Ring-in-Ring(s) Complexes Exhibiting Tunable Multicolor Photoluminescence

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Supporting Information

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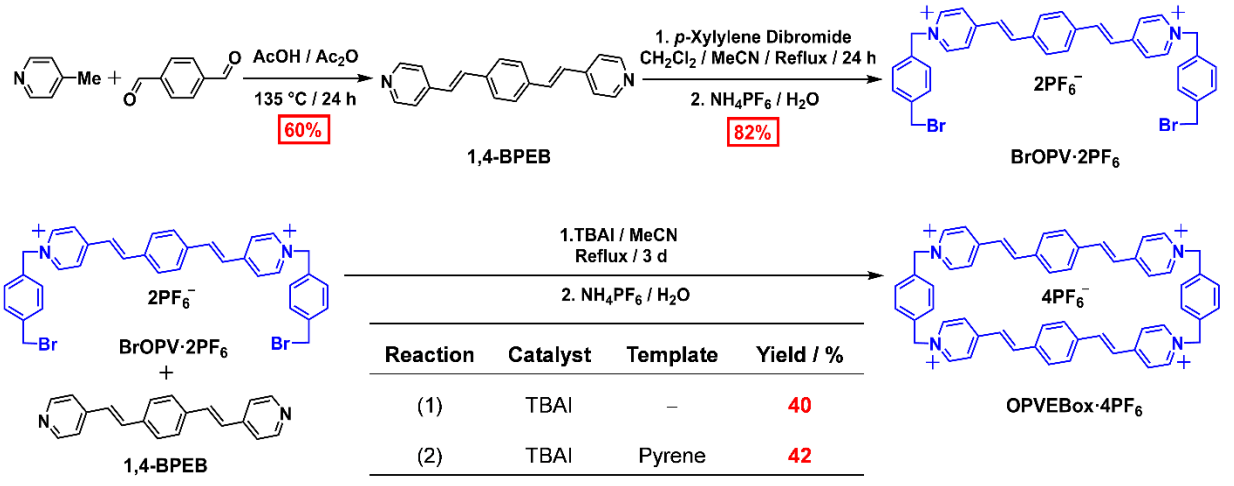
Section A. Materials / General Methods / Instruments

All solvents and reagents were obtained commercially and used without further purification unless noted otherwise. 1,4-Bis((*E*)-2-(pyridin-4-yl)vinyl)benzene (**1,4-BPEB**), 4,4'-((1*E*,1′*E*)-1,4-phenylenebis(ethene-2,1-diyl))bis(1-(4-(bromomethyl)benzyl)pyridin-1-ium) (**BrOPV**$^{2+}$) and 4,4'-((1*E*,1′*E*)-1,4-phenylenebis(ethene-2,1-diyl))bis(1-methylpyridin-1-ium) (**OPV**$^{2+}$) were prepared according to the previous literature procedures.[1] Thin-layer chromatography (TLC) was performed on silica gel 60 F254 (E Merck). Developed plates were visualized using UV light at wavelengths of 254 and 365 nm. Reverse-phase liquid chromatography was performed on Combiflash Rf 200 purification system, using C18-columns and a binary solvent system (MeCN with 0.1% TFA and H_2O with 0.1% TFA). Normal-phase column chromatography was carried out on silica gel 60F (Merck 9385, 0.040 − 0.063 mm). UV-Vis Absorption spectra were recorded in a conventional rectangular quartz cell (10 × 10 × 45 mm) on a UV-3600 Shimadzu spectrophotometer. Fluorescence spectra were measured in a rectangular quartz cell (10 × 10 × 45 mm) on a HORIBA FluoroMax-4 spectrometer, which was equipped with an integrating sphere for absolute fluorescence quantum yields determination and time-correlated single-photon counting (TCSPC) module for emission decays. All the photophysical (UV-Vis absorption and fluorescence spectroscopy) experiments were performed at 298 K in H_2O, except the nuclear magnetic resonance (NMR) experiments which were performed in CD_3CN and D_2O. NMR Spectra were recorded on a Bruker Avance III 600 MHz and Agilent 500 MHz spectrometers, with working frequencies of 600 and 500 MHz for ^{1}H NMR, as well as 150 and 125 MHz for ^{13}C NMR, respectively. 2D DOSY NMR Spectroscopy was conducted in D_2O with the concentration of **OPVEBox**·4Cl held at 0.2 mM. The spectrometer was set with the following parameters: the pulse sequence: Bruker pulse program dstebpgp3s; the relaxation delay (D1): 2 s; the diffusion time (D20): 0.06 s; the diffusion gradient pulse length (P30): 1.0 ms; the number of scan (ns): 16; the number of gradient steps: 32 steps with linear spacing; the gradient range: 2–85%. Single crystal X-ray diffraction studies were measured on a Bruker Kappa APEX2 CCD or a Rigaku XtaLAB Synergy diffractometer using Cu-Kα radiation (λ = 1.5407 Å) equipped with an Oxford cryostream variable temperature device, and data were collected using the Bruker APEX-II or Rigaku CrysAlis Pro program. Detailed experimental procedures are provided below in the appropriate sections. Cyclic voltammetry (CV) was performed on a Gamry Multipurpose instrument (Reference 600) interfaced to a PC with a three-electrode system under a N_2 atmosphere at 298 K. Microcalorimetric titrations were performed on a thermostated TA Nano Isothermal Titration Calorimeter at atmospheric pressure and 298 K, the data were analyzed with NanoAnalyze software. Electrospray ionization-mass spectra (ESI-MS) were measured on Waters Synapt G2 mass spectrometer. The specific experimental conditions were employed as follow: ESI capillary voltage, 2.0 kV; sample cone voltage, 20 V; extraction cone voltage, 0.1 V; source temperature, 120 ºC; desolvation temperature, 150 ºC; cone gas flow, 10 L/h; desolvation gas flow, 700 L/h (N_2).

Section B. Synthetic Protocols



Reaction	Catalyst	Template	Yield / %
(1)	TBAI	–	40
(2)	TBAI	Pyrene	42

Scheme S1. Synthetic routes of **OPVEBox**·$4PF_6$

OPVEBox•4PF$_6$: Two different reactions were carried out for the ring-closing step: (1) catalyst without template, (2) catalyst with a template.

(1) TBAI as a catalyst without template: **BrOPV**•$2PF_6$ (141 mg, 0.15 mmol) and **1,4-BPEB** (43 mg, 0.15 mmol) were dissolved in dry MeCN (75 mL), followed by adding 0.2 equiv of TBAI (11 mg, 0.03 mmol) as catalyst. The resulting mixture was heated at 80 ºC for 3 days under a N_2 atmosphere. After cooling to room temp, excess TBACl was added to quench the reaction resulting in a yellow precipitate which was collected by filtration and washed with Me_2CO and CH_2Cl_2. The crude precipitate was then subjected to reverse-phase C18 column chromatogram, starting with H_2O / 0.1 % TFA as eluent, followed by continuous addition of MeCN / 0.1% TFA over the course of 45 min. The fractions containing the desired product were combined, and followed by removal of MeCN by rotary evaporation under vacuum. The residual aqueous mixture was then treated with excess NH_4PF_6. The resulting yellow precipitate was separated by filtration and dried under vacuum yielding pure **OPVEBox**•$4PF_6$ (yield: 40%).

(2) TBAI as a catalyst and pyrene as a template: A solution of **BrOPV**•$2PF_6$ (141 mg, 0.15 mmol), **1,4-BPEB** (43 mg, 0.15 mmol), TBAI (11 mg, 0.03 mmol) and 6 equiv of pyrene (182 mg, 0.90 mmol) in dry MeCN (75 mL) was heated under reflux at 80 ºC for 3 days. After cooling to room temp, excess TBACl was added to quench the reaction. The resulting crude precipitate was separated by filtration, and then dissolved in H_2O in order to remove the pyrene template by continuous liquid-liquid extraction with $CHCl_3$ over 3 days. The color of aqueous phase changed

from brown to yellow. The aqueous phase was concentrated by rotary evaporation under vacuum and the resulting crude precipitate was then subjected to reverse-phase C18 column chromatography, starting with H_2O / 0.1 % TFA as eluent, followed by continuous addition of MeCN up to an eluent mixture of 99.9 % MeCN / 0.1% TFA over the course of 45 min. The fractions containing the desired product were combined and concentrated by rotary evaporation under vacuum. The residue was dissolved in H_2O and treated with excess NH_4PF_6 to afford a yellow precipitate, which after filtration and drying under a vacuum yielded pure **OPVEBox•**$4PF_6$ (yield: 42%).

^{1}H NMR (600 MHz, CD_3CN) δ 8.60 (d, *J* = 7.0 Hz, 2H), 7.90 (d, *J* = 7.0 Hz, 2H), 7.65 (d, *J* = 16.1 Hz, 3H), 7.58 (s, 2H), 7.26 (d, *J* = 16.4 Hz, 1H), 5.58 (s, 2H). ^{13}C NMR (150 MHz, CD_3CN) δ 154.9, 144.5, 141.6, 137.8, 137.1, 131.0, 129.8, 125.6, 124.7, 64.4. HRMS-ESI for **OPVEBox•**$4PF_6$; Calcd for $C_{56}H_{48}F_{24}N_4P_4$: *m/z* = 1211.2804 $[M - PF_6]^+$, 533.1598 $[M - 2PF_6]^{2+}$; Found: 1211.2807 $[M - PF_6]^+$, 533.1595 $[M - 2PF_6]^{2+}$.

OPVEBox•4Cl**:** A water-soluble counterpart of **OPVEBox•**4Cl was obtained by means of counterion exchange: Tetrabutylammonium chloride (TBACl, 300 mg) was added to a MeCN solution (4 mL) of **OPVEBox•**$4PF_6$ (100 mg). The resulting yellow precipitate was collected by centrifugation and washed with Me_2CO to give the desired compound **OPVEBox•**4Cl (67 mg) as a yellow powder (yield: 99%).

^{1}H NMR (600 MHz, D_2O) δ 8.74 (d, *J* = 6.6 Hz, 2H), 7.95 (d, *J* = 6.2 Hz, 2H), 7.64 (m, 5H), 7.26 (d, *J* = 16.3 Hz, 1H), 5.71 (s, 2H). ^{13}C NMR (125 MHz, D_2O) δ 153.9, 143.2, 140.2, 136.7, 135.9, 129.9, 128.7, 124.6, 123.8, 63.4. ESI-TOF for **OPVEBox•**4Cl; Calcd for $C_{56}H_{48}Cl_4N_4$: *m/z* = 194.10 $[M - 4Cl]^{4+}$, 258.46 $[M - 4Cl - H]^{3+}$, 423.16 $[M - 2Cl]^{2+}$, Found: 194.10 $[M - 4Cl]^{4+}$, 258.46 $[M - 4Cl - H]^{3+}$, 423.16 $[M - 2Cl]^{2+}$.

Section C. NMR Spectroscopy

(1) The ^{1}H NMR and ^{13}C NMR spectroscopy of the target products: OPVEBox•$4PF_6$ and OPVEBox•4Cl

Chemical shifts are reported in ppm relative to the signals corresponding to the residual non-deuterated solvents (CD_3CN: δ_H = 1.96 ppm and δ_C = 1.32 and 118.26 ppm; D_2O: δ_H = 4.79 ppm).

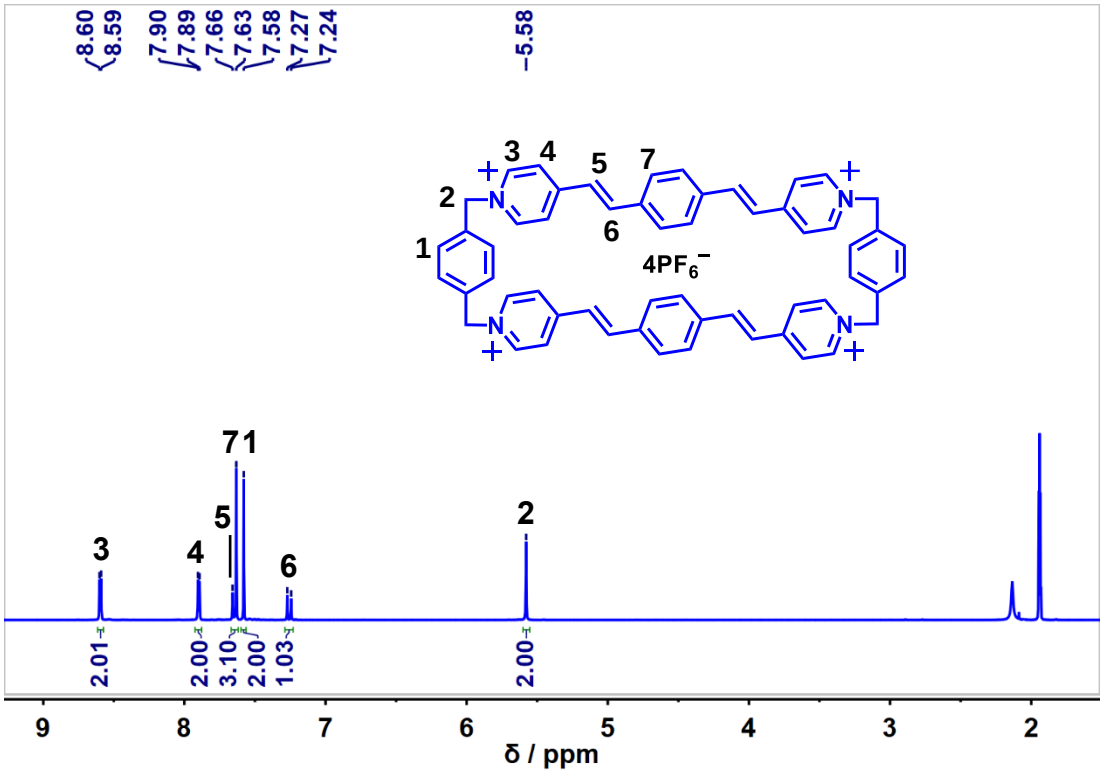


Figure S1. ^{1}H NMR spectrum (600 MHz, CD_3CN, 298 K) of **OPVEBox**•$4PF_6$

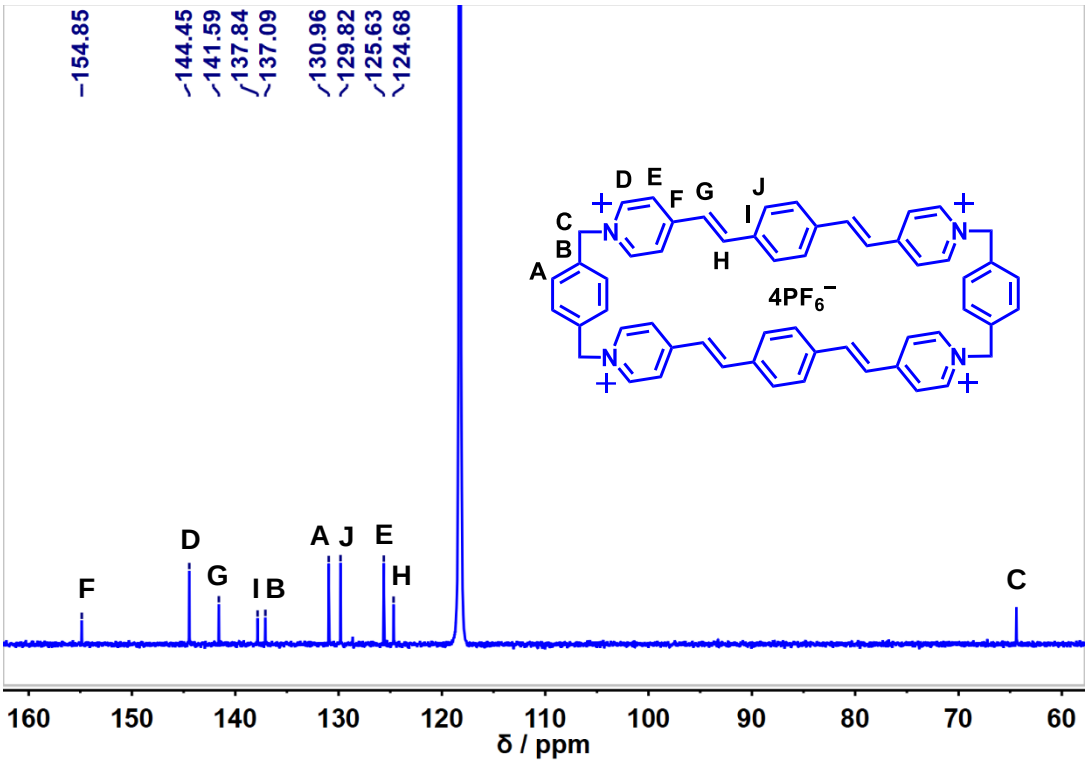


Figure S2. ^{13}C NMR spectrum (150 MHz, CD_3CN, 298 K) of **OPVEBox**•$4PF_6$

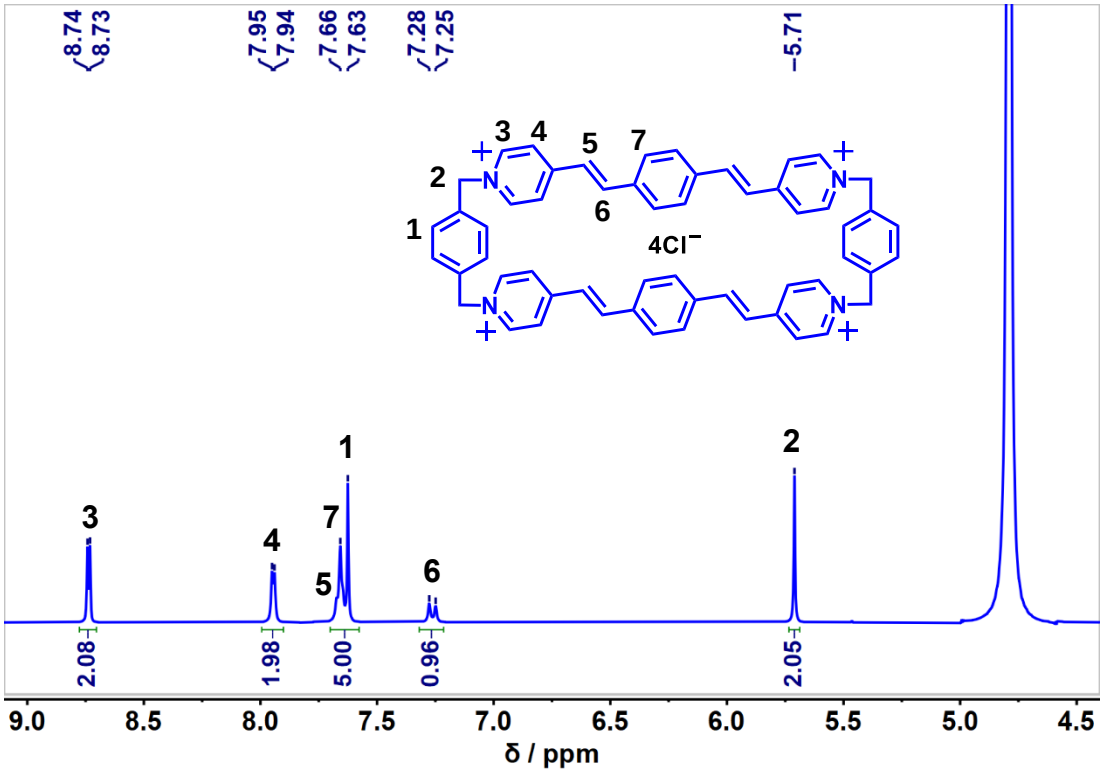


Figure S3. ^{1}H NMR spectrum (600 MHz, D_2O, 298 K) of **OPVEBox•**4Cl

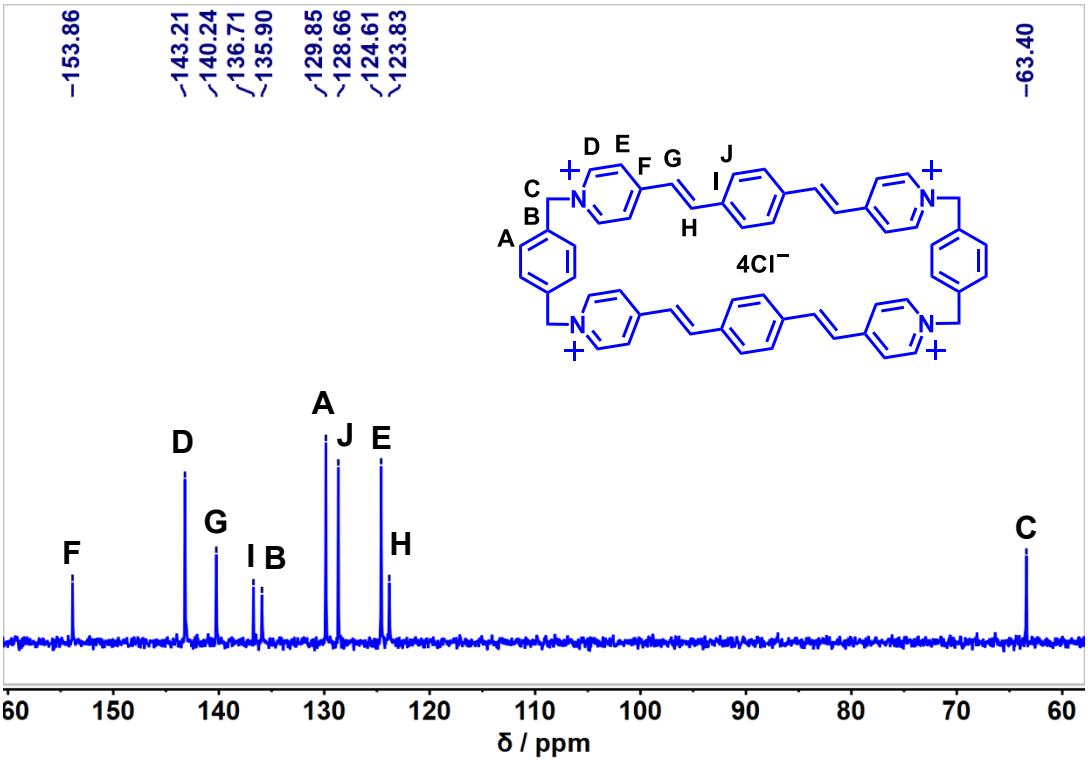


Figure S4. ^{13}C NMR spectrum (125 MHz, D_2O, 298 K) of **OPVEBox•**4Cl

(2) The two-dimensional COSY, ROESY, HSBC, HMQC NMR spectroscopy of OPVEBox•4PF$_6$. and OPVEBox•4Cl

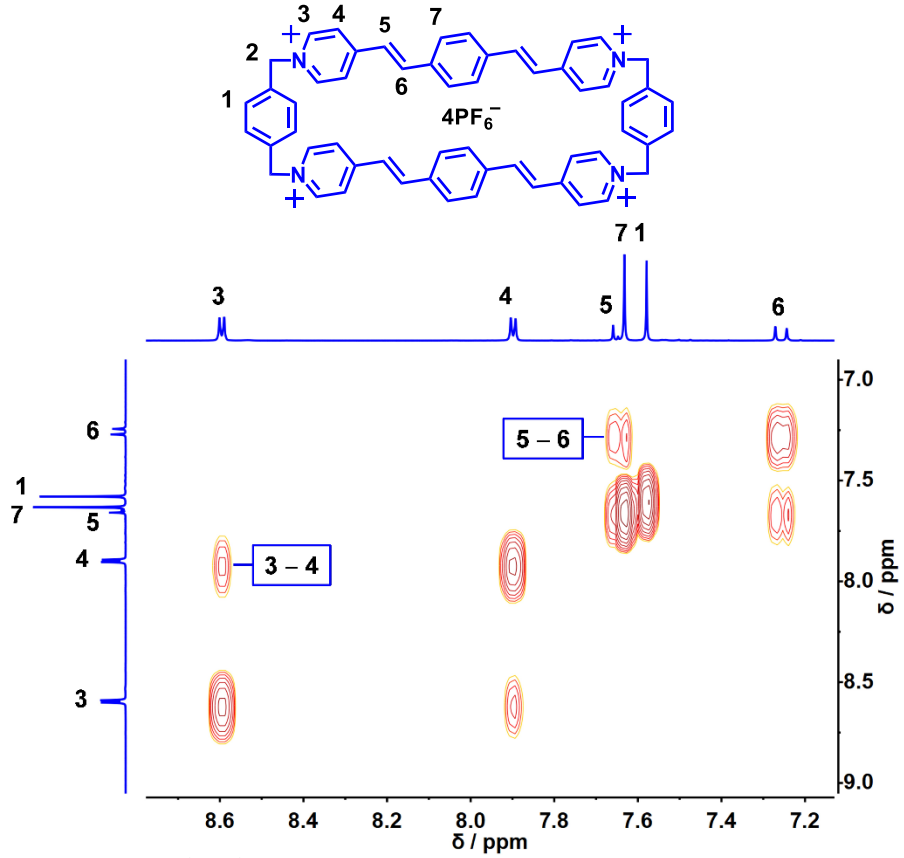


Figure S5. Annotated 2D ^{1}H–^{1}H COSY NMR spectrum (600 MHz, CD_3CN, 298 K) of **OPVEBox**•4PF$_6$

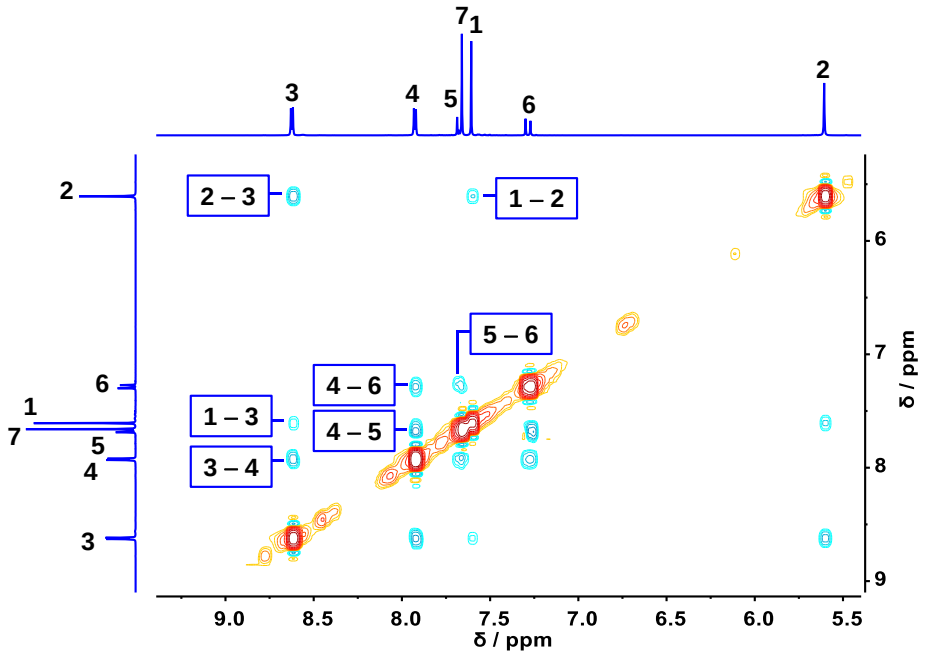


Figure S6. Annotated 2D ^{1}H–^{1}H ROESY NMR spectrum (600 MHz, CD_3CN, 298 K) of **OPVEBox**•4PF$_6$.

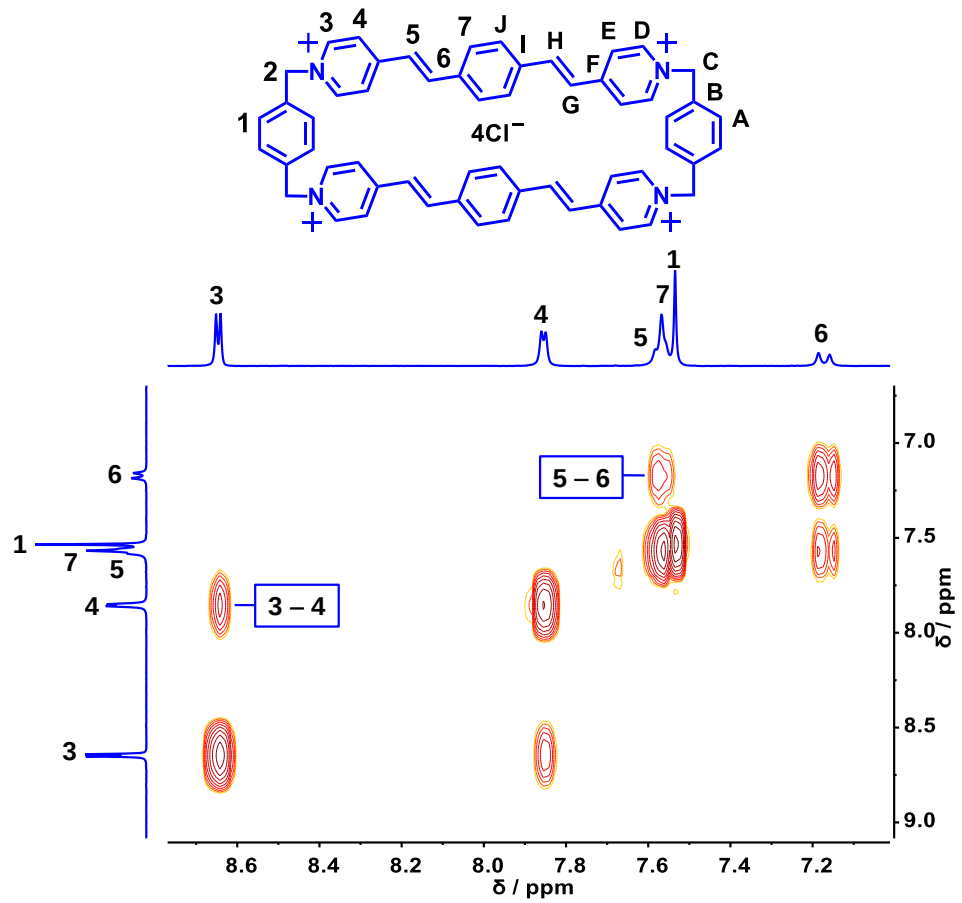


Figure S7. Annotated 2D ^{1}H–^{1}H COSY NMR spectrum (600 MHz, D_2O, 298 K) of **OPVEBox•**4Cl

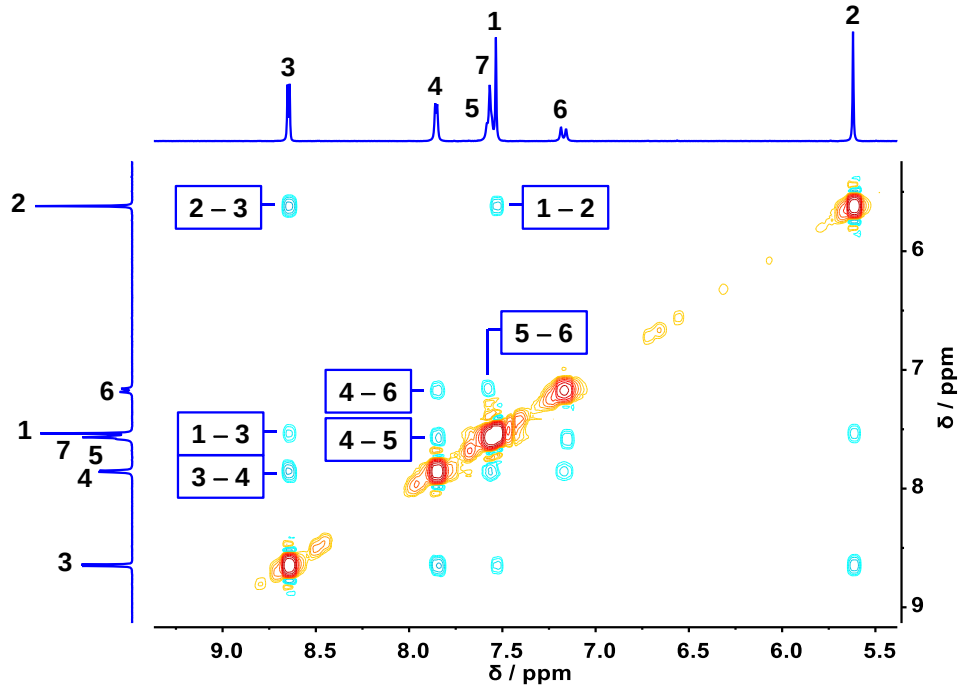


Figure S8. Annotated 2D ^{1}H–^{1}H ROESY NMR spectrum (600 MHz, D_2O, 298 K) of **OPVEBox•**4Cl

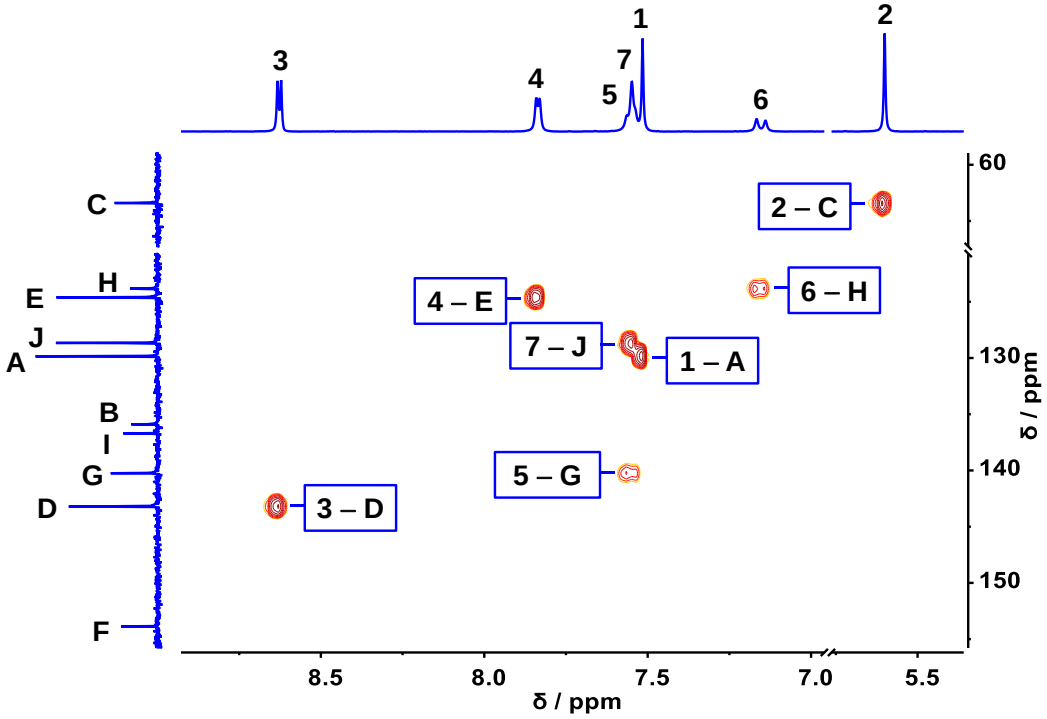


Figure S9. Annotated $^{1}H–^{13}C$ Heteronuclear Single Quantum Coherence (HSQC) NMR spectrum (600 MHz, D_2O, 298 K) of **OPVEBox•**4Cl

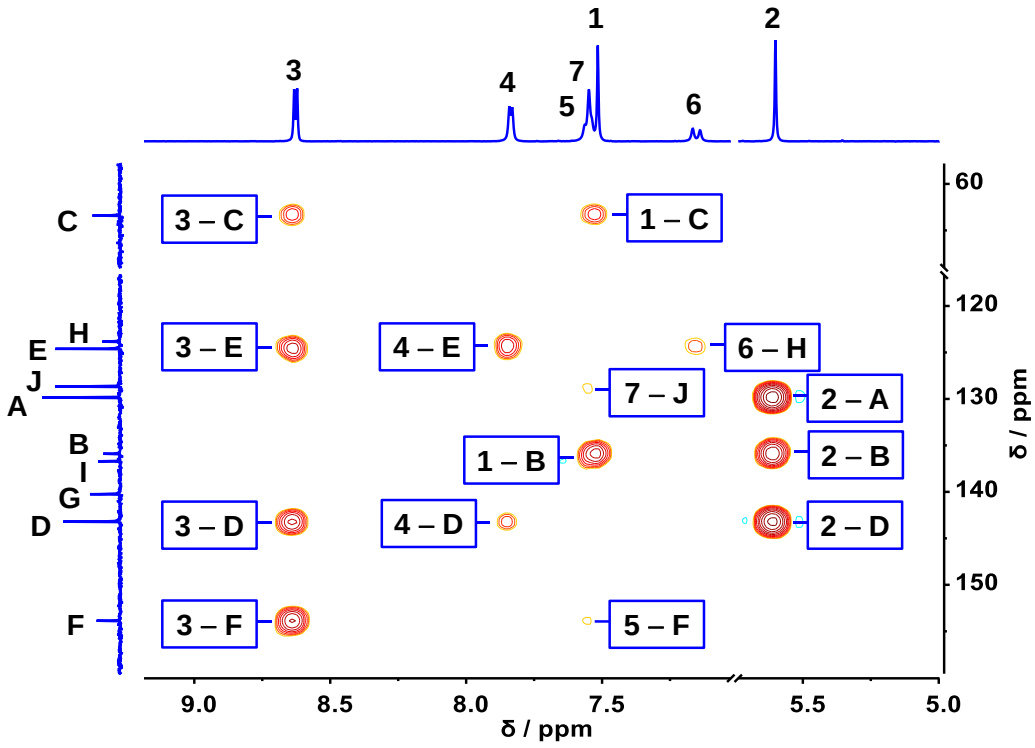


Figure S10. Annotated $^{1}H–^{13}C$ Heteronuclear Multiple Bond Coherence (HMBC) NMR spectrum (600 MHz, D_2O, 298 K) of **OPVEBox•**4Cl

(3) The one-dimensional ^{1}H NMR and two-dimensional ^{1}H–^{1}H COSY and ROESY NMR spectroscopy of OPVEBox^{4+}⊂CB[8] ring-in-ring complex

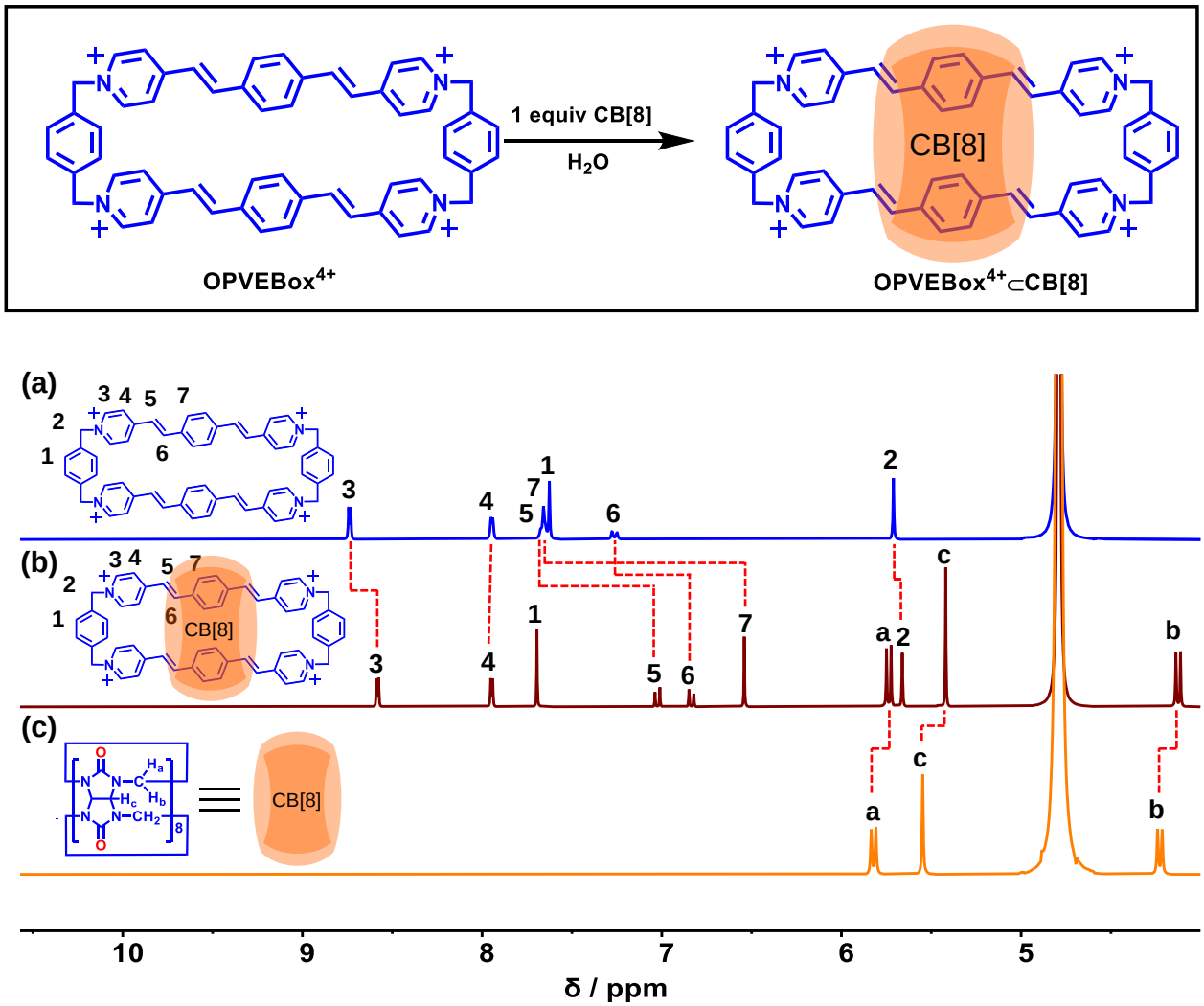


Figure S11. ^{1}H NMR Spectra (600 MHz, [**OPVEBox^{4+}**] = [**CB[8]**] = 2.0 × 10^{-4} M, D_2O, 298 K) of (a) **OPVEBox^{4+}**, (b) **OPVEBox^{4+}⊂CB[8]** ring-in-ring complex, and (c) **CB[8]** showing the chemical shift changes of **OPVEBox^{4+}** and **CB[8]** upon forming the binary **OPVEBox^{4+}⊂CB[8]** ring-in-ring complex. The chemical shifts of proton H-7 residing on the central phenylene groups and the protons (H-5 and H-6) residing on the C=C double bonds show large upfield shifts (Δδ = –0.64, –0.43 and –1.12 for H-5, H-6, and H-7, respectively), together with the small upfield shifts of the signal for protons on **CB[8]** (Δδ = –0.09, –0.11 and –0.13 for H-a, H-b, and H-c, respectively), indicating that **CB[8]** is bound in the middle of **OPVEBox^{4+}** to form the 1:1 ring-in-ring structure.

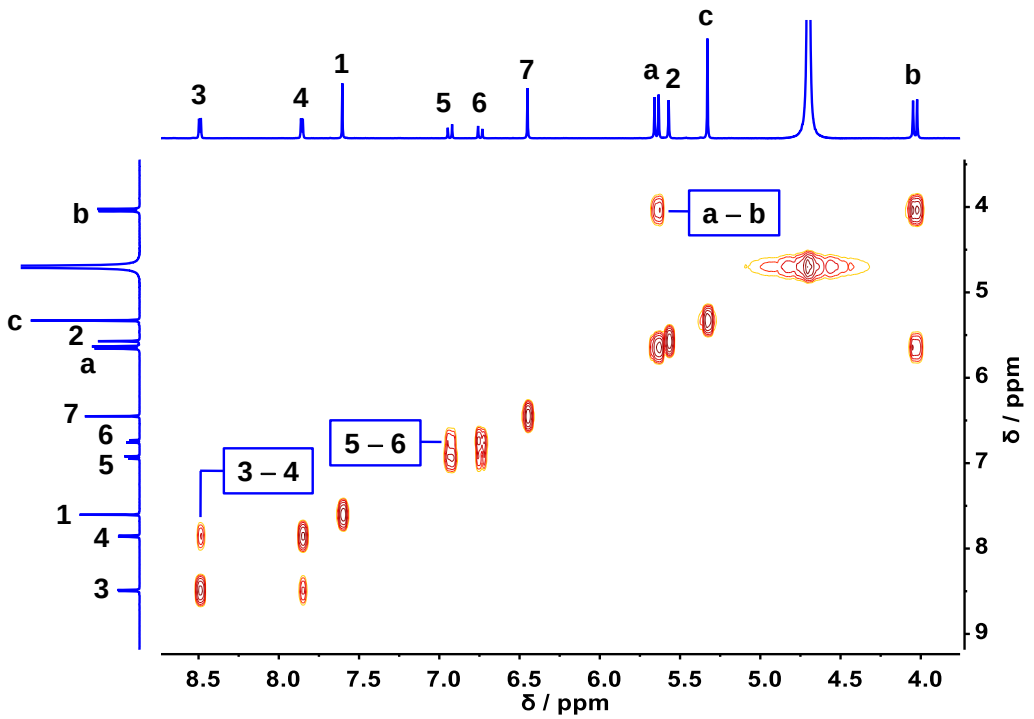


Figure S12. Annotated 2D ^{1}H–^{1}H COSY NMR spectrum (600 MHz, D_2O, 298 K) of **OPVEBox^{4+}⊂CB[8]** ring-in-ring complex

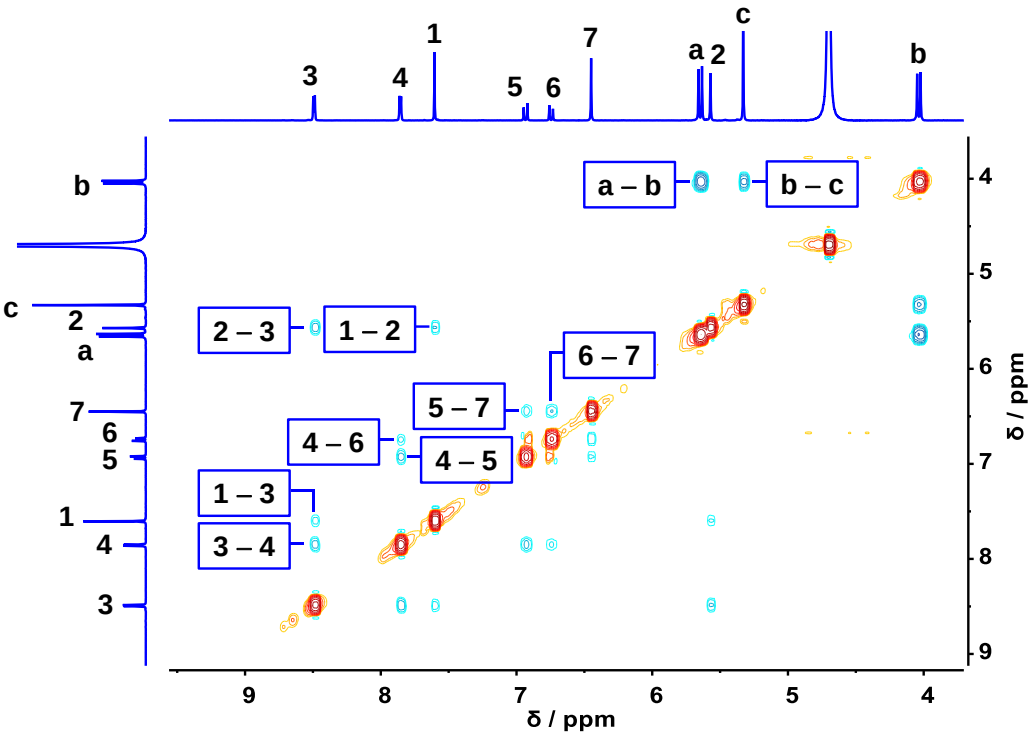


Figure S13. Annotated 2D ^{1}H–^{1}H ROESY NMR spectrum (600 MHz, D_2O, 298 K) of **OPVEBox^{4+}⊂CB[8]** ring-in-ring complex

(4) The one-dimensional ^{1}H NMR and two-dimensional ^{1}H–^{1}H COSY and ROESY NMR spectroscopy of OPVEBox^{4+}⊂2CB[8] ring-in-rings complex

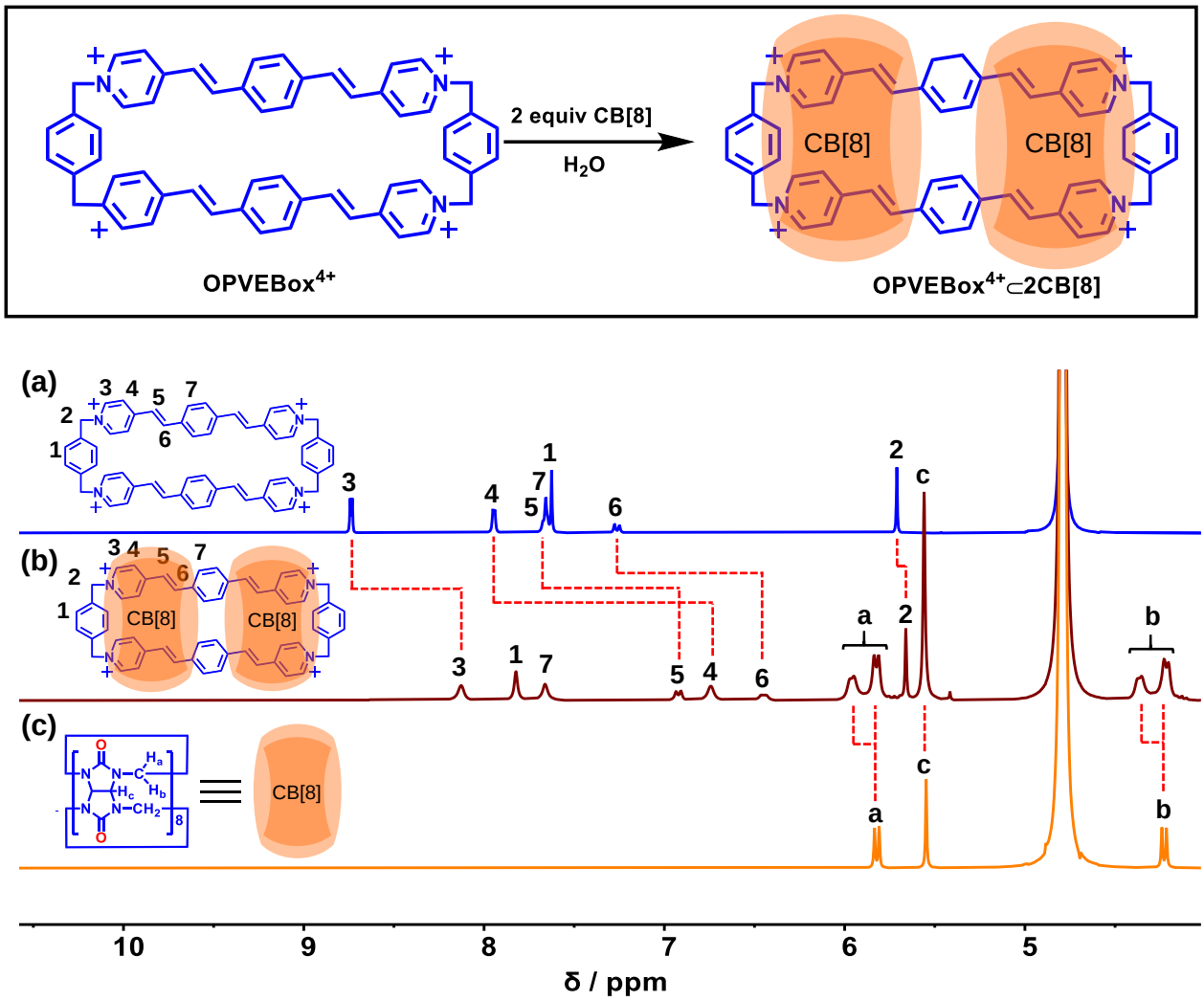


Figure S14. ^{1}H NMR Spectra (600 MHz, [**OPVEBox^{4+}**] = 2.0 × 10^{-4}, [**CB[8]**] = 4.0 × 10^{-4} M, D_2O, 298 K) of (a) **OPVEBox^{4+}**, (b) **OPVEBox^{4+}⊂2CB[8]** ring-in-rings complex, and (c) **CB[8]**, showing the chemical shift changes of **OPVEBox^{4+}** and **CB[8]** upon forming the **OPVEBox^{4+}⊂2CB[8]** ring-in-rings complex. All the protons residing on the pyridinium groups and the C=C double bonds display large upfield shifts (Δδ = –0.61, –1.20, –0.75 and –0.81 for H-3, H-4, H-5, and H-6, respectively), while the chemical shift of H-7 showed no change, indicating that two **CB[8]** molecules are bound to the two ends of **OPVEBox^{4+}** to form the 1:2 ring-in-rings superstructure. All the methylene protons (H-a and H-b) on **CB[8]** were split into two sets of peaks (δ = 5.96 / 5.82 and 4.36 / 4.22 for H-a and H-b, respectively), indicating that the centrosymmetric geometry of **CB[8]** molecules has been broken.

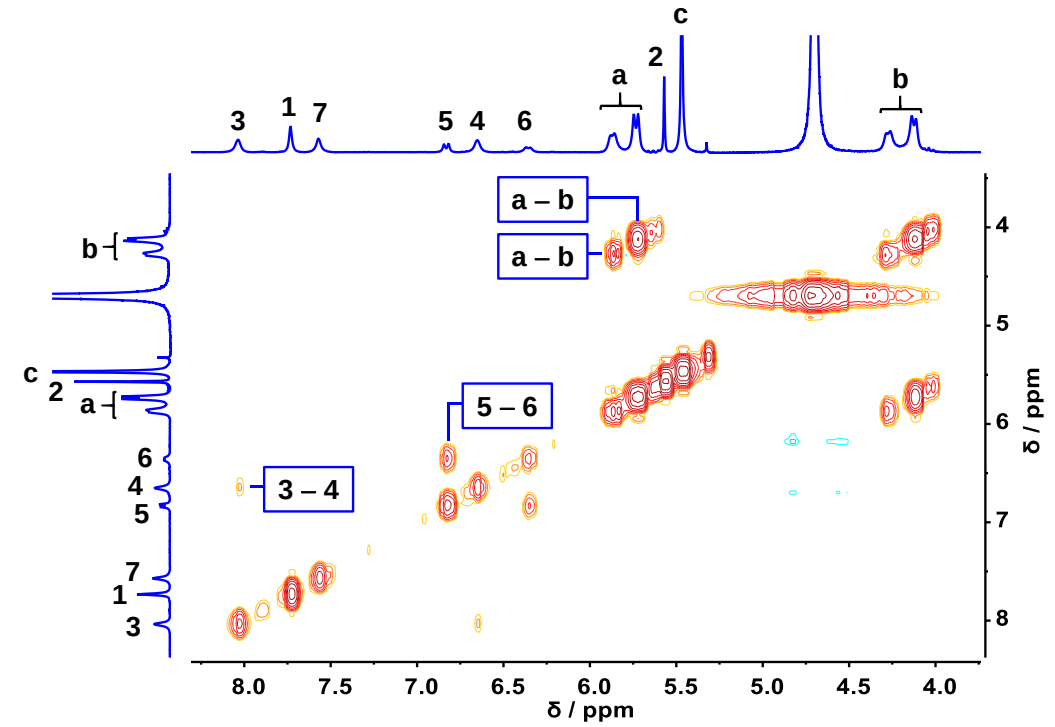


Figure S15. Annotated 2D ^{1}H–^{1}H COSY NMR spectrum (600 MHz, D_2O, 298 K) of **OPVEBox^{4+}⊂2CB[8]** ring-in-rings complex

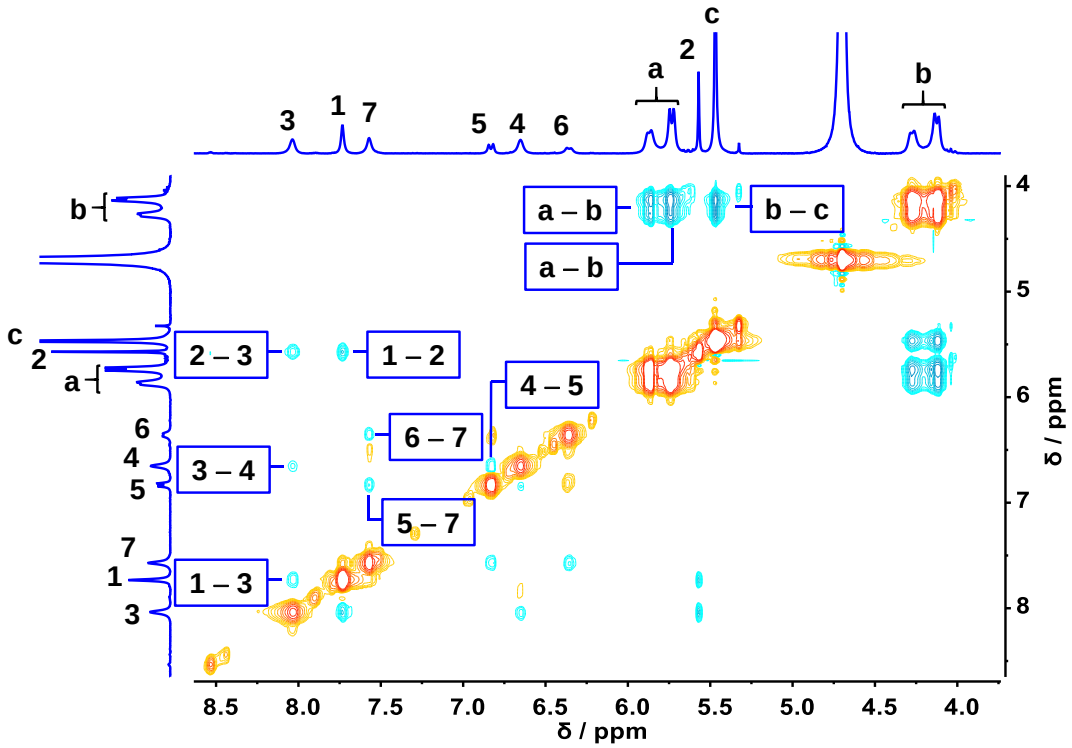


Figure S16. Annotated 2D ^{1}H–^{1}H ROESY NMR spectrum (600 MHz, D_2O, 298 K) of **OPVEBox^{4+}⊂2CB[8]** ring-in-rings complex

(5) The two-dimensional DOSY spectroscopy characterization of OPVEBox^{4+}

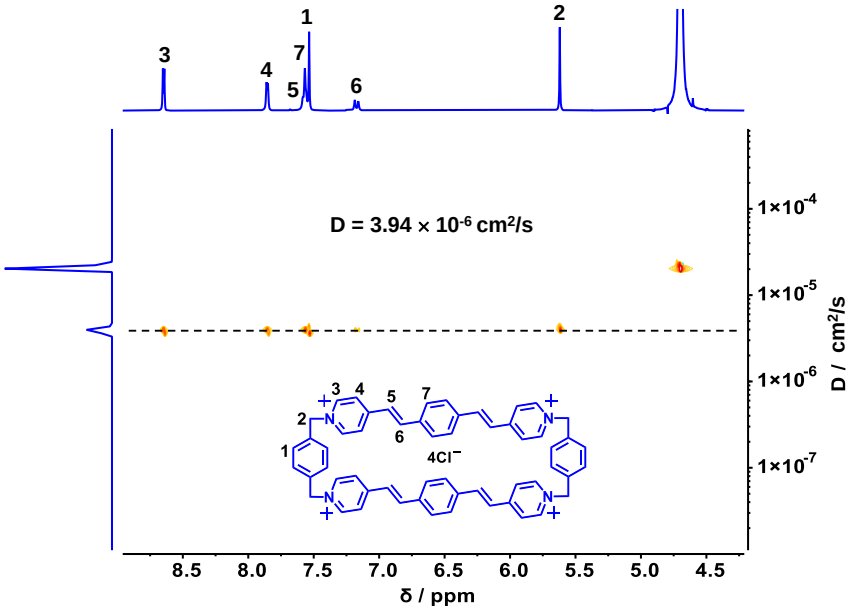


Figure S17. 2D DOSY spectrum (600 MHz, D_2O, 298 K) of **OPVEBox•**4Cl

(6) The ^{1}H NMR Titrations between OPVEBox^{4+}and CB[8]

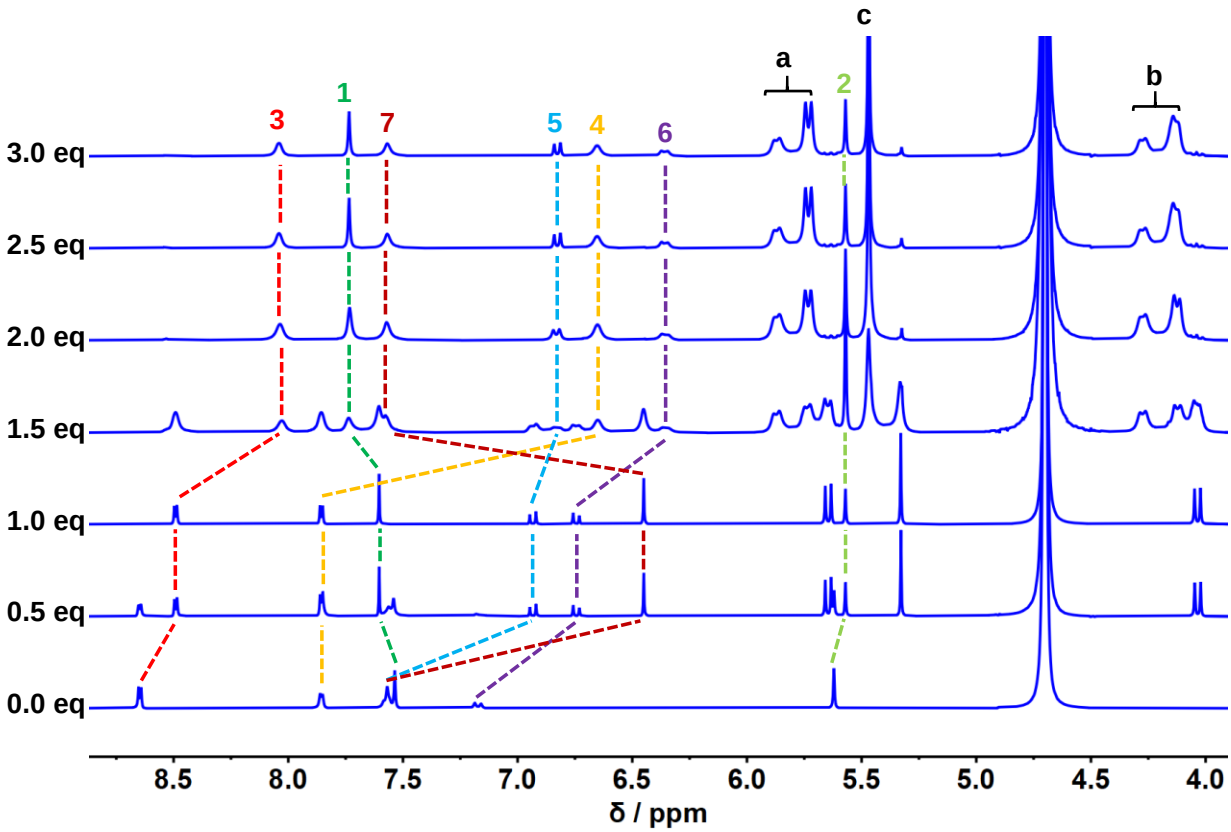


Figure S18. ^{1}H NMR Titration (600 MHz, H_2O, 298 K) of **OPVEBox^{4+}** upon addition different equiv of **CB[8]** ([**OPVEBox^{4+}**] = 2.0 × 10^{-4} M, [**CB[8]**] / [**OPVEBox^{4+}**] = 0 – 3 eq). The annotations show the chemical shift changes of the protons in **OPVEBox^{4+}** upon addition different equiv of **CB[8]**.

(7) The binding behavior OPVEBox^{4+} and γ-CD

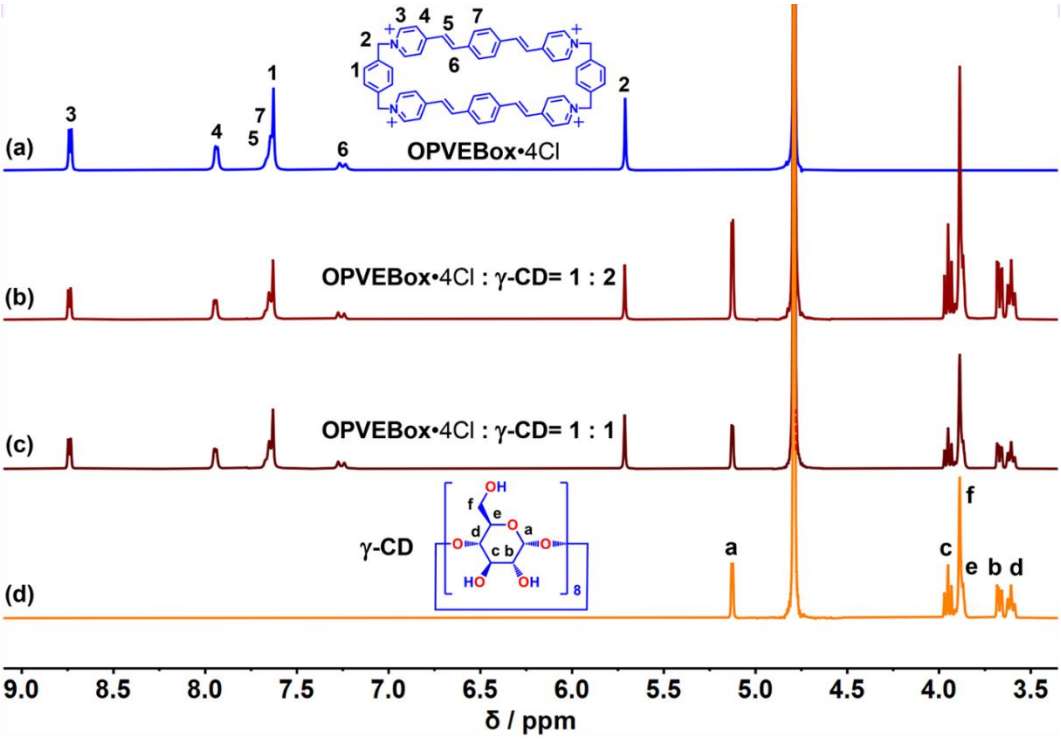


Figure S19. ^{1}H NMR Spectra (500 MHz, D_2O, 298 K) of (a) **OPVEBox•**4Cl, (b) **OPVEBox•**4Cl with 1 equiv of **γ-CD**, (c) **OPVEBox•**4Cl with 2 equiv of **γ-CD**, and (d) **γ-CD**.

(8) The binding behavior between OPV^{2+} and CB[8]

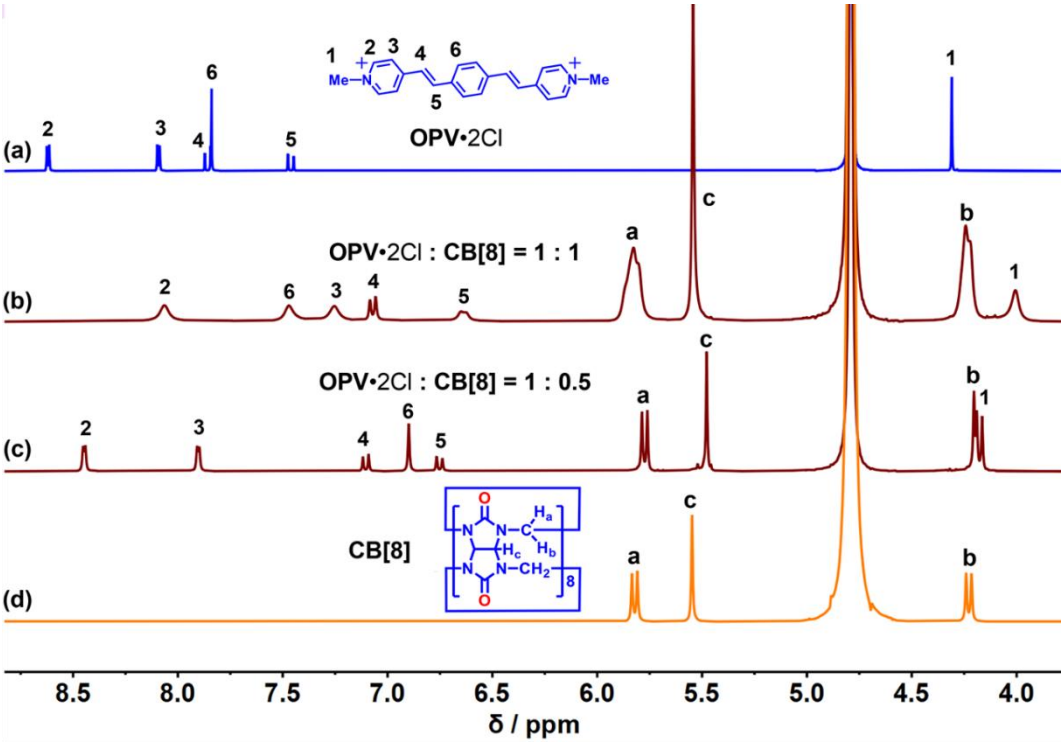


Figure S20. ^{1}H NMR Spectra (600 MHz, D_2O, 298 K) of (a) **OPV•**2Cl, (b) **OPV•**2Cl with 1 equiv of **CB[8]**, (c) **OPV•**2Cl with 0.5 equiv of **CB[8]**, and (d) **CB[8]**.

Section D. Mass Spectrometry

The mass spectrometry characterizations of OPVEBox•4Cl and ternary OPVEBox^{4+}⊂2CB[8] ring-in-rings complex

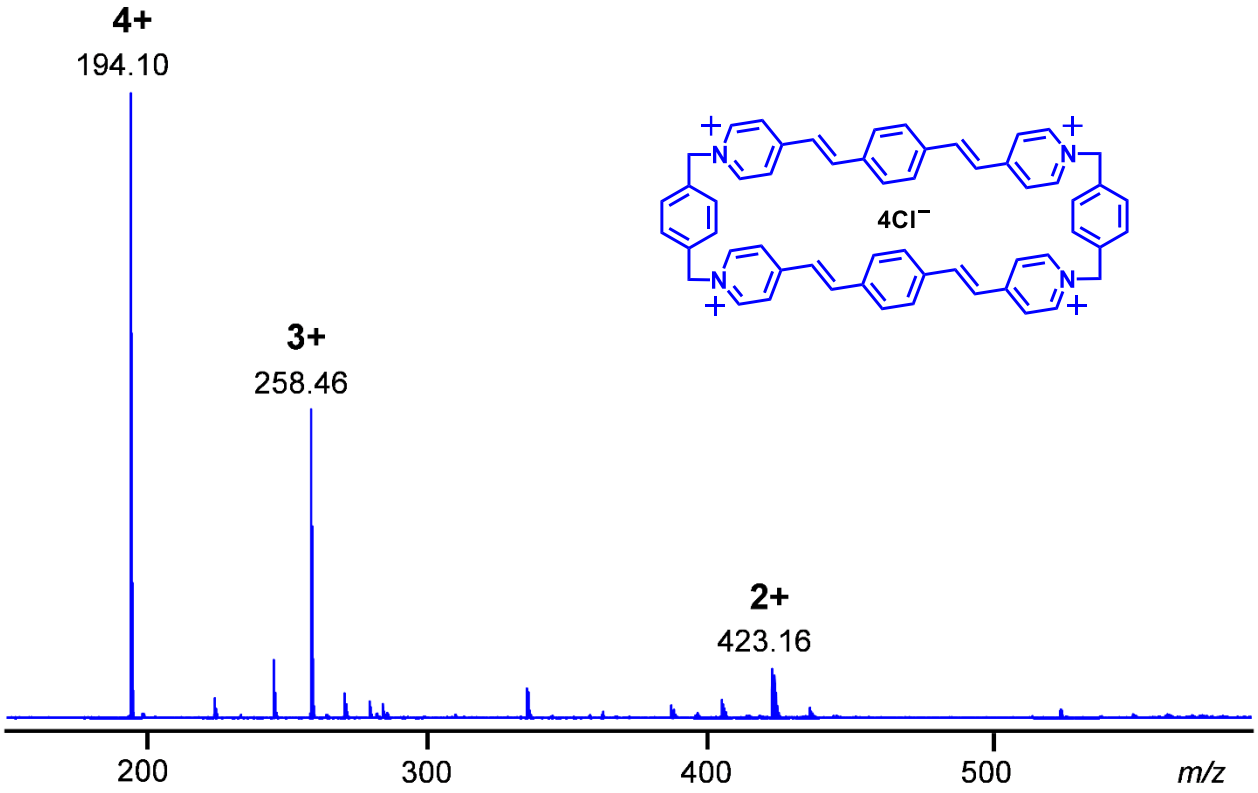


Figure S21. Electrospray ionization-mass spectrum (ESI-MS) of **OPVEBox•**4Cl

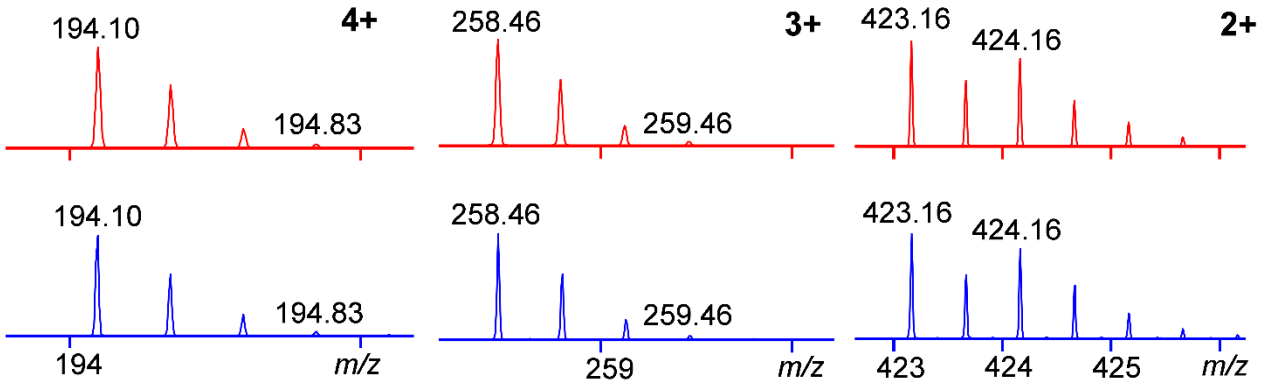


Figure S22. Calculated (red) and measured (blue) isotope patterns for different charged states observed from **OPVEBox•**4Cl

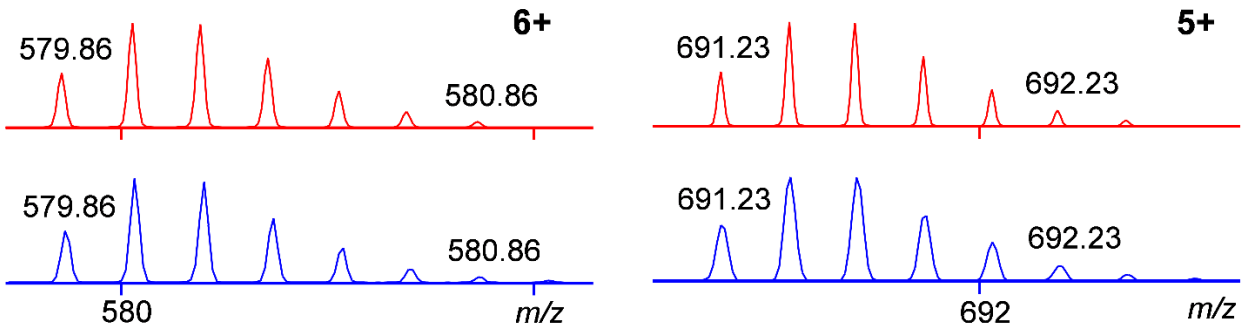


Figure S23. Calculated (red) and measured (blue) isotope patterns for different charged states observed from **OPVEBox^{4+}⊂2CB[8]** ring-in-rings complex

Section E. Crystallographic Characterization

All crystallographic data are available free of charge from the Cambridge Crystallographic Data Centre (CCDC) via www.ccdc.cam.ac.uk/data_request/cif.

(1) OPVEBox•4Cl

(a) Method. **OPVEBox•**4Cl (0.5 mg, 0.5 μmol) was dissolved in deionized H_2O (1.0 mL), and the resulting solution was passed through a 0.45-μm filter. Then the filter was added into two 1-mL tubes with volumes of 0.2 and 0.4 mL, respectively. The tubes were placed together in one 20-mL vial containing Me_2CO (~3 mL) and the vial was capped. Slow vapor diffusion of Me_2CO into the aqueous solution of **OPVEBox•**4Cl (0.5 mM) during 1 week, yielded yellow single crystals of **OPVEBox•**4Cl. A suitable crystal was mounted on a MITIGEN holder with Paratone oil on a XtaLAB Synergy, Single source at home / near, HyPix diffractometer. The crystal was kept at 100.01(10) K during data collection. Using Olex2[2], the structure was solved with the ShelXT[3] structure solution program using Intrinsic Phasing and refined with the XL[4] refinement package using Least Squares minimisation. The solid-state (super)structure of **OPVEBox•**4Cl is shown in Figure 1.

(b) Crystal Parameters. $[C_{58}H_{48}N_4\cdot(Cl)_4]\cdot(C_3H_6O)_2\cdot(H_2O)_6$. *M*r =1143.03. Yellow block (0.171 × 0.065 × 0.021 mm^3). Monoclinic, space group $P2_1/c$ (no. 14), a = 15.6756(7), b = 11.7857(4), c = 16.4783(8) Å, α = 90.000, β = 91.124(4), γ = 90.000°, V = 3043.7(2) Å^3, Z = 2, T = 100.01(10) K, μ(CuKα) = 2.215 mm^{-1}, *Dcalc* = 1.247 g/mm^3, 11277 reflections measured ($5.638 \leq 2\Theta \leq 103.66$),

3312 unique (R_{int} = 0.0668, R_{sigma} = 0.0775) which were used in all calculations. The final R_1 was 0.0554 (I > 2σ(I)) and wR_2 was 0.1523 (all data). CCDC Number: 2016357.

(c) Refinement Details. No special refinement necessary.

(2) OPVEBox•4PF$_6$

(a) Method. **OPVEBox**•4PF_6 (1.4 mg, 1.0 μmol) was dissolved in MeCN (1.0 mL), and the resulting solution was passed through a 0.45-μm filter when added into two 1-mL tubes with volumes of 0.2, and 0.4 mL, respectively. The tubes were placed together in one 20-mL vial containing *i*Pr_2O (~3 mL) and the vial was capped. Slow vapor diffusion of *i*Pr_2O into the MeCN solution of **OPVEBox**•4PF_6 (1.0 mM) over the course of 3 days, yielded yellow single crystals of **OPVEBox**•4PF_6. A suitable crystal was mounted on a MITIGEN holder in Paratone oil on a Kappa Apex 2 diffractometer. The crystal was kept at 100.03 K during data collection. Using Olex2[2], the structure was solved with the ShelXT[3] structure solution program using Intrinsic Phasing and refined with the XL[4] refinement package using Least Squares minimisation. The solid-state (super)structure of **OPVEBox**•4PF_6 is shown in Figure S24.

(b) Crystal Parameters. $C_{56}H_{48}N_4 \cdot (PF_6)_4$. *M*r = 1356.86. Yellow block (0.129 × 0.105 × 0.027 mm^3). Monoclinic, space group $P2_1/c$ (no. 14), a = 19.621(8), b = 12.649(4), c = 14.500(5) Å, α = 90.000, β = 107.270(15), γ = 90.000°, V = 3437(2) $Å^3$, Z= 2, T= 100.03 K, μ(CuKα)= 1.934 mm^{-1}, *Dcalc* = 1.303 g/mm^3, 7256 reflections measured (4.716 ≤ 2Θ ≤ 88.984), 2571 unique (R_{int} = 0.1535, R_{sigma} = 0.1765) which were used in all calculations. The final R_1 was 0.1395 (I > 2σ(I)) and wR_2 was 0.4034 (all data). CCDC Number: 2016358.

(c) Refinement Details. Rigid bond restraints (esd 0.01) were imposed on the displacement parameters as well as restraints on similar amplitudes (esd 0.05) separated by less than 1.7 Å globally. Distance restraints were imposed on the disordered atoms.

(d) Solvent Treatment Details.

The solvent masking procedure as implemented in Olex2 was used to remove the electronic contribution of solvent molecules from the refinement. As the exact solvent content is not known, only the atoms used in the refinement model are reported in the formula here. Total solvent accessible volume / cell = 693.0 $Å^3$ [20.2%], Total electron count / cell = 247.0.

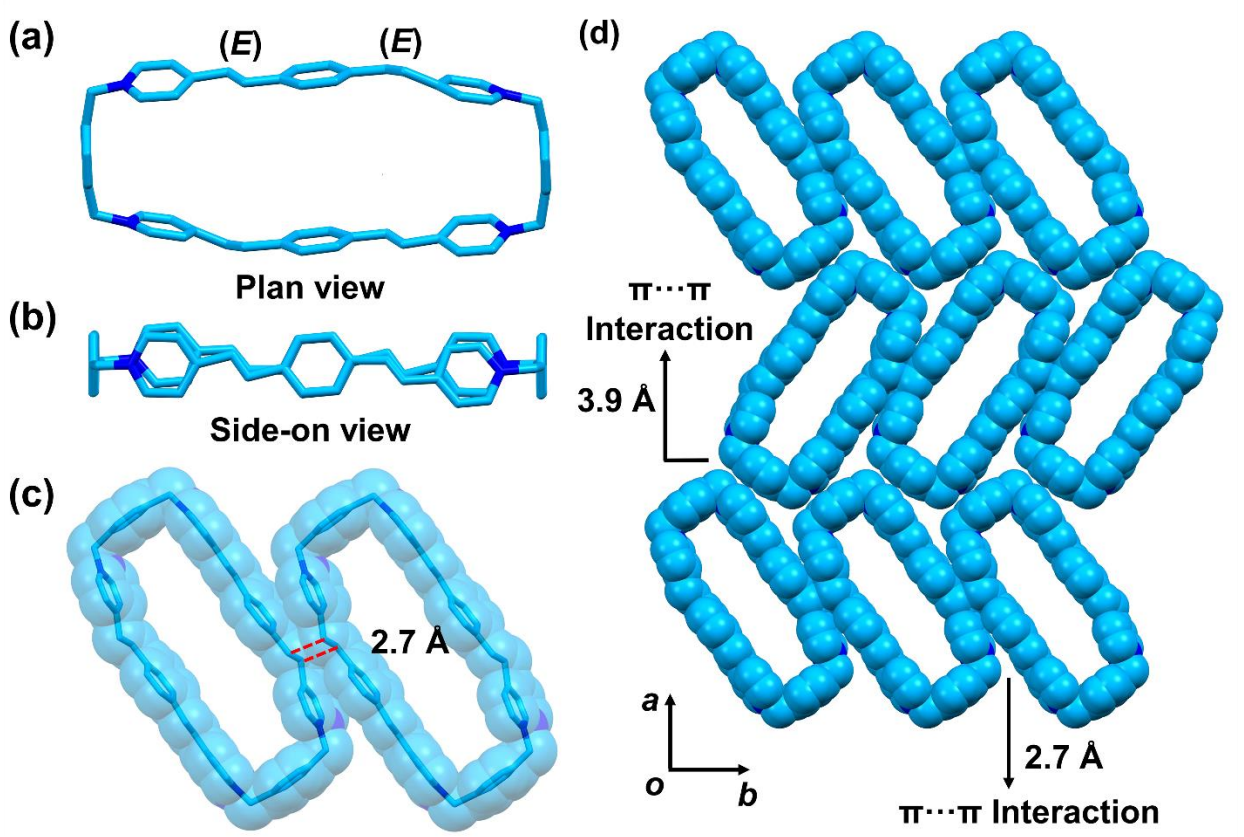


Figure S24. Solid-state (super)structure of **OPVEBox^{4+}** obtained from X-ray diffraction studies on single crystals of **OPVEBox•**4PF_6. (a − b) Capped-stick representations of different views showing the box-like geometry of **OPVEBox^{4+}**; (c) The solid-state superstructure showing the face-to-face stacking between the adjacent OPV^{2+} units in adjacent **OPVEBox^{4+}** molecules; (d) Solid-state superstructure of **OPVEBox^{4+}** revealing a herringbone type of packing and two kinds of [π···π] interactions. The hydrogen atoms, counterions and solvent molecules are omitted for the sake of clarity.

Section F. Cyclic Voltammetry

Cyclic voltammetry (CV) was performed on a Gamry Multipurpose instrument (Reference 600) interfaced to a PC under N_2 atmosphere at 298 K. The CV experiments were recorded with a glassy carbon working electrode (0.071 cm^2, Cypress system), and the electrode surface was polished routinely with alumina–water slurry on a felt surface immediately before use. The counter electrode was a Pt coil, and the reference electrode was a Ag/AgCl electrode. CV Experiments were carried out in a 0.1 M solution of $TBAPF_6$ electrolyte in DMF at a 0.1 V/s scan rate, and are referenced to the reversible Fc/Fc^+ couple ([ferrocene] = 0.5 mM).

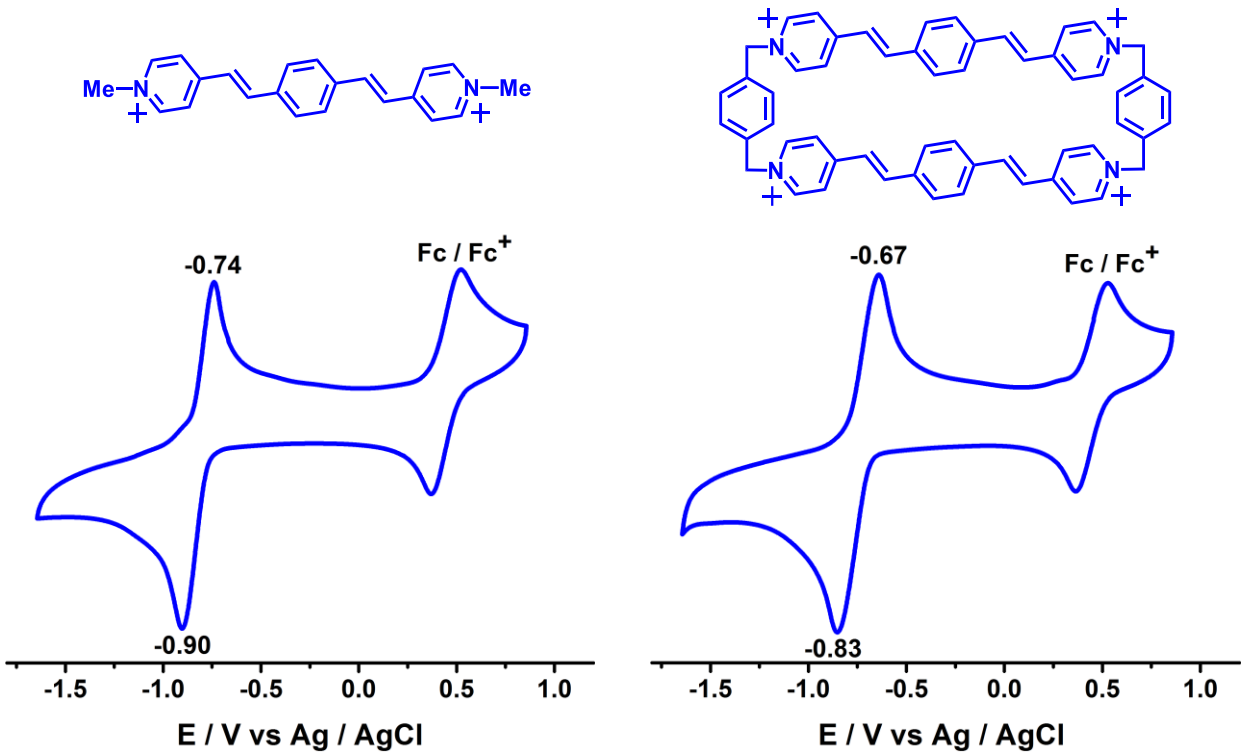


Figure S25. Cyclic voltammograms ([**OPV**$^{2+}$] = 1.0 mM, [**OPVEBox**$^{4+}$] = 0.5 mM) of **OPV**$^{2+}$ (left) and **OPVEBox**$^{4+}$ (right). The results show similar cyclic voltammogram with one set of reversible redox peaks, indicating the absence of electron communication between the pyridinium units.

Section G. Photophysical Characterization

(1) UV-Vis Spectroscopic Analysis

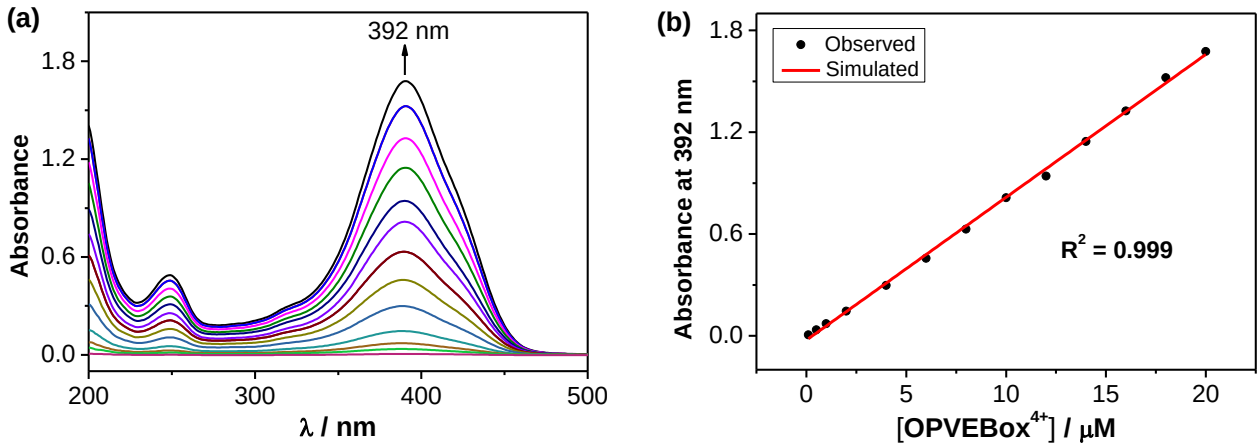


Figure S26. (a) UV-Vis Absorption spectra ([**OPVEBox**$^{4+}$] = 0.1–20.0 μM, H_2O, 298 K) of **OPVEBox**$^{4+}$ in different concentrations; (b) Absorbance changes at 392 nm with increasing concentration. The linear relation between absorbance and concentration indicates that there is no aggregation occurring for **OPVEBox**$^{4+}$ at the concentrations used in the analysis.

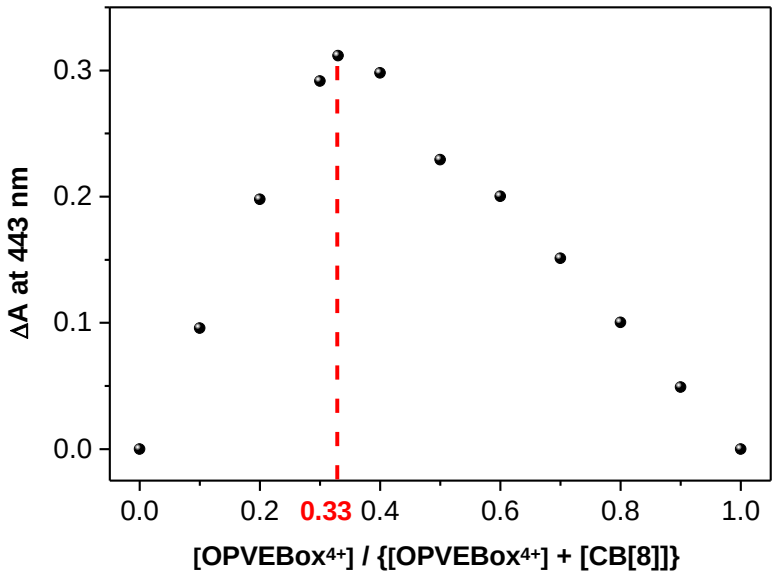


Figure S27. Job's experiment for **OPVEBox^{4+}** upon complexation with **CB[8]** in aqueous solution at 298 K. Absorbance intensity changes of **OPVEBox^{4+}** recorded at 443 nm was used to analyze the binding ratio. The total concentration of host and guest is constant ([**OPVEBox^{4+}**] + [**CB[8]**] = 100 μM).

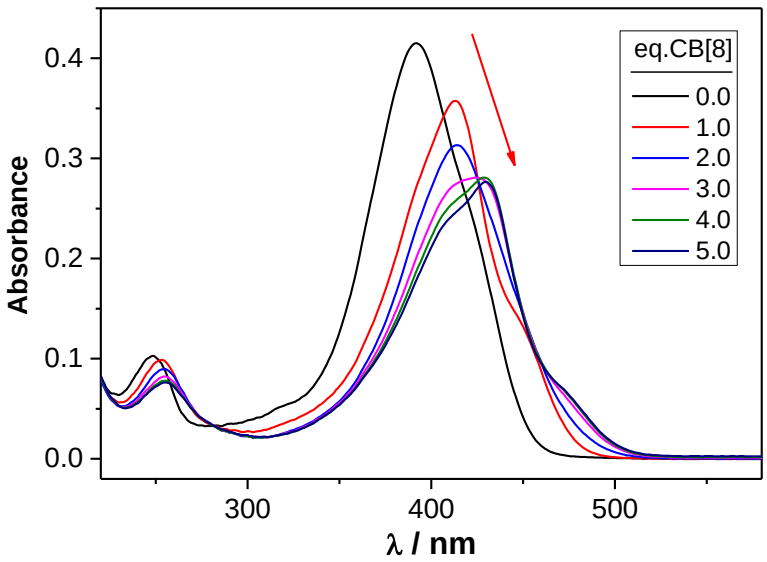


Figure S28. UV-Vis Absorption spectra ([**OPVEBox^{4+}**] = 4 μM, [**CB[8]**] = 0–20 μM, H_2O, 298 K) of **OPVEBox^{4+}** with adding different equiv of **CB[8]**. The maximum absorption peaks show obvious red shifts and decline.

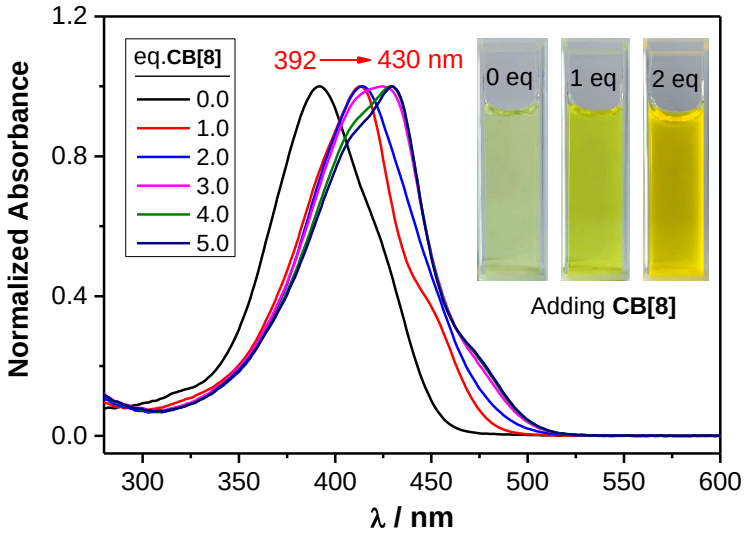


Figure S29. Normalized UV-Vis absorption spectra ([**OPVEBox**$^{4+}$] = 4 μM, [**CB[8]**] = 0–20 μM, H_2O, 298 K) of **OPVEBox**$^{4+}$ with adding different equiv of **CB[8]**. The maximum absorption wavelength red shifted from 392 to 430 nm.

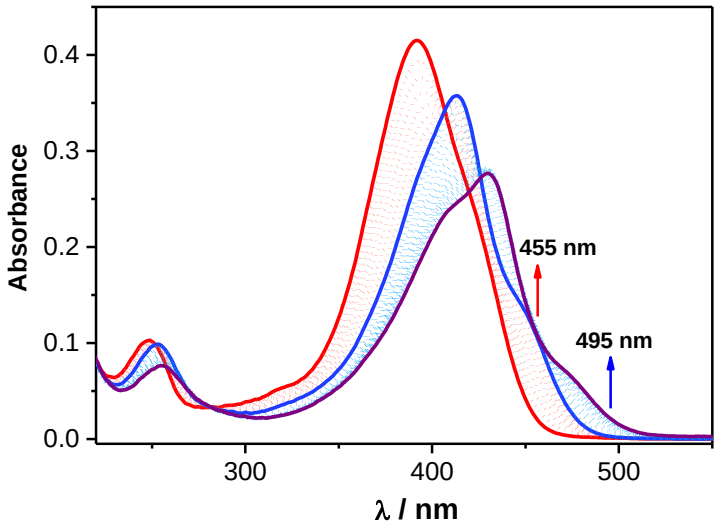


Figure S30. (a) UV-Vis Titration experiment ([**OPVEBox**$^{4+}$] = 4 μM, [**CB[8]**] = 0−20 μM, H_2O, 298 K) on adding **CB[8]** to a aqueous solution of **OPVEBox**$^{4+}$ at 298 K. A typical two-stage bonding process is uncovered. First stage (red curves): the formation of binary **OPVEBox**$^{4+}$⊂**CB[8]** ring-in-ring complex upon the addition of 1 equiv of **CB[8]**. Second stage (blue curves): the ternary **OPVEBox**$^{4+}$⊂**2CB[8]** ring-in-rings complex formed gradually upon continue to add 4 equiv of **CB[8]**.

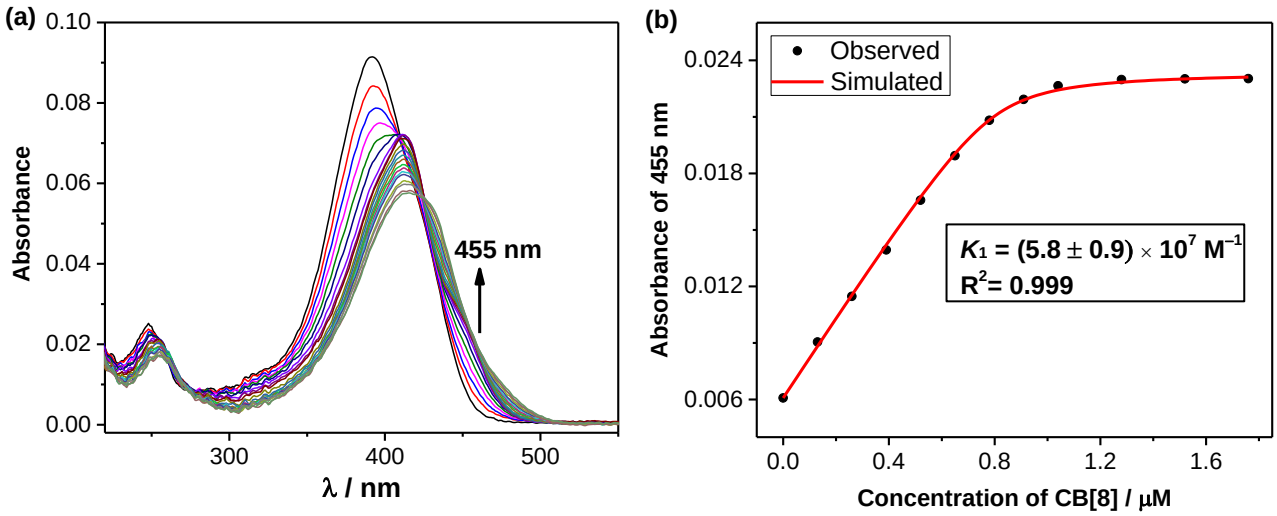


Figure S31. (a) UV-Vis Titration experiment ([**OPVEBox**$^{4+}$] = 0.8 μM, [**CB[8]**] = 0−1.76 μM, H_2O, 298 K) on adding **CB[8]** to a aqueous solution of **OPVEBox**$^{4+}$ at 298 K. (b) Nonlinear least-squares analysis of the absorbance intensity changes at 455 nm in the UV-Vis titration experiment as shown in (a), the first-stage binding constant (K_1) was determined to be 5.8×10^7 M^{-1}.

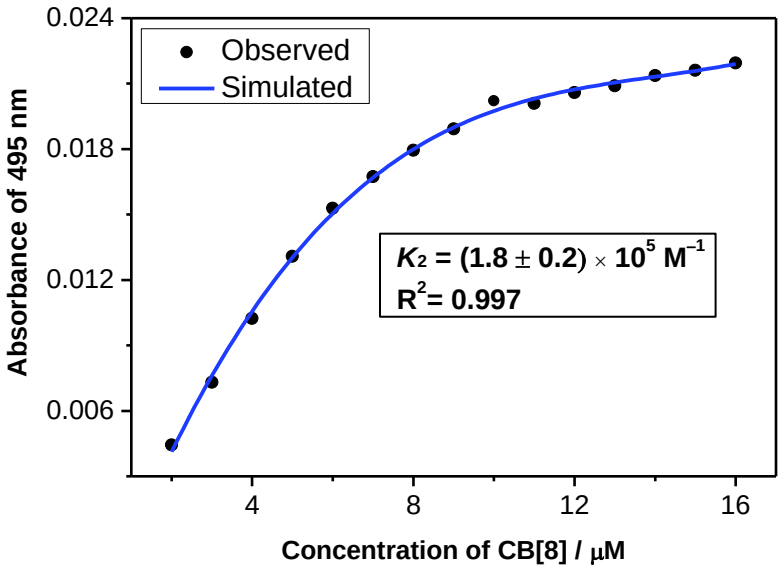


Figure S32. Nonlinear least-squares analysis of the absorbance intensity changes at 495 nm in the UV-Vis titration experiment as shown in Figure S30, in order to calculate the second-stage binding constant (K_2) for the formation of ternary **OPVEBox**$^{4+}$**⊂2CB[8]** ring-in-rings complex in aqueous solutions.

(2) ***Fluorescence Spectroscopic Analysis***

The excitation and emission spectra (Figures S33 and S34) were recorded for **OPVEBox^{4+}**. The red shift of emission spectra (Figure S35) upon the addition of different equiv of **CB[8]** to the aqueous solution of **OPVEBox•**4Cl. The fluorescence quantum yield (Figure S36 and Table S1) and lifetime (Table S2) changes of **OPVEBox•**4Cl upon the addition of different equiv of **CB[8]** in aqueous solutions.

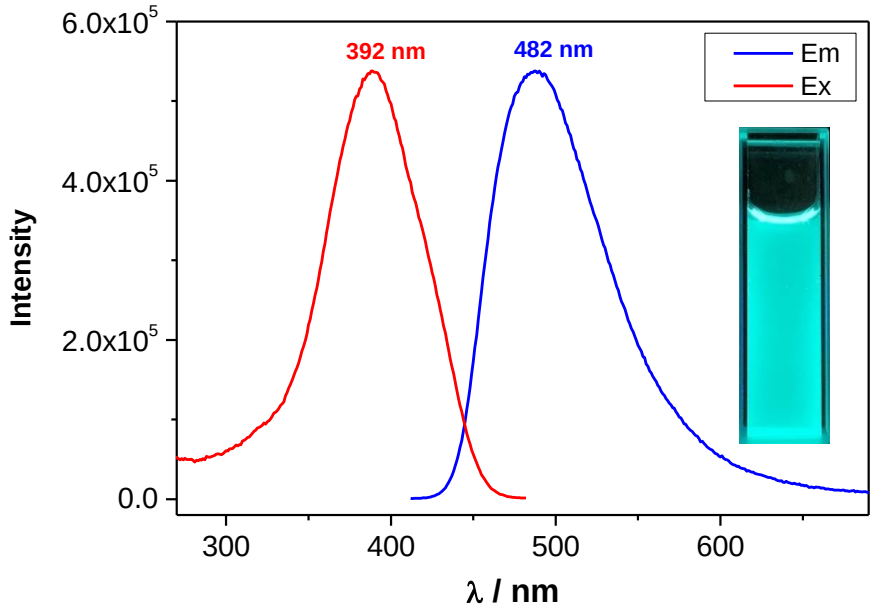


Figure S33. Excitation and emission spectra ([**OPVEBox^{4+}**] = 2 μM, H_2O, 298 K) of **OPVEBox^{4+}** in an aqueous solution

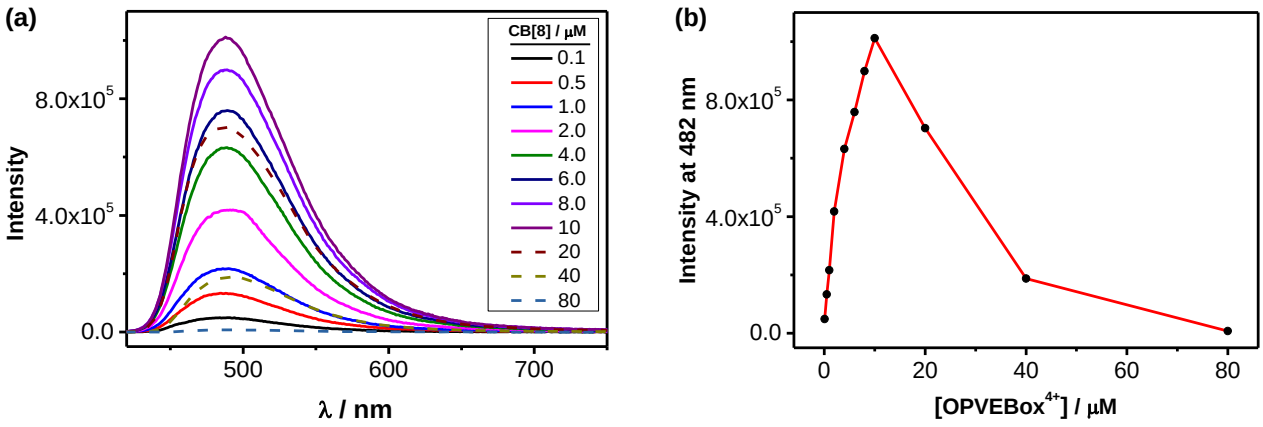


Figure S34. (a) Emission spectra ([**OPVEBox^{4+}**] = 0.1–80.0 μM, λex = 392 nm, H_2O, 298 K) of **OPVEBox^{4+}** in different concentration, (b) Emission intensity changes at 482 nm with increasing concentration, indicating there are no obvious aggregation for **OPVEBox^{4+}** at the concentration lower than 10.0 μM.

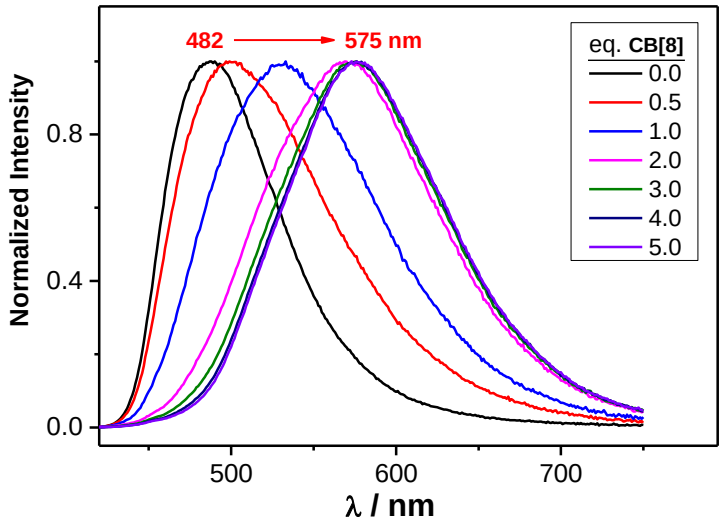


Figure S35. (a) Normalized emission spectra ([**OPVEBox**$^{4+}$] = 2 μM, [**CB[8]**] = 0−10 μM, λ_{ex} = 392 nm, H_2O, 298 K) of **OPVEBox**$^{4+}$ with adding different equiv of **CB[8]**.The maximum emission wavelength red shifted from 482 to 575 nm.

Table S1. The Fluorescence Quantum Yields of OPVEBox^{4+} (λ_{ex} = 392 nm) after Addition of 0–5 Equiv of CB[8] in Aqueous Solutions

Concentration of OPVEBox^{4+}	Sample	Quantum Yield / %
2 μM	**OPVEBox^{4+}**	2.35 ± 0.004
	1 equiv **CB[8]**	2.39 ± 0.008
	2 equiv **CB[8]**	8.14 ± 0.020
	3 equiv **CB[8]**	16.03 ± 0.051
	5 equiv **CB[8]**	18.55 ± 0.058
10 μM	**OPVEBox^{4+}**	2.50 ± 0.002
	1 equiv **CB[8]**	2.55 ± 0.002
	2 equiv **CB[8]**	13.87 ± 0.013
	3 equiv **CB[8]**	20.99 ± 0.021
	5 equiv **CB[8]**	29.58 ± 0.032

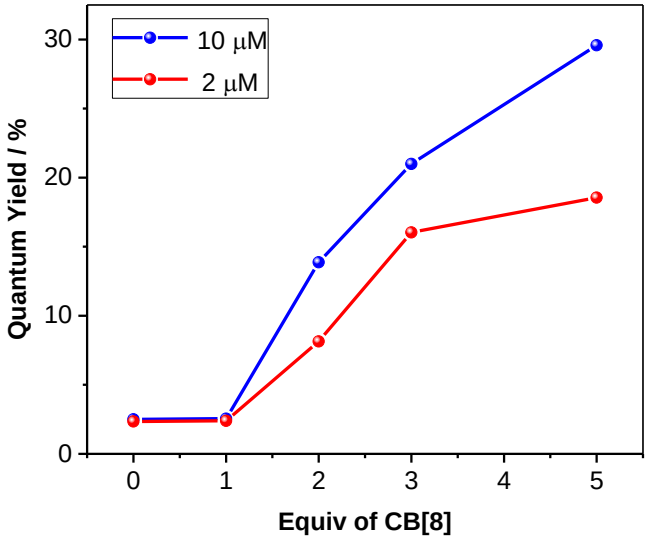


Figure S36. The fluorescence quantum yields of **OPVEBox^{4+}** ([**OPVEBox^{4+}**] = 2 or 10 μM) at two different concentrations with adding different equiv of **CB[8]** in aqueous solutions

Table S2. The Fluorescence Lifetimes of OPVEBox^{4+} (λ_{ex} = 374 nm, Laser) after Addition of 0–5 Equiv of CB[8] in Aqueous Solutions[a]

Concentration of OPVEBox^{4+}	**Sample**	**Lifetime** / ns (% contribution)		
		τ_1	τ_2	τ_{avg}
2 μM	**OPVEBox^{4+}**	0.33 (100)	–	0.33
	1 equiv **CB[8]**	0.59 (85.94)	8.11 (14.06)	5.80
	2 equiv **CB[8]**	0.67 (22.76)	11.68 (77.24)	11.50
	3 equiv **CB[8]**	0.74 (11.95)	11.98 (88.05)	11.89
	5 equiv **CB[8]**	0.75 (7.24)	11.79 (92.76)	11.74
10 μM	**OPVEBox^{4+}**	0.28 (100)	–	0.28
	1 equiv **CB[8]**	0.58 (86.53)	7.87 (13.47)	5.53
	2 equiv **CB[8]**	0.81 (9.98)	11.97 (90.02)	11.89
	3 equiv **CB[8]**	1.00 (5.74)	11.99 (94.26)	11.93
	5 equiv **CB[8]**	1.10 (4.77)	12.01 (95.23)	11.96

[a] The fluorescence decay traces of **OPVEBox^{4+}** with 0, 1, and 2–5 equiv of **CB[8]** were detected at 482, 533, 575 nm, respectively.

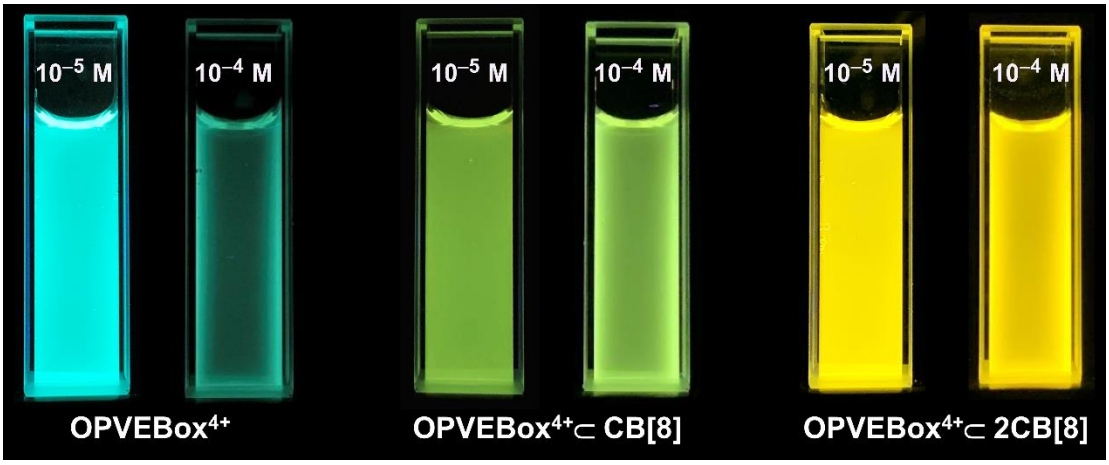


Figure S37. Fluorescent photographs of **OPVEBox^{4+}**, **OPVEBox^{4+}⊂CB[8]** and **OPVEBox^{4+}⊂2CB[8]** at the concentration of 10^{-5} and 10^{-4} M in aqueous solution, showing that both the binary and ternary ring-in-ring(s) complexes have highly fluorescent emission at relatively higher concentration (0.1 mM).

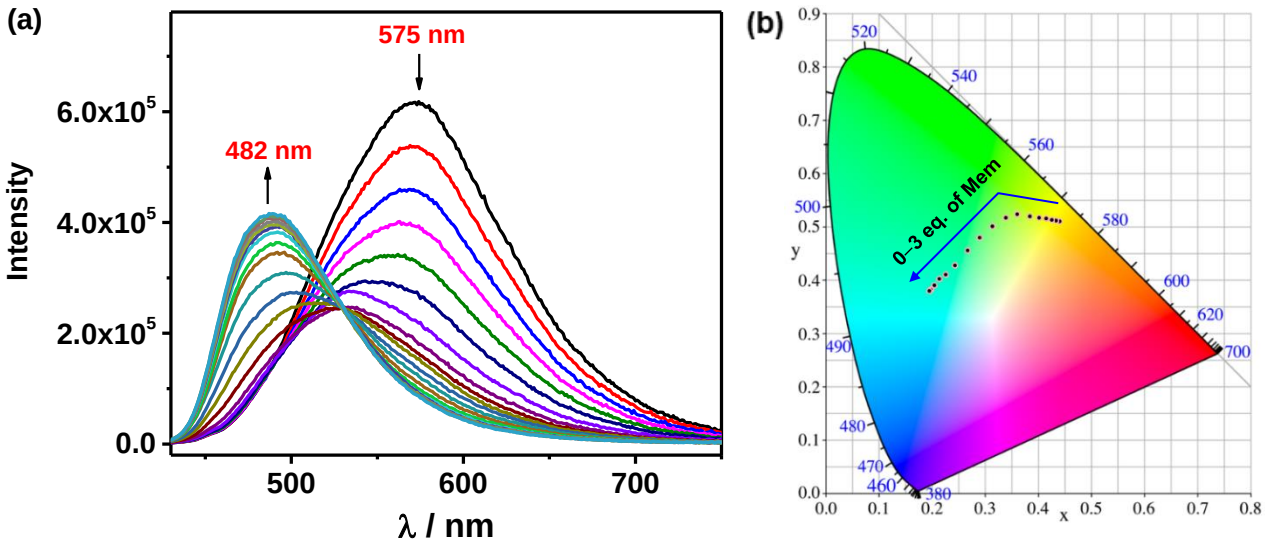


Figure S38. (a) Emission spectra recorded during the continuous addition of memantine hydrochloride (**Mem**) to an aqueous solution of **OPVEBox**•4Cl⊂**2CB[8]** ring-in-rings complex ([**OPVEBox**•4Cl] = 2 μM, [**CB[8]**] = 4 μM, [**Mem**] = 0 – 6 μM, λex = 392 nm, H_2O, 298 K). (b) The 1931 CIE chromaticity diagram illustrating the luminescent color changes, with the continuous addition of **Mem** to an aqueous solution of the ternary ring-in-rings complex corresponding to (a).

Section H. Isothermal Titration Calorimetry (ITC)

(1) Experiment methods and conditions

All microcalorimetric titrations were performed in a thermostated TA Nano Isothermal Titration

Calorimeter at atmospheric pressure and 298 K. The samples were dissolved in an aqueous NaCl (1.0 mM) solution, in order to improve the solubility of **CB[8]**, and the concentrations of sample were calibrated by UV-Vis absorption spectroscopy after filtered by a 0.45-filter. A solution of one reactant in a syringe was sequentially injected with stirring at 150 rpm into a solution of the other reactant in the sample cell with a constant volume of 185 μL. A representative titration curve is shown in Figure S39, each titration of reactant into the sample cell gave an apparent reaction heat caused by the formation of the inclusion complex. The reaction heat decreases gradually until a balance was reached, whereupon only the dilution heat was measured. The net reaction heat was obtained by subtracting the dilution heat from the apparent reaction heat. The resulting data were analyzed with NanoAnalyze software using a 1:1 binding model to give the complex stability constant (*K*a), standard molar reaction enthalpy (Δ*H*), and standard deviations. Generally, the first point of the titration curve was disregarded, as there is some liquid mixing near the tip of the injection needle before ITC run. Each titration experiment was duplicated independently two times. All isotherm fittings were used to calculate the average K_a and Δ*H*, and the titration isotherm showed in Figure S39 is one set of them. The standard free energy (Δ*G*) and entropy changes (Δ*S*) can be obtained according to the following equation:

$$\Delta G = -RT \ln K_a = \Delta H - T\Delta S$$

where *R* is the gas constant and *T* is the absolute temperature.

(2) Measurement of the thermodynamic parameters between OPVEBox^{4+} and CB[8]

Upon titrating **CB[8]** into the solution of **OPVEBox^{4+}**, a typical two-stage bonding process is uncovered. This process can be described using the following complexation equilibria:

$$\text{First-stage: } \mathbf{OPVEBox^{4+}} + \mathbf{CB[8]} \overset{K_1}{\rightleftharpoons} \mathbf{OPVEBox^{4+}\subset CB[8]}$$

$$\text{Second-stage: } \mathbf{OPVEBox^{4+}\subset CB[8]} + \mathbf{CB[8]} \overset{K_2}{\rightleftharpoons} \mathbf{OPVEBox^{4+}\subset 2CB[8]}$$

Hindering by the poor water solubility of **CB[8]**, it is difficult to obtain simultaneously the K_1 and K_2 in a continuous calorimetric titration manner. The value for K_1 can be determined to be 5.8×10^7 M^{-1} by analysis of the UV-Vis titration data. Such a high affinity between **OPVEBox^{4+}** and **CB[8]** indicates that the **OPVEBox^{4+}⊂CB[8]** complex is formed quantitatively at high concentration. Hence, we tried using the twice-independent single injection experiments to estimate the binding enthalpy for the formation of **OPVEBox^{4+}⊂CB[8]**. The experiment data are shown in Figure S40. On the other hand, when a solution of the **OPVEBox^{4+}⊂CB[8]** complex in a syringe was injected sequentially into a solution of **CB[8]** in the sample cell, the thermodynamic parameters of the second-stage recognition process were obtained. The experiment data are shown in Figure S39.

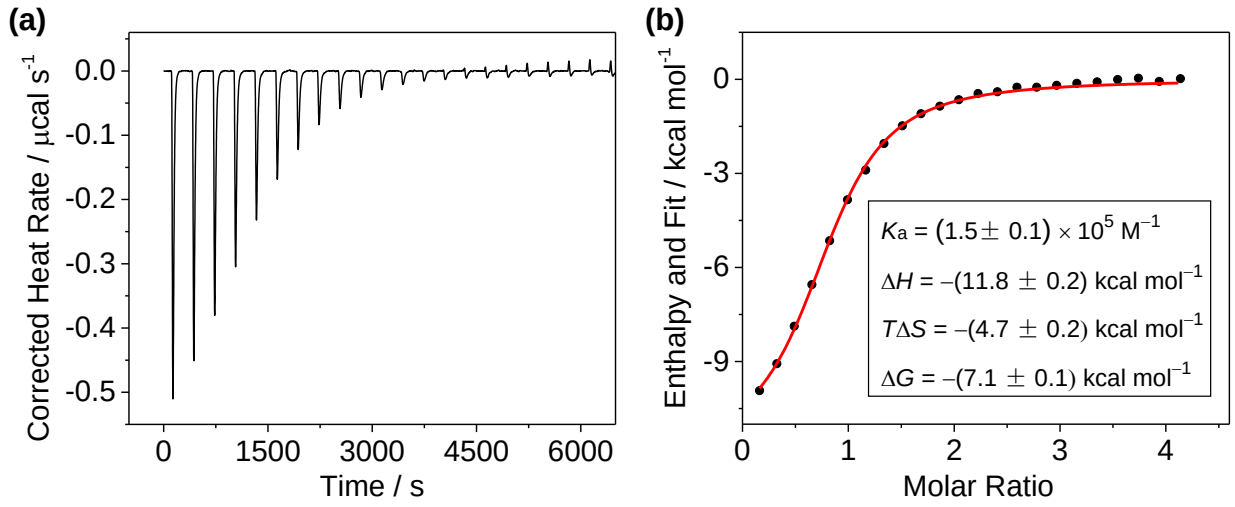


Figure S39. Microcalorimetric titration data (a) and fitted curves (b) upon the addition of **OPVEBox^{4+}⊂CB[8]** complex (836 μM in syringe) into **CB[8]** (50 μM in cell) in aqueous NaCl (1 mM) solution at 298 K. The result suggested that the ternary **OPVEBox^{4+}⊂2CB[8]** complex was formed and the bonding constant K_2 was found to be 1.5×10^5 M^{-1}.

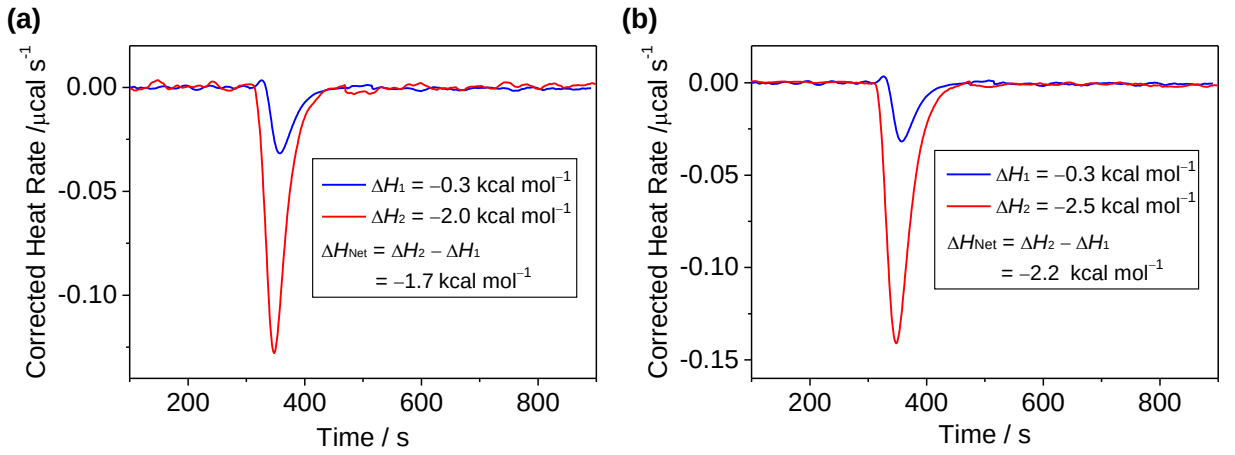


Figure S40. Twice-independent single injection experiments, in which adding 1 equiv of **OPVEBox^{4+}** (949 μM in syringe) into sample cell with (red line) or without (blue line) **CB[8]** (15 μM in cell) all at once in aqueous NaCl (1 mM) solution. The ΔH_1, ΔH_2 and ΔH_{Net} are represented as the dilution heat, apparent reaction heat and net reaction heat, respectively. The averaged binding enthalpy (ΔH_{Net}) for the formation of **OPVEBox^{4+}⊂CB[8]** complex was estimated to be –2.0 kcal mol^{-1}.

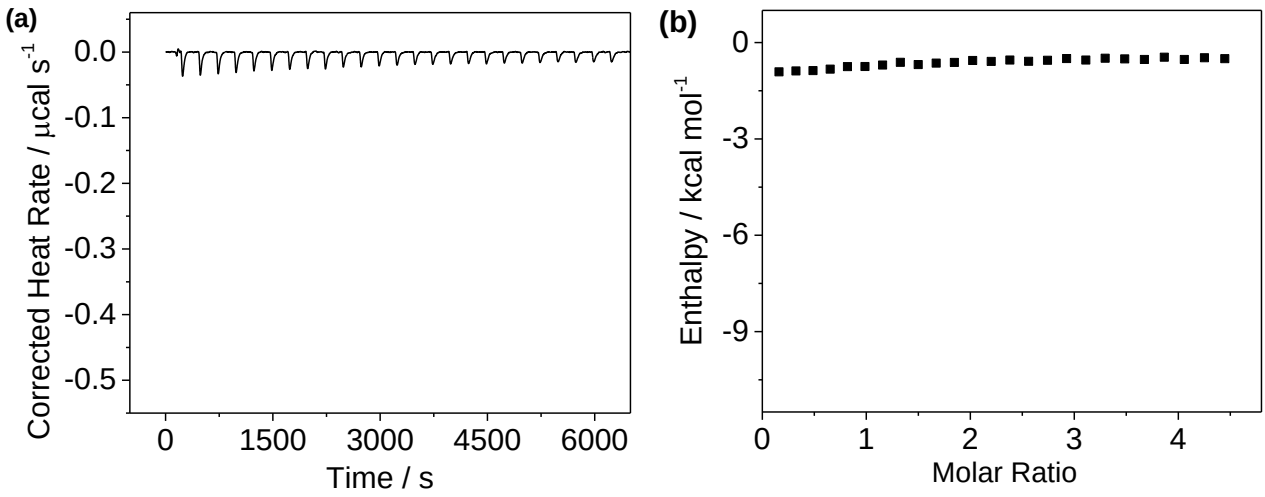


Figure S41. Microcalorimetric titration data (a) and the change of enthalpy (b) upon the addition of **CBPQT^{4+}** (1000 μM in syringe) into **CB[8]** (50 μM in cell) in aqueous NaCl (1 mM) solution at 298 K. There is no obvious enthalpy change, indicating that **CBPQT^{4+}** does not bind inside the cavity of **CB[8]** to form a ring-in-ring complex.

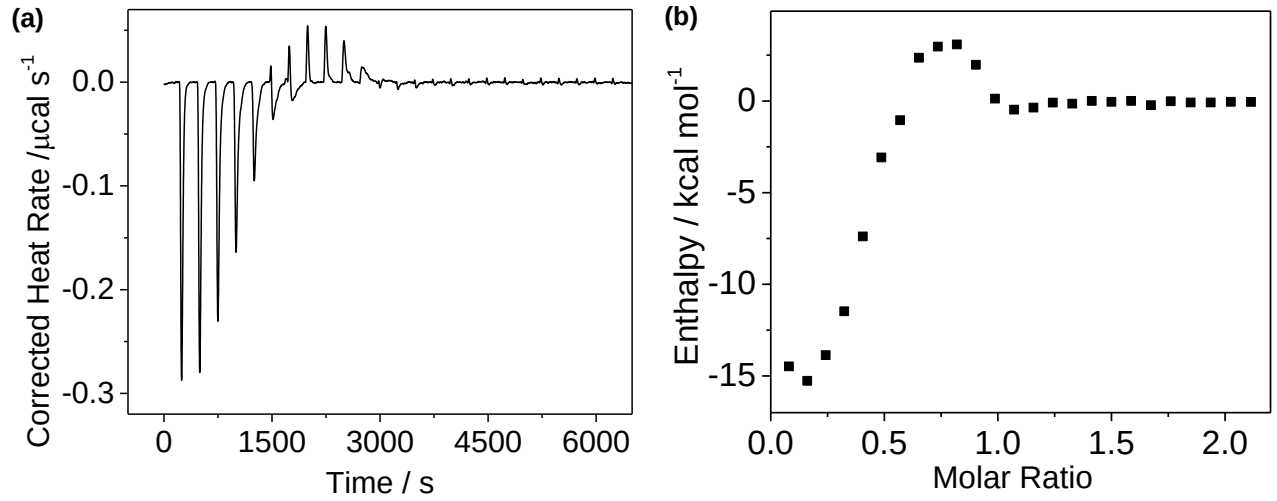


Figure S42. Microcalorimetric titration data (a) and the change of enthalpy (b) upon the addition of **OPVEBox^{4+}** (949 μM in syringe) into **CB[8]** (50 μM in cell) in aqueous NaCl (1 mM) solution at 298 K. The isotherm is too complex to fit with available programs.

Section I. Density Functional Theory Calculations

In order to gain a better understanding of the geometrical superstructure of the binary **OPVEBox^{4+}⊂CB[8]** and ternary **OPVEBox^{4+}⊂2CB[8]** ring-in-ring(s) complexes, as well as the electronic properties and frontier molecular orbitals for all the structures, DFT calculations have been carried out based on the crystal structures of **OPVEBox^{4+}** and **CB[8]**. Figures S43 and S44 show the DFT-optimized structures of the **OPVEBox^{4+}⊂CB[8]** and **OPVEBox^{4+}⊂2CB[8]**

complexes, respectively. Figures S45 and S46 show the electrostatic potential maps of **CB[8]** and **OPVEBox^{4+}**, as well as the **OPVEBox^{4+}⊂CB[8]** and **OPVEBox^{4+}⊂2CB[8]** complexes, respectively. Figures S47−S50 show the frontier molecular orbitals of **CB[8]**, **OPVEBox^{4+}**, **OPVEBox^{4+}⊂CB[8]** and **OPVEBox^{4+}⊂2CB[8]**, respectively. Tables S3 and S4 summarizes the energy levels for **CB[8]**, **OPVEBox^{4+}**, and their complexes in vacuum and water, respectively. Tables S5 and S6 summarizes the strain energy for the central **OPVEBox^{4+}** in ring-in-ring(s) complexes in vacuum and water, respectively

The xyz coordinates from the X-ray single crystals of the **OPVEBox^{4+}** and **CB[8]** were used as the starting geometries for their individual optimizations in vacuum. In order to construct the complexes, **OPVEBox^{4+}** was carefully manipulated in the molecular editor Avogadro program[5] (version 1.1.1) and threaded through the **CB[8]** structure until half of each loop was sitting on either side of the **CB[8]** molecule; this geometry formed the basis of **OPVEBox^{4+}⊂CB[8]** complex. This superstructure was initially energy minimized at the molecular mechanics (MM) level with the universal force field[6,7] (UFF) in Avogadro. In order to form **OPVEBox^{4+}⊂2CB[8]** complex, one **CB[8]** molecule was moved along to one end of **OPVEBox^{4+}** and another **CB[8]** was added to the other end. This complex was also energy minimized at the same level as **OPVEBox^{4+}⊂CB[8]**. All four (super)structures, i.e., **CB[8]**, **OPVEBox^{4+}**, **OPVEBox^{4+}⊂CB[8]**, **OPVEBox^{4+}⊂2CB[8]**, were optimized subsequently with density functional theory (DFT) in the Orca program[8] (version 4.1.2) using the hybrid generalized gradient approximation (GGA) Becke three-parameter Lee-Yang-Parr[9] (B3LYP) functional, and the Ahlrich's double zeta basis set with a polarization function[10] Def2-SVP. In order to speed up the DFT optimizations, the Coulomb integral and numerical chain-of-sphere integration for the HF exchange[11,12] (RIJCOSX) method was applied with the Def2/J auxiliary basis[13,14] (AuxJ). The Frontier Molecular Orbitals (FMO) were visualized in ChemCraft (version b574b). The electrostatic potential maps were computed with B3LYP and the Slater-type basis set[15] DZP in the Amsterdam Density Functional program[16] (version 2018.104) for **CB[8]**, **OPVEBox^{4+}** and **OPVEBox^{4+}⊂CB[8]** complex, while that of **OPVEBox^{4+}⊂2CB[8]** complex was computed at the B3LYP/SZ level on account of its size, as any larger basis was computationally intractable. Frozen cores were used as implemented in ADF (which for C, O and N relates to the 1s core being frozen) to reduce the computational cost. The optimized structures in vacuum were re-optimized at the same theoretical level with the Solvation Model based on Density[17] (SMD) variant of the Conductor-like Polarizable Continuum Model[18] (CPCM) in a water continuum, in the Orca program. These CPCM structures were found to have several stationary points that equilibrated and thus no single minimum was found; except for slight xyz displacements the overall structures in a water continuum remained chemically identical to their vacuum counterparts. These can therefore be considered as semi-optimized but serve the purpose of analyzing the FMO energies in experimental conditions.

(1) DFT Optimized Structures

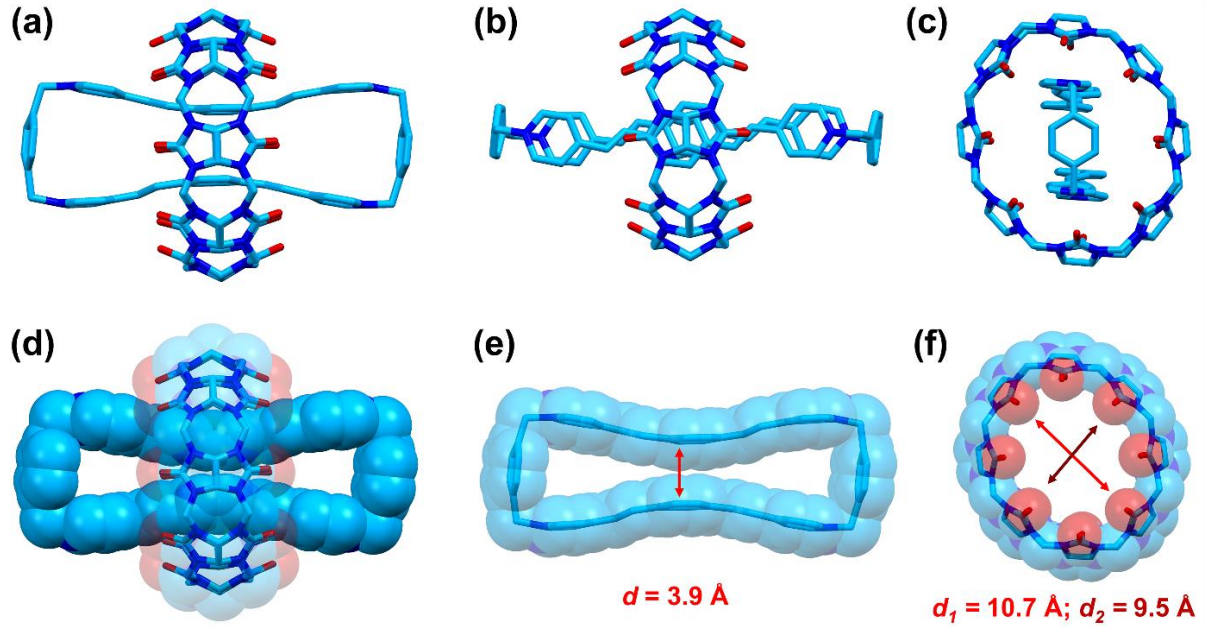


Figure S43. Optimized superstructure of the binary **OPVEBox^{4+}⊂CB[8]** ring-in-ring complex obtained from DFT calculations. (a–c) Capped-stick representations of different views of the **OPVEBox^{4+}⊂CB[8]** complex; (d–f) Space-filling representations showing geometries of **OPVEBox^{4+}⊂CB[8]**, as well as individual **OPVEBox^{4+}** and **CB[8]** in the complex, and the characteristic distances defining their geometrical dimensions.

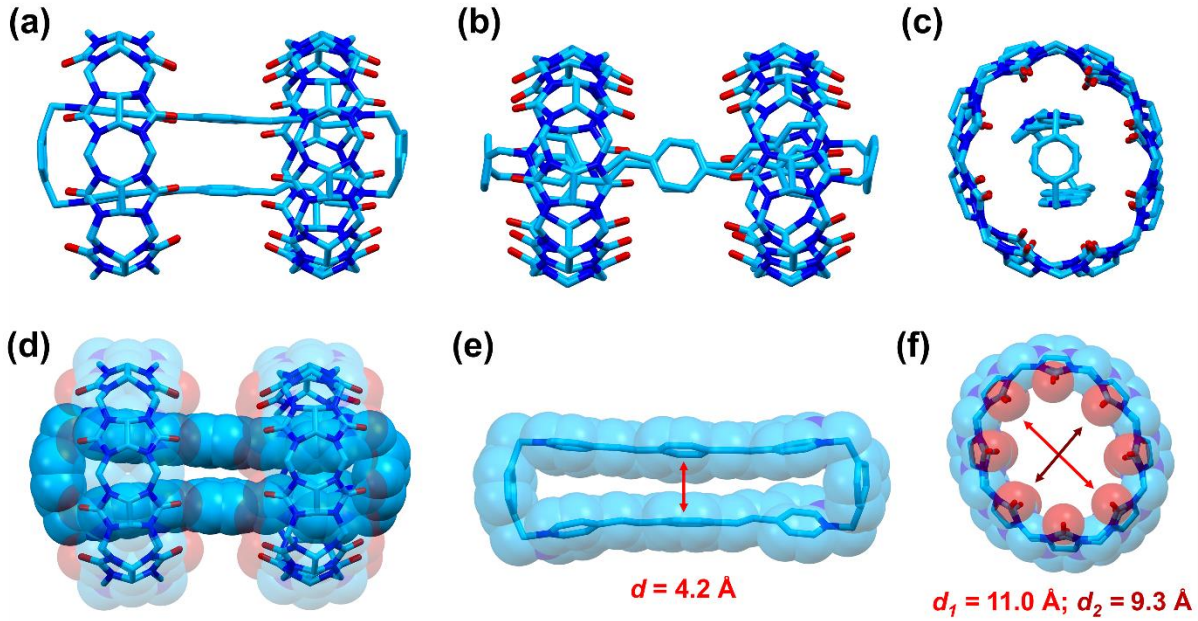


Figure S44. Optimized superstructure of the ternary **OPVEBox^{4+}⊂2CB[8]** ring-in-rings complex obtained from DFT calculations. (a–c) Capped-stick representations of different views of the **OPVEBox^{4+}⊂2CB[8]** complex; (d–f) Space-filling representations showing geometries of **OPVEBox^{4+}⊂2CB[8]**, as well as individual **OPVEBox^{4+}** and **CB[8]** in the complex, and the characteristic distances defining their geometrical dimensions.

(2) Electrostatic Potential Map Calculations

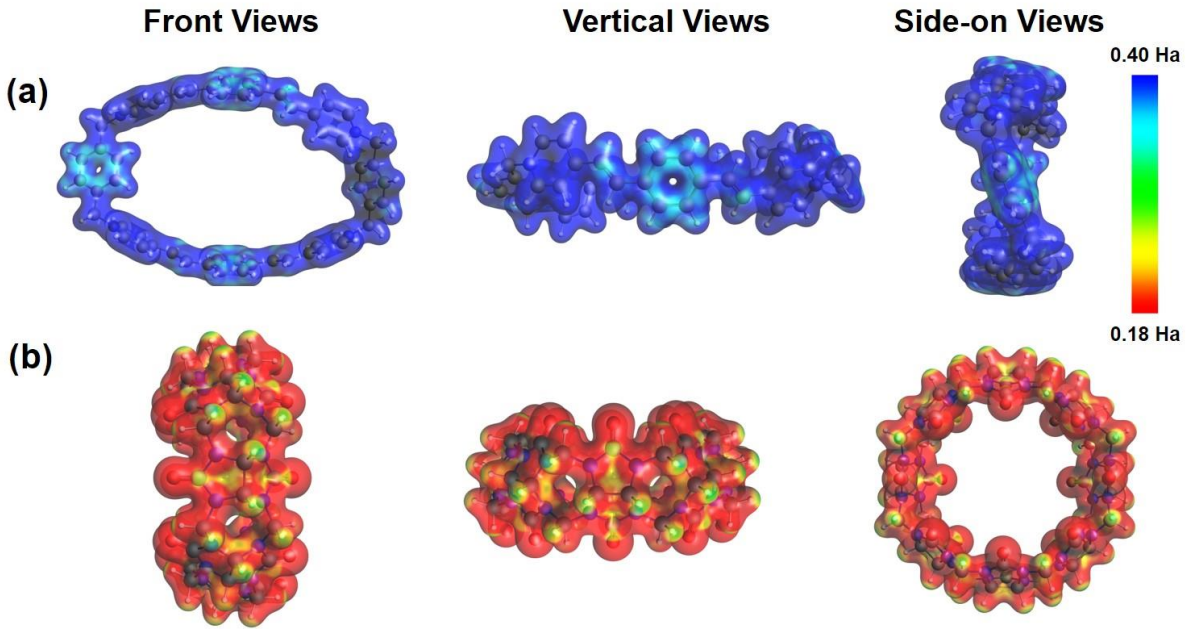


Figure S45. Different views of electrostatic potential maps of (a) **OPVEBox^{4+}** and (b) **CB[8]** obtained from DFT calculations. These maps demonstrate that the **OPVEBox^{4+}** is electron poor, while the **CB[8]** is related electron negative. Red and blue colors in the maps represent negative and positive electrostatic potentials, respectively.

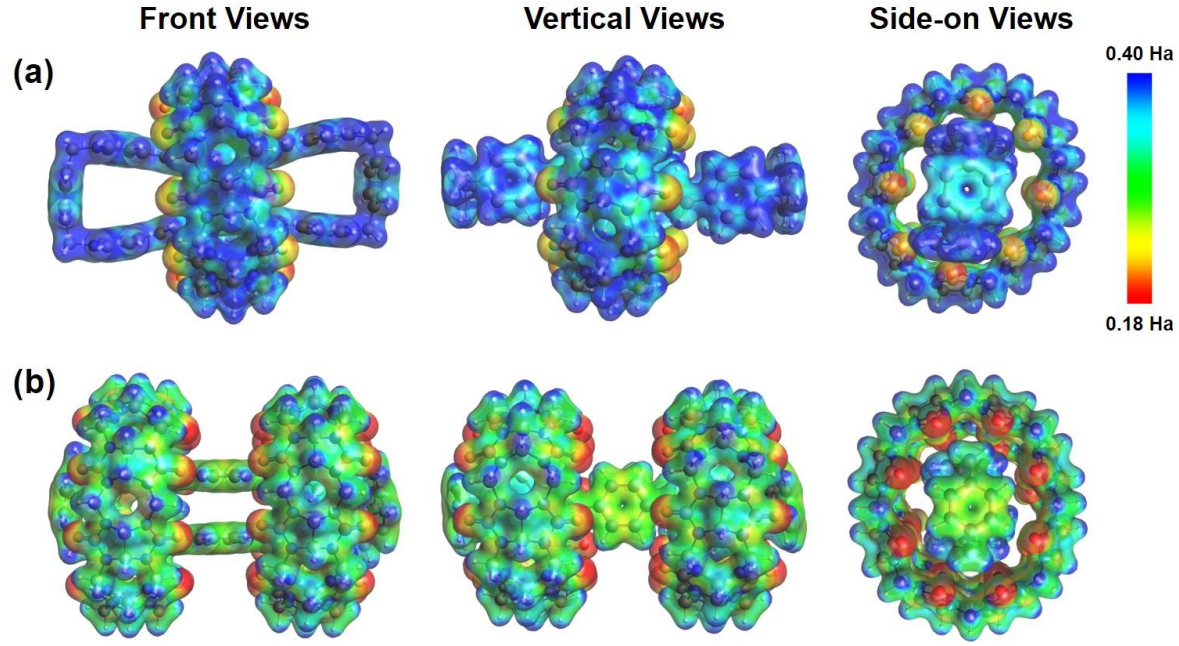


Figure S46. Different views of electrostatic potential maps for (a) the binary **OPVEBox^{4+}⊂CB[8]** and (b) ternary **OPVEBox^{4+}⊂2CB[8]** ring-in-ring(s) complexes obtained from DFT calculations. The maps demonstrate that when combing with one or two **CB[8]** molecules, the **OPVEBox^{4+}⊂CB[8]** and **OPVEBox^{4+}⊂2CB[8]** complexes become more and more electron rich. Red and blue colors in the maps represent negative and positive electrostatic potentials, respectively.

(3) Frontier Molecular Orbital Calculations

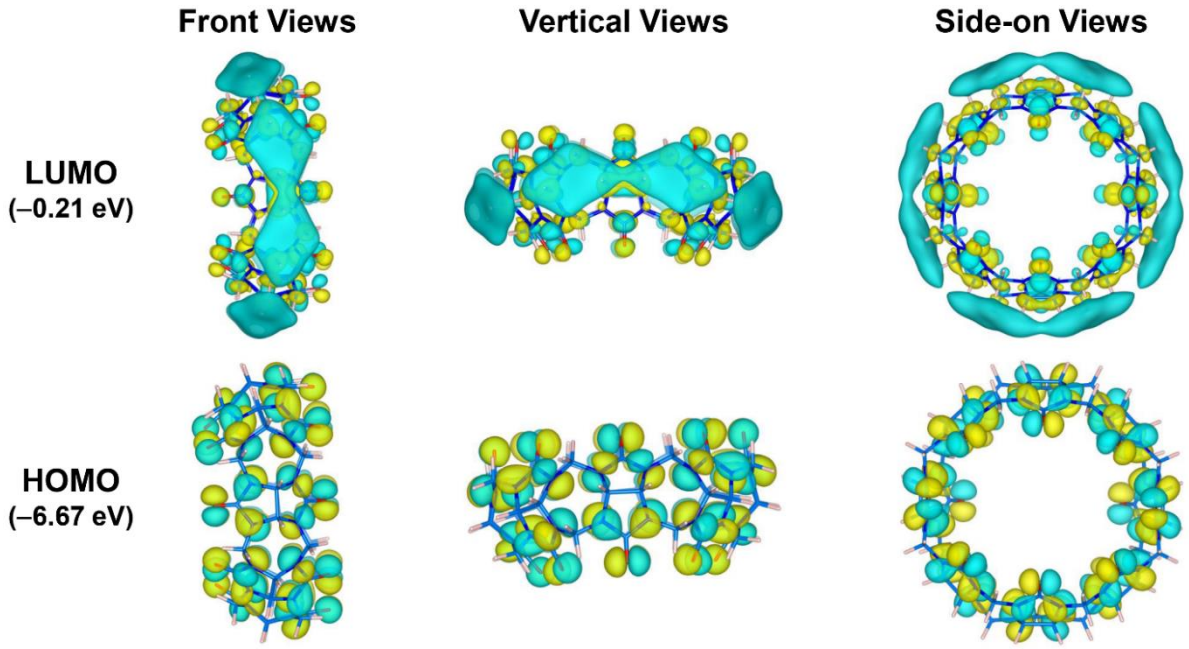


Figure S47. Different views of frontier molecular orbitals for **CB[8]**, which were calculated using the optimized geometry. The energy bandgap was calculated to be 6.46 eV.

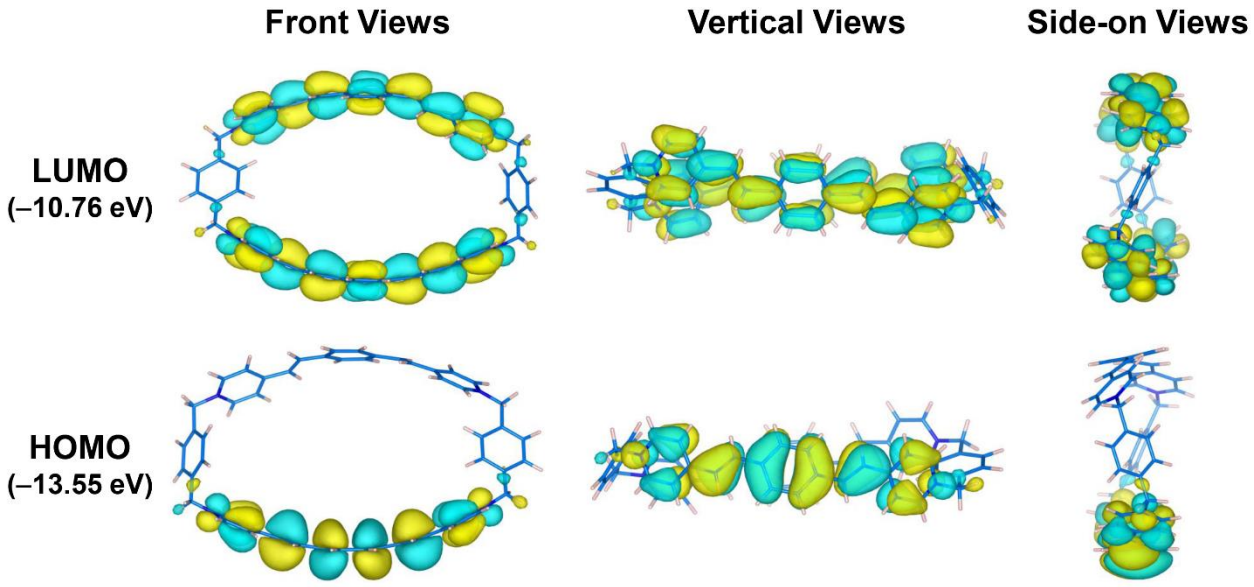


Figure S48. Different views of frontier molecular orbitals for **OPVEBox^{4+}**, which were calculated using the optimized geometry. The energy bandgap was calculated to be 2.79 eV. There is slight symmetry breaking, which results in the HOMO being localized on one side of the cyclophane.

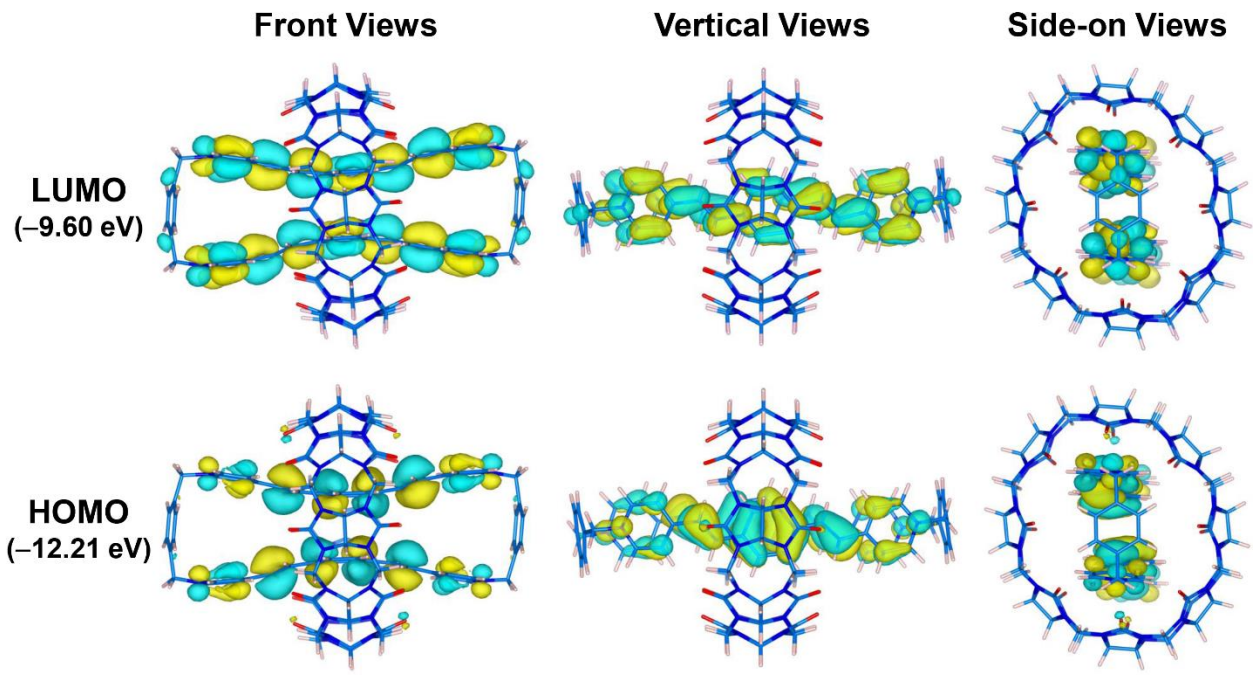


Figure S49. Different views of frontier molecular orbitals for binary **OPVEBox^{4+}⊂CB[8]** ring-in-ring complex, which were calculated using the optimized geometry. The energy bandgap was calculated to be 2.61 eV.

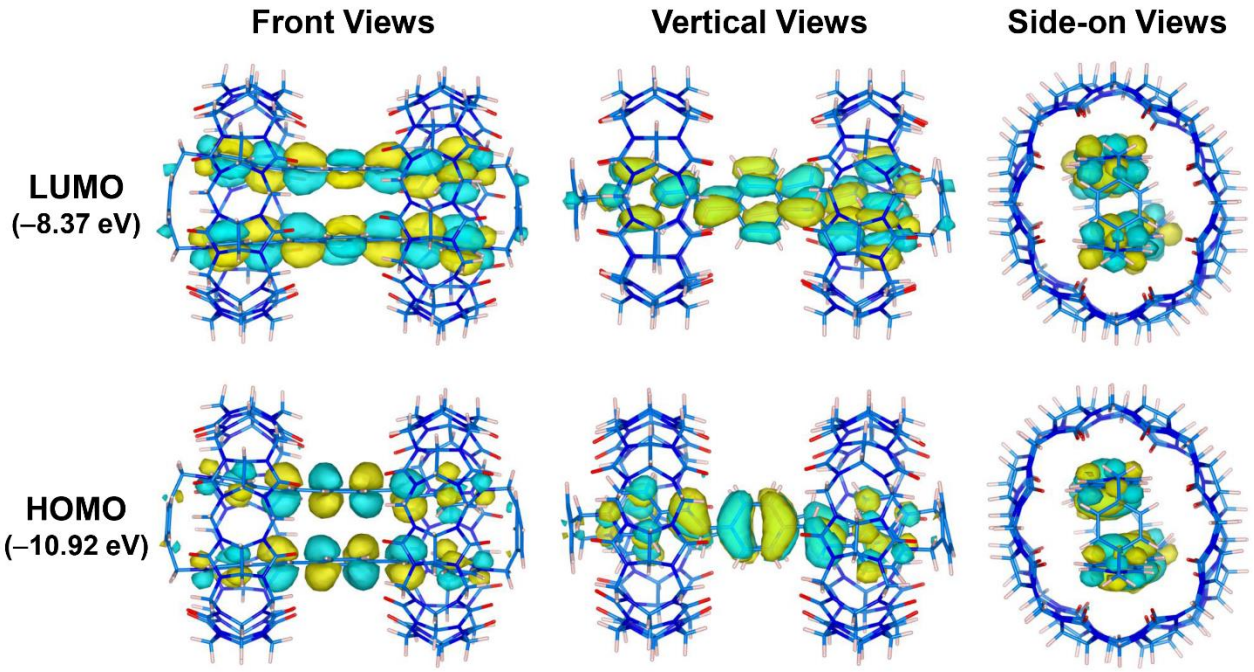


Figure S50. Different views of frontier molecular orbitals for ternary **OPVEBox^{4+}⊂2CB[8]** ring-in-rings complex, which were calculated using the optimized geometry. The energy bandgap was calculated to be 2.55 eV.

Table S3. The Calculated Energy Levels of the Frontier Molecular Orbitals in Vacuum

Energy / eV	CB[8]	$OPVEBox^{4+}$	$OPVEBox^{4+}$⊂CB[8]	$OPVEBox^{4+}$⊂2CB[8]
Ψ_{LUMO}	−0.21	−10.76	−9.60	−8.37
Ψ_{HOMO}	−6.67	−13.55	−12.21	−10.92
$\Delta E_{HOMO\text{-}LUMO}$	6.46	2.79	2.61	2.55

Table S4. The Calculated Energy Levels of the Frontier Molecular Orbitals in Water

Energy / eV	CB[8]	$OPVEBox^{4+}$	$OPVEBox^{4+}$⊂CB[8]	$OPVEBox^{4+}$⊂2CB[8]
Ψ_{LUMO}	0.54	−3.21	−3.10	−3.04
Ψ_{HOMO}	−6.82	−6.18	−5.81	−5.64
$\Delta E_{HOMO\text{-}LUMO}$	7.36	2.97	2.71	2.60

(4) Strain Energy Calculations

Table S5. The Calculated Strain Energy for the Central $OPVEBox^{4+}$ in Ring-in-Ring(s) Complexes in Vacuum

Strain Energy	$OPVEBox^{4+}$	$OPVEBox^{4+}$⊂CB[8]	$OPVEBox^{4+}$⊂2CB[8]
E / ha	–2377.4934	–2377.4478	–2377.4251
ΔE / kal mol^{-1}	–	28.59	42.85

Table S6. The Calculated Strain Energy for the Central $OPVEBox^{4+}$ in Ring-in-Ring(s) Complexes in Water

Strain Energy	$OPVEBox^{4+}$	$OPVEBox^{4+}$⊂CB[8]	$OPVEBox^{4+}$⊂2CB[8]
E / ha	–2378.3322	–2378.3354	–2378.3250
ΔE / kal mol^{-1}	–	–2.01	4.52

Section J. Cartesian Coordinates for the Optimized Structures

(1) In Vaccum

(a) CB[8]

H	11.145790	30.137660	-4.726710	N	14.890850	28.096560	-0.962540
H	8.717530	30.233430	-4.523130	C	5.076300	29.287440	-0.757560
H	12.834100	31.647930	-3.862140	C	6.141090	31.357560	-0.402960
H	12.786700	28.203600	-4.612570	H	17.586470	30.451800	-0.795770
C	10.782740	29.882270	-3.709150	C	6.542460	27.470070	-1.048860
H	14.514400	29.709960	-3.745880	H	16.707890	27.144070	-0.525560
H	7.202080	31.689540	-3.296480	O	6.376930	32.453210	0.045350
H	6.992670	28.383610	-4.166030	O	6.989410	26.353440	-0.951700
C	9.220520	29.914920	-3.586310	C	16.692130	30.826060	-0.260340
C	12.546430	31.475280	-2.802810	C	15.727080	27.350980	-0.046210
C	12.415750	27.927640	-3.604930	N	5.119020	30.501210	0.006150
N	11.224400	30.892380	-2.775780	N	5.666500	28.099040	-0.157650
N	11.112440	28.510170	-3.398590	H	16.730250	31.922990	-0.185890
H	12.491310	32.443410	-2.282950	H	15.211820	26.397920	0.144700
H	12.279670	26.837850	-3.540820	H	3.151280	30.571990	0.643280
H	5.498060	29.840890	-2.884440	H	3.964930	27.129190	0.597900
N	8.982740	30.898810	-2.553460	C	4.155660	30.861230	1.013060
N	8.877990	28.544650	-3.288880	H	17.936480	28.628380	0.959360
C	7.687740	31.496910	-2.315960	C	5.021050	27.324830	0.882960
C	7.535330	28.018850	-3.272220	H	4.204770	31.951630	1.150280
C	14.185700	29.514430	-2.704290	H	5.561270	26.367930	0.937640
C	10.156190	31.544540	-2.153700	N	16.708270	30.324310	1.091650
C	9.987140	27.704890	-3.249490	N	15.964380	27.975330	1.236310
H	7.859730	32.456000	-1.805150	C	17.001050	28.958760	1.457160
H	7.630100	26.923560	-3.310960	N	4.371990	30.280370	2.315660
N	13.584030	30.713510	-2.138060	N	5.039220	27.910020	2.204330
N	13.420810	28.302200	-2.645150	C	16.673230	31.182940	2.186320
H	16.309230	28.965520	-2.260450	C	15.554760	27.357250	2.421040
O	10.227470	32.524260	-1.452780	O	16.593550	32.387670	2.151960
O	9.972960	26.499980	-3.167010	O	14.841960	26.387620	2.509270
C	6.034740	29.583990	-1.947600	H	3.074320	28.628220	2.279860
N	6.788460	30.735580	-1.474930	C	4.086320	28.902680	2.644600
N	6.748280	28.350950	-2.110930	C	17.123980	29.017240	3.018710
C	15.369650	29.233620	-1.733950	H	18.139610	28.760590	3.386150
C	14.473920	31.359480	-1.272850	O	4.570920	32.293400	3.456170
C	13.823020	27.463610	-1.605990	C	4.507520	31.087360	3.441510
H	4.036310	29.073650	-1.079890	O	6.387760	26.300460	3.204370
O	14.380150	32.487010	-0.853090	C	5.669550	27.267700	3.274030
O	13.372200	26.372500	-1.354520	N	16.822790	30.396600	3.324960
N	15.531200	30.479140	-1.041660	N	16.182790	28.022030	3.477820

C	4.206750	28.871780	4.207180
N	4.480350	30.246690	4.550370
N	5.255670	27.905500	4.446880
H	16.970000	32.088160	4.462910
H	15.680710	26.494100	4.768900
C	17.033810	31.000840	4.617600
C	16.210510	27.457530	4.807930
H	3.274480	28.537280	4.708310
H	18.042580	30.730800	4.989830
H	17.269680	27.278150	5.092410
H	4.425210	31.866380	5.799060
H	6.031570	26.362800	5.571210
N	16.077180	30.644660	5.632360
N	15.558900	28.239750	5.838600
C	4.484630	30.771980	5.893300
C	5.504140	27.312970	5.742630
O	14.790790	32.576240	5.557330
O	14.265050	26.488920	6.669150
H	3.596850	30.390400	6.434090
C	15.042030	31.492470	6.025640
H	4.527240	27.103500	6.228600
C	14.696390	27.613280	6.744650
C	16.136170	29.444850	6.416850
N	5.650310	30.461430	6.682590
O	6.782630	32.471400	6.421530
N	6.332060	28.089500	6.641540
O	7.882220	26.398700	7.055120
H	17.179110	29.249410	6.741120
C	6.701820	31.357310	6.877560
C	7.414580	27.486460	7.289950
C	5.838210	29.232020	7.395960
N	14.403040	30.879260	7.107830
N	14.482680	28.508930	7.792710
C	15.175770	29.749890	7.603030
O	10.938710	32.590890	7.024260
O	11.289000	26.620600	8.870580
H	4.907730	28.957030	7.934610
N	7.604190	30.747110	7.755220
N	7.808750	28.350910	8.311230
H	13.301470	32.585770	7.405730
H	13.626350	27.090060	9.020810
C	11.022570	31.633410	7.753830
C	11.253220	27.826270	8.932770
C	7.024710	29.551790	8.351250
C	13.489570	31.639400	7.934270
C	13.699650	28.186000	8.959520
N	12.204880	31.022900	8.180900
H	8.672480	32.495440	7.849280
N	12.346980	28.686270	8.963220
H	15.709730	30.034870	8.533290
H	8.977480	26.921690	9.227730
N	9.962110	30.977850	8.385650
N	10.112790	28.613500	9.063440
C	8.631640	31.542000	8.396670
C	8.820250	28.009400	9.276600
C	11.978440	30.055900	9.231680
H	13.969960	31.858320	8.911850
H	14.233300	28.579190	9.846530
H	6.700570	29.763990	9.390970
C	10.415950	29.997750	9.345320
H	8.341600	31.741250	9.450830
H	8.443270	28.291570	10.280300
H	12.469780	30.401880	10.164910
H	10.041950	30.270040	10.354470

(b) OPVEBox^{4+}

H	-6.312880	4.247277	-0.538720
H	-4.764450	2.441943	-0.032410
H	-7.122610	6.526215	-0.120640
C	-5.998020	4.760495	0.374112
H	-5.375980	1.972575	1.556233
C	-4.712950	2.683110	1.040236
C	-6.461330	6.056248	0.613113
H	-2.514910	3.767629	0.165685
C	-5.152210	4.118202	1.294271
N	-3.330230	2.397498	1.514123
C	-2.281430	3.077076	0.978171
H	-6.160070	8.840997	1.183339
C	-6.079380	6.754348	1.770896
H	-3.972760	0.937184	2.865147
C	-3.103630	1.486606	2.498996
C	-4.782280	4.811060	2.454520

C	-1.001150	2.914483	1.464087
H	-0.195180	3.495077	1.010920
C	-6.590520	8.180815	1.951017
C	-5.230770	6.116313	2.685228
H	-4.829900	10.056490	2.447471
H	-4.132210	4.343613	3.198703
H	-7.683590	8.221563	1.820297
C	-1.842460	1.283157	3.019106
C	-0.735450	2.038771	2.550474
H	-4.903250	6.621884	3.595846
H	-1.736600	0.549186	3.818827
C	-5.291760	9.718080	3.376856
N	-6.268530	8.779868	3.267826
H	1.295296	2.739166	2.728274
C	0.581107	2.033617	3.161852
H	-4.105710	10.952510	4.642813
C	-4.900230	10.204400	4.607007
C	-6.917860	8.353530	4.387184
H	-7.725960	7.635157	4.233861
C	0.931426	1.319217	4.267791
H	0.214072	0.597554	4.672851
H	3.191232	2.914572	3.814311
C	-5.485830	9.717384	5.803480
C	-6.556250	8.796267	5.641656
C	3.170306	2.394778	4.774290
C	2.132226	1.482409	5.078535
H	-4.133780	10.881480	7.005814
H	-7.116690	8.414883	6.496301
H	4.936735	3.403956	5.459814
C	-4.919580	10.124510	7.075995
C	4.163423	2.670868	5.704732
C	2.207922	0.777001	6.304754
H	1.449915	0.025067	6.540291
C	4.167468	2.053758	6.979740
C	3.198560	1.055326	7.234840
C	-5.180170	9.550597	8.282966
H	-5.944840	8.768144	8.345335
H	-3.409550	11.610120	8.935825
H	3.202697	0.504985	8.177085
H	5.799794	3.305914	7.640284
C	5.089794	2.551627	7.995618
C	-3.504670	10.824700	9.688961
C	-4.433390	9.771971	9.517022
H	-1.969370	11.686250	10.918950
C	-2.690260	10.871190	10.813080
C	-4.569500	8.825250	10.562220
C	5.062506	2.242524	9.321516
H	-5.324770	8.038936	10.480690
H	7.081568	4.249163	9.188959
H	4.354490	1.488025	9.673449
C	6.766971	3.933138	10.184690
C	-2.742090	9.853027	11.796760
C	-3.735370	8.854549	11.672010
C	5.811229	2.901599	10.375680
H	-3.862880	8.099201	12.450640
H	-1.149580	10.765000	12.948960
H	8.051197	5.390175	11.143120
C	-1.717030	9.834667	12.836350
C	7.322512	4.586724	11.266870
C	5.539157	2.553058	11.725030
H	4.849106	1.739710	11.957440
C	-1.350980	8.742293	13.560440
H	-1.887280	7.802800	13.402230
N	6.981428	4.267195	12.543270
H	6.254819	7.391382	12.964110
C	6.118590	3.242189	12.768120
H	0.332545	10.767450	14.610800
C	-0.205040	8.646770	14.445820
C	0.598783	9.738995	14.860010
H	8.273704	5.734958	13.292380
H	4.527281	8.635271	14.186220
C	5.890395	6.996073	13.917130
H	5.898237	3.006785	13.810780
C	7.517192	5.051649	13.700760
H	-0.392500	6.481792	14.668580
C	0.200309	7.366959	14.907290
C	4.912070	7.705147	14.614570
C	1.750494	9.524992	15.592150
H	2.390556	10.347340	15.918290
C	6.437447	5.814147	14.449150
H	8.034540	4.345960	14.366770
C	1.359682	7.209215	15.634080
N	2.144243	8.272956	15.947400
C	4.443678	7.245699	15.859010
H	1.708301	6.233754	15.978030
C	5.979791	5.363832	15.694810
C	3.431685	8.041693	16.667620
H	3.830538	9.031890	16.930840
C	4.987320	6.067783	16.388720
H	6.414816	4.470093	16.151520
H	3.195501	7.525968	17.609580
H	4.651394	5.697041	17.361510

(c) OPVEBox^{4+}⊂CB[8]

H	-4.472230	4.296714	-1.458780	H	4.498483	9.433895	4.187355
H	-4.598720	1.775709	-1.188180	H	-0.036680	3.219233	3.364744
H	-5.265910	6.537650	-0.816430	H	4.112293	-0.187830	3.744890
C	-5.235390	4.390380	-0.680740	N	2.678780	8.378558	4.117547
C	-5.014210	1.917906	-0.181550	C	-1.023980	2.947867	3.747805
H	-5.672150	1.067355	0.042129	C	4.725851	7.206065	4.348701
C	-5.686450	5.660488	-0.316370	C	-6.310330	6.999695	3.712547
H	-2.494110	2.555528	-0.629350	C	3.313998	0.529768	4.005733
C	-5.725780	3.249346	-0.027710	O	-1.075630	9.511704	4.230824
N	-3.875340	1.882802	0.788245	N	3.888072	1.856749	4.112727
C	-2.657300	2.372000	0.434261	C	4.008931	8.562150	4.661638
C	-6.638470	5.812838	0.703718	C	5.383763	3.677390	4.358262
H	-6.736650	7.989941	0.590432	H	-7.359880	6.743849	3.867544
C	-6.766600	3.395922	0.902520	H	5.953864	1.503161	4.286766
H	-5.090430	1.128040	2.309676	O	0.458956	0.341425	4.380745
H	-0.735170	3.057718	1.058027	N	1.065694	10.016420	4.972094
C	-1.696900	2.654218	1.381767	C	-4.025030	7.234790	4.475680
C	-4.121300	1.579100	2.093154	C	5.172806	2.162891	4.707831
H	-4.467390	8.110935	1.187676	C	-0.321450	10.070480	5.004682
C	-7.220610	4.666016	1.264431	H	6.922608	5.806325	5.154467
C	-6.901980	7.177868	1.311536	C	-5.386350	6.929186	4.732837
H	-7.211400	2.516617	1.377283	H	2.284907	11.670590	5.431225
H	4.918588	5.427380	2.290600	H	-2.630930	10.974740	5.347760
H	-7.923330	7.271751	1.703966	C	-1.299070	3.045412	5.076239
H	3.152202	5.086078	2.210680	H	-2.280560	2.736838	5.447539
C	-4.683010	7.771089	2.201468	H	1.174222	4.268110	4.798034
H	-8.012910	4.759062	2.012840	N	2.620281	0.058956	5.181744
C	-3.205060	1.848023	3.082853	N	5.109393	6.711434	5.654742
C	4.003292	5.249149	2.887123	C	1.234851	-0.011710	5.240780
C	-1.971410	2.480233	2.763498	H	-2.012650	7.555728	5.111029
O	1.521205	6.735870	2.949690	N	5.568169	4.302795	5.653609
H	1.017537	9.091976	3.132645	C	1.674679	10.902160	5.942842
N	-5.960160	7.382196	2.453442	C	6.072826	5.647693	5.845016
O	2.276635	2.952617	2.851141	N	4.091915	8.663338	6.102522
H	2.347117	10.286970	3.345170	C	-2.955980	7.119552	5.442722
H	-2.704690	8.064451	2.952689	N	-0.694460	10.906190	6.046425
H	2.578775	0.563775	3.189119	H	4.380093	10.719350	6.329418
H	5.620648	7.321777	3.708420	H	-2.050040	12.495460	6.111334
C	2.514521	7.130201	3.519608	H	-5.730930	6.658212	5.733010
C	-3.715310	7.719237	3.178872	H	-1.020930	-0.863630	5.770990
N	3.714127	6.437681	3.659919	C	-2.055760	11.391150	6.186979
H	-3.442440	1.553897	4.107284	C	0.910402	4.009281	5.824491
C	1.776268	9.471516	3.831530	H	3.947128	-1.350740	5.995688
C	3.317150	2.947728	3.476867	N	5.233781	2.145188	6.158072
N	4.168914	4.031858	3.652733	C	4.768715	7.590488	6.680728
H	6.267203	3.862310	3.718514	C	-0.358650	3.455094	6.107310

O	-4.364270	9.679802	6.386570
H	0.389398	12.605060	6.641652
C	3.844922	9.888987	6.829320
C	0.448735	11.502070	6.709237
C	3.263431	-0.545390	6.325391
C	5.499600	3.392281	6.698836
N	2.451519	10.259250	6.983001
N	0.898920	-0.616260	6.449948
O	-2.826770	0.489631	6.585534
H	6.431822	5.715014	6.881973
H	5.888261	0.187878	6.454745
C	-0.437940	-1.118240	6.667657
H	-0.395740	7.314143	6.373538
C	-3.056390	6.598868	6.693429
H	-0.401760	-2.219230	6.783568
C	5.249592	0.936795	6.957799
H	2.813097	4.632695	6.596713
H	-4.006730	6.173551	7.030196
N	-2.741860	11.001550	7.397841
C	1.831814	4.220111	6.842102
C	-3.887060	10.213160	7.365398
N	3.955333	0.352345	7.229911
C	2.062413	-1.069530	7.184987
H	4.255982	9.753073	7.839171
O	5.041221	7.462618	7.853667
C	-0.695550	3.228111	7.462241
H	2.047197	-2.172140	7.281601
H	-1.691090	2.853976	7.709263
O	5.674461	3.645925	7.875533
C	-2.342010	0.124319	7.638454
N	0.681391	11.095720	8.079535
C	-0.689590	7.108013	7.404134
C	1.880417	10.416690	8.240531
H	-6.156880	9.342956	7.951389
H	-4.717400	0.788511	8.039702
O	-6.135870	6.894743	8.003452
N	-1.143180	-0.555020	7.799524
O	-5.503000	3.078709	8.025414
C	-1.996680	6.654916	7.694899
H	5.695433	1.197736	7.927232
C	1.535070	3.885819	8.184926
N	-4.416980	10.188620	8.648905
C	0.228044	3.432557	8.475734
H	-2.508710	12.713190	8.597497
C	-2.524120	11.610560	8.693945
C	3.425593	0.327682	8.513481
N	2.280140	-0.460350	8.481033
H	-6.893950	4.826084	8.997288
H	1.229632	7.686249	8.170643
C	-5.711220	9.604041	8.920864
O	2.365141	10.051150	9.293391
C	0.233980	7.312418	8.417644
N	-2.913020	0.282167	8.895979
C	-4.306420	0.652475	9.049574
H	-0.059760	12.759780	9.096042
C	-0.023790	11.658740	9.211530
C	-5.961030	7.148550	9.180115
C	-5.230660	2.950718	9.198379
N	-1.360760	11.156910	9.428987
C	-2.293540	6.320834	9.037755
H	-6.350030	10.352910	9.423817
H	3.545101	4.367435	8.849486
C	-0.910450	-0.960930	9.169922
H	-4.841700	-0.177940	9.549293
H	-3.274930	5.908516	9.283167
H	-0.065750	3.226435	9.506351
C	-3.725310	11.086580	9.553404
C	2.594860	3.941936	9.186305
H	-0.851080	-2.063900	9.237810
O	3.902876	0.861032	9.492278
N	-5.695280	8.395722	9.720710
N	-4.553430	1.878056	9.776477
C	-6.534880	4.893404	10.034220
H	-4.409130	11.891940	9.882832
H	0.559079	11.403660	10.108140
C	1.594060	-0.849900	9.691922
N	0.232781	-0.364860	9.832523
C	-2.136340	-0.360820	9.936220
H	5.269513	3.882228	10.146280
N	-6.030040	6.238254	10.225520
H	1.588217	-1.954210	9.767511
N	-5.571580	3.829556	10.224430
C	-0.103060	7.085746	9.772591
C	-1.696920	10.552550	10.638200
C	-1.372240	6.531878	10.055430
H	-7.384590	4.734896	10.724870
N	-3.082360	10.482510	10.697310

H	-2.746720	-1.129160	10.447790
C	2.494642	3.420967	10.436900
H	2.169272	-0.433580	10.531160
H	1.551330	2.984797	10.768640
C	-0.140190	0.470756	10.874360
N	-1.527340	0.524895	10.906960
C	-5.634640	8.378271	11.170970
H	1.819082	7.803441	10.432240
C	4.925080	3.611268	11.146510
O	-0.921140	10.199080	11.498200
C	-4.470620	1.979060	11.217420
H	-1.636060	6.273024	11.081880
C	0.837467	7.495332	10.803610
C	-5.845650	6.863841	11.520780
C	-5.187520	3.335162	11.530370
H	-6.415800	9.038068	11.591760
H	-4.960290	1.107276	11.691510
H	6.898695	3.796657	12.011600
N	-4.350040	8.684573	11.766250
C	3.563792	3.305662	11.403820
O	0.614024	1.029529	11.648190
C	-3.776180	10.011650	11.873230
N	-3.140560	2.162542	11.761740
H	-6.729110	6.679052	12.160530
C	5.849179	3.540733	12.166680
H	-6.082060	3.219496	12.171020
H	-4.574650	10.729130	12.133850
N	-4.630810	6.509505	12.226400
C	-2.237940	1.069649	12.047600
N	-4.175590	4.103771	12.218640
C	-3.779080	7.593671	12.402210
C	-2.976100	3.411070	12.359230
H	-3.041110	9.977831	12.689990
C	0.562468	7.593186	12.132040
H	-2.808670	0.254118	12.533940
H	-0.424930	7.322273	12.515170
H	-1.479180	1.449243	12.746430
O	-2.738760	7.588942	13.028250
C	-4.464860	5.292104	12.991740
C	3.254236	2.821070	12.700620
O	-1.982730	3.805448	12.929020
H	2.981389	8.986184	11.772080
N	5.499143	3.158203	13.425820
H	2.243655	2.475776	12.926870
H	7.552193	5.781357	13.866440
H	-5.380070	5.113567	13.588310
C	1.510190	8.060565	13.116190
H	-3.613750	5.455225	13.668140
C	4.222058	2.769189	13.677900
H	7.462390	3.268674	14.175130
C	2.744016	8.692337	12.796590
C	6.441061	3.362580	14.567630
H	6.750688	8.023826	14.501930
C	6.759856	5.874428	14.614810
H	0.274053	7.483567	14.821890
C	1.235877	7.886712	14.497970
H	4.006549	2.429328	14.691710
C	3.660469	8.961110	13.786120
H	6.275775	2.550536	15.288780
C	6.305855	7.144537	14.976690
H	4.629689	9.411888	13.569410
C	6.177569	4.727625	15.175410
C	2.196436	8.168910	15.445320
N	3.414566	8.657711	15.091110
C	5.265055	7.291144	15.906930
H	2.033369	7.985483	16.508970
C	5.225549	4.879993	16.195490
H	5.211445	9.473140	15.837060
C	4.553516	8.622599	16.060810
H	4.804947	4.002837	16.695510
C	4.774581	6.150114	16.559920
H	4.138124	8.764806	17.067470
H	4.011459	6.243804	17.337990

(d) OPVEBox^{4+}⊂2CB[8]

H	-4.666680	3.998761	-2.384580	C	-2.156920	3.125608	0.999594
H	-4.502320	1.526840	-1.741570	C	0.196734	-0.627550	0.249435
H	0.959356	1.975079	-2.832980	H	-7.535440	2.214027	0.319254
H	-0.823510	2.166857	-2.938780	H	0.451482	9.166450	-1.051100
C	-5.507210	4.092192	-1.691010	C	-7.171340	6.816126	0.294247
H	-5.565210	6.238152	-1.862890	C	-4.445500	1.733587	1.542694
O	-1.903660	4.336107	-2.521190	H	-5.389920	1.210229	1.688080
C	0.040434	2.198310	-2.259480	H	-4.375600	10.283660	-0.981480
H	-1.783470	6.739751	-2.681210	N	1.654145	3.781954	0.165337
H	-0.157240	7.493538	-2.797080	H	-8.155980	6.953818	0.753550
C	-5.113510	1.752292	-0.859410	C	-0.331620	8.786824	-0.367480
C	-6.014090	5.357087	-1.395670	N	1.340886	1.404571	0.664171
H	-2.854800	3.025757	-1.048880	C	2.250557	2.521206	0.561032
H	-5.660000	0.848242	-0.573110	N	-2.848560	-1.667950	1.137167
O	-2.317200	0.587137	-1.903670	N	1.270046	5.994007	0.239720
C	-5.986860	2.970743	-0.997860	H	2.208947	7.851782	0.078438
H	2.218549	3.861010	-1.859670	C	-4.214640	-1.427630	1.177002
C	-0.814510	4.530187	-2.022250	C	-4.894060	7.228754	1.174079
C	-0.880180	7.005567	-2.113970	N	-2.543530	9.635934	-0.269080
N	0.142291	3.557561	-1.750610	H	-8.439290	4.454635	0.841154
H	-2.847560	-1.601510	-0.924900	H	-3.244900	11.585710	-0.479680
H	1.742109	6.257164	-1.793670	C	-3.643130	10.586860	-0.219520
N	-0.161580	1.159105	-1.269140	N	-6.167610	6.843304	1.420379
C	-1.326920	0.399708	-1.229190	C	-2.396000	2.775775	2.352036
H	1.752074	0.302914	-1.080320	C	1.645408	4.892364	1.004372
N	-0.298680	5.764846	-1.633150	C	-3.606840	2.069479	2.588237
C	-3.025760	2.759031	-0.006760	H	-0.906780	10.938380	-0.071580
N	-4.145560	2.048559	0.257709	C	1.463130	7.344953	0.722588
C	1.361130	4.120845	-1.209760	C	-1.220240	9.923795	0.240896
O	-3.536270	8.050975	-1.645430	N	0.310560	-0.323440	1.658694
H	-1.581870	-2.653880	-0.203440	H	-6.622080	-1.533670	1.880272
C	1.066288	5.659555	-1.152650	N	0.273974	8.166070	0.791090
C	-7.003270	5.497671	-0.410460	H	-2.927560	7.551431	1.919056
C	-7.117060	3.093507	-0.177090	H	2.691133	2.671854	1.556886
C	-2.108620	-1.685840	-0.114810	O	-6.365320	9.808666	0.275762
C	0.893224	0.596217	-0.446880	H	-1.945420	-3.214330	2.238301
N	-1.143900	-0.617330	-0.300750	C	1.022582	0.846980	1.901409
H	-6.953820	7.688911	-0.331080	C	-3.930960	7.202401	2.163268
H	0.688572	-1.592630	0.020633	C	-2.346210	-2.194320	2.393157
N	-1.278850	7.965448	-1.098750	N	-4.655660	-1.659470	2.476108
H	-4.680610	7.554598	0.155481	H	-0.542940	3.675129	2.958155
C	-2.565590	8.497267	-1.069060	H	0.392177	-2.257840	2.438303
O	-4.911280	-1.094920	0.242811	H	-3.894090	1.762712	3.594102
H	-1.259090	3.682448	0.735184	O	-7.673000	0.686952	2.191115
H	3.050358	2.267550	-0.159670	C	-1.413280	3.142899	3.349579
C	-7.626460	4.357880	0.117593	H	1.860519	7.265888	1.744893

C	-6.063410	-1.653470	2.819601
C	0.014115	-1.257860	2.722404
O	1.941158	4.906811	2.178747
N	-4.356260	10.676150	1.040404
C	-6.492650	6.378382	2.652217
C	-5.697950	10.325760	1.145596
H	-6.326370	-2.625980	3.276143
N	-1.380670	-1.376180	3.089032
H	-7.518820	6.034650	2.771132
N	-1.047430	9.758247	1.667431
C	-0.123730	8.764695	1.986258
C	-3.603260	-2.156650	3.336981
O	1.348092	1.281126	2.980435
H	-3.878470	-3.150780	3.739463
C	-4.230050	6.763587	3.479222
H	-8.111140	10.406110	1.870286
C	-7.355650	0.424458	3.331974
H	0.549692	-0.901050	3.614345
N	-6.496380	-0.598690	3.722300
C	-5.570190	6.333286	3.677789
H	-9.276890	2.033638	3.407147
H	1.067709	4.005086	4.283401
C	-1.452840	2.856754	4.681078
H	-3.550610	12.413560	1.909715
O	-9.013500	8.202440	2.368853
C	-3.882840	11.399540	2.205529
O	-9.195250	4.442429	3.035586
O	0.280474	8.493239	3.093870
H	-2.319270	2.330071	5.093362
H	-1.181740	11.752610	2.263646
C	-1.868400	-0.856420	4.281047
N	-6.140910	10.697260	2.408696
C	-1.455980	10.749270	2.643578
H	-2.246150	7.224568	4.198890
N	-3.192240	-1.276900	4.412330
C	-7.543960	10.652290	2.779622
C	-3.209510	6.810467	4.508318
N	-2.858970	10.747840	2.990029
H	7.242203	7.886422	6.623331
H	5.591985	7.169481	6.555496
H	-5.909280	5.974268	4.649172
C	0.815522	3.775113	5.319786
N	-7.797030	1.077704	4.480921
C	-8.974220	1.927994	4.458601
H	-10.224200	6.606529	3.686267
C	-5.127920	11.408030	3.162840
C	-0.425120	3.183531	5.659730
H	-7.848680	11.651970	3.140495
O	-1.249860	-0.194700	5.081933
C	-8.651590	8.542347	3.475202
H	-0.894190	10.538020	3.565095
C	-6.341080	-0.668030	5.156237
C	-9.083130	4.399209	4.242561
H	-9.786860	1.421889	5.016505
H	-6.594780	-1.682420	5.518981
O	3.747142	8.450348	7.492064
C	6.439342	7.404242	7.215415
H	-5.485680	12.426830	3.407370
N	-7.904950	9.668473	3.783023
H	2.883589	10.646080	8.122646
C	-3.892370	-1.140280	5.670357
N	-8.812750	3.265024	5.001706
O	5.281363	4.832934	6.761736
H	-4.216330	-2.142990	6.012837
H	2.706089	4.510686	6.032095
C	-3.293970	10.410750	4.271917
N	-5.047290	-0.261010	5.664514
H	6.186177	2.588460	6.470271
C	-3.393700	6.438616	5.806764
C	-7.307700	0.439775	5.691126
C	1.745968	4.067899	6.307140
H	4.014630	11.957590	8.615060
H	9.013376	6.465455	7.658874
C	-9.827310	6.738214	4.703108
H	-0.925240	7.752219	5.934521
C	4.667826	8.872811	8.151397
N	-4.640030	10.753550	4.357607
N	-8.935640	7.878617	4.663743
N	5.959607	8.341509	8.207033
H	-4.353530	5.998906	6.092259
H	7.676364	9.547961	8.382410
H	7.889665	2.131197	6.829053
N	-9.224760	5.478227	5.110462
N	6.932574	6.144026	7.730887
C	6.345481	4.946704	7.329497
C	-0.680510	2.887913	7.020681
H	-8.154000	0.033806	6.277683

C	3.582172	10.979300	8.903468	C	-0.479140	7.448539	8.010441
H	-3.174930	-0.724440	6.392703	C	-6.975910	2.148410	7.547484
H	-1.627200	2.416624	7.296136	H	-4.614970	10.492290	6.397049
H	9.307465	4.034729	7.712716	H	-9.375420	8.927388	6.436475
O	-2.614030	9.945800	5.156460	C	5.135766	1.271194	8.333238
C	6.958918	2.550602	7.251347	H	-9.983120	5.352840	7.066346
N	4.651885	10.006610	8.962458	N	-7.898320	5.617286	7.162459
H	-10.665600	6.955959	5.390185	H	-0.999510	11.216080	10.664990
C	8.259883	5.947242	8.281983	C	8.602437	7.673513	10.145400
N	7.212315	3.917701	7.660379	C	-2.874250	6.023475	8.165418
C	6.856917	9.145070	9.007780	H	3.748759	12.833750	10.963940
H	6.272498	11.283210	9.356433	C	2.514132	4.118850	8.645541
C	-5.128820	0.849028	6.505085	C	-7.010480	4.618051	7.543929
O	0.801282	10.322180	9.291644	H	0.005291	2.940491	9.041891
C	-7.731050	9.845389	5.209680	H	-3.832470	5.506050	8.236652
C	-1.251200	7.286430	6.866105	O	-5.312330	8.368312	7.302984
N	-6.462310	1.257178	6.530009	H	8.130703	0.475694	8.760496
C	-2.473940	6.576285	6.925365	N	8.597429	4.069610	9.693845
C	8.427984	4.384561	8.285826	H	-7.760410	1.613732	8.118392
C	-8.796210	3.551054	6.424343	C	3.260965	11.889460	11.272580
C	1.485237	3.785595	7.670401	N	5.980446	10.023680	11.022690
N	-6.384160	9.687942	5.717265	H	3.149973	-0.176960	8.699077
C	5.926867	10.257730	9.592161	N	0.936104	11.432340	11.329980
C	-5.357350	10.706080	5.613932	H	9.686714	2.290305	9.554834
C	-8.500310	8.624102	5.830361	C	-7.790940	6.975285	7.659066
O	4.252462	1.635149	7.594622	H	-6.140660	2.394185	8.218716
C	0.248683	3.185957	8.007454	C	7.296411	1.004674	9.259609
H	-8.144540	10.823020	5.523938	C	8.688574	5.209256	10.480890
C	-9.070620	5.093670	6.496070	O	-5.999870	4.765552	8.194624
H	9.353491	8.178118	9.508827	H	-0.723740	12.629770	11.746730
N	2.805563	11.156190	10.113830	C	-0.487950	11.561910	11.575360
H	-9.562940	2.945127	6.944232	C	6.891304	9.023499	11.361850
O	-4.215550	1.347209	7.124048	H	5.968100	11.998650	11.698380
C	1.439143	10.891670	10.148480	H	8.989076	7.610435	11.172700
H	-5.817940	11.695210	5.801112	H	4.713098	5.558818	9.812049
N	-7.513750	3.407007	7.078127	N	5.023682	0.336004	9.360164
C	-6.278030	8.642986	6.630678	C	8.922413	2.748863	10.208270
N	6.468579	1.670092	8.283499	C	-0.875600	6.878241	9.245658
N	-7.508110	7.987501	6.666058	H	1.687003	13.180330	12.233480
H	3.356131	4.685930	8.236702	O	-2.220350	9.286134	11.373590
N	8.425657	6.311289	9.673693	C	-2.090000	6.158849	9.300661
H	0.442875	8.031258	7.960734	C	1.950151	12.113080	12.105560
N	7.403261	8.491878	10.178700	H	-6.956670	6.985190	8.375772

H	-8.729220	7.239132	8.182634	H	-0.731840	5.451327	11.590590
C	2.537307	3.742901	9.955893	C	1.471352	11.767110	14.593790
C	5.555117	11.013720	11.994050	H	2.856004	2.583361	12.375040
C	3.825507	-0.451510	9.522948	N	1.232746	0.002849	12.003830
H	4.085057	-1.525760	9.445864	H	-4.322610	8.855766	14.401700
N	4.122427	11.156850	12.184600	C	3.435747	-0.865000	12.016580
N	7.808136	1.827958	10.341170	H	1.395766	8.601574	12.348600
H	1.735209	3.103529	10.330470	H	3.671868	-1.934120	11.851180
C	6.295684	0.031997	9.980231	H	-3.541110	3.575858	12.935930
O	1.174660	0.640020	9.773756	N	0.285927	10.949280	14.752160
H	6.551343	-1.035290	9.834192	C	-3.174350	5.962145	13.578640
O	8.951881	5.246492	11.665020	C	-0.192820	0.073214	12.236020
C	4.671334	4.925857	10.698990	C	-1.965010	10.196740	14.770190
H	9.348499	2.894221	11.211380	N	5.712057	4.299576	12.761750
O	7.205680	8.694061	12.483950	C	5.907002	-0.399760	12.480380
N	-1.016270	10.783940	12.675390	H	6.103096	-1.467780	12.271480
H	-2.455610	5.762462	10.248390	C	-1.528710	2.083674	12.798350
C	-1.914560	9.740195	12.449960	H	-2.820640	10.713350	15.245940
H	0.649384	7.922962	10.353850	N	-3.173220	7.113871	14.354370
C	3.608339	4.002742	10.894490	N	4.493349	-0.239760	12.779810
C	-0.051070	7.085300	10.430370	C	4.697683	3.434758	13.003780
H	5.984897	10.721730	12.963030	H	2.119380	11.565400	15.458800
H	-3.883230	8.224350	12.774230	H	-0.545560	-0.914810	12.592660
N	2.256432	11.522950	13.392880	H	7.624634	4.985909	13.324890
N	3.090150	-0.234930	10.757030	C	0.660048	6.586432	12.786010
C	3.538807	10.986510	13.434070	H	6.667548	7.200286	14.074500
C	1.768441	0.198607	10.730730	C	1.371704	7.781739	13.066680
H	6.475989	5.787138	11.531250	C	2.161060	-0.640190	12.902690
C	7.334852	1.417539	11.582570	N	-0.629490	1.086520	13.172030
N	6.421521	0.389460	11.378560	H	6.461791	-0.099230	13.380720
C	5.675414	5.059018	11.638620	C	-3.181720	3.518678	13.973680
O	-3.350220	5.901580	12.382990	N	-2.984500	4.876766	14.430230
H	-1.266340	12.246210	14.170740	C	6.784965	4.480841	13.814190
H	-0.666180	0.303960	11.270630	C	0.155905	10.036760	15.792330
O	-1.862190	2.361036	11.668620	N	-2.000540	2.678598	13.968540
C	-0.968590	11.185040	14.064090	H	1.729604	-1.583310	13.291090
N	-2.426640	9.354720	13.687100	N	-1.146360	9.559609	15.781780
C	-3.514770	8.407563	13.794190	H	4.760886	2.863524	13.929330
C	-0.086300	6.333941	11.567630	C	4.034086	0.325571	13.961740
H	1.174439	12.832400	14.605420	H	7.105403	3.473955	14.103480
C	3.650215	3.286429	12.119540	C	6.042147	6.659588	14.788940
O	7.678851	1.855845	12.658220	H	-3.956100	3.038542	14.602950
O	4.058602	10.468480	14.401740	N	2.646684	0.175935	14.001300

H	0.163712	4.663160	13.687650	N	-1.640490	5.069759	16.477530
C	0.688319	5.610293	13.816060	C	-1.075770	6.269872	16.900990
C	-3.068360	6.831572	15.771160	N	-0.631280	2.872594	15.989200
H	2.566948	8.860389	14.523560	C	0.695187	2.438657	15.991680
C	2.011688	7.956935	14.277670	H	-2.305680	1.621182	15.763090
H	4.887738	8.405539	15.275190	H	-0.892510	8.677907	17.625480
O	1.020703	9.727439	16.583800	C	5.420997	4.608505	15.922560
C	6.157182	5.269352	14.929080	H	1.523554	-0.579120	15.599950
C	-0.504460	0.952292	14.604860	H	2.619029	0.796703	15.966150
H	-3.966050	7.203922	16.300920	C	4.137338	6.627271	16.279700
O	4.714071	0.852515	14.817490	H	5.577052	3.540779	16.103640
C	-2.919470	5.267738	15.820710	O	-0.072830	6.382624	17.573330
N	-1.873060	7.306179	16.438590	O	1.604963	2.941129	16.616420
C	5.036841	7.339991	15.470470	H	1.416692	5.084302	15.795740
C	-1.646490	8.686992	16.825290	C	-1.165650	3.794810	16.980170
C	-1.478770	2.042896	15.160730	C	2.767417	7.202977	16.518950
N	0.784863	1.321506	15.159980	H	2.756245	8.279438	16.721730
H	-0.773350	-0.073820	14.922110	C	4.397955	5.285327	16.590470
H	-2.589730	9.105338	17.220730	H	-0.363140	4.013379	17.698840
C	1.904800	0.394666	15.233180	H	-1.993310	3.288277	17.511750
C	1.358719	5.831930	15.003810	H	3.739879	4.734300	17.268190
N	1.990638	7.004462	15.241230	H	2.201710	6.693398	17.306890
H	-3.723260	4.770608	16.397260				

(2) In Water

(a) CB[8]

H	11.147940	29.884370	-4.728450	C	6.273080	31.392700	-0.330570
H	8.736268	30.245820	-4.501580	H	17.577330	30.312020	-0.833070
H	12.943480	31.404890	-3.966910	C	6.486095	27.572560	-1.041350
H	12.627420	28.039970	-4.477940	H	16.675630	27.151650	-0.459830
C	10.772130	29.793750	-3.697030	O	6.616653	32.441300	0.196392
H	14.466850	29.548810	-3.732480	O	6.931939	26.440200	-0.933680
H	7.271528	31.686350	-3.255880	C	16.701060	30.751450	-0.332900
H	6.955899	28.516390	-4.152410	C	15.703880	27.333830	0.032391
C	9.229687	29.899660	-3.579970	N	5.185163	30.629250	0.033460
C	12.606750	31.371200	-2.916610	N	5.656475	28.215990	-0.130830
C	12.314240	27.810610	-3.445810	H	16.795910	31.843850	-0.335550
N	11.249140	30.892940	-2.894170	H	15.228710	26.368700	0.243829
N	11.054180	28.464760	-3.177070	H	3.272195	30.728540	0.794502
H	12.607890	32.387630	-2.505100	H	3.844671	27.371930	0.485303
H	12.149950	26.731160	-3.348530	C	4.299474	30.977540	1.108661
H	5.524043	30.005490	-2.841880	H	17.924430	28.614870	0.981473
N	9.045153	30.880390	-2.519670	C	4.894494	27.426580	0.820894
N	8.828578	28.549160	-3.270220	H	4.376820	32.058720	1.272537
C	7.767805	31.514830	-2.284290	H	5.324511	26.417910	0.820305
C	7.463646	28.088290	-3.274860	N	16.696860	30.316040	1.040742
C	14.161910	29.379440	-2.687850	N	15.939590	27.992080	1.296946
C	10.231820	31.520270	-2.206110	C	17.002470	28.971870	1.466482
C	9.898603	27.721660	-3.014670	N	4.579845	30.329180	2.369245
H	7.961240	32.484460	-1.810720	N	4.910348	27.906810	2.177773
H	7.482125	26.995900	-3.367110	C	16.442530	31.163020	2.095676
N	13.556960	30.595340	-2.138740	C	15.611840	27.381210	2.494387
N	13.389950	28.174290	-2.567370	O	16.157740	32.349210	2.016583
H	16.265790	28.800550	-2.238050	O	14.864890	26.422120	2.628315
O	10.350160	32.491710	-1.472420	H	3.056995	28.878790	2.279583
O	9.841241	26.534590	-2.728660	C	4.086675	28.991010	2.654131
C	6.038149	29.690730	-1.919690	C	17.115890	29.104600	3.007476
N	6.875592	30.778350	-1.415780	H	18.145360	29.012160	3.388039
N	6.686467	28.423230	-2.107850	O	5.004613	32.266740	3.578323
C	15.343650	29.125690	-1.730080	C	4.736486	31.075650	3.523442
C	14.468480	31.253150	-1.321160	O	6.356507	26.330860	3.079155
C	13.749980	27.432430	-1.463140	C	5.607118	27.290230	3.195964
H	4.043698	29.233650	-1.041170	N	16.604510	30.441520	3.264715
O	14.363180	32.394280	-0.897290	N	16.303250	28.020180	3.501888
O	13.218280	26.393910	-1.097320	C	4.207454	28.889750	4.196941
N	15.533000	30.404240	-1.103630	N	4.499712	30.244850	4.595574
N	14.837500	28.054470	-0.873780	N	5.280797	27.924040	4.382056
C	5.085504	29.421340	-0.737080	H	16.772820	32.193480	4.330880

H	15.903720	26.547350	4.881635
C	16.872670	31.117130	4.513617
C	16.325420	27.559510	4.865436
H	3.290775	28.532550	4.691816
H	17.905370	30.895040	4.830208
H	17.376570	27.518650	5.198881
H	4.377396	31.798170	5.940398
H	6.018238	26.334400	5.467535
N	15.995610	30.770320	5.596223
N	15.558650	28.355030	5.807670
C	4.488400	30.707410	5.959964
C	5.530595	27.297330	5.660111
O	14.535550	32.558080	5.412512
O	14.318080	26.574140	6.653072
H	3.618674	30.264640	6.468588
C	14.899050	31.524350	5.954681
H	4.563583	27.112580	6.160705
C	14.746160	27.714880	6.736469
C	16.117660	29.577830	6.387921
N	5.661335	30.393510	6.737215
O	6.802129	32.394460	6.482652
N	6.391641	28.049680	6.546339
O	8.027157	26.409140	6.802786
H	17.164320	29.410230	6.687038
C	6.715007	31.261680	6.930693
C	7.488824	27.452190	7.144799
C	5.874354	29.129720	7.385179
N	14.314720	30.920770	7.055307
N	14.539550	28.582210	7.788474
C	15.169840	29.854670	7.572920
O	10.822720	32.554780	7.051607
O	11.427030	26.654150	8.430923
H	4.960482	28.800300	7.905211
N	7.640654	30.634440	7.756575
N	7.849262	28.225650	8.226803
H	13.202710	32.613700	7.425604
H	13.774340	27.165040	9.077069
C	10.951410	31.609130	7.816067
C	11.346400	27.842690	8.702681
C	7.057985	29.419730	8.330822
C	13.412350	31.654680	7.913854
C	13.773280	28.255990	8.965743
N	12.146560	31.002540	8.159789
H	8.563358	32.448210	8.077603
N	12.399500	28.691570	8.961022
H	15.685670	30.192820	8.485889
H	9.113707	26.814080	9.025082
N	9.940177	30.984590	8.515667
N	10.176090	28.566760	8.844995
C	8.575987	31.444030	8.517937
C	8.927350	27.890840	9.113510
C	11.971670	30.041020	9.238746
H	13.906180	31.848730	8.882454
H	14.277970	28.707450	9.833148
H	6.756861	29.601670	9.374559
C	10.429390	29.909510	9.343870
H	8.232901	31.504390	9.565089
H	8.604952	28.122770	10.142110
H	12.450190	30.415700	10.157170
H	10.042650	30.012950	10.370080

(b) OPVEBox^{4+}

H	-6.679060	4.171015	-0.690640
H	-4.948380	2.415475	-0.226860
H	-7.392170	6.513691	-0.326320
C	-6.295270	4.724174	0.169908
H	-5.718740	1.964666	1.301898
C	-5.000230	2.656986	0.842625
C	-6.697820	6.044662	0.375209
H	-2.715210	3.406741	-0.094160
C	-5.408330	4.100671	1.061523
N	-3.681000	2.388162	1.447398
C	-2.579750	2.942195	0.882365
H	-6.250930	8.860909	0.859258
C	-6.210780	6.779088	1.467492
H	-4.520700	1.374723	3.064232
C	-3.598580	1.796294	2.664456
C	-4.925990	4.833884	2.150500
C	-1.369980	2.942643	1.539749
H	-0.511630	3.414934	1.060920

C	-6.660760	8.216741	1.648729
C	-5.316760	6.159644	2.347572
H	-4.690700	9.872946	2.060337
H	-4.230070	4.390461	2.864341
H	-7.755720	8.293639	1.599929
C	-2.412750	1.767619	3.364266
C	-1.255700	2.385292	2.834536
H	-4.901550	6.693799	3.202180
H	-2.413960	1.299728	4.347850
C	-5.115600	9.544716	3.008737
N	-6.219040	8.763476	2.942896
H	0.751865	3.136702	3.074981
C	-0.015760	2.539408	3.573011
H	-3.661410	10.499250	4.239369
C	-4.556870	9.877658	4.224737
C	-6.806260	8.308384	4.080744
H	-7.695540	7.691492	3.952333
C	0.195075	2.062474	4.825303
H	-0.573300	1.437439	5.289383
H	2.345674	3.753044	4.356260
C	-5.093810	9.362523	5.425204
C	-6.276850	8.592671	5.318785
C	2.358116	3.259171	5.328945
C	1.341508	2.342324	5.677057
H	-3.556530	10.308560	6.599545
H	-6.781690	8.191897	6.197140
H	4.126627	4.307948	5.956378
C	-4.377260	9.590412	6.666298
C	3.362664	3.577048	6.232078
C	1.404541	1.726287	6.947629
H	0.629719	1.010037	7.231131
C	3.403492	2.989898	7.516817
C	2.413057	2.038311	7.846835
C	-4.570950	8.893635	7.813265
H	-5.353030	8.128971	7.852492
H	-2.695230	10.826630	8.461923
H	2.415842	1.555080	8.824643
H	5.086295	4.217857	8.085401
C	4.420374	3.435550	8.460227
C	-2.789480	10.022170	9.193627
C	-3.740750	8.994936	9.007593
H	-1.226090	10.822130	10.433040
C	-1.958990	10.021970	10.305260
C	-3.846270	7.992677	9.999389
C	4.557678	3.002233	9.737084
H	-4.597070	7.206827	9.886084
H	6.537393	4.994429	9.448421
H	3.899645	2.218730	10.118380
C	6.417384	4.571184	10.445030
C	-2.019030	8.982702	11.261790
C	-2.996200	7.977196	11.098100
C	5.484020	3.544080	10.713380
H	-3.100090	7.184099	11.841320
H	-0.515540	9.924992	12.497930
H	7.895678	5.905448	11.297590
C	-1.054240	8.983260	12.354340
C	7.185592	5.095339	11.462520
C	5.431998	3.060221	12.040760
H	4.744867	2.258512	12.312790
C	-0.734740	7.915319	13.124600
H	-1.204370	6.947489	12.931290
N	7.081515	4.626197	12.729010
H	6.502294	7.663311	13.363790
C	6.223201	3.618447	13.018360
H	0.546569	10.081380	14.367650
C	0.281469	7.917944	14.162690
C	0.872212	9.090856	14.684410
H	8.496110	6.013361	13.390160
H	4.656532	8.671733	14.662900
C	6.171130	7.189325	14.291300
H	6.181572	3.289779	14.056290
C	7.790008	5.309639	13.845040
H	0.316195	5.744964	14.330980
C	0.741479	6.686056	14.682170
C	5.132357	7.756504	15.024690
C	1.884514	9.003939	15.617300
H	2.377519	9.883397	16.031870
C	6.782068	6.003039	14.726950
H	8.358252	4.551079	14.397360
C	1.755499	6.655317	15.613120
N	2.317406	7.801942	16.068020
C	4.680568	7.142781	16.204170
H	2.158870	5.724600	16.012310
C	6.357956	5.413220	15.922500
C	3.500602	7.710037	16.956920
H	3.702552	8.720750	17.333680
C	5.307040	5.976306	16.653160
H	6.835687	4.496515	16.276480
H	3.233587	7.074255	17.809760
H	4.958981	5.493244	17.569190

(c) OPVEBox^{4+}⊂CB[8]

H	-4.607720	4.393425	-1.381200	H	4.427922	9.306256	4.172536
H	-4.658900	1.865446	-1.133920	H	0.117293	3.480243	3.149304
H	-5.501450	6.601852	-0.724200	H	4.366941	-0.239930	3.983417
C	-5.382170	4.454983	-0.612460	N	2.770131	8.010467	4.203861
C	-5.038060	2.009771	-0.115880	C	-0.869950	3.259116	3.563557
H	-5.624350	1.130619	0.175149	C	4.968759	7.147006	4.300219
C	-5.888030	5.700835	-0.241580	C	-6.542900	6.895169	3.791936
H	-2.609570	2.799770	-0.718090	C	3.601162	0.542419	4.101637
C	-5.816930	3.294076	0.041364	O	-1.056120	9.057390	4.283615
N	-3.861970	2.091223	0.794399	N	4.248002	1.829454	4.117048
C	-2.700710	2.634910	0.355398	C	4.099613	8.377527	4.665507
C	-6.839220	5.802223	0.783569	C	5.804461	3.587286	4.333232
H	-6.978760	7.974475	0.714298	H	-7.596480	6.662801	3.946844
C	-6.836770	3.387389	0.998801	H	6.283304	1.399472	4.401182
H	-4.988720	1.386056	2.401909	O	0.726341	0.666719	4.333445
H	-0.783920	3.422294	0.844460	N	1.080829	9.532934	5.060223
C	-1.699690	2.979643	1.238665	C	-4.245370	7.035414	4.524185
C	-4.044510	1.849168	2.118075	C	5.519122	2.110831	4.749339
H	-4.688300	7.991369	1.266515	C	-0.297670	9.629057	5.056300
C	-7.347060	4.633342	1.366474	H	7.192830	5.821059	5.005143
C	-7.136400	7.143622	1.412008	C	-5.608000	6.766509	4.794264
H	-7.204800	2.486311	1.495516	H	2.233829	11.268330	5.376104
H	5.462344	5.389117	2.316214	H	-2.594990	10.605110	5.323671
H	-8.152850	7.207377	1.816200	C	-1.107810	3.384789	4.892175
H	3.750108	4.969959	2.014169	H	-2.105250	3.160334	5.275361
C	-4.904140	7.645549	2.276694	H	1.511008	4.238325	4.596942
H	-8.106180	4.698072	2.150213	N	2.807115	0.249567	5.265022
C	-3.084590	2.181520	3.043669	N	5.365203	6.623404	5.594722
C	4.496373	5.160337	2.794434	C	1.431456	0.330065	5.268614
C	-1.881540	2.811050	2.630973	H	-2.218910	7.270129	5.156185
O	1.839806	6.331939	2.893371	N	5.965640	4.264713	5.603587
H	1.034857	8.570729	3.242727	C	1.687045	10.506780	5.954395
N	-6.190120	7.313395	2.548167	C	6.400567	5.629352	5.746800
O	2.686416	2.936630	2.809620	N	4.248495	8.486469	6.096233
H	2.273045	9.858452	3.379947	C	-3.181930	6.879836	5.486566
H	-2.904050	7.817661	2.995302	N	-0.668680	10.519920	6.037115
H	2.933294	0.520665	3.231814	H	4.392700	10.550170	6.293161
H	5.860651	7.397619	3.704556	H	-2.005960	12.109150	6.103217
C	2.787051	6.823557	3.487823	H	-5.944450	6.465767	5.786823
C	-3.927060	7.527882	3.237038	H	-0.912200	-0.275400	5.757557
N	4.069503	6.321952	3.532573	C	-2.021050	11.007790	6.167446
H	-3.267490	1.927185	4.088066	C	1.197414	4.086224	5.629701
C	1.782093	9.020090	3.907293	H	3.961774	-1.194710	6.245566
C	3.729687	2.913492	3.445349	N	5.512712	2.169880	6.201000
N	4.629671	3.950697	3.566110	C	4.996545	7.457778	6.632616
H	6.711882	3.709449	3.721551	C	-0.135000	3.717522	5.913639

O	-4.447830	9.455049	6.369885
H	0.416672	12.176160	6.727771
C	3.937300	9.693229	6.817700
C	0.470297	11.076030	6.734041
C	3.339986	-0.315390	6.478677
C	5.771208	3.432642	6.682412
N	2.531782	9.958949	6.988923
N	0.989819	-0.100790	6.510254
O	-2.709770	1.082755	6.539903
H	6.820582	5.740367	6.753801
H	5.979137	0.189561	6.610500
C	-0.367050	-0.561690	6.664976
H	-0.645240	6.983833	6.391153
C	-3.322800	6.400133	6.745052
H	-0.372710	-1.662410	6.764234
C	5.415435	1.019427	7.065954
H	3.145123	4.510667	6.441651
H	-4.291900	6.029459	7.091584
N	-2.700710	10.610440	7.374737
C	2.111396	4.241510	6.662784
C	-3.904350	9.930003	7.353229
N	4.070163	0.586765	7.348306
C	2.070437	-0.654350	7.304937
H	4.383600	9.608946	7.815009
O	5.307847	7.326781	7.806950
C	-0.528140	3.588729	7.263818
H	1.917214	-1.737120	7.444132
H	-1.567750	3.356384	7.492645
O	5.862784	3.753496	7.861056
C	-2.245620	0.705668	7.607138
N	0.695899	10.589710	8.084406
C	-0.940740	6.817214	7.426901
C	1.933091	9.995607	8.228858
H	-6.221030	9.222843	7.981875
H	-4.612740	1.383113	7.949094
O	-6.372830	6.802887	8.186470
N	-1.070680	0.009803	7.781634
O	-5.644280	3.559728	8.182503
C	-2.264420	6.440142	7.739998
H	5.881938	1.283917	8.022109
C	1.738771	4.019285	8.008327
N	-4.403720	9.922730	8.642315
C	0.387877	3.725878	8.289953
H	-2.315690	12.310130	8.539592
C	-2.438980	11.221300	8.659499
C	3.541234	0.616736	8.623144
N	2.316646	-0.022510	8.584213
H	-7.399150	4.878427	9.373048
H	1.016379	7.276028	8.172541
C	-5.752880	9.503575	8.932630
O	2.431934	9.610738	9.277354
C	-0.001080	6.976626	8.428748
N	-2.836400	0.861883	8.844517
C	-4.242060	1.161184	8.956268
H	0.018068	12.249900	9.139068
C	0.020599	11.147790	9.227208
C	-6.205480	7.117943	9.356912
C	-5.397120	3.293231	9.349107
N	-1.326310	10.677310	9.415733
C	-2.581420	6.155390	9.086607
H	-6.309120	10.346970	9.373374
H	3.761480	4.348773	8.711010
C	-0.868950	-0.413450	9.150401
H	-4.769180	0.271029	9.345201
H	-3.586610	5.804553	9.321386
H	0.049776	3.601702	9.318752
C	-3.677440	10.831880	9.508679
C	2.764523	4.040175	9.037684
H	-0.800210	-1.511910	9.202546
O	4.078207	1.086012	9.612962
N	-5.857440	8.368784	9.815224
N	-4.550720	2.292396	9.794127
C	-6.915190	4.967204	10.352930
H	-4.318410	11.689270	9.770699
H	0.592631	10.856420	10.116390
C	1.591743	-0.359960	9.782093
N	0.252797	0.182296	9.853195
C	-2.108770	0.166273	9.886632
H	5.345933	3.972673	10.056130
N	-6.386210	6.303742	10.455370
H	1.536077	-1.458980	9.878660
N	-5.948720	3.902070	10.454130
C	-0.345640	6.788793	9.785880
C	-1.723570	10.214510	10.659320
C	-1.647550	6.336142	10.096830
H	-7.671660	4.824920	11.139620
N	-3.099600	10.262050	10.699810

H	-2.745110	-0.609870	10.340990
C	2.572406	3.620420	10.311450
H	2.155662	0.044722	10.631420
H	1.586302	3.286950	10.636420
C	-0.157820	0.944319	10.927740
N	-1.536040	1.010357	10.913620
C	-5.825400	8.449396	11.264270
H	1.615739	7.421472	10.401430
C	4.985605	3.698807	11.047130
O	-0.985780	9.876211	11.568740
C	-4.551610	2.180063	11.241790
H	-1.923880	6.136957	11.133360
C	0.634390	7.143456	10.793600
C	-6.176060	6.997367	11.710840
C	-5.420720	3.383540	11.695550
H	-6.542090	9.205394	11.619460
H	-4.955220	1.203582	11.553430
H	6.966136	3.752613	11.913150
N	-4.524150	8.676542	11.856370
C	3.613481	3.465342	11.301560
O	0.574319	1.444228	11.771030
C	-3.851360	9.948834	11.884630
N	-3.273050	2.420931	11.874230
H	-7.080840	6.927958	12.334070
C	5.904715	3.553569	12.060620
H	-6.241990	3.107143	12.374160
H	-4.596290	10.741640	12.058710
N	-5.011020	6.598573	12.473180
C	-2.286150	1.395413	12.088790
N	-4.468360	4.232476	12.381760
C	-4.044430	7.577269	12.532560
C	-3.229770	3.637453	12.524900
H	-3.146540	9.931672	12.724890
C	0.401799	7.233770	12.125510
H	-2.788590	0.501392	12.498270
H	-0.576280	6.974484	12.539320
H	-1.568590	1.773744	12.826420
O	-2.977620	7.499175	13.124580
C	-4.877890	5.357574	13.186190
C	3.265554	3.005804	12.592570
O	-2.278830	4.087089	13.146230
H	2.789868	8.618852	11.641180
N	5.527804	3.154082	13.303250
H	2.233658	2.742836	12.823430
H	7.505268	5.711343	13.672020
H	-5.840170	5.117822	13.666230
C	1.391892	7.701564	13.068860
H	-4.118090	5.506954	13.962460
C	4.229141	2.868751	13.564780
H	7.486924	3.199352	14.053370
C	2.591223	8.352229	12.680010
C	6.468999	3.302619	14.446140
H	6.649557	7.952403	14.279360
C	6.745904	5.806661	14.452450
H	0.268180	7.068197	14.830850
C	1.186002	7.523802	14.456660
H	3.992876	2.540058	14.576120
C	3.530782	8.688397	13.625570
H	6.275710	2.485827	15.151410
C	6.262610	7.070071	14.794980
H	4.474590	9.163341	13.359930
C	6.209879	4.660339	15.055160
C	2.165098	7.876465	15.360020
N	3.328741	8.433851	14.944360
C	5.243633	7.203551	15.748670
H	2.056612	7.705073	16.430750
C	5.260194	4.801520	16.076460
H	5.097751	9.369453	15.586300
C	4.488874	8.505265	15.875760
H	4.851279	3.917770	16.572210
C	4.783003	6.065238	16.424030
H	4.094033	8.669874	16.884720
H	4.009077	6.157638	17.190030

(d) OPVEBox^{4+}⊂2CB[8]

H	-4.048305	4.018274	-2.211001	C	-1.986700	2.624441	1.132694
H	-4.287489	1.506092	-1.847619	C	0.138544	-1.022260	0.557671
H	1.393594	1.611805	-2.299368	H	-7.282345	2.419356	0.174072
H	-0.337352	1.902629	-2.638800	H	1.282539	8.567049	-0.364603
C	-4.935559	4.166047	-1.591038	C	-6.499429	6.971251	0.384760
H	-4.727741	6.310295	-1.590945	C	-4.478500	1.523136	1.440550
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H	-3.464055	4.597172	16.677094				

Section K. References

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