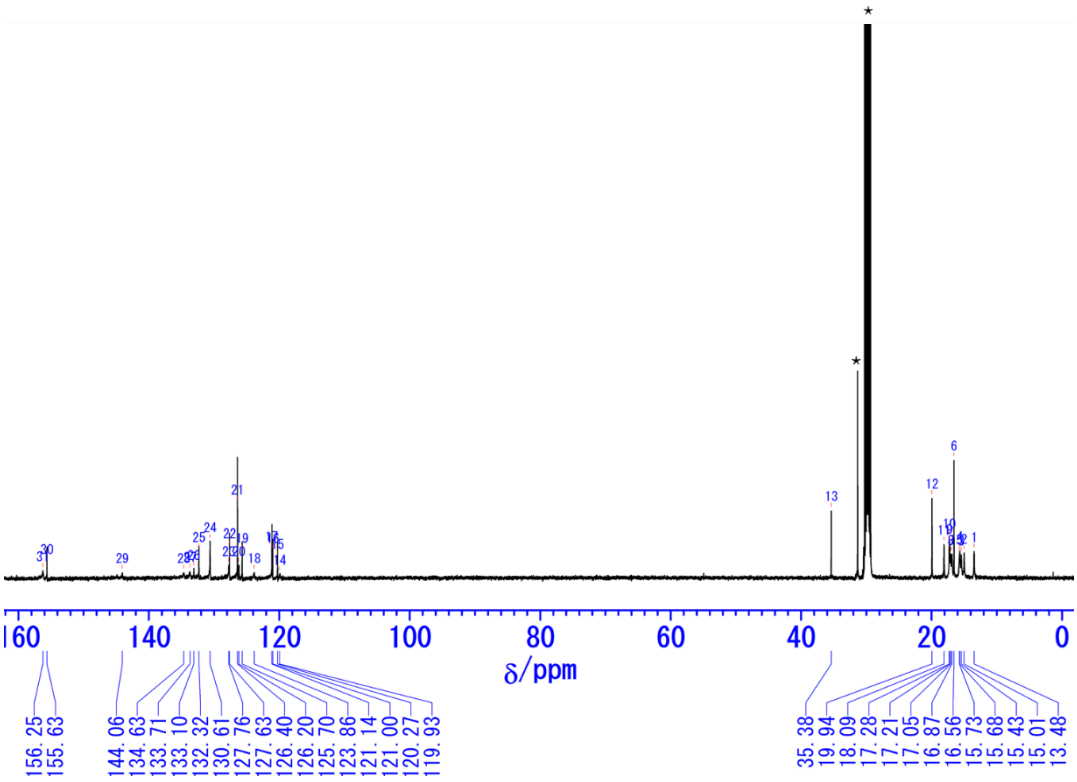


Figure S3d. ^{13}C-NMR spectrum of **3d**$^{+}$ in acetone-d_6.

3e$^+$

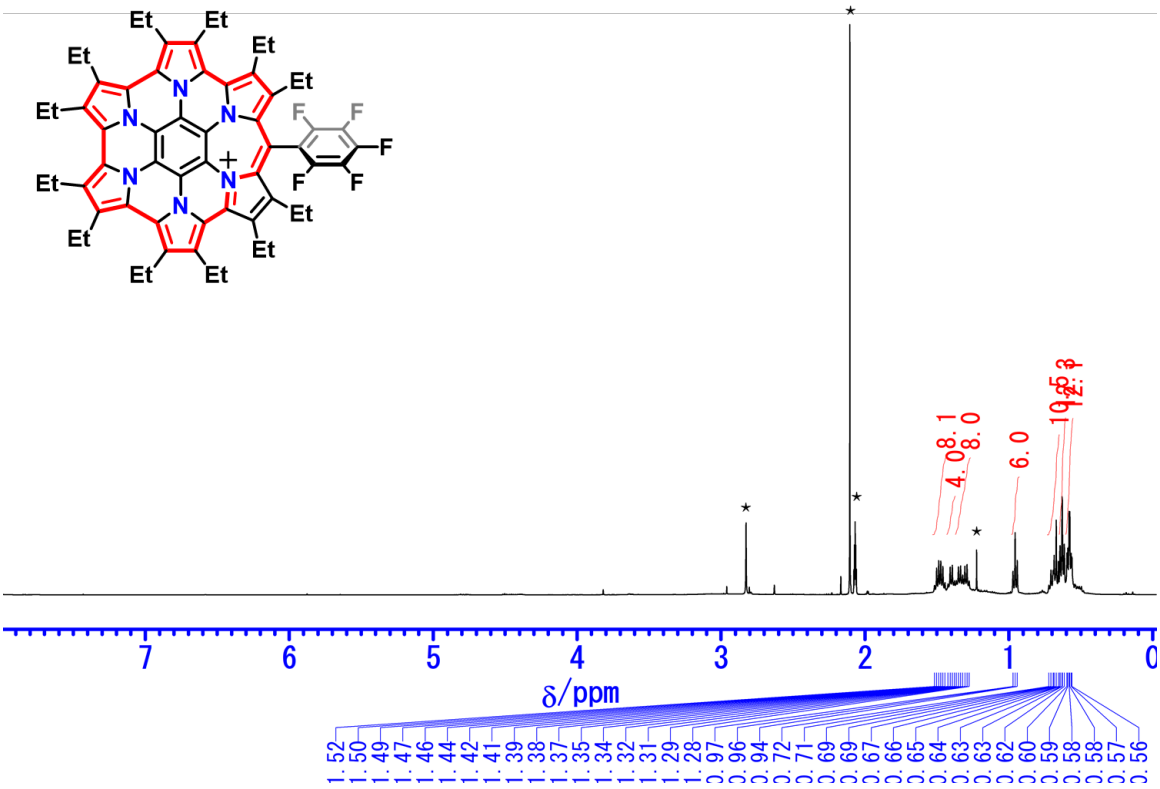


Figure S3e. ^{1}H-NMR spectrum of **3e**$^+$ in acetone-d_6.

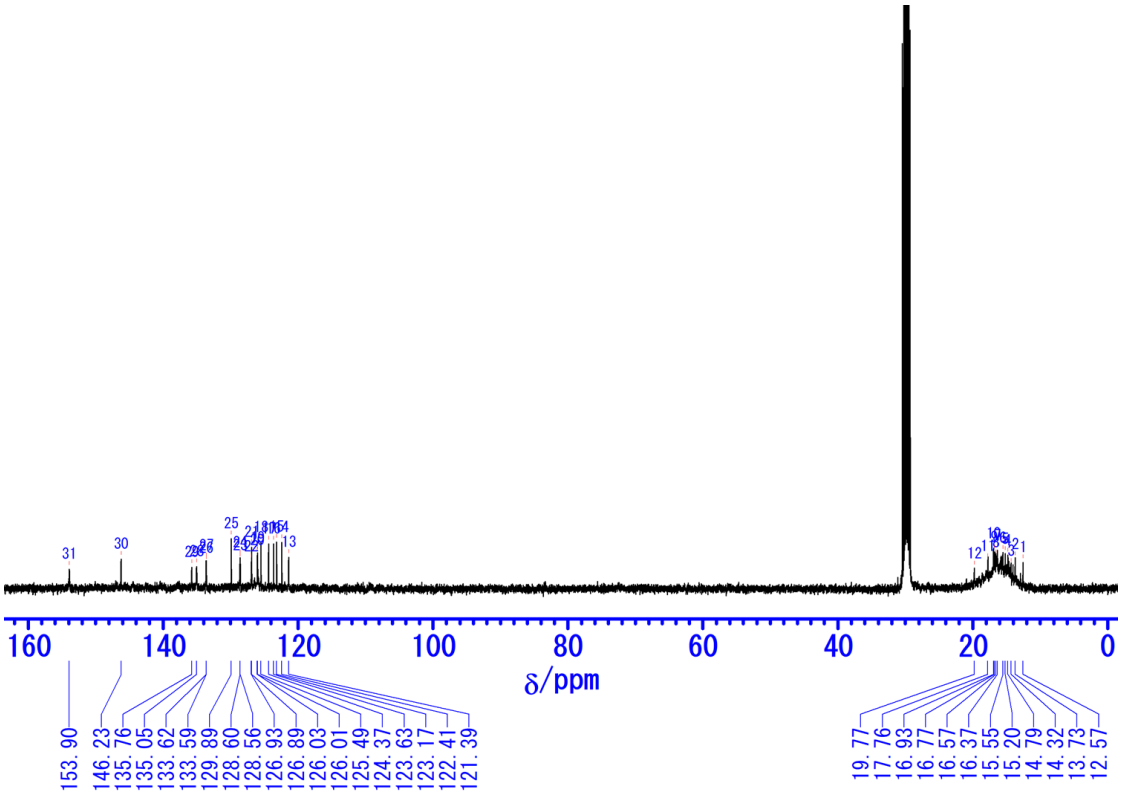


Figure S3f. ^{13}C-NMR spectrum of **3e**$^+$ in acetone-d_6.

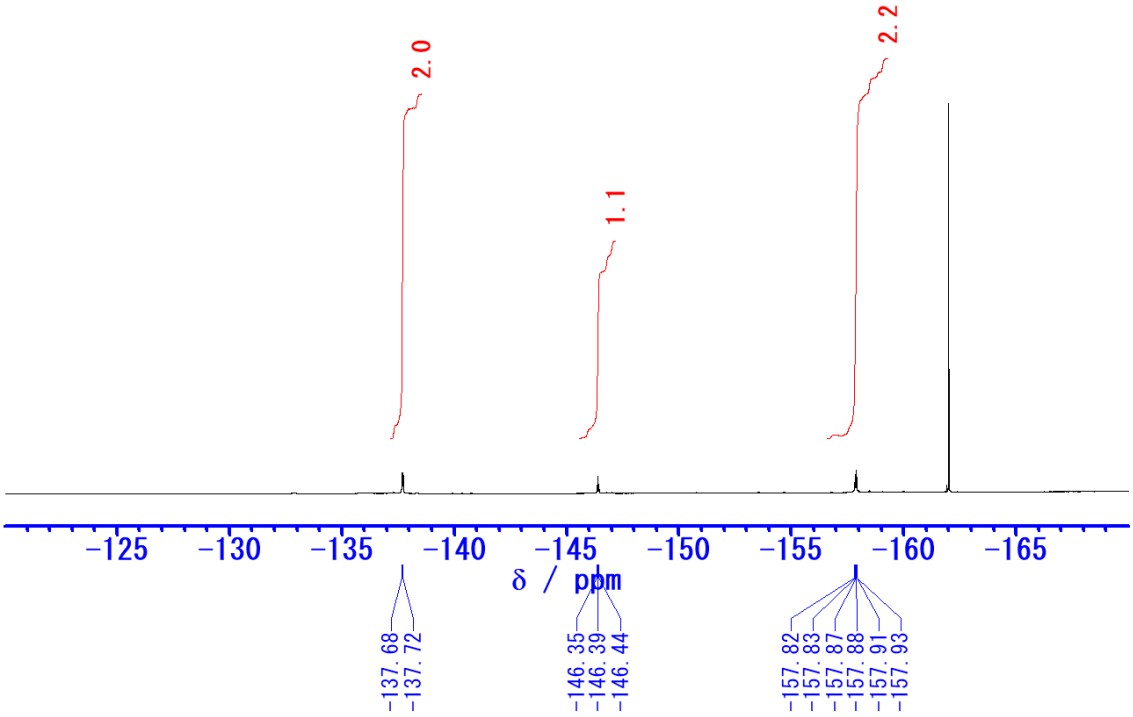


Figure S3g. ^{19}F-NMR spectrum of **3e**$^{+}$ in acetone-d_6.

3c^{3+}

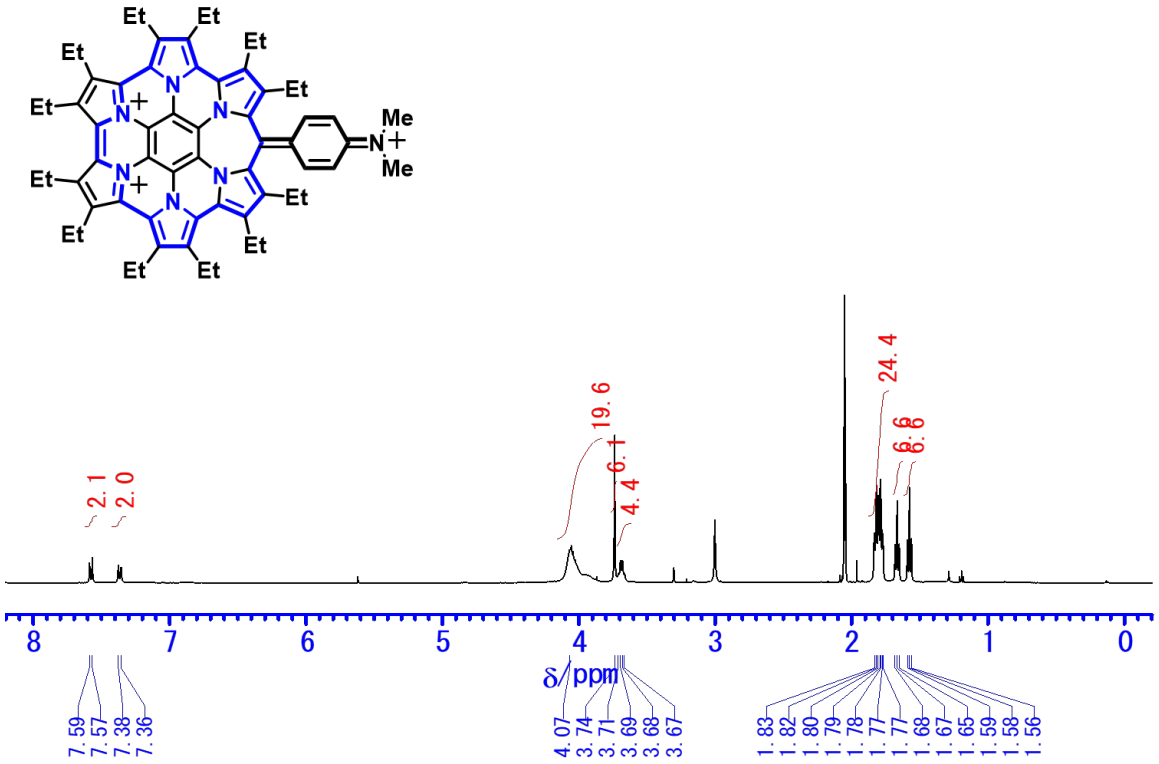


Figure S3h. ^{1}H-NMR spectrum of **3c**$^{3+}$ in acetone-d_6.

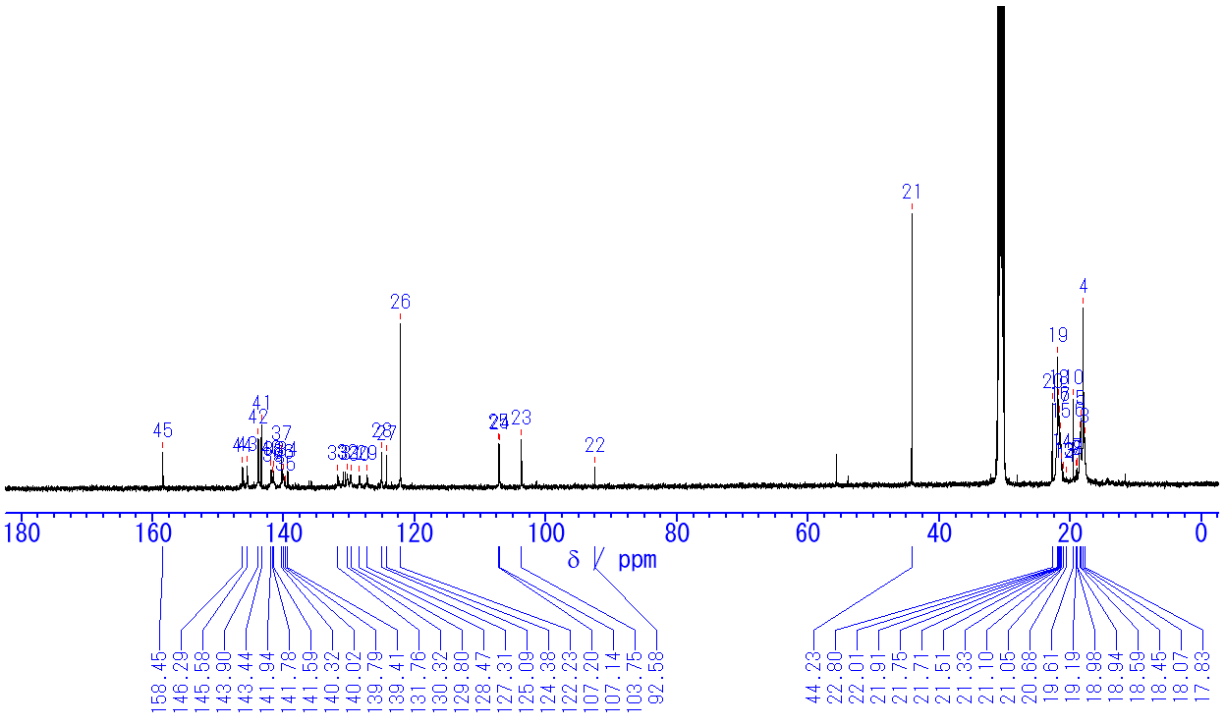


Figure S3i. ^{13}C-NMR spectrum of **3c**$^{3+}$ in acetone-d_6.

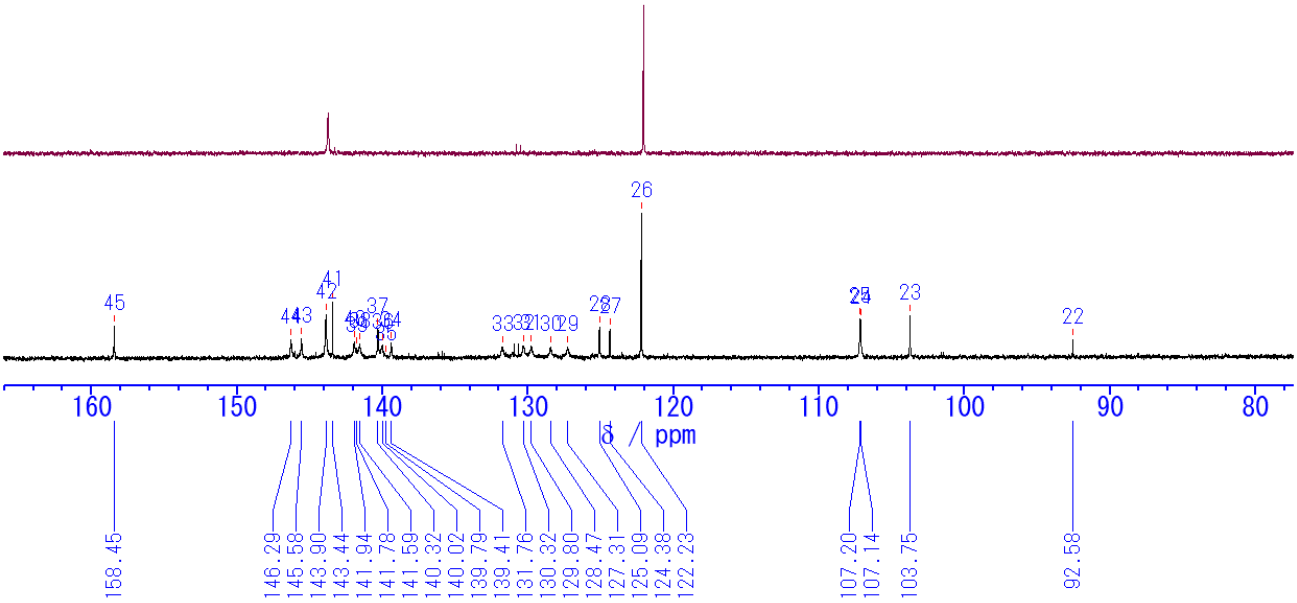


Figure S3j. DEPT 90 (upper) and ^{13}C-NMR (lower) spectra of **3c**$^{3+}$ in acetone-d_6.

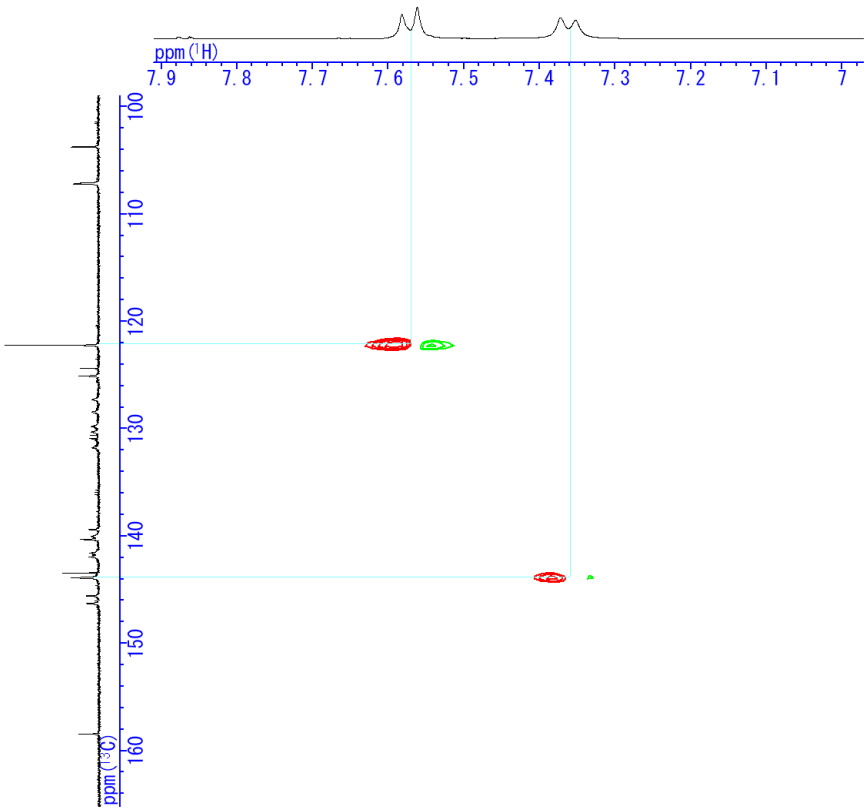


Figure S3k. HSQC spectrum of **3c**$^{3+}$ in acetone-d_6.

3e^{3+}

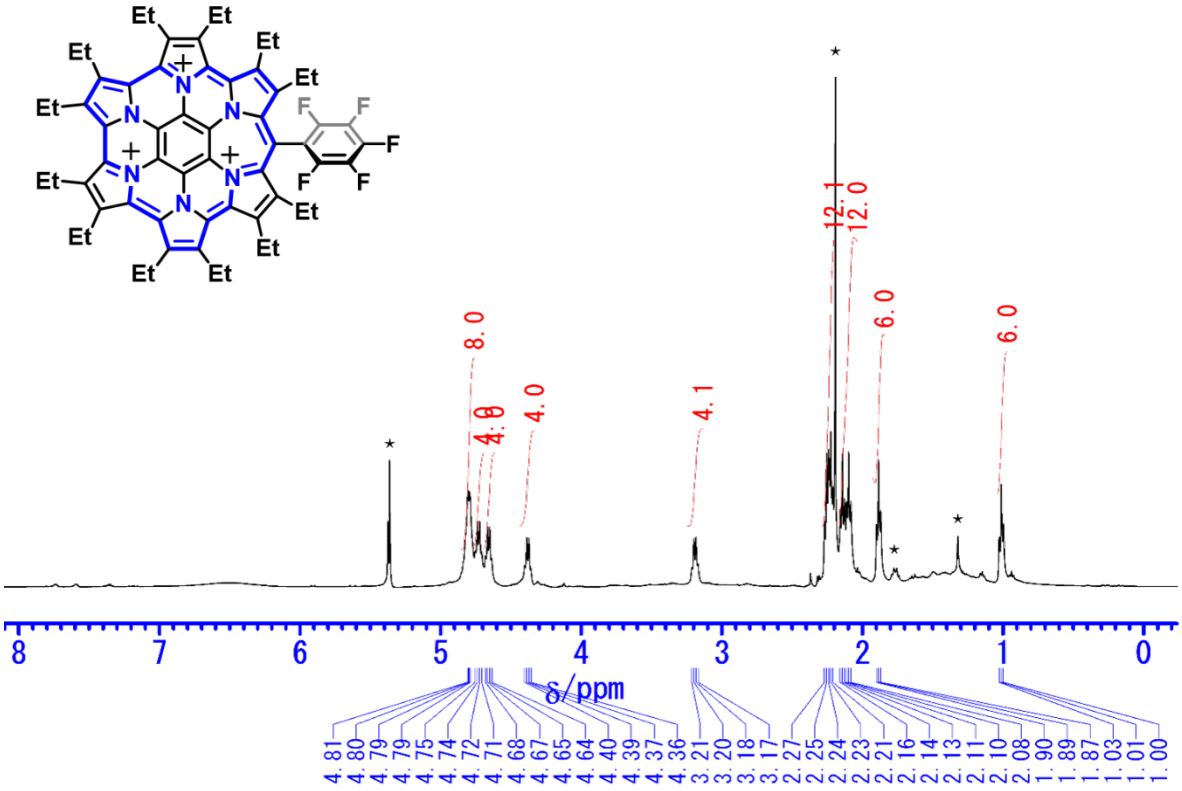


Figure S3l. ^{1}H-NMR spectrum of **3e**$^{3+}$ in CD_2Cl_2.

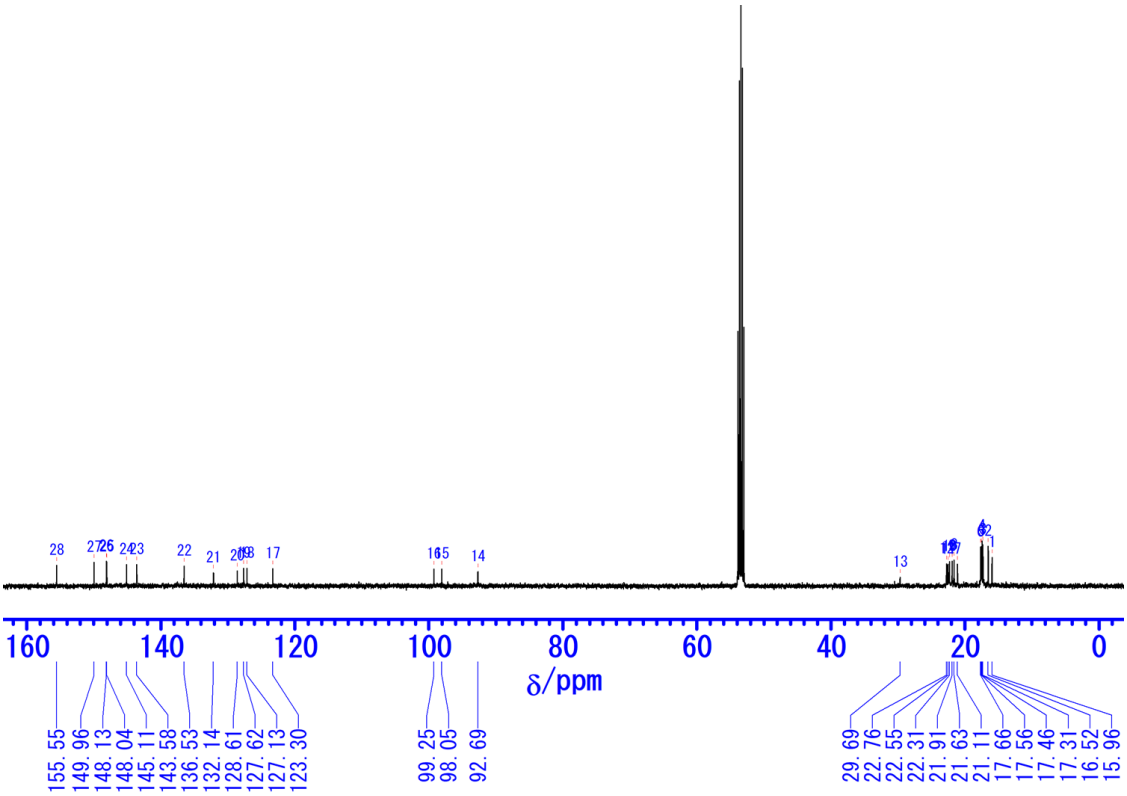


Figure S3m. ^{13}C-NMR spectrum of **3e**$^{3+}$ in CD_2Cl_2.

S4. COSY and NOESY spectra of $3c^+$, $3d^+$ and $3e^+$

$3c^+$

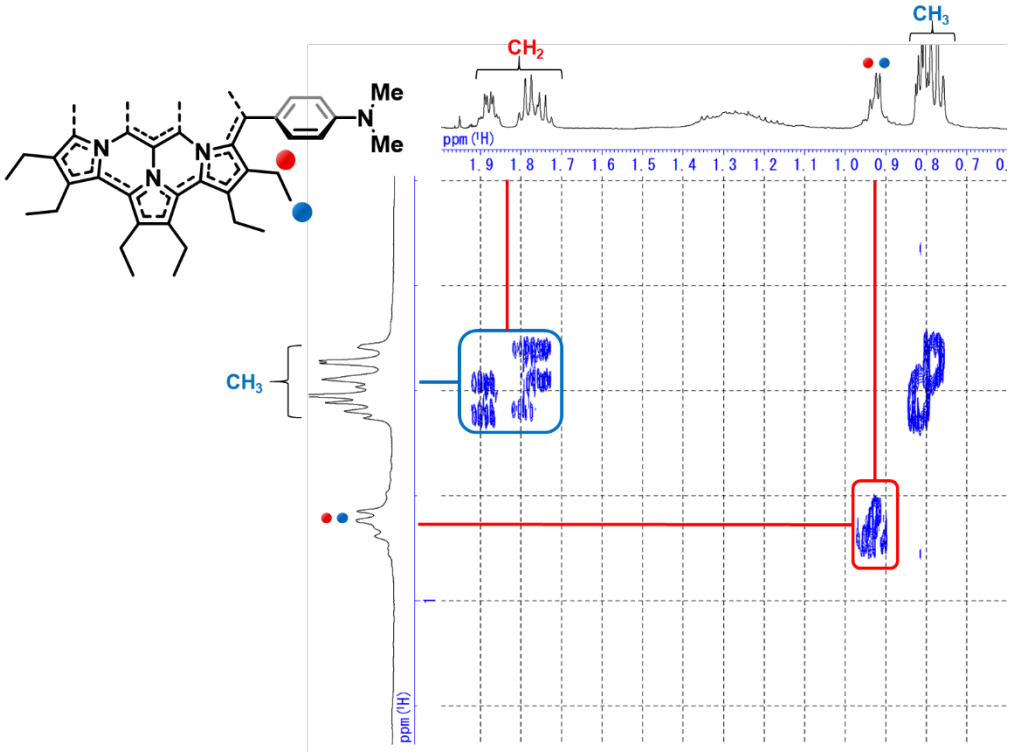


Figure S4a. ^{1}H-^{1}H COSY spectrum of **3c**$^+$ in acetone-d_6.

$3d^+$

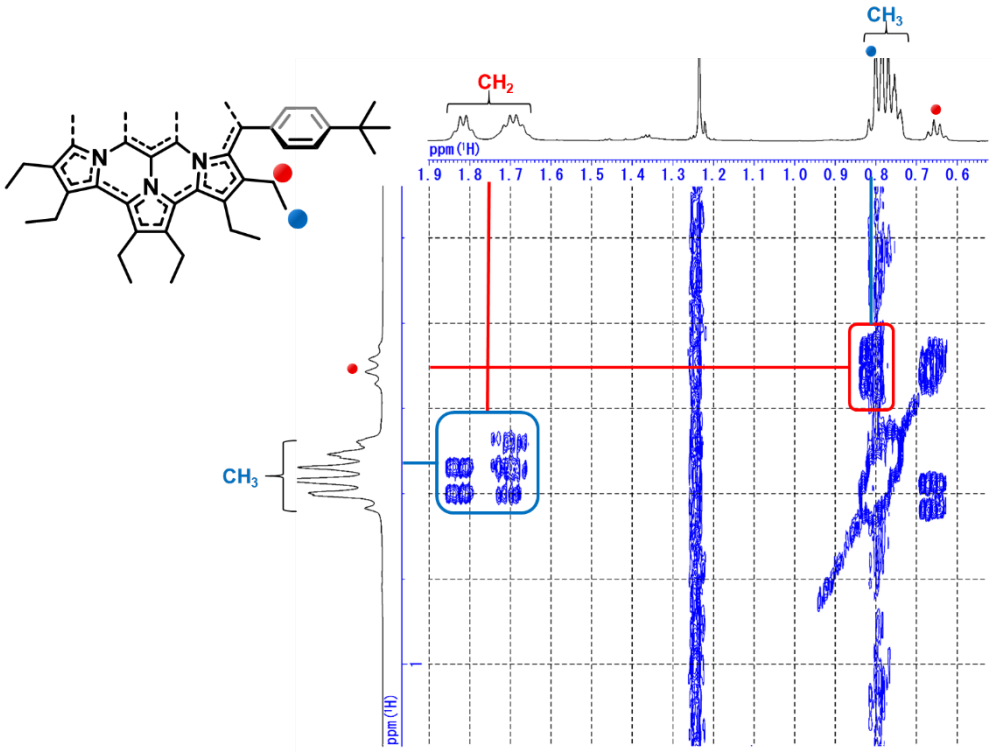


Figure S4b. ^{1}H-^{1}H COSY spectrum of **3d**$^+$ in acetone-d_6.

3e$^+$

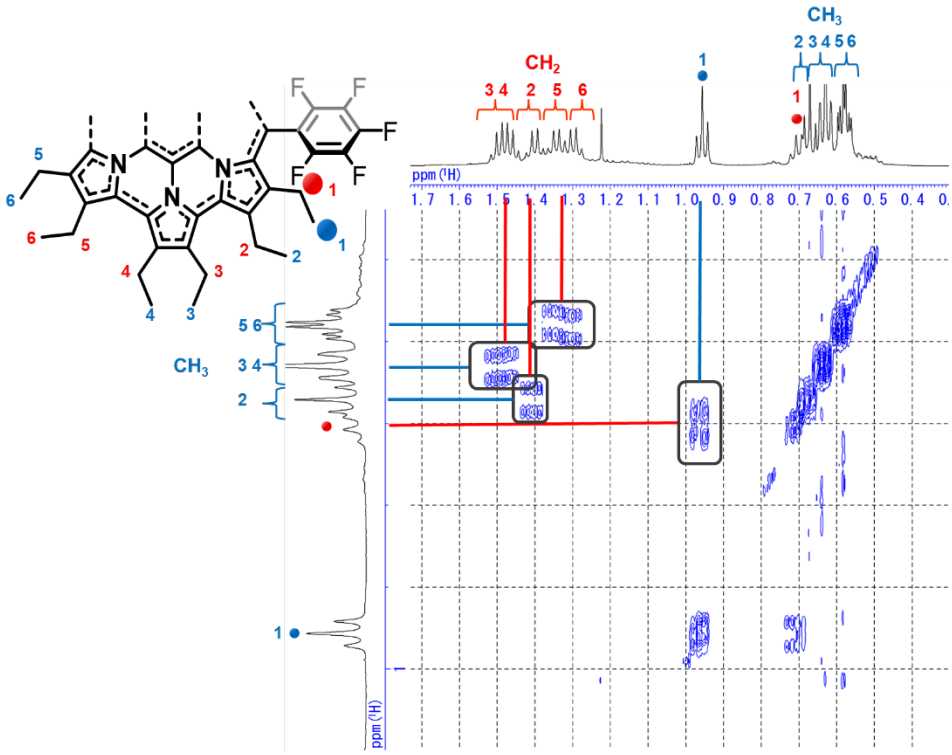


Figure S4c. ^{1}H-^{1}H COSY spectrum of **3e**$^+$ in acetone-d_6.

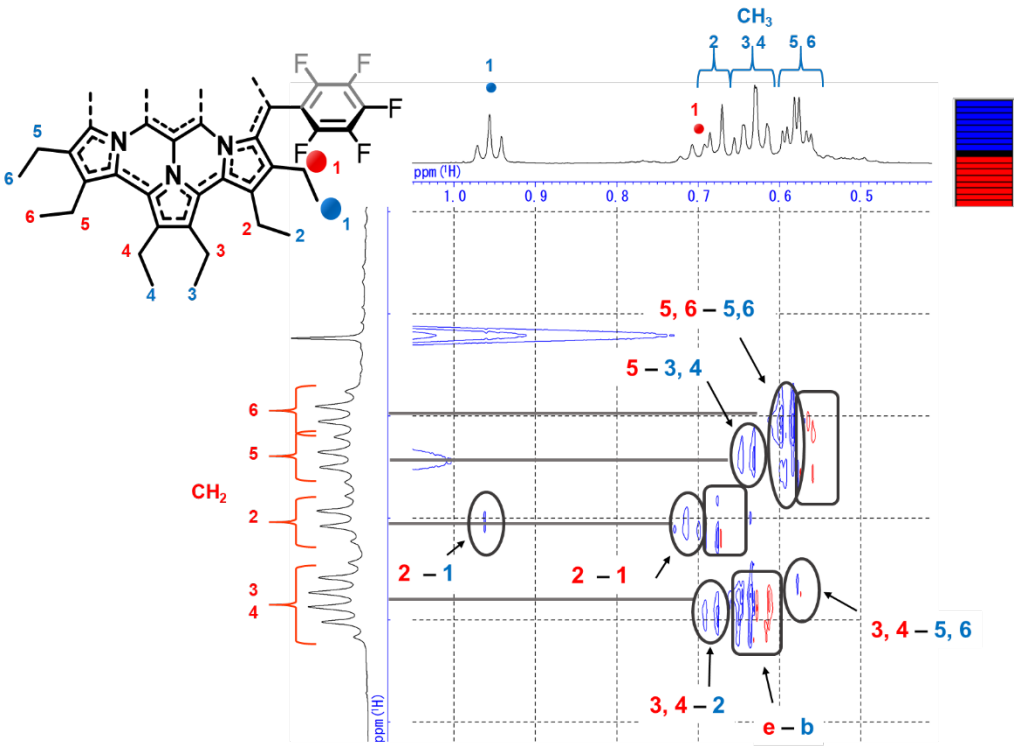


Figure S4d. ^{1}H-^{1}H NOESY spectrum of **3e**$^+$ in acetone-d_6.

S5. Mass spectra

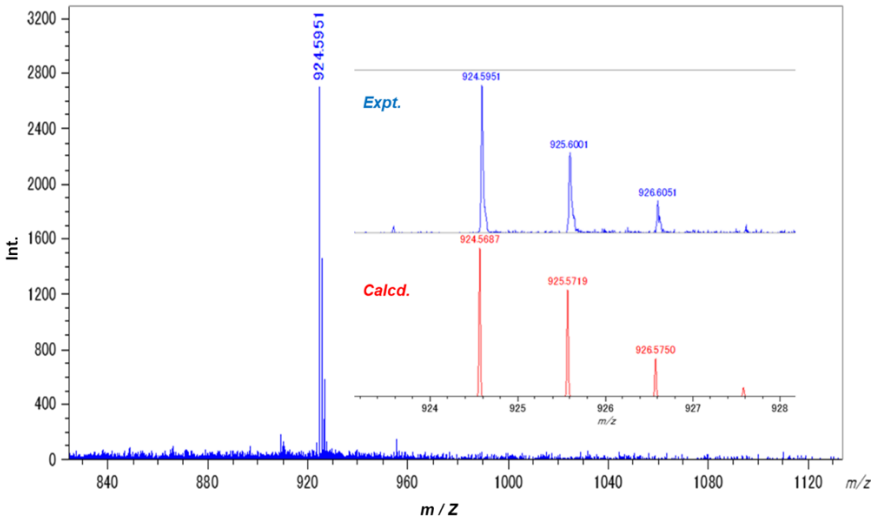


Figure S5a. LDI-TOF MS spectrum of **3c**$^{+}$.

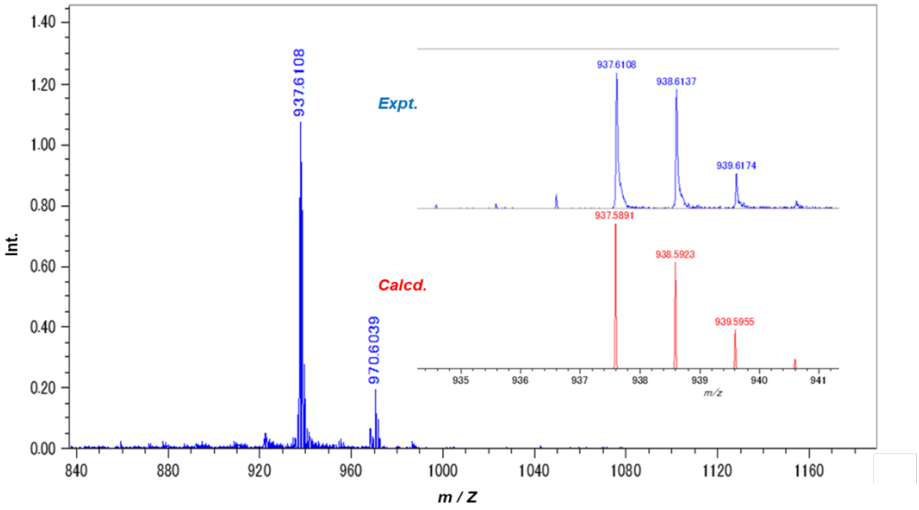


Figure S5b. LDI-TOF MS spectrum of **3d**$^{+}$.

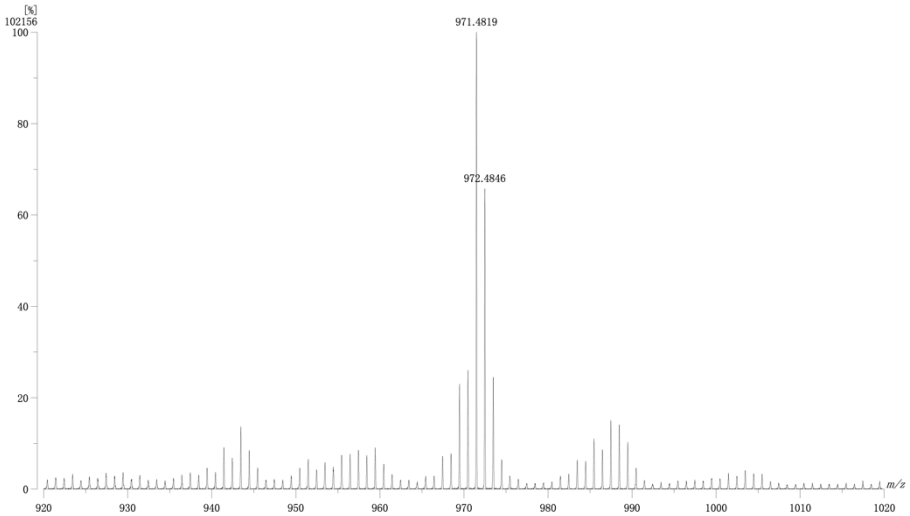


Figure S5c. FAB MS spectrum of **3e**$^{+}$.

S6. X–ray crystal structures and bond lengths

X-ray diffraction analysis was performed using a Rigaku VariMax with Saturn diffractometer using multilayer mirror monochromated Mo Kα radiation (λ=0.71073 Å) at 100 K. The crystals were mounted in cryoloops. Data collection was performed using CrystalClear software. Data reduction was performed using CrystalClear or CrysAlisPro software. The data were corrected for Lorentz polarization and absorption effects. The structures were solved using SHELXT 2014/5[1] or -2018/3[2] and expanded using the Fourier technique. All calculations were performed using Olex2[3] software. SHELXL-2018/3[2] were used for structure refinement. The data were validated using PLATON.

Table S6a. Crystallographic refinement data for **3c**$^+$, **3d**$^+$ **and 3e**$^+$.

	3c$^+$	**3d**$^+$ *	**3e**$^+$
Formula	$C_{63}H_{70}N_7 \cdot SbF_6 \cdot C_7H_8O \cdot 2CHCl_3$	$C_{65}H_{73}N_6 \cdot SbF_6 \cdot C_7H_8O$	$C_{61}H_{60}F_5N_6 \cdot SbF_6 \cdot 3C_7H_8O$
Formula weight	1507.88	1282.17	1532.30
Size	0.25 × 0.04 × 0.01	0.25 × 0.04 × 0.03	0.22 × 0.06 × 0.01
Radiation	Mo*Ka*	Mo*Ka*	Mo*Ka*
Temperature [K]	100	100	100
Crystal system	monoclinic	orthorhombic	monoclinic
Space group	$P2_1/c$ (#14)	*Fdd2* (#43)	$P2_1/n$ (#14)
a [Å]	15.9748(7)	43.9853(6)	19.1475(5)
b [Å]	12.9194(4)	47.1290(6)	13.0806(3)
c [Å]	34.5124(10)	13.0964(2)	28.6942(7)
a [°]	90	90	90
b [°]	101.007(4)	90	101.915(2)
g [°]	90	90	90
V [Å^3]	6991.8(4)	27148.6(7)	7031.9(3)
Z	4	16	4
ρ [g·cm^{-3}]	1.432	1.255	1.447
μ [mm^{-1}]	0.689	0.469	0.478
F(000)	3104	10688	3168
No. of reflections	132811 (Total)	131511 (Total)	132290 (Total)
measured	21689 (Unique)	20726 (Unique)	21665 (Unique)
R_{int}	0.1171	0.0852	0.0752
R_1 ($I > 2.00\sigma(I)$)	0.1194	0.0489	0.0840
wR_2 (All reflections)	0.3281	0.0948	0.2173
GOF	1.075	1.038	1.101
CCDC No.	2232453	2232452	2232451

***** The refinement was performed by using the Platon SQUEEZE program.

Table S6b. Crystallographic refinement data for $\mathbf{3c}^{3+}$.

	$\mathbf{3c}^{3+}$
Formula	$2C_{63}H_{70}N_7 \cdot 6SbF_6 \cdot 2C_7H_8O \cdot 5C_3H_6O$
Formula weight	3771.67
Size	0.17×0.08× 0.01
Radiation	Mo*Ka*
Temperature [K]	100
Crystal system	monoclinic
Space group	*C*2/*c* (#15)
a [Å]	55.5390(14)
b [Å]	8.6589(3)
c [Å]	32.5046(8)
a [°]	90
b [°]	90.397(2)
g [°]	90
V [Å^3]	15631.3(8)
Z	4
ρ [g·cm^{-3}]	1.603
μ [mm^{-1}]	1.125
F(000)	7600
No. of reflections measured	72644 (Total)
	22603 (Unique)
R_{int}	0.1198
R_1 ($I > 2.00\sigma(I)$)	0.0896
wR_2 (All reflections)	0.2449
GOF	1.027
CCDC No.	2232450

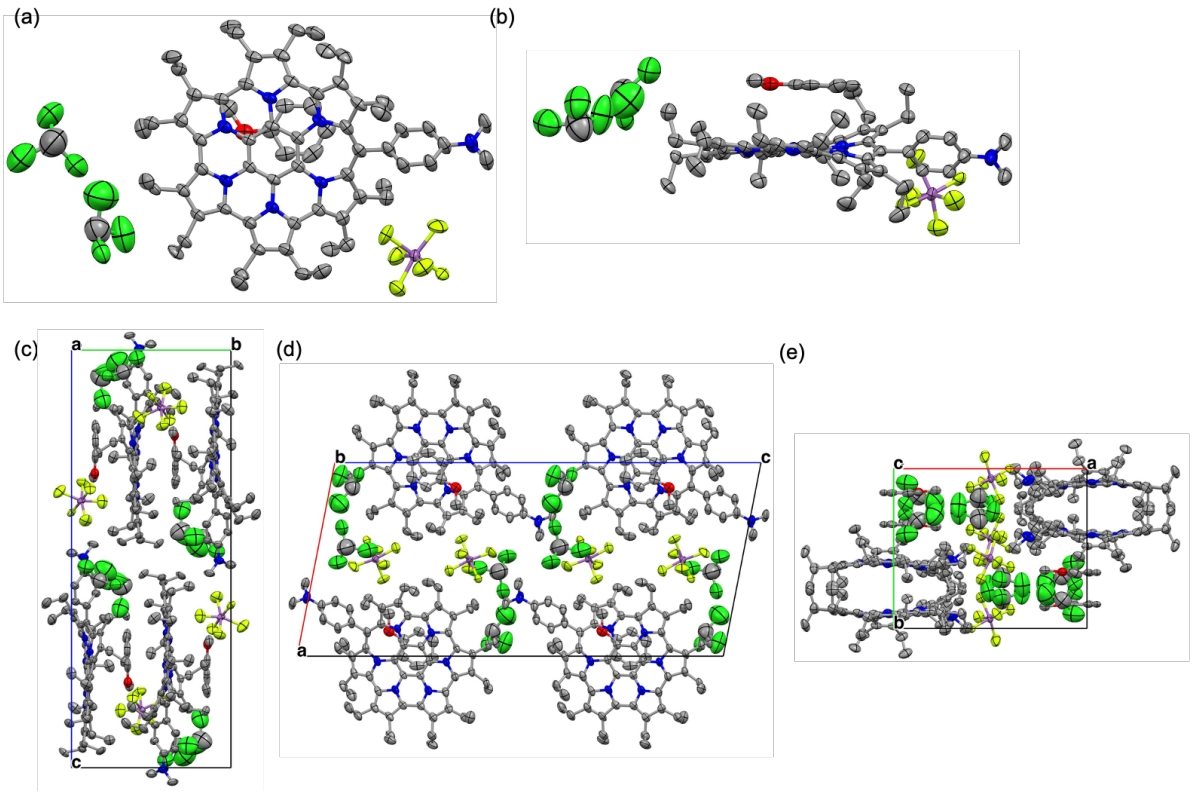


Figure S6a. X-ray crystal structures of $\mathbf{3c}^{+}$ from (a) top and (b) side. Packing structures of $\mathbf{3c}^{+}$: views along the (c) *a* axis, (d) *b* axis, and (e) *c* axis. Thermal ellipsoids are scaled to 50% probability. Hydrogen and disordered atoms with lower occupancy are omitted for clarity.

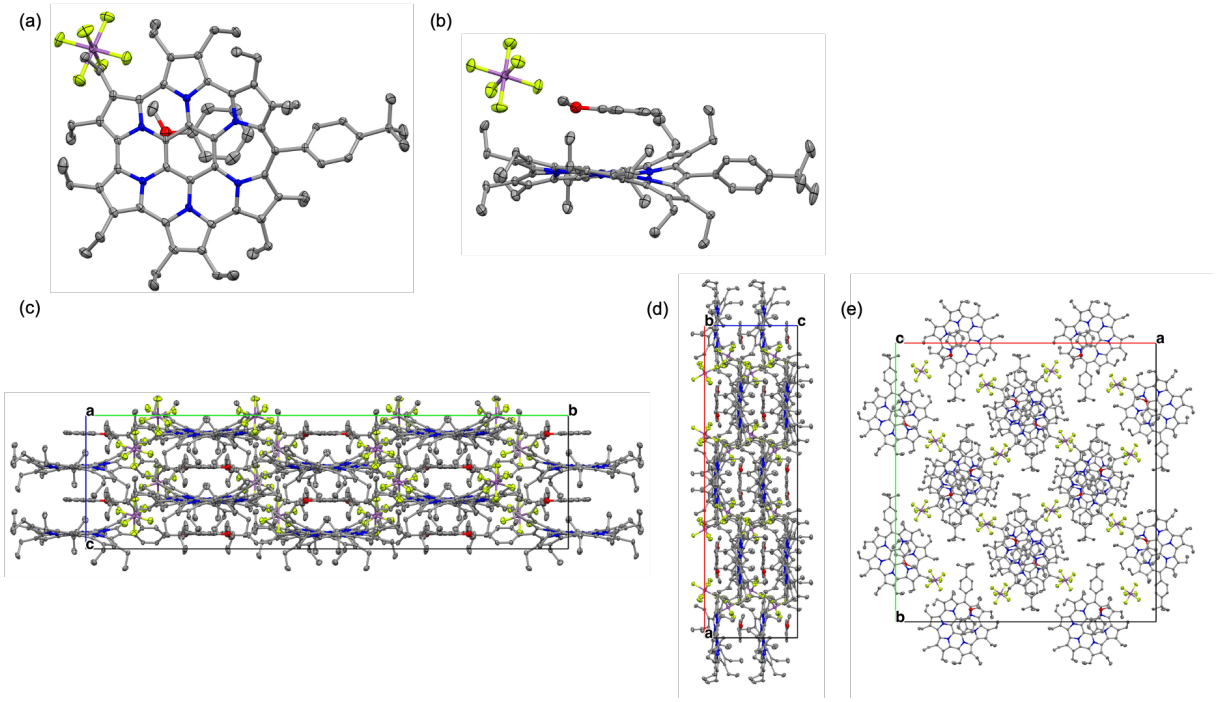


Figure S6b. X-ray crystal structures of $\mathbf{3d}^{+}$ from (a) top and (b) side. Packing structures of $\mathbf{3d}^{+}$: views along the (c) *a* axis, (d) *b* axis, and (e) *c* axis. Thermal ellipsoids are scaled to 50% probability. Hydrogen and disordered atoms with lower occupancy are omitted for clarity.

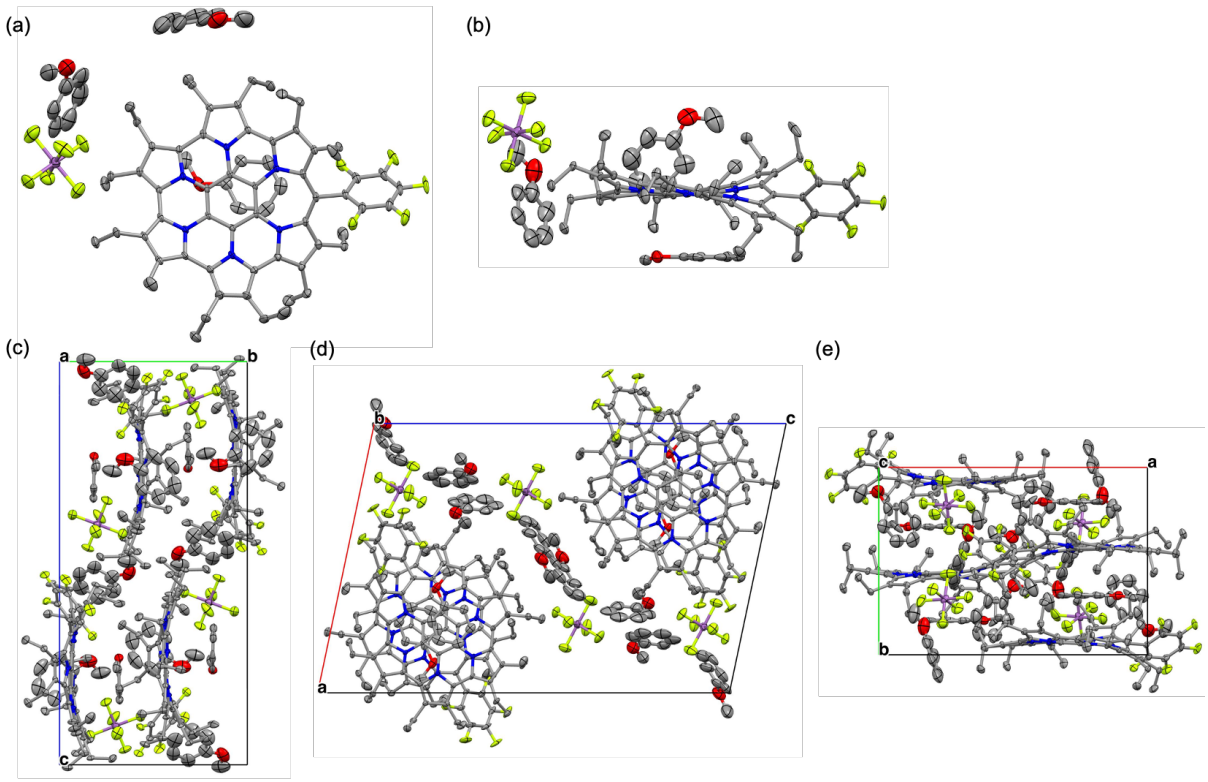


Figure S6c. X-ray crystal structures of **3e**$^{+}$ from (a) top and (b) side. Packing structures of **3e**$^{+}$: views along the (c) *a* axis, (d) *b* axis, and (e) *c* axis. Thermal ellipsoids are scaled to 50% probability. Hydrogen and disordered atoms with lower occupancy are omitted for clarity.

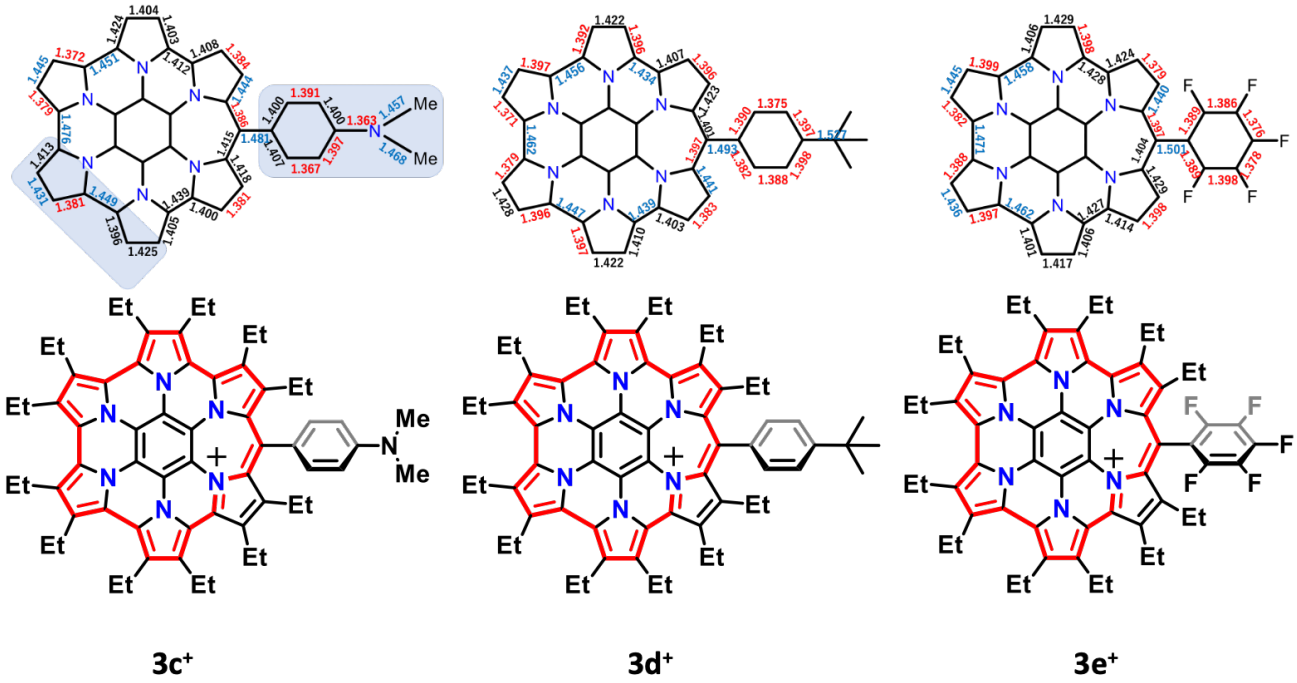


Figure S6d. Selected bond lengths (Å) of **3c**$^{+}$–**3e**$^{+}$ from the single crystal structure analyses. For the bond lengths in **3c**$^{+}$ highlighted in blue, the lengths with higher occupancy are picked up.

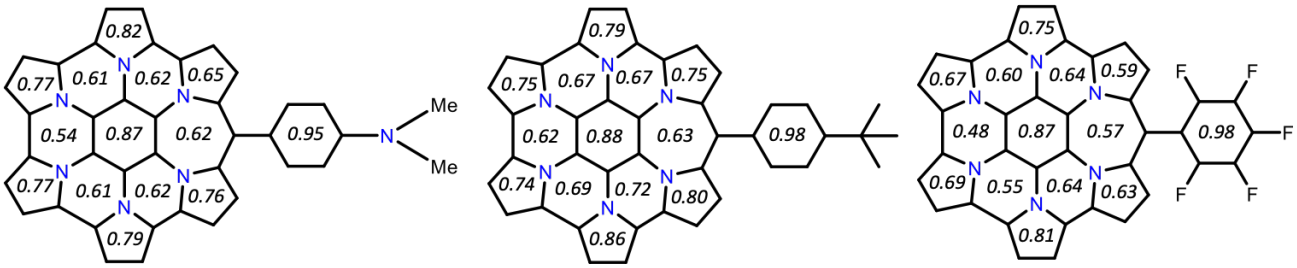


Figure S6e. HOMA values of the crystal structures of **3c**$^{+}$–**3e**$^{+}$. The values for **3c**$^{+}$ is calculated based on the structure with higher occupancy as indicated in Figure 6d.

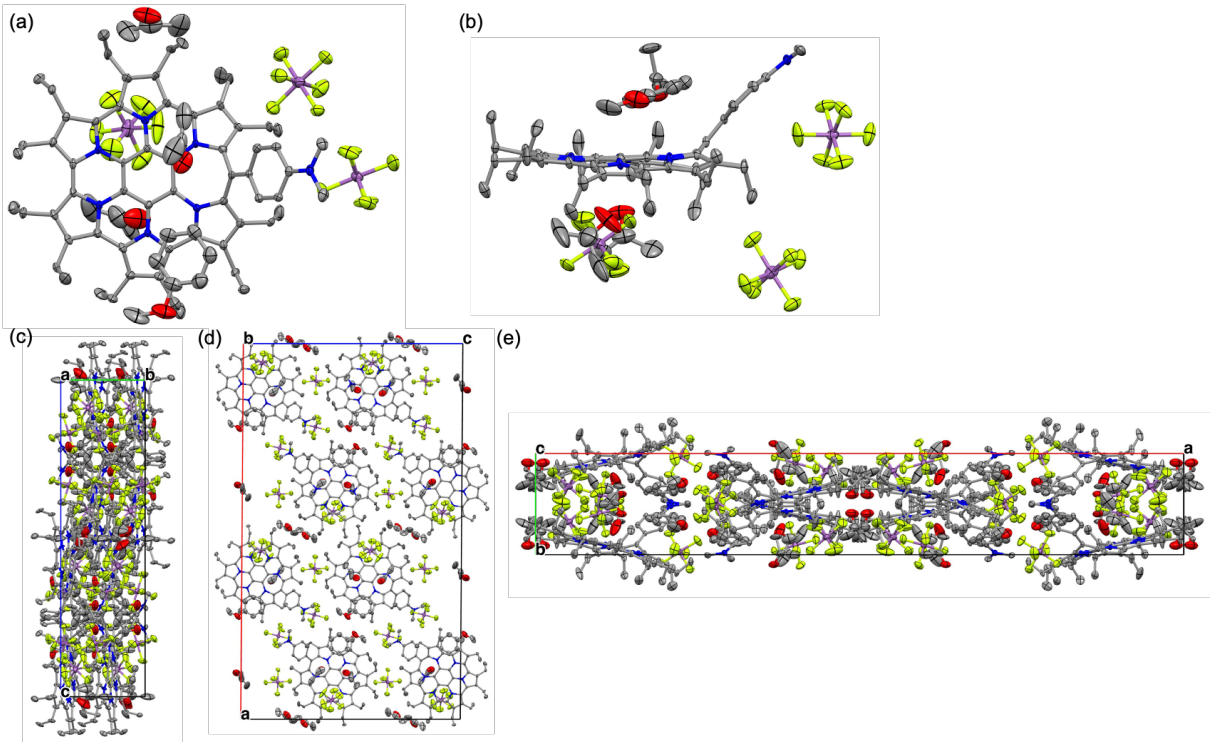


Figure S6f. X-ray crystal structures of **3c**$^{3+}$ from (a) top and (b) side. Packing structures of **3c**$^{3+}$: views along the (c) *a* axis, (d) *b* axis, and (e) *c* axis. Thermal ellipsoids are scaled to 50% probability. Hydrogen and disordered atoms with lower occupancy are omitted for clarity.

S7. ACID plots of $3c^{+}$, $3d^{+}$, $3e^{+}$, $3c^{3+}$ and $3e^{3+}$

ACID plots (CSGT/B3LYP/6-31+G(d)) of **3c**$^{+}$, **3d**$^{+}$, **3e**$^{+}$, **3c**$^{3+}$ and **3e**$^{3+}$ were calculated by using the method developed by Herges based on the optimized ground-state geometries.[4] For ACID calculations, the magnetic field is aligned perpendicular to the molecular plane and directed out of the image. Isovalue is 0.04 and the blue and red arrows indicate the diatropic (clockwise) and paratropic (counterclockwise) ring current, respectively. Et groups are replaced with H atoms.

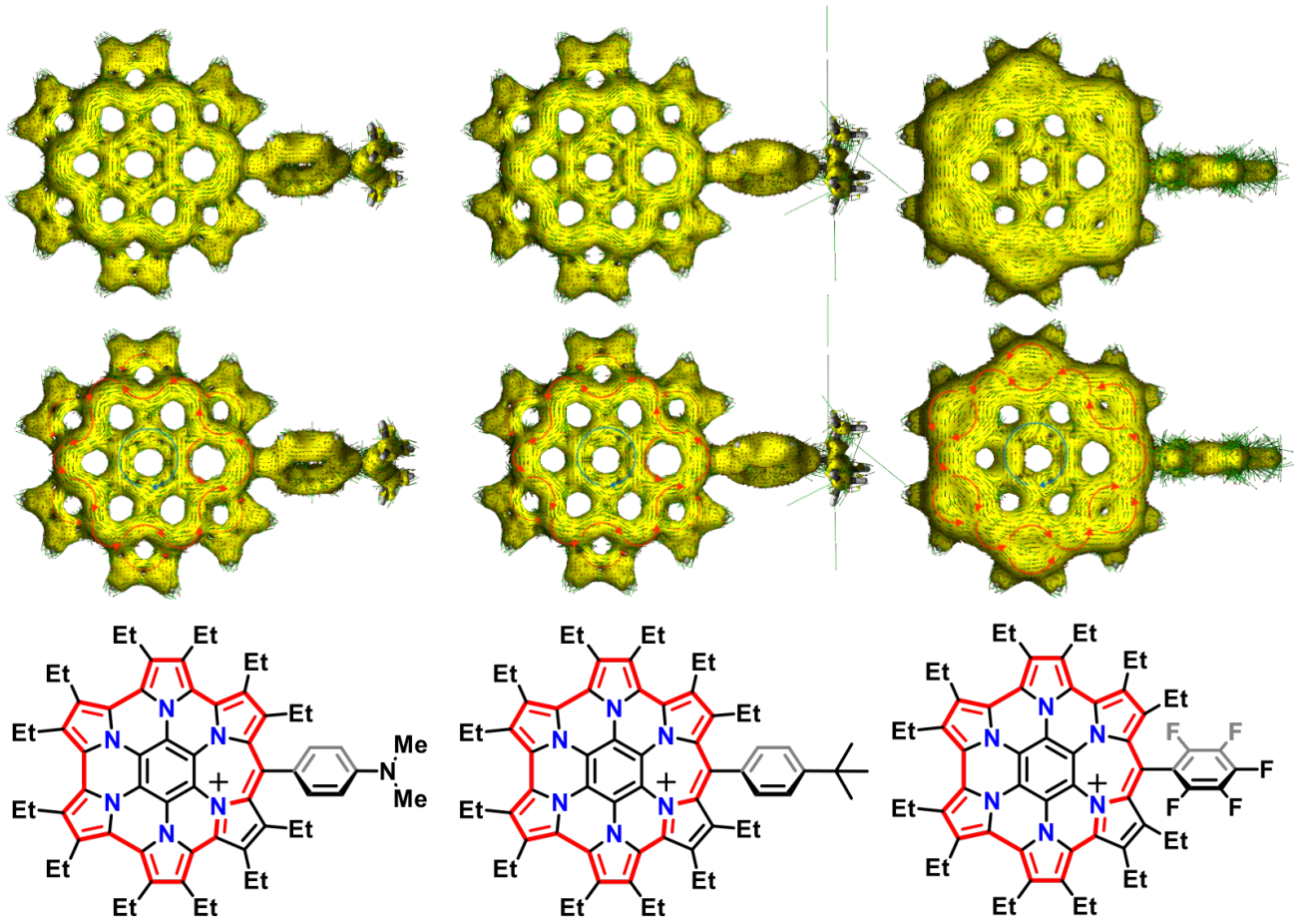


Figure S7a. AICD plots of **3c**$^{+}$, **3d**$^{+}$, and **3e**$^{+}$.

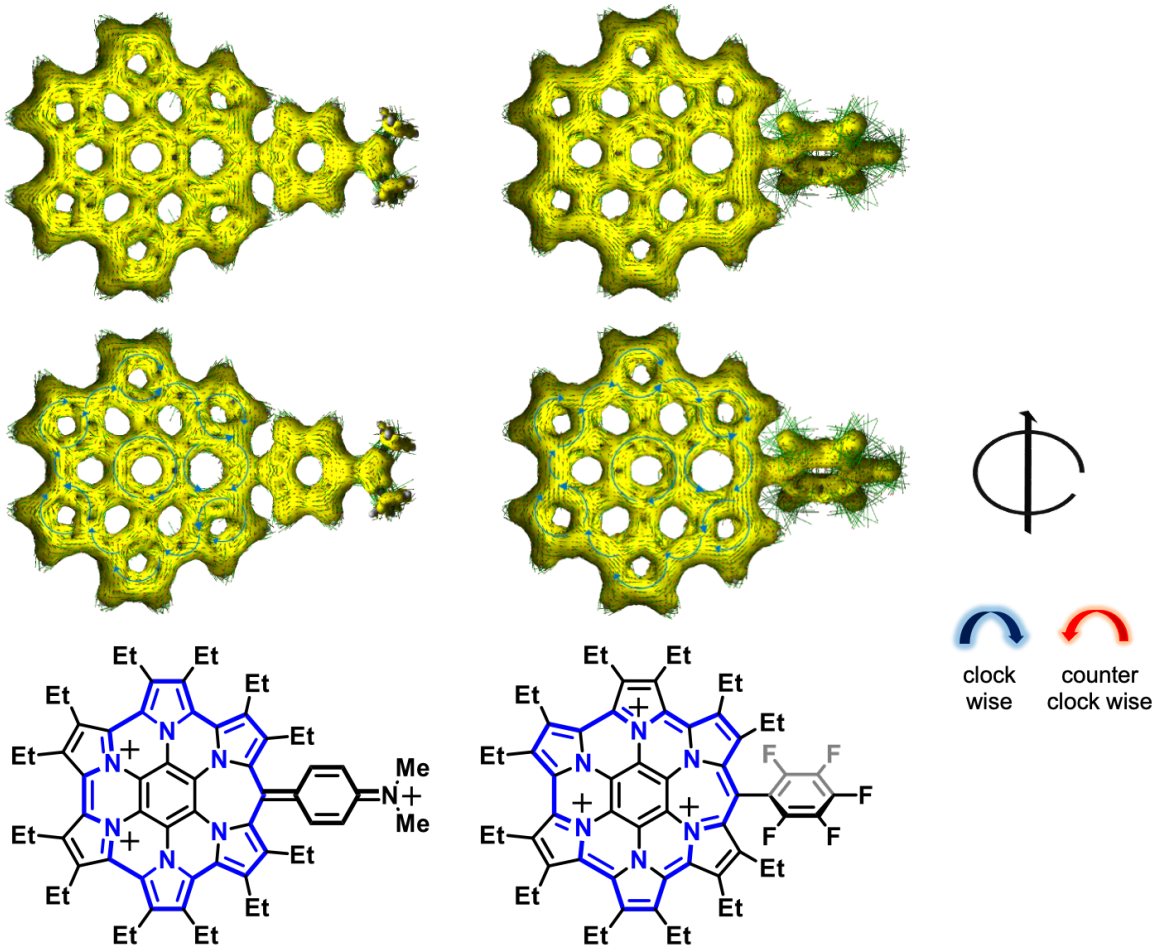


Figure S7b. AICD plots of $\mathbf{3c}^{3+}$ and $\mathbf{3e}^{3+}$.

S8. Solvatochromism of $3c^+$ and dipole moments of $3c^+$, $3d^+$ and $3e^+$

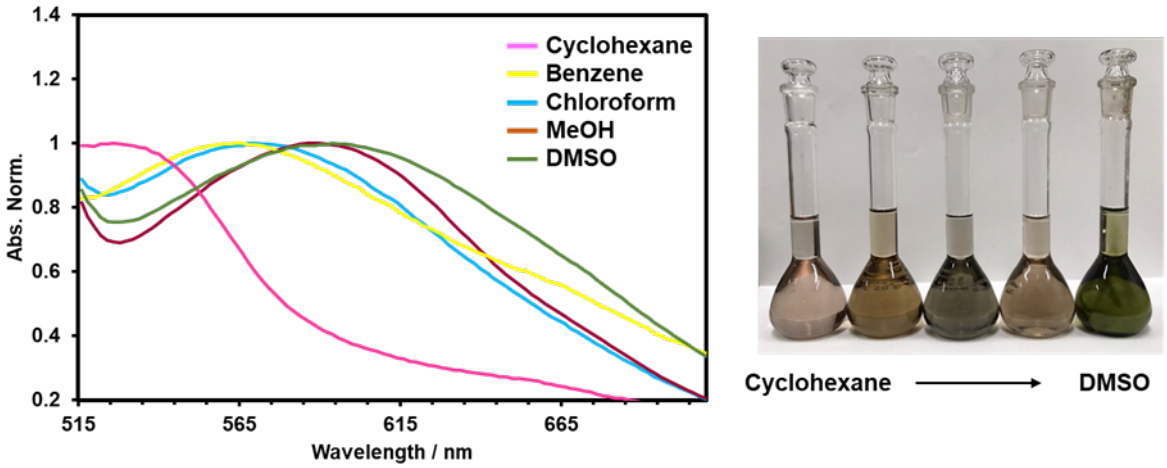


Figure S8a. Absorption spectra of **3c**$^+$ in various solvents and their photographs of the solutions ([**3c**$^+$] = 5.9×10^{-3} mM): cyclohexane, benzene, chloroform, methanol and *N,N*-dimethylformamide (DMF).

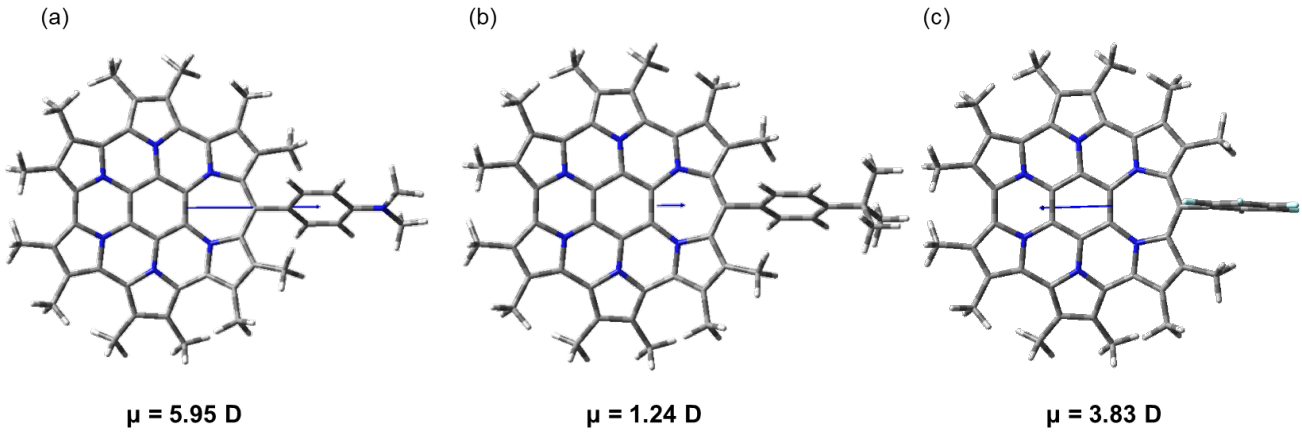
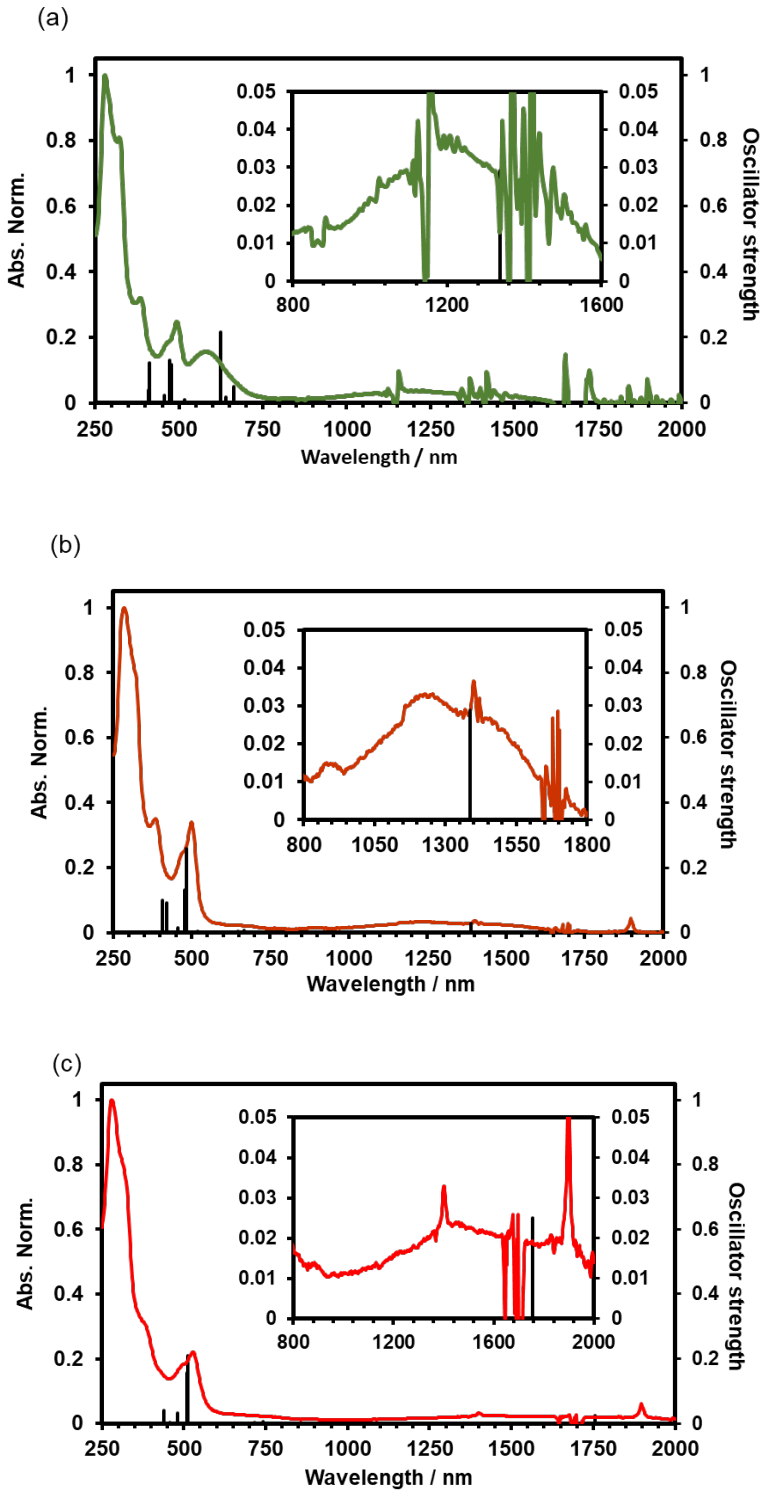


Figure S8b. Dipole moments of (a) **3c**$^+$, (b) **3d**$^+$ and (c) **3e**$^+$ calculated at the B3LYP/6-31G(d)) level of theory.

S9. TD-DFT calculations

The GAUSSIAN 09 series of programs was used for all calculation.[5] All molecules were fully optimized using the hybrid density functional at B3LYP level of theory with the 6-31G+(d) basis set. Frequency calculations were conducted to ensure that these structures were indeed local minima. TD-DFT calculations were performed at the B3LYP/6-31G+(d) level of the theory under vacuum.



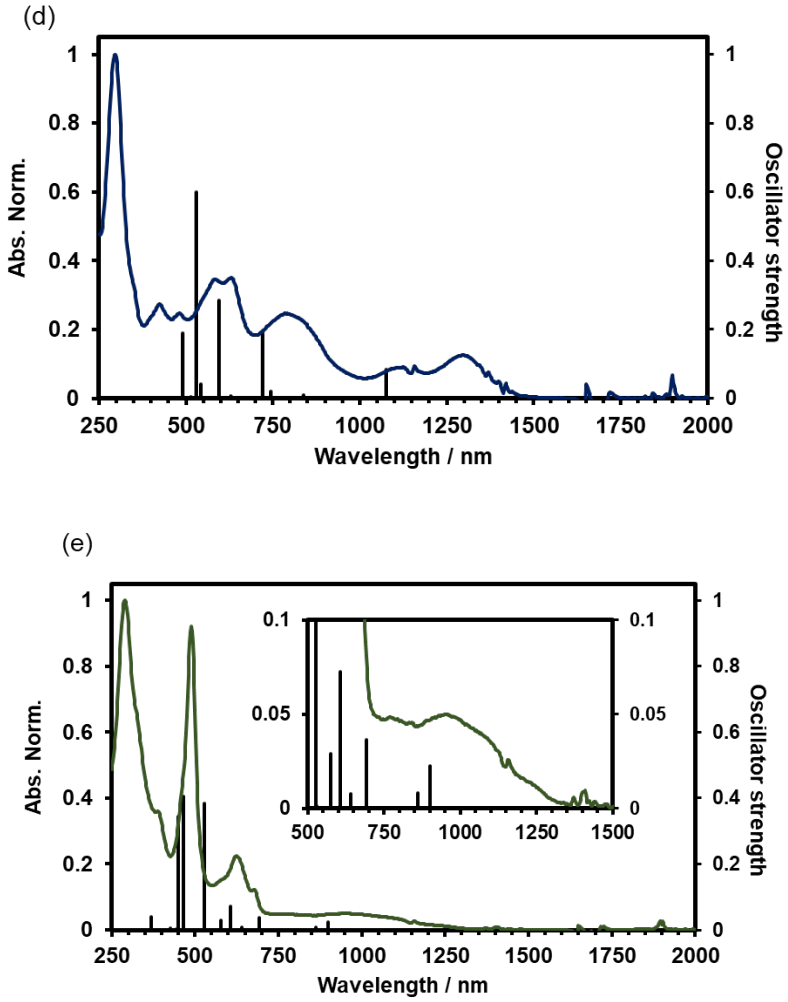


Figure S9. UV/Vis/NIR spectra in CH_2Cl_2 and the TD-DFT results of (a) **3c**$^{+}$, (b) **3d**$^{+}$, (c) **3e**$^{+}$, (d) **3c**$^{3+}$ and (e) **3e**$^{3+}$.

Table S9. TD-DFT results of (a) **3c**$^{+}$, (b) **3d**$^{+}$, (c) **3e**$^{+}$, (d) **3c**$^{3+}$ and (e) **3e**$^{3+}$

(a) **3c**$^{+}$ (Et groups were replaced to Me groups)

No.	Wavelength (nm)	Osc. Strength	Major contributions
1	1337.20 nm	0.0291	HOMO->LUMO (99%)
2	663.47 nm	0.0496	H-1->LUMO (57%), H-2->LUMO (40%)
3	639.03 nm	0.0182	H-3->LUMO (92%)
4	624.72 nm	0.2162	H-2->LUMO (58%), H-1->LUMO (36%)
5	517.77 nm	0.0101	HOMO->L+1 (98%)
6	477.43 nm	0.1181	H-4->LUMO (82%)
7	471.34 nm	0.1291	H-5->LUMO (86%)
8	457.31 nm	0.0225	HOMO->L+2 (90%)
9	411.49 nm	0.1215	HOMO->L+3 (73%)
10	410.53 nm	0.0397	H-6>LUMO (98%)

(b) **3d**$^{+}$ (Et groups were replaced to Me groups)

No.	Wavelength (nm)	Osc. Strength	Major contributions
1	1387.51 nm	0.0288	HOMO->LUMO (99%)
2	666.75 nm	0.0083	H-1->LUMO (95%)
3	647.27 nm	0.0039	H-2->LUMO (97%)
4	519.23 nm	0.0045	HOMO->L+1 (97%)
5	483.90 nm	0.2573	H-3->LOMO (91%)
6	477.74 nm	0.1327	H-4->LUMO (88%)
7	456.72 nm	0.0140	HOMO->L+2 (93%)
8	421.32 nm	0.0909	H-5->LUMO (89%)
9	407.52 nm	0.1004	HOMO->L+3 (66%)
10	406.47 nm	0.0135	H-6>LUMO (79%)

(c) **3e**$^{+}$ (Et groups were replaced to Me groups)

No.	Wavelength (nm)	Osc. Strength	Major contributions
1	1756.47nm	0.0251	HOMO->LUMO (100%)
2	740.86nm	0.0065	H-1->LUMO (96%)
3	715.35 nm	0.0037	H-2->LUMO (97%)
4	566.05 m	0.0010	HOMO->L+1 (97%)
5	532.99nm	0.0004	HOMO->L+2 (87%)
6	511.39 nm	0.2085	H-3->LOMO (84%)
7	508.91 nm	0.1574	H-4->LOMO (86%)
8	479.83nm	0.0315	HOMO->L+3 (82%), HOMO->L+5 (10%)
9	456.50nm	0.0024	HOMO->L+4 (83%), HOMO->L+5 (11%)
10	439.42 nm	0.0388	H-5->LUMO (81%), HOMO->L+4 (16%)

(d) **3c**$^{3+}$ (Et groups were replaced to Me groups)

No.	Wavelength (nm)	Osc. Strength	Major contributions
1	1076.50 nm	0.0825	HOMO->LUMO (93%)
2	838.64 nm	0.0089	H-1->LUMO (83%), H-3->LUMO (11%)
3	743.17 nm	0.0189	H-2->LUMO (95%)
4	719.86 nm	0.1907	HOMO->L+1 (81%), H-3->LUMO (12%)
5	629.82 nm	0.0068	H-2->L+1 (95%)
6	595.96 nm	0.2854	H-3->LUMO (66%), H-2-> L+1 (12%)
7	542.53 nm	0.0420	H-4->LUMO (75%), H-3-> L+1 (20%)
8	530.55 nm	0.5999	H-2->L+1 (76%), HOMO->L+1 (11%)
9	514.86 nm	0.0033	H-5>LUMO (97%)
10	489.81 nm	0.1886	H-2-> L+1 (73%), H-4>LUMO (17%)

(e) **3e**$^{3+}$ (Et groups were replaced to Me groups)

No.	Wavelength (nm)	Osc. Strength	Major contributions
1	900.26 nm	0.0228	HOMO->LUMO (80%), H-3->LUMO (13%)
2	861.54 nm	0.0085	H-1->LUMO (88%)
3	724.12 nm	0.0001	H-2->LUMO (97%)
4	692.07 nm	0.0366	H-3->LUMO (75%), H-1->L+1 (13%)
5	677.17 nm	0.0002	HOMO->L+1 (71%), H-4->LUMO (27%)
6	641.72 nm	0.0080	H-1->L+1 (79%)
7	607.21 nm	0.0727	H-4->LUMO (47%), H-3->L+1 (25%), HOMO->L+1 (14%)
8	604.73 nm	0.0008	H-2->L+1 (96%)
9	576.68 nm	0.0292	H-5->LUMO (77%), H-4->L+1 (17%)
10	530.22 nm	0.0015	H-6->LUMO (96%)

S10. Optimized structures and molecular orbitals

The GAUSSIAN 09[5] series of programs was used for all calculations. All molecules were fully optimized using the hybrid density functional at the B3LYP level of theory with the 6-31G(d) basis set. Frequency calculations were conducted to ensure that these structures were indeed local minima. Visualization of the results was performed by use of Gauss View 5.0 software.

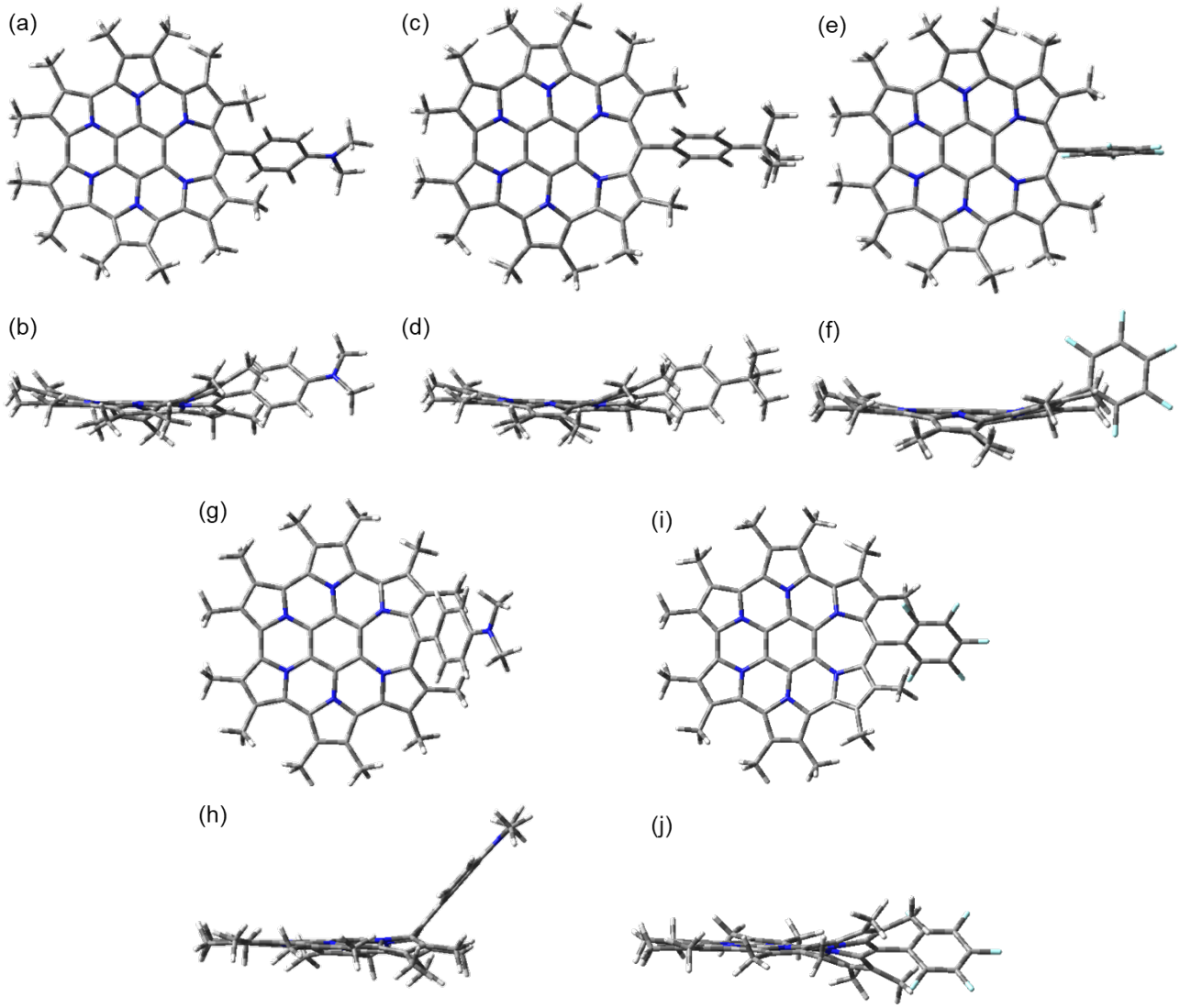


Figure S10a. Optimized structures of (a, b) **3c**$^{+}$, (c, d) **3d**$^{+}$, (e, f) **3e**$^{+}$, (g, h) **3c**$^{3+}$ and (i, j) **3e**$^{3+}$ from top and side views. Ethyl groups were replaced with methyl groups to simplify the calculation.

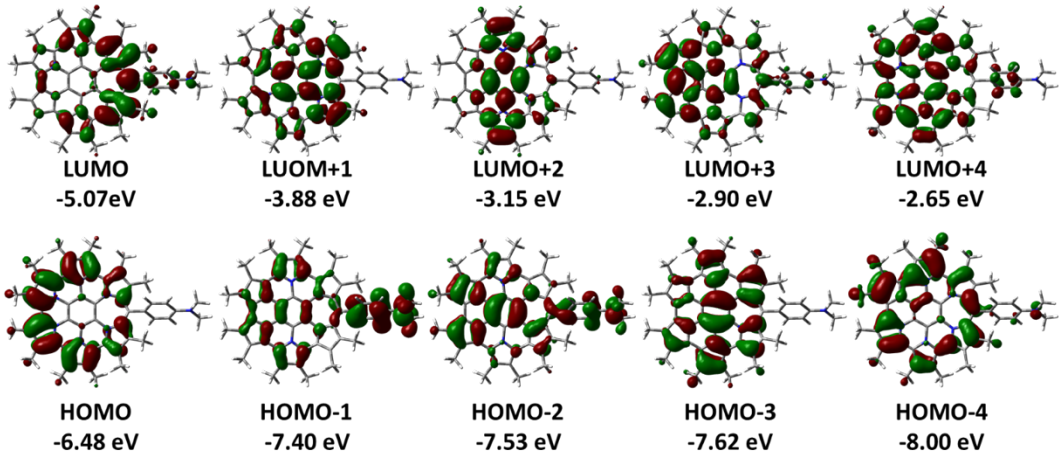


Figure S10b. Frontier molecular orbitals (isovalue = 0.02) and orbital energies of **3c**$^{+}$.

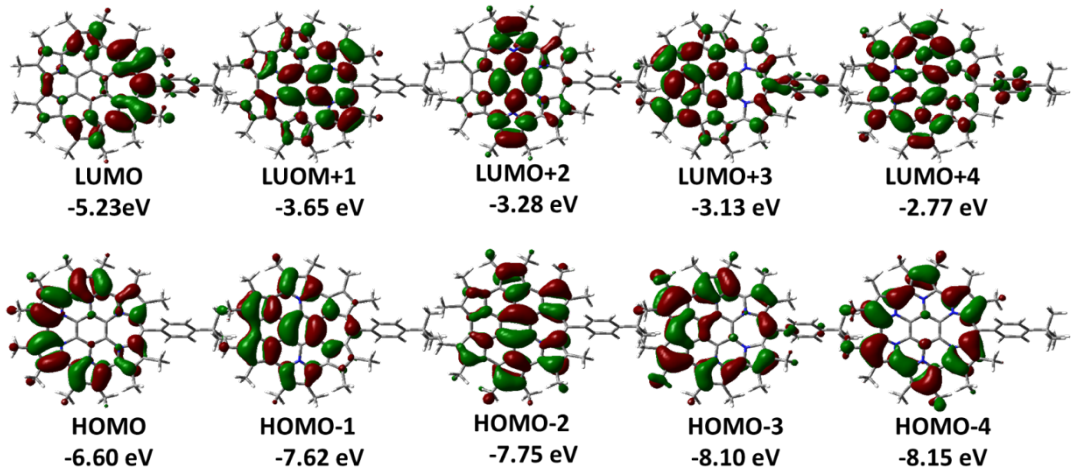


Figure S10c. Frontier molecular orbitals (isovalue = 0.02) and orbital energies of **3d**$^{+}$.

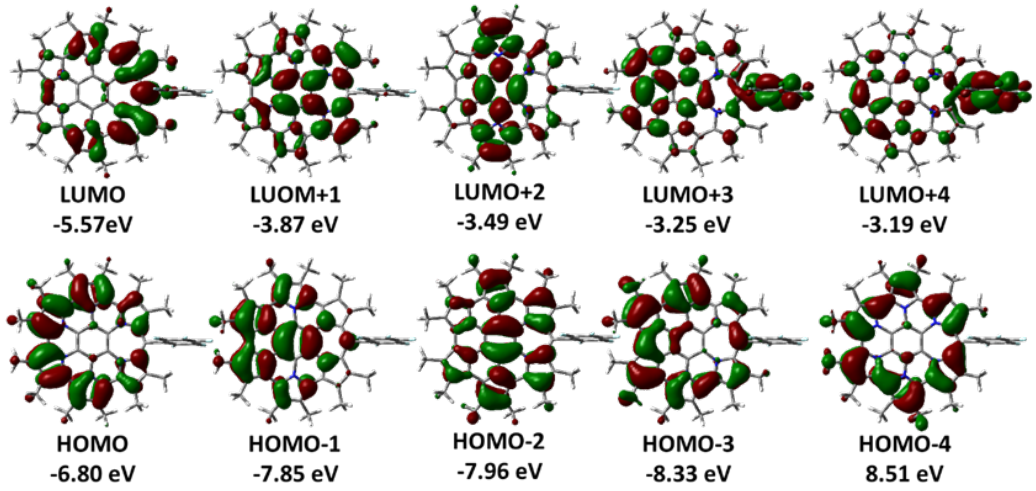


Figure S10d. Frontier molecular orbitals (isovalue = 0.02) and orbital energies of **3e**$^{+}$.

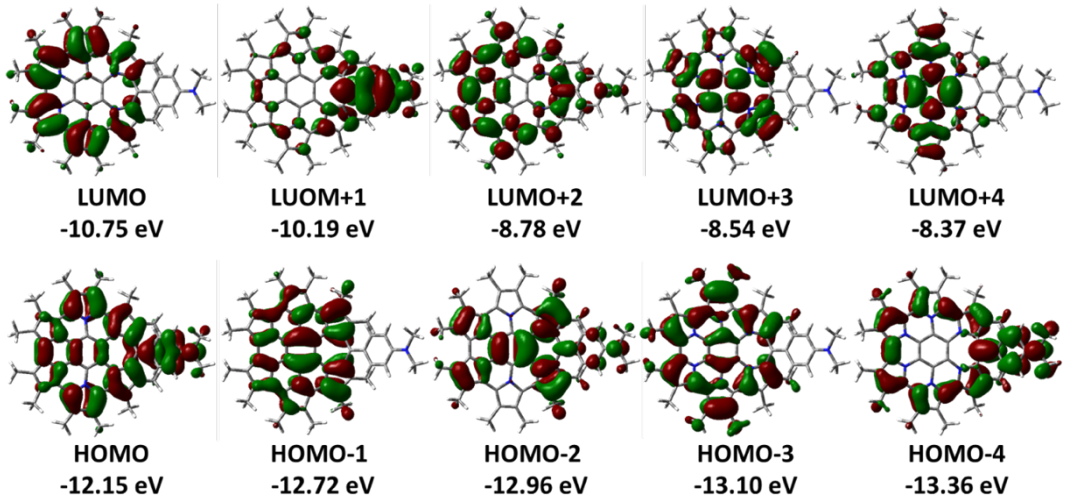


Figure S10e. Frontier molecular orbitals (isovalue = 0.02) and orbital energies of **3c**$^{3+}$.

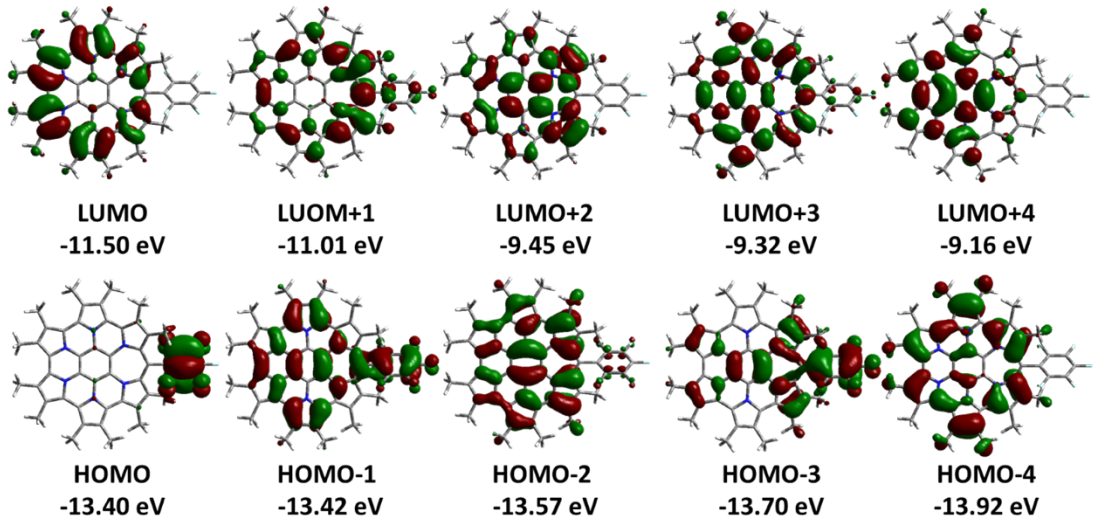


Figure S10f. Frontier molecular orbitals (isovalue = 0.02) and orbital energies of **3e**$^{3+}$.

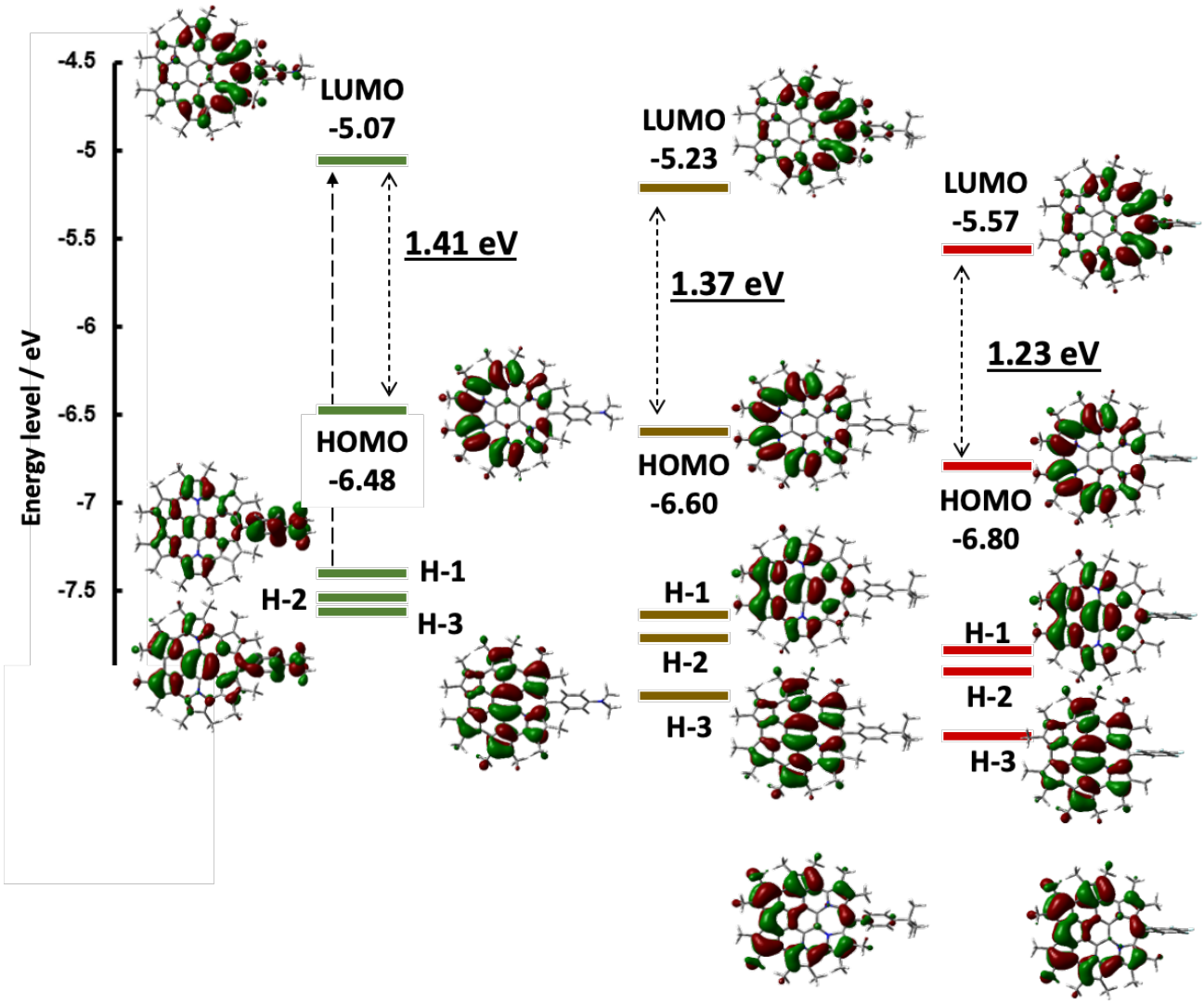


Figure S10g. Comparison of the molecular orbitals and the energies of **3c**$^{+}$–**3e**$^{+}$ (from left to right).

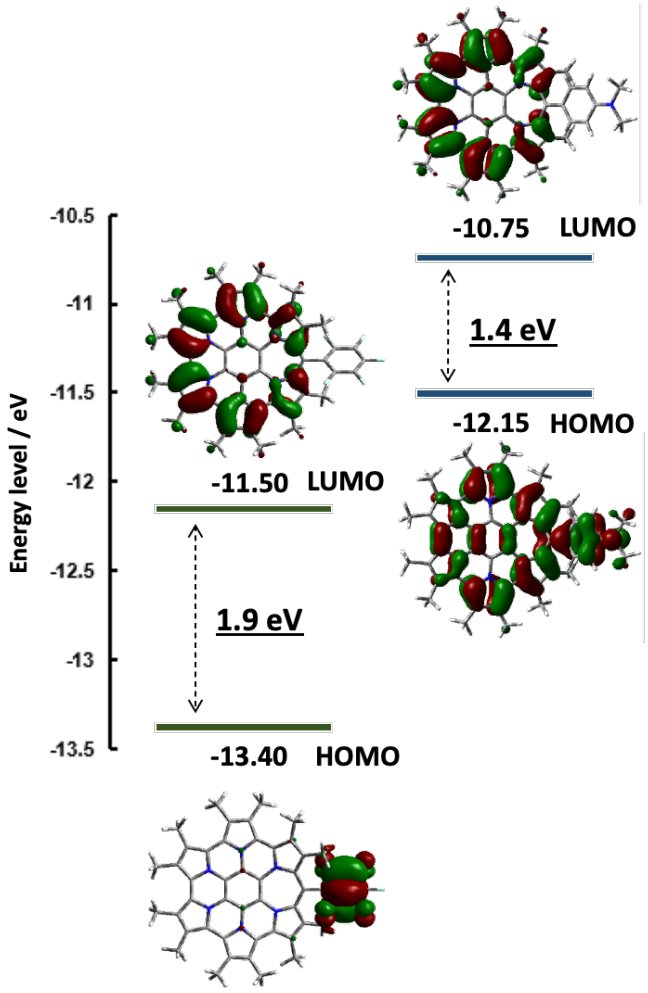


Figure S10h. Comparison of the molecular orbitals and the energies of **3e**$^{3+}$ (left) and **3c**$^{3+}$ (right).

S11. Cyclic voltammogram and differential pulse voltammogram

Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) of **3c**$^{+}$ were measured under following conditions: 0.1 M $TBAPF_6$ in CH_2Cl_2, $Ag/AgNO_3$ reference electrode, Pt working electrode and Pt counter electrode, scan rate: 100 mV s^{-1}; V *vs.* Fc/Fc^{+}.

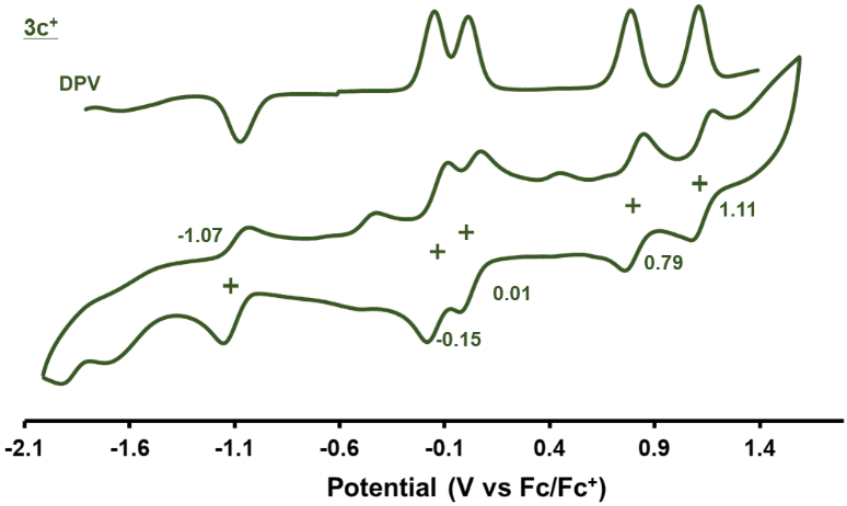


Figure S11. CV and DPV of **3c**$^{+}$ with wide measuring range.

S12. Bond lengths of the optimized structures of **3c**$^{+}$ and **3c**$^{3+}$

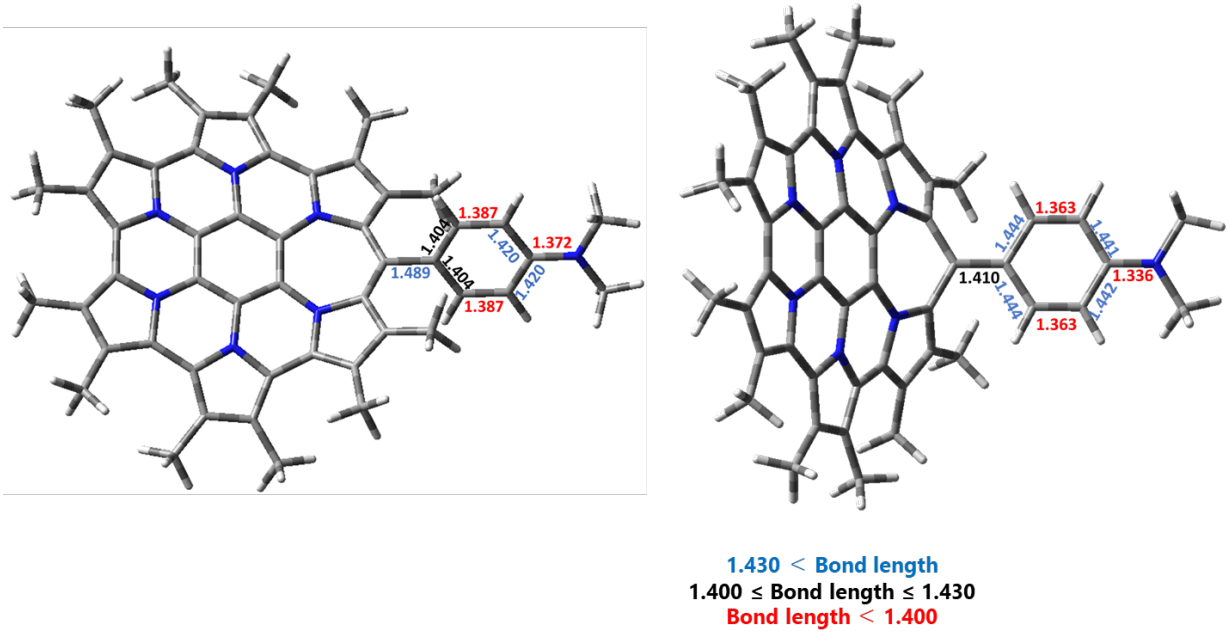


Figure S12. Bond lengths (Å) of **3c**$^{+}$ (left) and **3c**$^{3+}$ (right) for the optimized structure. Ethyl groups were replaced with methyl groups to simplify the calculation.

S13. Atomic coordinates of optimized structures

Atomic coordinates of the optimized structures calculated at the B3LYP/6-31G(d) level of theory are shown. Ethyl groups are replaced with methyl groups and hydrogen atoms to simplify the calculations.

3c^{+}-H (Et groups are replaced with H atoms)

C	-3.10719	0.68962	0.05134	N	0.00743	4.39563	4.90981	C -1.18048 -0.10103 0.4456
C	-3.11007	-0.68502	0.08918	N	-3.24924	2.84882	1.86832	C -1.48637 -1.31472 0.92418
C	-1.90757	-1.37393	0.01086	C	-2.82265	1.85701	1.18807	C -1.24625 -2.40761 0.18396
C	-0.65798	-0.71706	-0.11039	C	-1.456	1.16229	1.28592	C -0.39993 -1.10155 -1.50331
C	-0.65583	0.70652	-0.16901	C	-0.38504	1.67911	2.25836	C -0.63486 0.00063 -0.77429
C	-1.90147	1.37281	-0.06699	N	-0.47747	2.64674	3.08514	H 1.17963 0.23232 1.73517
N	-2.01357	2.74869	-0.18094	C	0.81738	1.08575	2.32115	H 2.53079 1.54037 3.58852
N	-4.30862	1.35218	0.12965	C	1.50528	1.74116	3.2565	H -5.76639 2.14526 -0.05407
N	-4.31011	-1.34676	0.18358	C	0.65928	2.68386	3.6875	H -3.66286 0.58589 -0.39102
N	-2.02743	-2.75069	-0.0268	C	-4.44746	3.05638	1.44595	H 2.95548 3.34026 5.43382
C	-0.96838	3.53862	-0.65034	C	-4.81219	2.20191	0.48313	H 2.23531 5.40486 6.94102
C	-1.53426	4.77055	-1.03304	C	-3.74586	1.41881	0.3177	H -7.55382 6.11909 2.64522
C	-2.92461	4.71372	-0.73907	C	0.93308	3.58131	4.63725	H -7.18627 4.08022 0.98289
C	-3.21118	3.45174	-0.2038	C	1.98855	3.85744	5.41674	H -4.79163 8.77008 6.44564
C	-4.4142	2.7406	0.17735	C	1.62468	4.90295	6.18054	H -6.65149 7.92974 4.74403
C	-5.71724	3.02358	0.57295	C	0.36811	5.20793	5.82565	H 0.30915 7.42498 7.80117
C	-6.41197	1.77439	0.73299	N	-1.63497	6.14488	5.66558	H -2.08102 8.57351 7.63609
C	-5.52603	0.73924	0.43529	N	-3.93892	6.31113	4.65293	H -1.93574 -1.41079 1.9264
C	-5.54569	-0.7199	0.35947	N	-4.69646	4.73641	2.84335	H -1.51494 -3.38351 0.61863
C	-6.49169	-1.7431	0.39068	C	-5.51019	5.63446	3.24396	H 0.04899 -0.95135 -2.49635
C	-5.80647	-2.99794	0.26665	C	-6.64956	5.50579	2.54871	H -0.3806 0.99556 -1.17625
C	-4.44819	-2.73432	0.10428	C	-6.46289	4.47353	1.70722	C -0.69868 -2.33323 -1.04556
C	-3.21773	-3.46399	-0.13139	C	-5.21887	4.02961	1.9368	N -0.42768 -3.5947 -1.88631
C	-2.86085	-4.77107	-0.49827	C	-3.63258	7.14621	5.56304	C -0.7825 -4.79104 -1.10928
C	-1.44079	-4.84414	-0.57364	C	-4.70215	7.93703	5.73759	C 0.22692 -3.36633 -3.18255
C	-1.94964	5.3149	4.75663	C	-5.64607	7.51122	4.8746	H -0.02077 -4.9834 -0.38287
C	-3.16243	5.40229	4.22346	C	-5.11473	6.47656	4.20727	H -1.71641 -4.62971 -0.6126
C	-3.51184	4.53724	3.2638	C	-0.5009	6.14164	6.2334	H -0.86859 -5.6308 -1.76676
C	-2.6925	3.55664	2.79141	C	-0.50997	7.13859	7.13024	H 1.168 -3.87517 -3.20143
C	-1.43964	3.46593	3.34194	C	-1.72289	7.72093	7.04602	H -0.39649 -3.74017 -3.96772
C	-1.11775	4.36372	4.31546	C	-2.40698	7.05764	6.10158	H 0.38575 -2.31741 -3.32202

$3c^{+}$-Me (Et groups are replaced with Me groups)

C	2.51647	-0.6741	0.09638	C	-2.18359	3.50351	0.25872	H	3.37808	6.51342	-0.30479
C	2.50353	0.70039	0.05442	C	-3.08205	2.46553	0.50029	H	4.02948	5.50671	-1.60556
C	1.29248	1.37015	-0.05204	C	-4.56283	-2.84104	-0.76164	H	2.61623	6.51848	-1.88978
C	0.04999	0.69365	-0.11945	H	-5.13391	-3.04752	0.15084	C	-0.00215	5.96543	-1.35316
C	0.0641	-0.73091	-0.09595	H	-5.06743	-2.03178	-1.28753	H	-1.00859	5.67251	-1.65606
C	1.31782	-1.37636	0.02989	H	-4.62903	-3.73057	-1.3934	H	-0.09017	6.78667	-0.63121
N	1.44398	-2.75501	-0.00384	C	-2.52484	-5.0252	-0.53145	H	0.49435	6.37562	-2.23911
N	3.72555	-1.31756	0.20327	H	-2.60502	-5.44348	-1.54182	C	-2.41321	4.95959	0.53988
N	3.69582	1.38004	0.09964	H	-1.78915	-5.61278	0.01848	H	-1.47599	5.46565	0.77834
N	1.39528	2.74337	-0.17063	H	-3.48995	-5.18015	-0.04167	H	-2.87553	5.48525	-0.30407
C	0.40376	-3.58478	-0.41479	C	0.35523	-6.04452	-1.34802	H	-3.07919	5.09094	1.39707
C	0.98222	-4.83433	-0.71854	H	0.0097	-6.7795	-0.61061	C	-4.43875	2.72702	1.09585
C	2.3726	-4.74307	-0.43791	H	-0.4882	-5.78259	-1.98692	H	-5.20651	2.9022	0.33394
C	2.64837	-3.44516	0.01229	H	1.08694	-6.5566	-1.97929	H	-4.78428	1.91599	1.73507
C	3.84597	-2.6992	0.34023	C	3.38256	-5.82663	-0.67771	H	-4.39256	3.6303	1.70969
C	5.15333	-2.94252	0.74812	H	4.36488	-5.4075	-0.90638	C	-4.51088	-0.08507	0.22767
C	5.83519	-1.67821	0.82451	H	3.49506	-6.4927	0.18715	C	-5.07015	-0.68776	1.35832
C	4.93738	-0.67399	0.4638	H	3.09229	-6.45487	-1.525	C	-5.35585	0.48382	-0.72992
C	4.94016	0.77819	0.29714	C	5.76437	-4.25979	1.12761	C	-6.45518	-0.72585	1.52307
C	5.87506	1.81097	0.25419	H	5.00108	-5.00481	1.35951	H	-4.42454	-1.13327	2.10868
C	5.17445	3.04914	0.06536	H	6.40766	-4.66913	0.33797	C	-6.73916	0.4623	-0.54914
C	3.81696	2.76243	-0.06306	H	6.38996	-4.15113	2.01994	H	-4.93445	0.94833	-1.61602
C	2.57524	3.46365	-0.32403	C	7.2606	-1.52534	1.27011	C	-7.29826	-0.14659	0.57466
C	2.19853	4.74739	-0.75301	H	7.97052	-1.59626	0.43568	H	-6.8741	-1.20338	2.3841
C	0.77804	4.80084	-0.8156	H	7.42799	-0.57051	1.77171	H	-7.3766	0.91667	-1.27861
C	0.29099	3.54656	-0.41918	H	7.52851	-2.31466	1.9791	N	-8.75659	-0.17805	0.75685
N	-1.09206	1.53922	-0.14884	C	7.37167	1.71383	0.33957	C	-9.24761	1.18322	1.01517
C	-2.43545	1.21937	0.18356	H	7.74167	1.79489	1.37022	H	-9.09724	1.7877	0.14517
C	-3.0225	-0.0526	0.04972	H	7.73757	0.77137	-0.07211	H	-10.2912	1.14763	1.24872
C	-2.43417	-1.29938	-0.24183	H	7.84051	2.51962	-0.23297	H	-8.7118	1.6052	1.83963
N	-1.04614	-1.60148	-0.24017	C	5.85204	4.38965	0.06732	C	-9.39115	-0.7052	-0.45985
C	-3.11144	-2.5423	-0.48914	H	6.22622	4.67539	-0.92471	H	-8.93956	-1.63926	-0.7216
C	-2.17089	-3.56541	-0.51735	H	5.18346	5.18007	0.4121	H	-10.43612	-0.85157	-0.28236
C	-0.88904	-2.98534	-0.40775	H	6.71333	4.37922	0.74223	H	-9.25964	-0.00848	-1.26121
C	-0.96475	2.93011	-0.15785	C	3.10553	5.87373	-1.1539				

$3d^{+}$-H (Et groups are replaced with H atoms)

C	-1.94964	5.3149	4.75663	N	-4.69646	4.73641	2.84335	H	2.23531	5.40486	6.94102
C	-3.16243	5.40229	4.22346	C	-5.51019	5.63446	3.24396	H	-7.55382	6.11909	2.64522
C	-3.51184	4.53724	3.2638	C	-6.64956	5.50579	2.54871	H	-7.18627	4.08022	0.98289
C	-2.6925	3.55664	2.79141	C	-6.46289	4.47353	1.70722	H	-4.79163	8.77008	6.44564
C	-1.43964	3.46593	3.34194	C	-5.21887	4.02961	1.9368	H	-6.65149	7.92974	4.74403
C	-1.11775	4.36372	4.31546	C	-3.63258	7.14621	5.56304	H	0.30915	7.42498	7.80117
N	0.00743	4.39563	4.90981	C	-4.70215	7.93703	5.73759	H	-2.08102	8.57351	7.63609
N	-3.24924	2.84882	1.86832	C	-5.64607	7.51122	4.8746	H	-1.92207	-1.41222	1.89658
C	-2.82265	1.85701	1.18807	C	-5.11473	6.47656	4.20727	H	-1.4973	-3.36852	0.5821
C	-1.456	1.16229	1.28592	C	-0.5009	6.14164	6.2334	H	0.03666	-0.99938	-2.47483
C	-0.38504	1.67911	2.25836	C	-0.50997	7.13859	7.13024	H	-0.38569	0.9637	-1.16838
N	-0.47747	2.64674	3.08514	C	-1.72289	7.72093	7.04602	C	-0.42768	-3.5947	-1.88631
C	0.81738	1.08575	2.32115	C	-2.40698	7.05764	6.10158	C	-0.57003	-3.25531	-3.38169
C	1.50528	1.74116	3.2565	C	-1.18048	-0.10103	0.4456	H	0.23827	-2.62187	-3.68218
C	0.65928	2.68386	3.6875	C	-1.48637	-1.31472	0.92418	H	-0.54831	-4.15791	-3.95592
C	-4.44746	3.05638	1.44595	C	-1.24625	-2.40761	0.18396	H	-1.49897	-2.75034	-3.54596
C	-4.81219	2.20191	0.48313	C	-0.69868	-2.33323	-1.04556	C	-1.44228	-4.69032	-1.50973
C	-3.74586	1.41881	0.3177	C	-0.39993	-1.10155	-1.50331	H	-1.2537	-5.02278	-0.51033
C	0.93308	3.58131	4.63725	C	-0.63486	0.00063	-0.77429	H	-2.4344	-4.29455	-1.57273
C	1.98855	3.85744	5.41674	H	1.17963	0.23232	1.73517	H	-1.34369	-5.51487	-2.18449
C	1.62468	4.90295	6.18054	H	2.53079	1.54037	3.58852	C	1.00026	-4.09993	-1.60825
C	0.36811	5.20793	5.82565	H	-5.76639	2.14526	-0.05407	H	1.09912	-4.3359	-0.56929
N	-1.63497	6.14488	5.66558	H	-3.66286	0.58589	-0.39102	H	1.18861	-4.97631	-2.19254
N	-3.93892	6.31113	4.65293	H	2.95548	3.34026	5.43382	H	1.7052	-3.33862	-1.86974

$3d^{+}$-Me (Et groups are replaced with Me groups)

C	2.51647	-0.6741	C	-3.08205	2.46553	H	2.61623	6.51848	-1.88978
C	2.50353	0.70039	C	-4.56283	-2.84104	C	-0.00215	5.96543	-1.35316
C	1.29248	1.37015	H	-5.13391	-3.04752	H	-1.00859	5.67251	-1.65606
C	0.04999	0.69365	H	-5.06743	-2.03178	H	-0.09017	6.78667	-0.63121
C	0.0641	-0.73091	H	-4.62903	-3.73057	H	0.49435	6.37562	-2.23911
C	1.31782	-1.37636	C	-2.52484	-5.0252	C	-2.41321	4.95959	0.53988
N	1.44398	-2.75501	H	-2.60502	-5.44348	H	-1.47599	5.46565	0.77834
N	3.72555	-1.31756	H	-1.78915	-5.61278	H	-2.87553	5.48525	-0.30407
N	3.69582	1.38004	H	-3.48995	-5.18015	H	-3.07919	5.09094	1.39707
N	1.39528	2.74337	C	0.35523	-6.04452	C	-4.43875	2.72702	1.09585
C	0.40376	-3.58478	H	0.0097	-6.7795	H	-5.20651	2.9022	0.33394
C	0.98222	-4.83433	H	-0.4882	-5.78259	H	-4.78428	1.91599	1.73507
C	2.3726	-4.74307	H	1.08694	-6.5566	H	-4.39256	3.6303	1.70969
C	2.64837	-3.44516	C	3.38256	-5.82663	C	-4.51088	-0.08507	0.22767
C	3.84597	-2.6992	H	4.36488	-5.4075	C	-5.07015	-0.68776	1.35832
C	5.15333	-2.94252	H	3.49506	-6.4927	C	-5.35585	0.48382	-0.72992
C	5.83519	-1.67821	H	3.09229	-6.45487	C	-6.45518	-0.72585	1.52307
C	4.93738	-0.67399	C	5.76437	-4.25979	H	-4.42454	-1.13327	2.10868
C	4.94016	0.77819	H	5.00108	-5.00481	C	-6.73916	0.4623	-0.54914
C	5.87506	1.81097	H	6.40766	-4.66913	H	-4.93445	0.94833	-1.61602
C	5.17445	3.04914	H	6.38996	-4.15113	C	-7.29826	-0.14659	0.57466
C	3.81696	2.76243	C	7.2606	-1.52534	H	-6.8741	-1.20338	2.3841
C	2.57524	3.46365	H	7.97052	-1.59626	H	-7.3766	0.91667	-1.27861
C	2.19853	4.74739	H	7.42799	-0.57051	C	-8.82604	-0.17955	0.76553
C	0.77804	4.80084	H	7.52851	-2.31466	C	-9.2263	-1.4848	1.47808
C	0.29099	3.54656	C	7.37167	1.71383	H	-8.85409	-1.47215	2.48117
N	-1.09206	1.53922	H	7.74167	1.79489	H	-10.2928	-1.56964	1.49443
C	-2.43545	1.21937	H	7.73757	0.77137	H	-8.8101	-2.3195	0.95372
C	-3.0225	-0.0526	H	7.84051	2.51962	C	-9.2629	1.02581	1.61867
C	-2.43417	-1.29938	C	5.85204	4.38965	H	-9.0298	1.9326	1.10069
N	-1.04614	-1.60148	H	6.22622	4.67539	H	-10.31737	0.97575	1.79327
C	-3.11144	-2.5423	H	5.18346	5.18007	H	-8.74506	1.00659	2.55482
C	-2.17089	-3.56541	H	6.71333	4.37922	C	-9.51668	-0.11263	-0.60929
C	-0.88904	-2.98534	C	3.10553	5.87373	H	-9.34221	0.84677	-1.04976
C	-0.96475	2.93011	H	3.37808	6.51342	H	-9.11867	-0.87504	-1.24586
C	-2.18359	3.50351	H	4.02948	5.50671	H	-10.56902	-0.26313	-0.48749

3e$^+$-H (Et groups are replaced with H atoms)

C	-1.94964	5.3149	C	1.62468	4.90295	6.18054	C	-0.69868	-2.33323	-1.04556
C	-3.16243	5.40229	4.22346	C	0.36811	5.20793	5.82565	C	-0.39993	-1.10155	-1.50331
C	-3.51184	4.53724	3.2638	N	-1.63497	6.14488	5.66558	C	-0.63486	0.00063	-0.77429
C	-2.6925	3.55664	2.79141	N	-3.93892	6.31113	4.65293	H	1.17963	0.23232	1.73517
C	-1.43964	3.46593	3.34194	N	-4.69646	4.73641	2.84335	H	2.53079	1.54037	3.58852
C	-1.11775	4.36372	4.31546	C	-5.51019	5.63446	3.24396	H	-5.76639	2.14526	-0.05407
N	0.00743	4.39563	4.90981	C	-6.64956	5.50579	2.54871	H	-3.66286	0.58589	-0.39102
N	-3.24924	2.84882	1.86832	C	-6.46289	4.47353	1.70722	H	2.95548	3.34026	5.43382
C	-2.82265	1.85701	1.18807	C	-5.21887	4.02961	1.9368	H	2.23531	5.40486	6.94102
C	-1.456	1.16229	1.28592	C	-3.63258	7.14621	5.56304	H	-7.55382	6.11909	2.64522
C	-0.38504	1.67911	2.25836	C	-4.70215	7.93703	5.73759	H	-7.18627	4.08022	0.98289
N	-0.47747	2.64674	3.08514	C	-5.64607	7.51122	4.8746	H	-4.79163	8.77008	6.44564
C	0.81738	1.08575	2.32115	C	-5.11473	6.47656	4.20727	H	-6.65149	7.92974	4.74403
C	1.50528	1.74116	3.2565	C	-0.5009	6.14164	6.2334	H	0.30915	7.42498	7.80117
C	0.65928	2.68386	3.6875	C	-0.50997	7.13859	7.13024	H	-2.08102	8.57351	7.63609
C	-4.44746	3.05638	1.44595	C	-1.72289	7.72093	7.04602	F	-2.0366	-1.43235	2.15133
C	-4.81219	2.20191	0.48313	C	-2.40698	7.05764	6.10158	F	-1.563	-3.61997	0.68629
C	-3.74586	1.41881	0.3177	C	-1.18048	-0.10103	0.4456	F	-0.46112	-3.43906	-1.78258
C	0.93308	3.58131	4.63725	C	-1.48637	-1.31472	0.92418	F	0.15097	-0.91723	-2.72194
C	1.98855	3.85744	5.41674	C	-1.24625	-2.40761	0.18396	F	-0.3236	1.21861	-1.26636

3e$^+$-Me (Et groups are replaced with Me groups)

C	-0.93632	-3.57803	-0.24695	C	-3.92332	5.79127	-1.04419	C	-0.67953	-6.04331	-1.06015
N	0.47447	-1.57505	-0.10809	H	-4.91047	5.3695	-1.24613	H	0.32762	-5.77774	-1.38555
C	1.83018	-1.25494	0.17701	H	-4.02809	6.51042	-0.22184	H	-0.59402	-6.8296	-0.29986
C	2.4342	0.00019	-0.03034	H	-3.62701	6.36341	-1.9284	H	-1.18917	-6.49035	-1.92058
C	1.85088	1.23773	-0.36822	C	-6.31263	4.3696	0.8675	C	1.76009	-4.96698	0.75722
N	0.46368	1.55309	-0.3722	H	-5.54024	5.11867	1.05196	H	0.81487	-5.44682	1.01646
C	2.53643	2.46169	-0.67686	H	-6.95077	4.73605	0.05293	H	2.22423	-5.54849	-0.04836
C	1.60358	3.49064	-0.75122	H	-6.93984	4.32571	1.7644	H	2.4158	-5.05224	1.62842
C	0.31925	2.9271	-0.61128	C	-7.83787	1.66693	1.19013	C	3.84117	-2.74086	1.10091
C	0.33078	-2.96223	-0.03642	H	-8.54829	1.67269	0.35313	H	4.58398	-2.90276	0.313
C	1.54816	-3.52751	0.38809	H	-8.01059	0.75813	1.7696	H	4.20128	-1.92272	1.72239
C	2.46787	-2.49046	0.54384	H	-8.10018	2.51414	1.83094	H	3.82387	-3.645	1.71445
C	3.98912	2.73307	-0.96072	C	-7.9859	-1.62447	0.49159	C	3.92933	0.01497	0.10303
H	4.57162	2.90817	-0.05016	H	-8.3399	-1.62253	1.53101	C	4.53405	0.57941	1.23429
H	4.46952	1.91435	-1.49437	H	-8.35003	-0.7124	0.01486	C	4.73448	-0.54092	-0.90049
H	4.07112	3.62795	-1.58271	H	-8.47152	-2.46655	-0.01033	C	5.92353	0.57731	1.36442
C	1.96474	4.94707	-0.82709	C	-6.49633	-4.32933	0.35635	C	6.12439	-0.52211	-0.77975
H	2.06944	5.31793	-1.85364	H	-6.89026	-4.66768	-0.61124	C	6.72106	0.03148	0.35566
H	1.21965	5.56239	-0.3218	H	-5.82922	-5.10589	0.73434	F	3.76323	1.11374	2.20529
H	2.9196	5.12102	-0.3235	H	-7.34574	-4.27229	1.04399	F	6.5748	1.18272	2.62177
C	-0.89679	5.92566	-1.74984	C	-3.78433	-5.90498	-0.83493	F	8.06551	0.03948	0.47765
H	-0.55167	6.71431	-1.06983	H	-4.04421	-6.50901	0.04384	F	6.99795	-1.11841	-1.89908
H	-0.05045	5.60998	-2.36013	H	-4.71438	-5.54811	-1.28199	F	4.15596	-1.084	-1.99268
H	-1.62167	6.39026	-2.42458	H	-3.31499	-6.58204	-1.55485				

3c^{3+}-H (Et groups are replaced with H atoms)

C -2.31424 -0.68195 0.14062
C -2.31252 0.68825 0.13025
C -1.14752 1.37182 -0.17265
C 0.07452 0.70883 -0.40236
C 0.07244 -0.71523 -0.39485
C -1.15203 -1.37212 -0.15905
N 1.14591 1.55767 -0.7346
C 2.48392 1.24282 -0.9203
C 3.0816 -0.00727 -0.46669
C 2.48159 -1.26154 -0.9042
N 1.14183 -1.57015 -0.71814
N -1.27499 2.73701 -0.29162
N -3.48131 1.35641 0.39055
N -3.48737 -1.34267 0.4003
N -1.28463 -2.73766 -0.26824
C 0.95115 2.92016 -1.10627
C 2.14862 3.36864 -1.69116
C 3.10163 2.33496 -1.55617
C 3.09776 -2.36401 -1.52395
C 2.14195 -3.39627 -1.64853
C 0.94448 -2.9368 -1.07204
C -0.28619 -3.56441 -0.71164
C -0.80573 -4.89654 -0.65683
C -2.14794 -4.82696 -0.25351
C -2.47259 -3.46167 0.00737
C -3.6164 -2.7184 0.38819
C -4.98706 -2.97976 0.76794
C -5.64019 -1.75972 0.94196
C -4.69076 -0.69344 0.72718
C -4.67998 0.71625 0.74823
C -5.59987 1.78931 1.04587
C -4.94707 3.00526 0.83896
C -3.59725 2.73304 0.39593
C -2.45684 3.46848 -0.00922
C -2.13064 4.82932 -0.29006
C -0.79173 4.88997 -0.70566
C -0.27644 3.55572 -0.74928
C 4.23848 -0.00354 0.33928
C 4.84262 1.21612 0.82087
C 5.97119 1.22799 1.58472
C 6.62797 0.0031 1.96651
C 5.97277 -1.22531 1.59149
C 4.83917 -1.21927 0.83543
N 7.76179 0.00716 2.67334
C 8.47683 -1.24038 2.99803
C 8.35368 1.26212 3.17313
H 4.37749 2.16481 0.58661
H 6.37266 2.17956 1.90839
H 6.35409 -2.17109 1.95455
H 4.3603 -2.16765 0.62818
H 8.49394 -1.91012 2.1367
H 9.50626 -0.99488 3.25602
H 8.0106 -1.74504 3.85198
H 8.79215 1.83822 2.35119
H 7.60202 1.86572 3.68705
H 9.13886 1.01803 3.88668
H -0.26541 5.80147 -0.89817
H -2.77432 5.68204 -0.23135
H 2.34541 4.28552 -2.20644
H 4.0932 2.37305 -1.95646
H -5.37292 3.97173 1.01062
H -6.60926 1.68498 1.38523
H -6.67933 -1.65734 1.17564
H -5.43731 -3.93857 0.91918
H -2.79414 -5.677 -0.18464
H -0.27901 -5.81122 -0.83246
H 2.33692 -4.31954 -2.15297
H 4.08988 -2.41 -1.92204

3c^{3+}-Me (Et groups are replaced with Me groups)

C -0.80242 0.70443 -0.9784	C 0.23983 -4.66823 -1.83257	H 0.59534 6.61955 -2.51792
C -0.89075 -0.6294 -0.97508	C 0.71047 -3.43652 -2.10176	H 0.0367 6.62609 -0.31402
C 0.01336 -1.33362 -1.66822	C 3.53445 -0.30336 -5.73279	H -1.602 6.25146 -0.93401
C 0.9873 -0.76417 -2.42479	C 3.51643 -1.4279 -6.48988	H -0.98815 5.65659 0.69766
C 1.07269 0.60155 -2.43523	C 3.90467 -1.52826 -7.77358	H -3.14233 5.04543 0.00769
C 0.18104 1.29358 -1.67627	C 4.27736 -0.4639 -8.5037	H -4.28944 4.35492 1.10536
N 1.79492 -1.5985 -2.9814	C 4.11104 0.69575 -7.84399	H -2.67866 4.78004 1.77034
C 2.74541 -1.38145 -3.81291	C 3.71638 0.75511 -6.55821	H -5.38455 1.8063 1.41217
C 3.13299 -0.2399 -4.41329	N 4.67272 -0.55613 -9.75606	H -4.27128 1.00843 2.65068
C 2.87896 0.95771 -3.84856	C 5.16532 1.98608 -4.50656	H -4.39084 2.72821 2.58063
N 1.97269 1.32036 -3.01414	C 3.88835 4.38 -3.27449	H -5.39875 -0.32762 1.1343
N -0.12985 -2.62287 -1.54597	C 1.3861 5.84167 -2.43484	H -5.60264 -2.00962 1.40005
N -1.83267 -1.17912 -0.31686	C -0.74015 5.83249 -0.36905	H -4.69408 -1.11227 2.64947
N -1.65174 1.38126 -0.31182	C -3.20103 4.36408 0.88058	H -4.77426 -3.84669 1.27039
N 0.20935 2.59323 -1.5567	C -4.39567 1.83374 1.9209	H -3.89602 -4.57497 -0.05512
C 1.72523 -2.87464 -2.7792	C -4.85991 -1.20092 1.55307	H -3.17243 -4.45919 1.63882
C 2.80354 -3.48139 -3.30047	C -3.75591 -3.94263 0.84624	H -1.74259 -5.57859 0.63318
C 3.48522 -2.50715 -3.90592	C -1.56181 -5.71844 -0.45121	H -2.49975 -5.93051 -1.00973
C 3.74378 1.98674 -3.97682	C 0.60407 -5.98586 -2.4619	H -0.95079 -6.6464 -0.47479
C 3.19652 3.05095 -3.38413	C 3.32347 -4.88296 -3.1513	H -0.29249 -6.62686 -2.6118
C 2.06119 2.59782 -2.82788	C 4.89201 -2.69322 -4.44089	H 0.96678 -5.8454 -3.50072
C 1.1419 3.28833 -2.12934	C 5.13088 0.63342 -10.5924	H 1.32252 -6.56569 -1.84205
C 0.84596 4.57005 -1.83928	C 4.72377 -1.87778 -10.51494	H 2.9993 -5.53253 -3.99306
C -0.22123 4.5778 -1.01265	H 3.13133 -2.38409 -6.10808	H 4.43338 -4.92176 -3.15548
C -0.63778 3.3071 -0.86862	H 3.88017 -2.53479 -8.22328	H 3.06038 -5.30581 -2.15962
C -1.62826 2.6556 -0.2328	H 4.24615 1.65762 -8.3651	H 5.55123 -3.03386 -3.61076
C -2.68079 3. 0.52838	H 3.50626 1.78322 -6.23252	H 4.95044 -3.46344 -5.2426
C -3.26464 1.85444 0.93197	H 5.54253 0.98822 -4.81574	H 5.38409 -1.7573 -4.78089
C -2.60349 0.83689 0.34707	H 5.32459 2.72325 -5.32542	H 5.60634 1.43202 -9.9837
C -2.71108 -0.50932 0.3257	H 5.85711 2.26283 -3.679	H 5.91529 0.3262 -11.31976
C -3.56626 -1.42418 0.82207	H 4.99289 4.29416 -3.34651	H 4.2672 1.05334 -11.15604
C -3.09516 -2.64265 0.48404	H 3.59243 5.06244 -4.10028	H 5.53619 -2.52335 -10.1106
C -1.98296 -2.4452 -0.24726	H 3.73586 4.82766 -2.2708	H 3.74672 -2.40832 -10.46202
C -1.07423 -3.22034 -0.87043	H 2.2072 6.27818 -1.82524	H 4.92174 -1.72096 -11.59835
C -0.8363 -4.53612 -1.02847	H 1.68112 5.69226 -3.49348	

3e^{3+}-H (Et groups are replaced with H atoms)

C 3.02371 -0.66304 0.00627	C 2.8239 -4.52736 -0.00141	C -6.63387 0.00165 0.12256
C 3.02105 0.66466 0.00543	C 3.1053 -3.21638 0.0067	C -5.98693 -0.00581 -1.05949
C 1.84878 1.3099 -0.0222	N 4.14564 -1.2586 0.03171	C -4.64674 -0.00879 -1.13274
C 0.63889 0.68419 -0.04867	N 4.14091 1.26355 0.03012	H -3.36085 -2.65554 -0.14047
C 0.64115 -0.6873 -0.04772	N 1.99437 2.57425 -0.02144	H -1.51608 -4.54423 -0.10563
C 1.85273 -1.31074 -0.02051	C 3.09625 3.21801 0.00261	H -1.52576 4.53747 -0.11212
N 2.00237 -2.57482 -0.0181	C 2.81435 4.52894 -0.00716	H -3.36622 2.64496 -0.14476
N -0.34725 1.51486 -0.07286	C 1.47341 4.6257 -0.03913	H 0.89442 -5.54987 -0.04819
C -1.60965 1.33055 -0.10041	C 1.01192 3.367 -0.04671	H 3.54232 -5.35606 0.01421
C -2.36983 -0.00438 -0.09167	C 5.26918 0.67548 0.05621	H 3.53239 5.358 0.00747
C -1.60687 -1.33762 -0.09829	C 6.20524 1.63633 0.07636	H 0.8839 5.55028 -0.05546
N -0.34403 -1.51898 -0.0707	C 5.5528 2.81578 0.05989	H 7.29222 1.49075 0.10097
C -2.27515 -2.50161 -0.11801	C 4.24349 2.52766 0.03049	H 6.00491 3.81508 0.06847
C -1.34905 -3.46058 -0.09966	C 4.25035 -2.52255 0.03364	H 6.01591 -3.80406 0.07321
C -0.18791 -2.79649 -0.06991	C 5.56069 -2.80616 0.06337	H 7.29646 -1.47627 0.10278
C -0.19347 2.79298 -0.07376	C 6.20987 -1.62475 0.07836	F -3.79979 0.00634 2.3111
C -1.35622 3.4542 -0.10465	C 5.27151 -0.66614 0.05705	F -6.47176 0.0128 2.4411
C -2.28024 2.49319 -0.1219	C -3.90992 -0.00478 -0.01326	F -7.98211 0.00518 0.19144
C 1.01905 -3.36649 -0.04227	C -4.52914 0.00208 1.17509	F -6.65881 -0.00961 -2.23041
C 1.48285 -4.62454 -0.03311	C -5.86953 0.00543 1.23289	F -4.03303 -0.01488 -2.33517

3e^{3+}-Me (Et groups are replaced with Me groups)

C -3.10719 0.68962 0.05134	C 1.60358 3.49064 -0.75122	H -8.47152 -2.46655 -0.01033
C -3.11007 -0.68502 0.08918	C 0.31925 2.9271 -0.61128	C -6.49633 -4.32933 0.35635
C -1.90757 -1.37393 0.01086	C 0.33078 -2.96223 -0.03642	H -6.89026 -4.66768 -0.61124
C -0.65798 -0.71706 -0.11039	C 1.54816 -3.52751 0.38809	H -5.82922 -5.10589 0.73434
C -0.65583 0.70652 -0.16901	C 2.46787 -2.49046 0.54384	H -7.34574 -4.27229 1.04399
C -1.90147 1.37281 -0.06699	C 3.98912 2.73307 -0.96072	C -3.78433 -5.90498 -0.83493
N -2.01357 2.74869 -0.18094	H 4.57162 2.90817 -0.05016	H -4.04421 -6.50901 0.04384
N -4.30862 1.35218 0.12965	H 4.46952 1.91435 -1.49437	H -4.71438 -5.54811 -1.28199
N -4.31011 -1.34676 0.18358	H 4.07112 3.62795 -1.58271	H -3.31499 -6.58204 -1.55485
N -2.02743 -2.75069 -0.0268	C 1.96474 4.94707 -0.82709	C -0.67953 -6.04331 -1.06015
C -0.96838 3.53862 -0.65034	H 2.06944 5.31793 -1.85364	H 0.32762 -5.77774 -1.38555
C -1.53426 4.77055 -1.03304	H 1.21965 5.56239 -0.3218	H -0.59402 -6.8296 -0.29986
C -2.92461 4.71372 -0.73907	H 2.9196 5.12102 -0.3235	H -1.18917 -6.49035 -1.92058
C -3.21118 3.45174 -0.2038	C -0.89679 5.92566 -1.74984	C 1.76009 -4.96698 0.75722
C -4.4142 2.7406 0.17735	H -0.55167 6.71431 -1.06983	H 0.81487 -5.44682 1.01646
C -5.71724 3.02358 0.57295	H -0.05045 5.60998 -2.36013	H 2.22423 -5.54849 -0.04836
C -6.41197 1.77439 0.73299	H -1.62167 6.39026 -2.42458	H 2.4158 -5.05224 1.62842
C -5.52603 0.73924 0.43529	C -3.92332 5.79127 -1.04419	C 3.84117 -2.74086 1.10091
C -5.54569 -0.7199 0.35947	H -4.91047 5.3695 -1.24613	H 4.58398 -2.90276 0.313
C -6.49169 -1.7431 0.39068	H -4.02809 6.51042 -0.22184	H 4.20128 -1.92272 1.72239
C -5.80647 -2.99794 0.26665	H -3.62701 6.36341 -1.9284	H 3.82387 -3.645 1.71445
C -4.44819 -2.73432 0.10428	C -6.31263 4.3696 0.8675	C 3.92933 0.01497 0.10303
C -3.21773 -3.46399 -0.13139	H -5.54024 5.11867 1.05196	C 4.53405 0.57941 1.23429
C -2.86085 -4.77107 -0.49827	H -6.95077 4.73605 0.05293	C 4.73448 -0.54092 -0.90049
C -1.44079 -4.84414 -0.57364	H -6.93984 4.32571 1.7644	C 5.92353 0.57731 1.36442
C -0.93632 -3.57803 -0.24695	C -7.83787 1.66693 1.19013	C 6.12439 -0.52211 -0.77975
N 0.47447 -1.57505 -0.10809	H -8.54829 1.67269 0.35313	C 6.72106 0.03148 0.35566
C 1.83018 -1.25494 0.17701	H -8.01059 0.75813 1.7696	F 3.76323 1.11374 2.20529
C 2.4342 0.00019 -0.03034	H -8.10018 2.51414 1.83094	F 6.5748 1.18272 2.62177
C 1.85088 1.23773 -0.36822	C -7.9859 -1.62447 0.49159	F 8.06551 0.03948 0.47765
N 0.46368 1.55309 -0.3722	H -8.3399 -1.62253 1.53101	F 6.99795 -1.11841 -1.89908
C 2.53643 2.46169 -0.67686	H -8.35003 -0.7124 0.01486	F 4.15596 -1.084 -1.99268

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