Electronic Supplementary Information

Complexation with pagoda[n]arene (n=4, 5) protects ferrocenium from oxidation

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1. Materials and methods

1.1 General Methods

All reagents involved in this research were commercially available and used without further purification unless noted otherwise. Solvents were either employed as purchased or dried before use by standard laboratory procedures. Ferrocene (**Fc**), ferrocenium hexafluorophosphate (**Fc**$^+$), and bis(cyclopentadienyl)Cobalt(III) hexafluorophosphate were purchased from Sigma Aldrich. The electrolyte *n*-Bu_4NPF_6 (TCI Chemicals) was dried in vacuo before its use in electrochemical experiments. Pagoda[4]arene and Pagoda[5]arene were synthesized according to the existing method.[1,2]

^{1}H NMR spectra were measured by Bruker DMX 500 spectrometer. All chemical shifts are reported in ppm with residual solvents or TMS (tetramethylsilane) as the internal standards. Electrospray ionization mass spectra (ESI-MS) were recorded on the Matrix Assisted Laser Desorption/Ionization, Time of Flight, MALDI-TOF.

1.2 FL Spectroscopy

The Fluorescence spectra were recorded on RF-6000 SHIMADZU. **Fc**$^+$ is unstable in organic solvents, so all solvents are purged with argon to remove the dissolved oxygen.

1.3 Cyclic voltammetry[3]

Cyclic voltammetry was performed on a CS Electrochemical Workstation model CS150M. A three-electrode configuration in a single-compartment cell (5 mL) was used including a freshly polished glassy carbon working electrode, a platinum-wire

counter-electrode and a silver-wire pseudoreference electrode. All solutions were argon-purged beforehand during the measurements. The cyclic voltammetry analysis was carried out in a mixed solution of chloroform and acetonitrile ($CHCl_3/CH_3CN$ = 4/1, v/v) containing 0.1 M *n*-Bu_4NPF_6 (Tetrabutylammonium hexafluorophosphate).

1.4 Data Analysis and Fitting[4]

All fittings were performed in a nonlinear manner, the complexation process of the Pagoda[n]arenes (*H*) with the guest (*G*) was expressed by the following equation according to a 1:1 host-guest binding stoichiometry.

$$[G] + [HG] = [G]_0$$

$$K_a = \frac{[HG]}{[H][G]}$$

$$[HG] = \frac{K_a[H][G]_0}{1 + K_a[H]}$$

$$[H] = \frac{(K_a[H]_0 - K_a[G]_0 - 1) + \sqrt{(K_a[G]_0 - K_a[H]_0 + 1)^2 + 4K_a[H]_0}}{2K_a}$$

$$F = F_{HG} + (F_H - F_{HG})\frac{[H]}{[H]_0}$$

$$= F_{HG} + (F_H - F_{HG})\frac{([H]_0 - [G]_0 - 1/K_a) + \sqrt{([H]_0 + [G]_0 + 1/K_a)^2 - 4[H]_0[G]_0}}{2[H]_0}$$

K_a is the binding constant for the complexation process, and it can be obtained by analyzing the sequential changes of fluorescence intensity of Pagoda[n]arenes at various concentrations of guest. Here, $[G]_0$ is the initial concentration of guest and constant, $[H]_0$ is the initial concentration of Pagoda[n]arenes and constant, $[HG]$ is the

concentrations of the complex formed by the host and guest. [*H*] is the concentration of the host, [*G*] is the concentrations of the guest. *F* is the fluorescence intensity of the whole system after adding the guest to the pagoda[n]arenes. F_{HG} is the fluorescence intensity of the complex formed by the host and guest. F_H is the fluorescence intensity of the pagoda[n]arenes.

1.5 DFT calculations

Calculations were performed using M06-2X/GEN functional combined with 6-31G(d) and LAN2DZ basis sets (Fe, Co, LAN2DZ, others, 6-31G(d)) in Gaussian 09. All the structures were optimized and certified without imaginary frequencies. In demand of considering basis set superposition error (BSSE, using key word "counterpoise=2") towards complex interaction.

2. ^{1}H NMR spectrum of P5 and P4

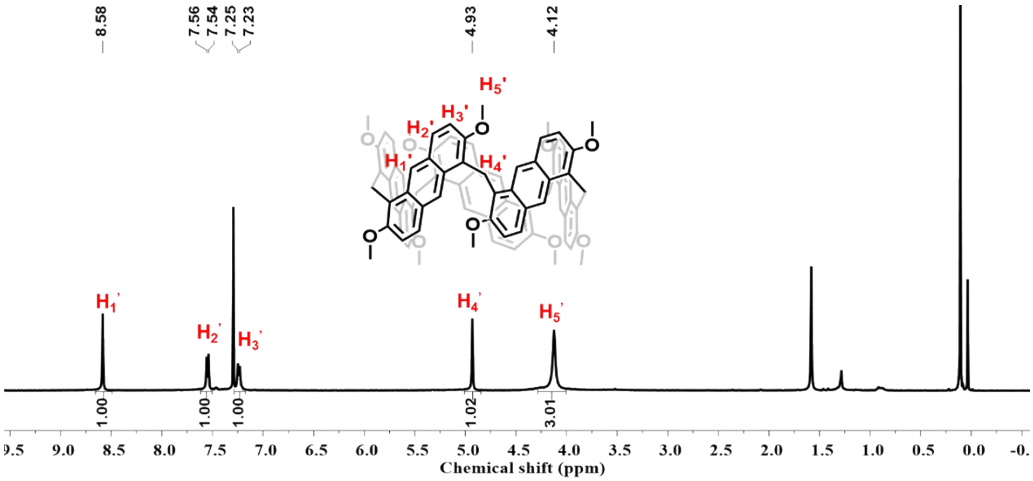


Fig. S1 ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 298K) of **P5**.

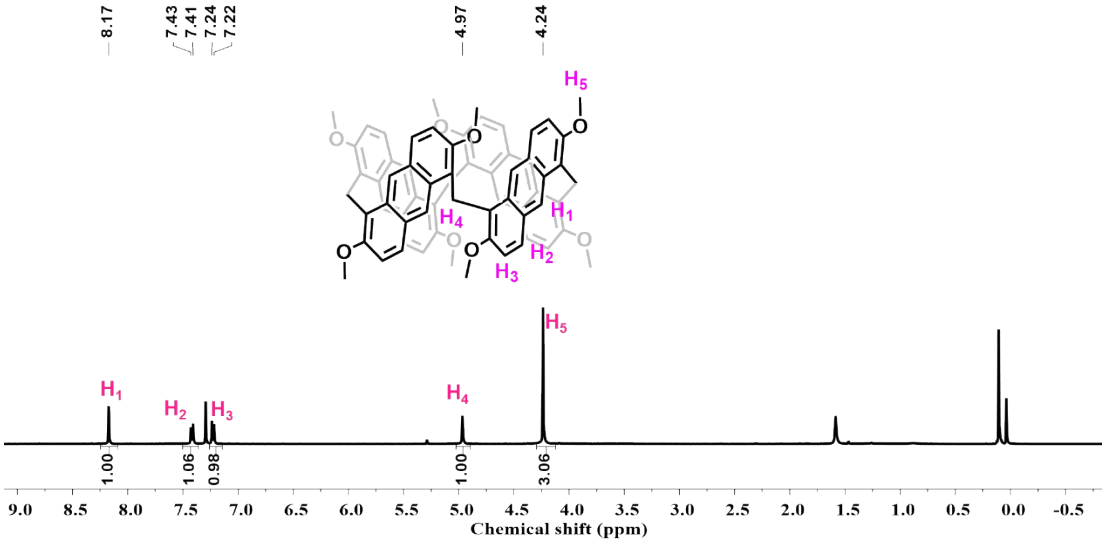


Fig. S2 ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 298K) of **P4**.

3. UV-vis spectra

3.1. UV-vis spectra of Fc^+

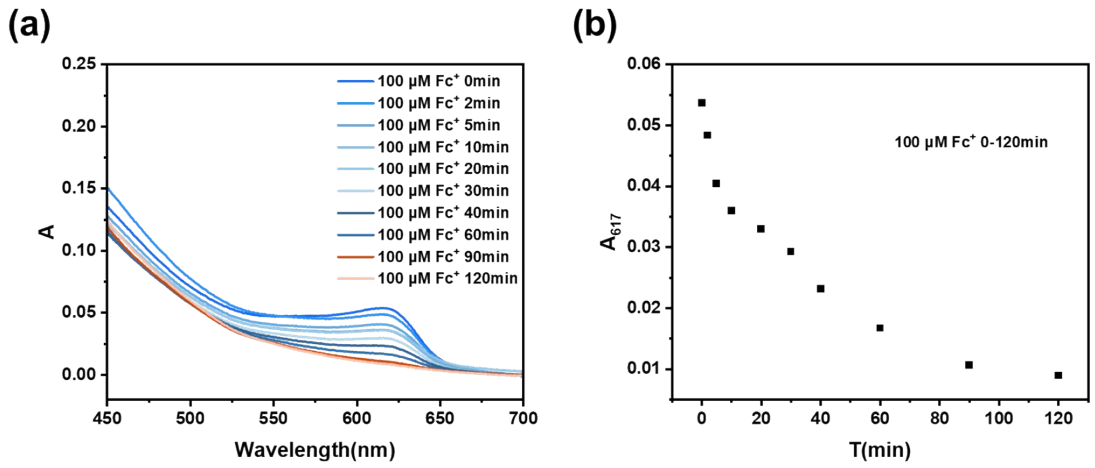


Fig. S3 The UV-vis spectra of (a) **Fc**$^+$ with time (0-120 min). (b) Plot of absorption of **Fc**$^+$ at 617 nm versus time. $CHCl_3/CH_3CN$ (4/1, v/v).

3.2. UV-vis spectra of Fc^+ with P5

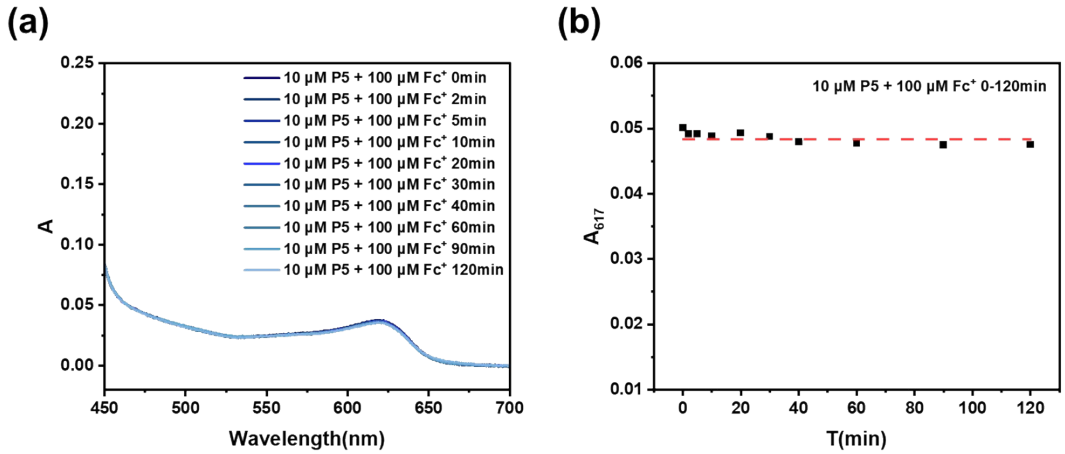


Fig. S4 The UV-vis spectra of (a) **Fc^+@P5** with time (0-120min). (b) Plot of absorption of **Fc^+@P5** at 617 nm versus time. $CHCl_3/CH_3CN$ (4/1, v/v).

3.3. UV-vis spectra of Fc^+ with P4

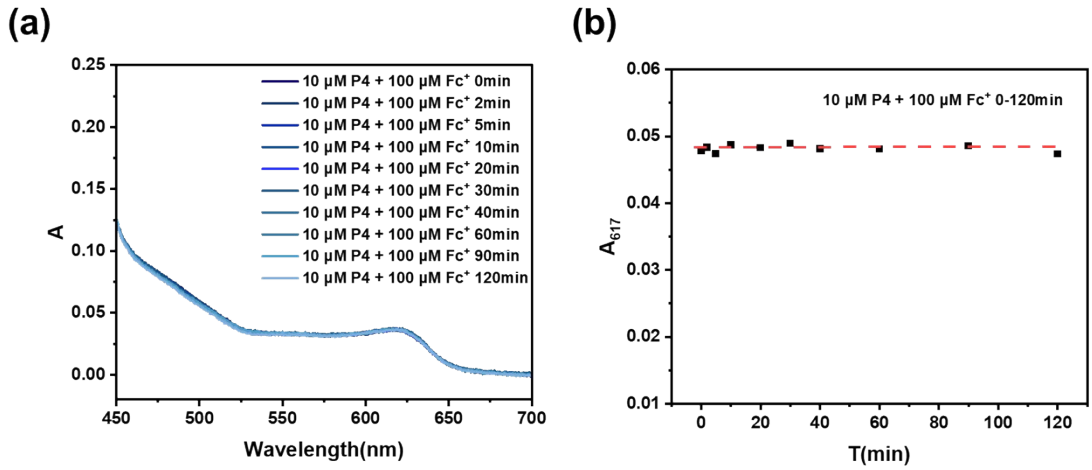


Fig. S5 The UV-vis spectra of (a) **Fc^+@P4** with time (0-120min). (b) Plot of absorption of **Fc^+@P4** at 617 nm versus time. $CHCl_3/CH_3CN$ (4/1, v/v).

3.4. UV-vis spectra of host-guest complexes

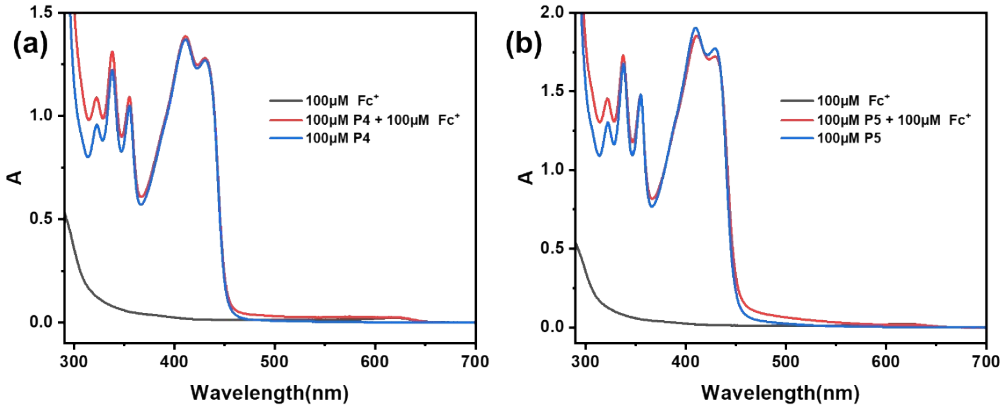


Fig. S6 The UV-vis spectra of (a) **P4**, **Fc**$^{+}$ and **Fc**$^{+}$**@P4**, (b) **P4**, **Fc**$^{+}$ and **Fc**$^{+}$**@P4**. Solvent: $CHCl_3/CH_3CN$ (4/1, v/v).

4. ^{1}H NMR study about the complexation of Fc with P4 and P5 respectively

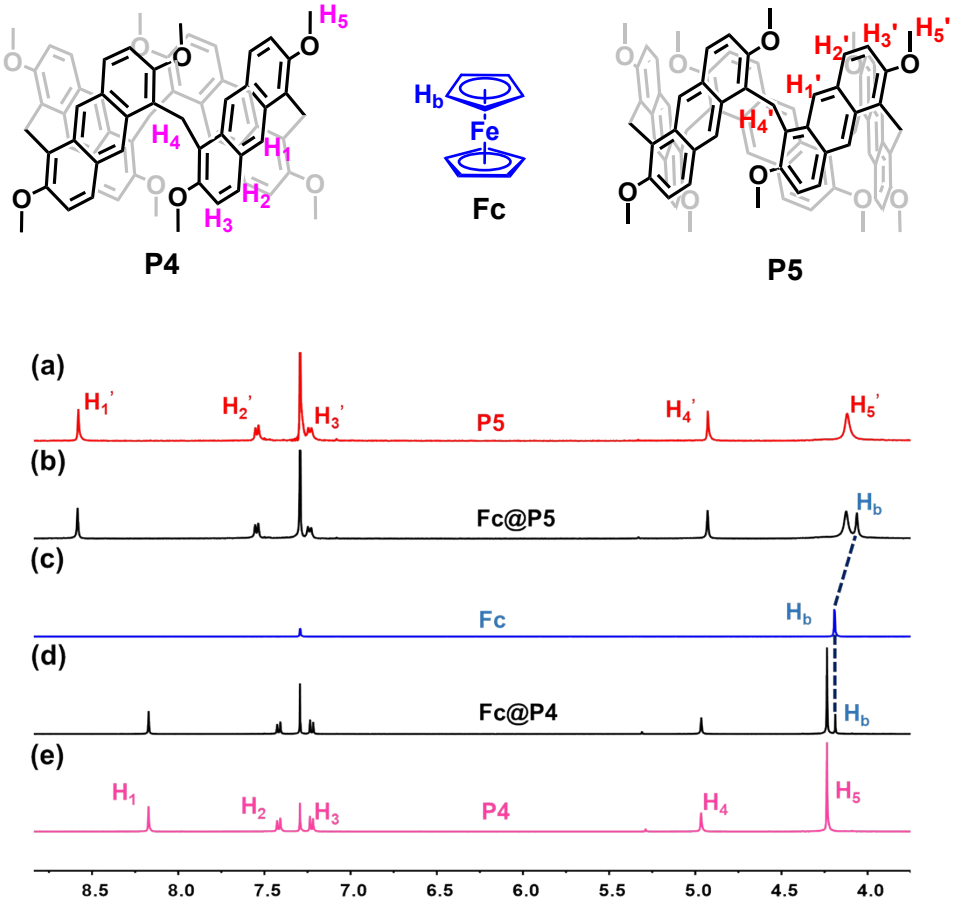


Fig. S7 Partial ^{1}H NMR spectrum ($CDCl_3$, 298K) of (a) **P5** (1 mM), (b) **Fc** (1 mM)

+**P5** (1 mM), (c) **Fc** (1 mM), (d) **Fc** (1 mM) +**P4** (1 mM), (e) **P4** (1 mM).

5. ^{1}H NMR study about the complexation of Cob$^+$ with P5

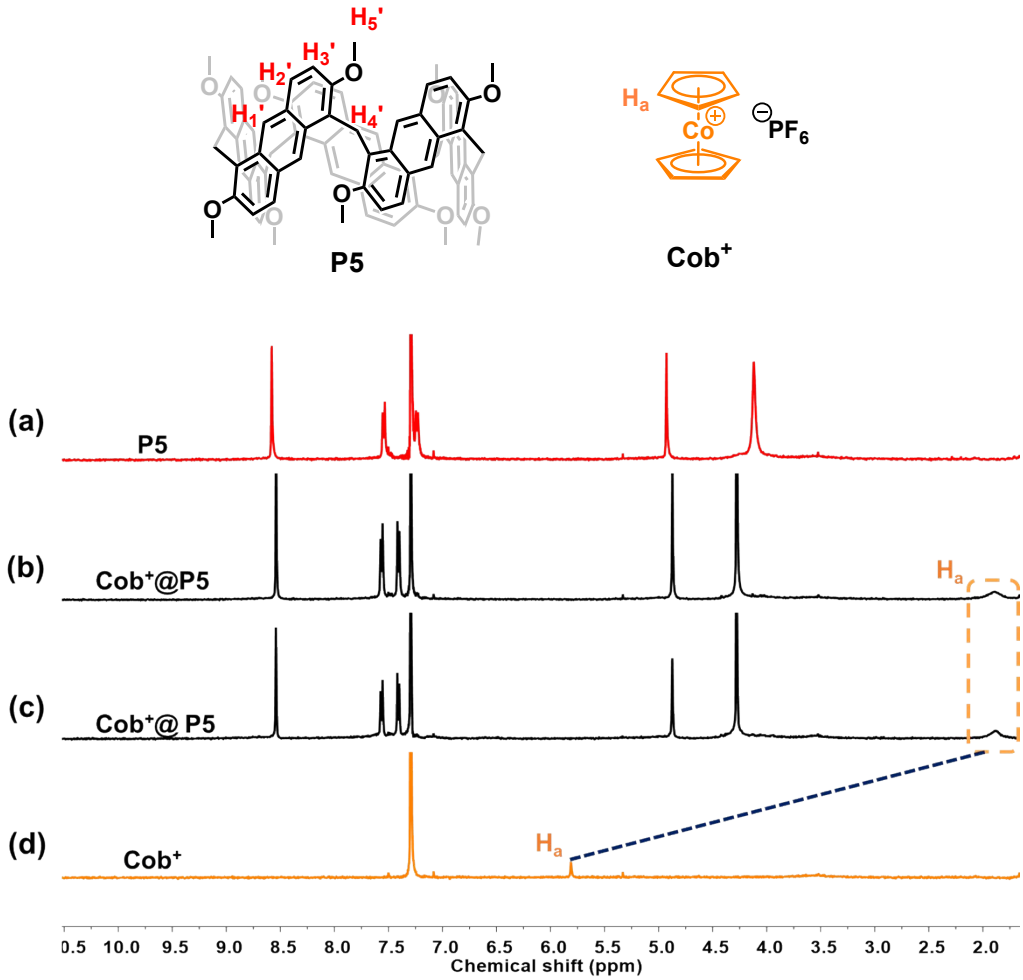


Fig. S8 Partial ^{1}H NMR spectrum ($CDCl_3$, 298K) of (a) **P5** (1 mM), (b) **Cob**$^+$ (1 mM) +**P5** (1 mM), (c) **Cob**$^+$ (1 mM) + **P5** (2 mM), (d) **Cob**$^+$ (1 mM).

6. The fluorescence titration experiments of P5 and P4 with Fc respectively.

Excitation at 330 nm, the fluorescent titration experiments were performed with a constant concentration of **P5** and **P4** (1×10^{-6} M) and varying concentrations of **Fc** in $CHCl_3/CH_3CN$ (4/1, v/v). The binding constants are determined by measuring the emission intensities of **P5** and **P4**.

6.1. P5 and P4 with Fc

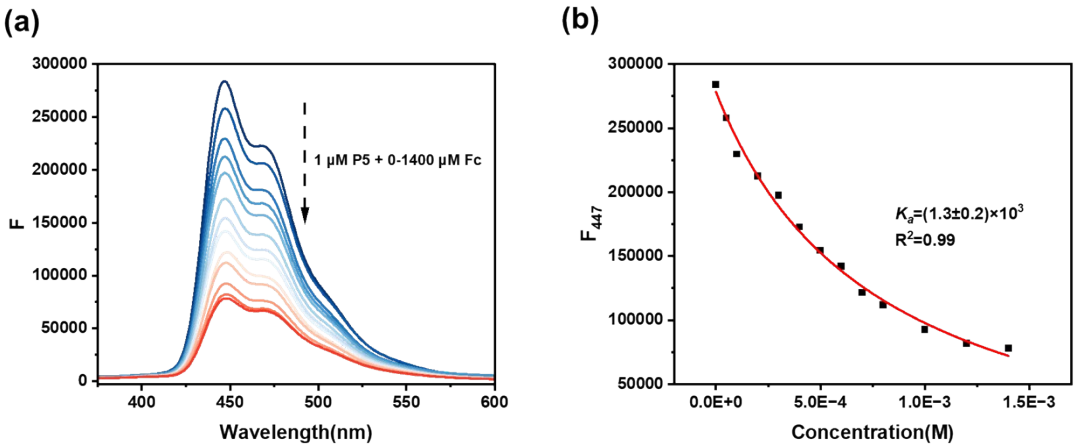


Fig. S9 (a) Fluorescent titrations of **P5** (1.0×10^{-6}M) with various equivalence of **Fc** ($CHCl_3/CH_3CN$=4/1, v/v) (λ_{ex}=330 nm). (b) Curve fit of the titration data of **P5** (1.0×10^{-6} M) when titrated with **Fc**.

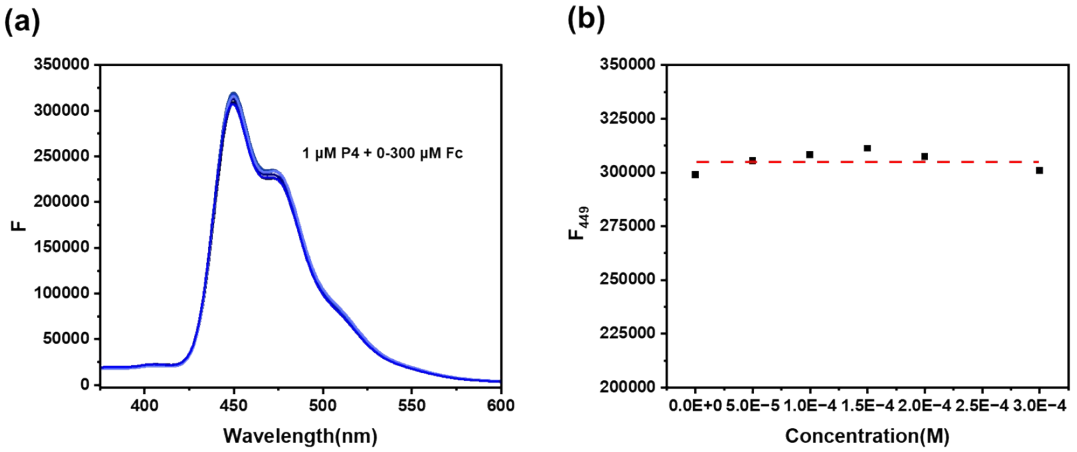


Fig. S10 (a) Fluorescent titrations of **P4** (1.0×10^{-6} M) with various equivalence of **Fc** ($CHCl_3/CH_3CN$=4/1, v/v) (λ_{ex}=330 nm). (b) Curve fit of the titration data of **P4** (1.0×10^{-6} M) when titrated with **Fc**.

6.2. P5 and P4 with Cob^+

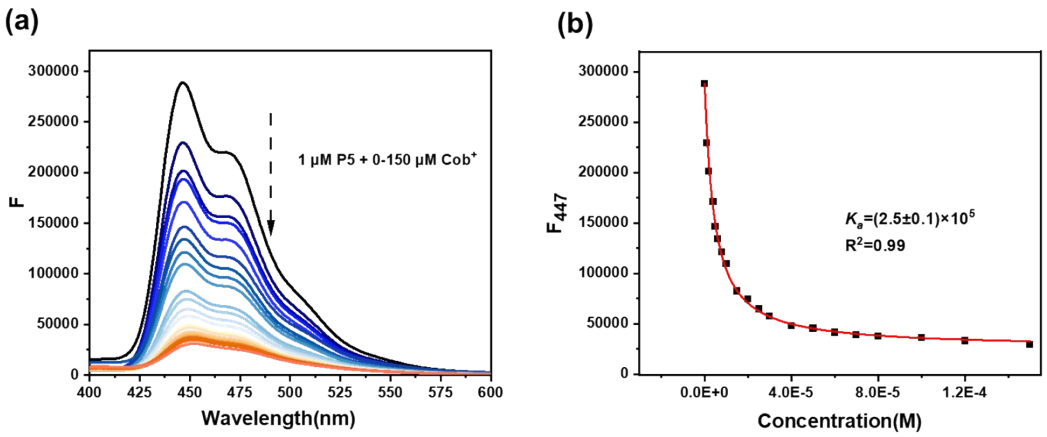


Fig. S11 (a) Fluorescent titrations of **P5** (1.0×10^{-6}M) with various equivalence of **Cob**$^+$ ($CHCl_3/CH_3CN$=4/1, v/v) (λ_{ex}=330 nm). (b) Curve fit of the titration data of **P5** (1.0×10^{-6} M) when titrated with **Cob**$^+$.

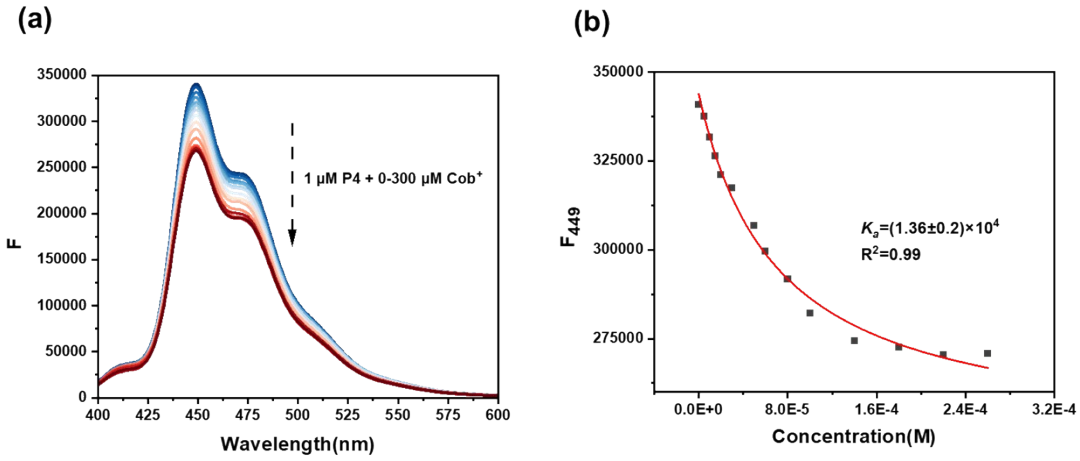


Fig. S12 (a) Fluorescent titrations of **P4** (1.0×10^{-6} M) with various equivalence of **Cob**$^+$ ($CHCl_3/CH_3CN$=4/1, v/v) (λ_{ex}=330 nm). (b) Curve fit of the titration data of **P4** (1.0×10^{-6} M) when titrated with **Cob**$^+$.

7. Job' plot of P5 and P4 with Fc^+ and Cob^+ respectively

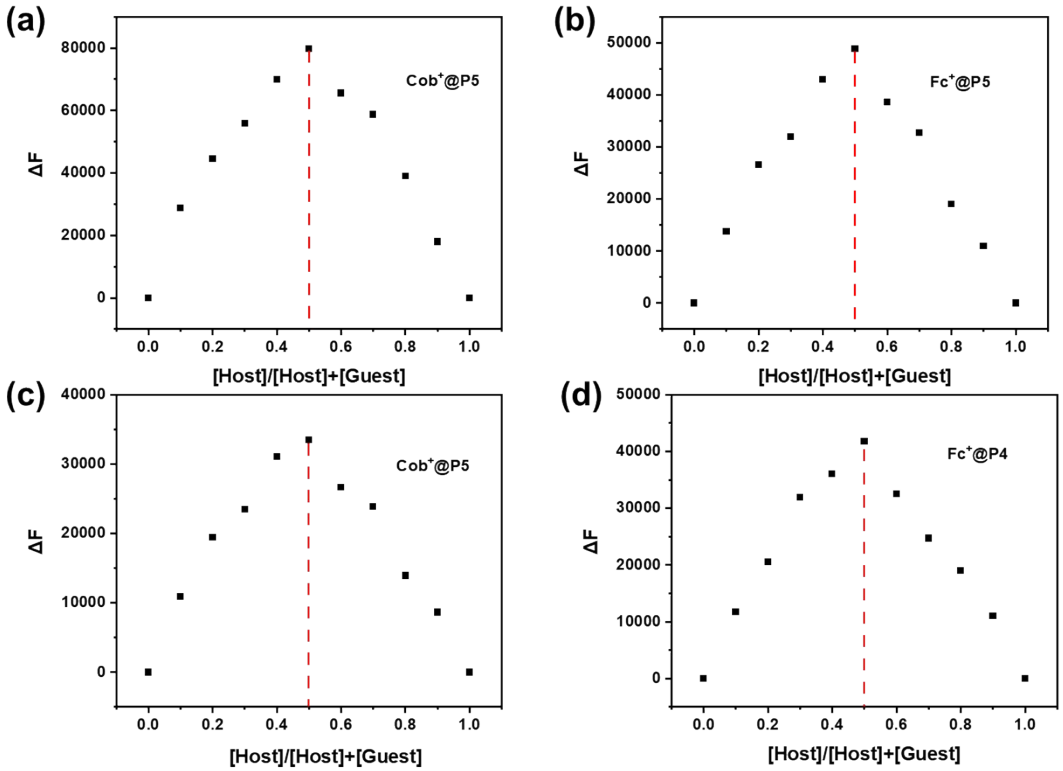


Fig. S13 Job' plot of (a) **Cob^+@P5**, (b) **Fc^+@P5**, (c) **Cob^+@P4** and (d) **Fc^+@P4**, the total concentration of the host and the guest is fixed: [Host]+[Guest] = 1.0 mmol/L.

8. HR-ESI-MS of host-guest complexes

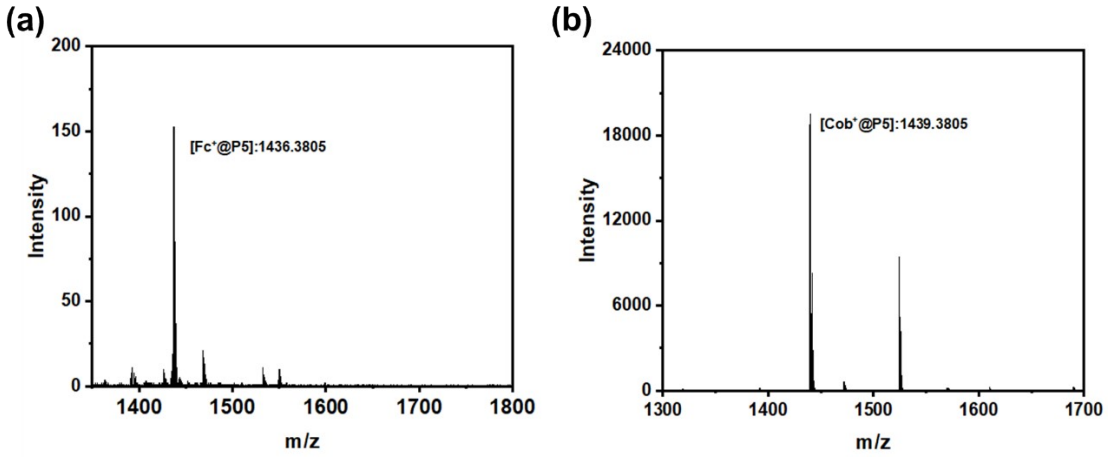


Fig. S14 HR-ESI-MS spectra of an equimolar mixture of (a) **Fc^+@P5**, (b) **Cob^+@P5**.

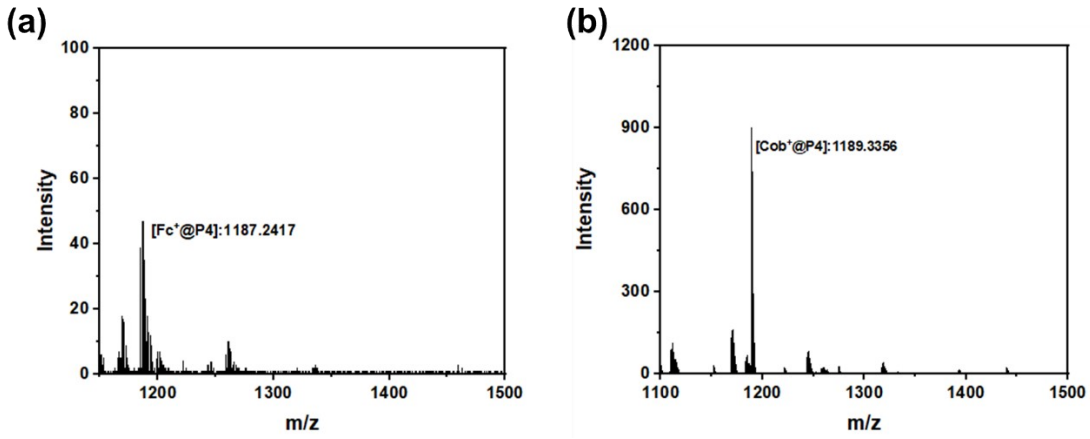


Fig. S15 HR-ESI-MS spectra of an equimolar mixture of (a) **Fc**$^{+}$@**P4**, (b) **Cob**$^{+}$@**P4**.

9. Stability test of Fc^{+}

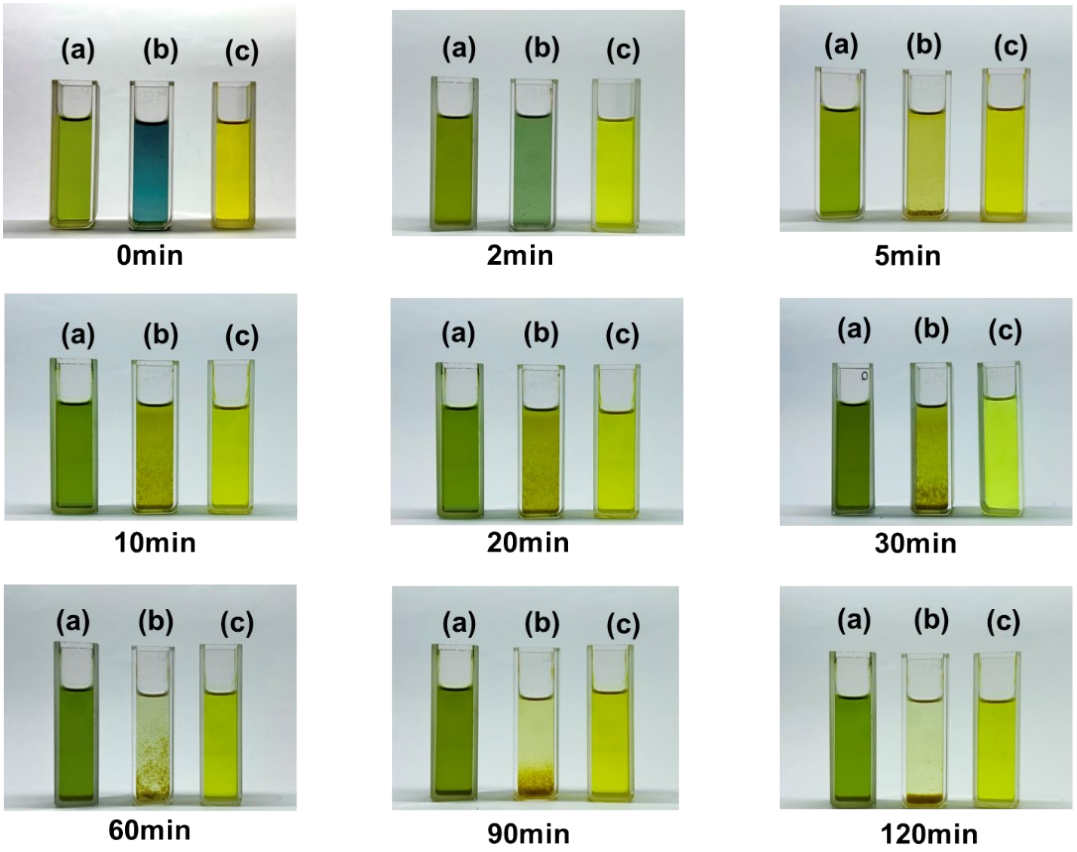


Fig. S16 Stability test in $CHCl_3/CH_3CN$ (4/1, v/v) (a) **P4** (1 mM) and **Fc**$^{+}$ (1 mM). (b) **Fc**$^{+}$ (1 mM). (c) **P4** (1 mM).

10. AIM Analysis of the Complexes

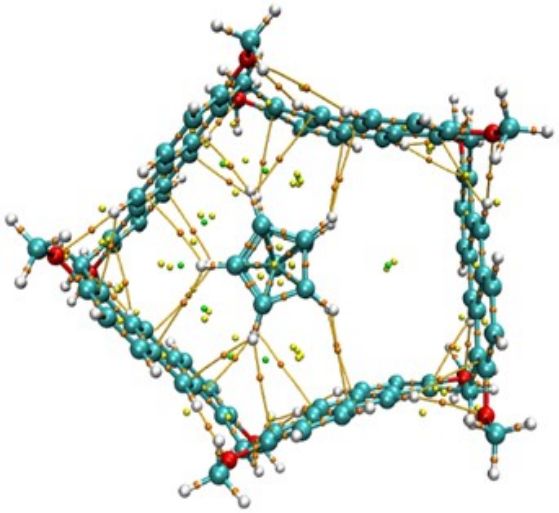


Fig. S17 AIM analysis of [**Cob**$^{+}$@**P5**]-I.

Table S1. The computed electron density values (ρ), the corresponding Laplacian values ($\nabla^2\rho$), and the eigenvalues ($\lambda1 < \lambda2 < \lambda3, \nabla^2\rho = \lambda1 + \lambda2 + \lambda3$) for selected bond critical points of [**Cob**$^{+}$@**P5**]-I.

Interaction	ρ	$\nabla^2\rho$	λ_1	λ_2	λ_3
C-H···π(1)	0.0052	0.0152	-0.0034	-0.0022	0.0208
C-H···π(2)	0.0027	0.0087	-0.0015	-0.0003	0.0105
C-H···π(3)	0.0044	0.0145	-0.0031	-0.0019	0.0195
C-H···π(4)	0.0043	0.0142	-0.0028	-0.0020	0.0191
C-H···π(5)	0.0044	0.0145	-0.0031	-0.0019	0.0195
C-H···π(6)	0.0043	0.0142	-0.0028	-0.0020	0.0190
C-H···π(7)	0.0027	0.0087	-0.0015	-0.0003	0.0105
C-H···π(8)	0.0052	0.0152	-0.0034	-0.0022	0.0208
C-H···π(9)	0.0067	0.0228	-0.0048	-0.0004	0.0280

C-H···π(10)	0.0071	0.0227	-0.0053	-0.0046	0.0326
C-H···π(11)	0.0043	0.0147	-0.0023	-0.0017	0.0187
C-H···π(12)	0.0040	0.0122	-0.0027	-0.0014	0.0163
C-H···π(13)	0.0043	0.0147	-0.0023	-0.0017	0.0186
C-H···π(14)	0.0040	0.0122	-0.0027	-0.0014	0.0163
C-H···π(15)	0.0071	0.0227	-0.0053	-0.0046	0.0326
C-H···π(16)	0.0067	0.0228	-0.0048	-0.0004	0.0280

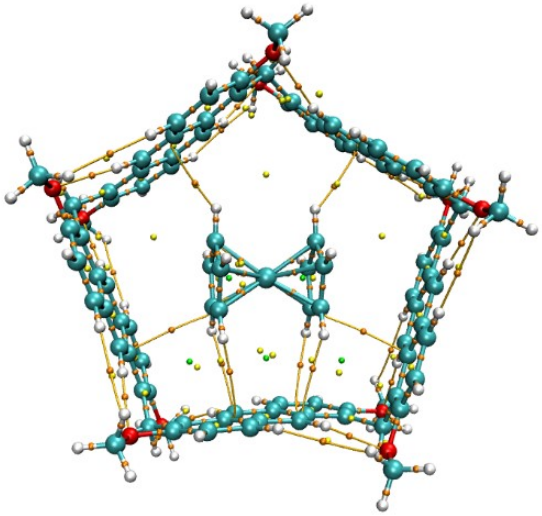


Fig. S18 AIM analysis of [**Cob**$^{+}$@**P5**]-II.

Table S2. The computed electron density values (ρ), the corresponding Laplacian values ($\nabla^2\rho$), and the eigenvalues ($\lambda1 < \lambda2 < \lambda3, \nabla^2\rho = \lambda1 + \lambda2 + \lambda3$) for selected bond critical points of [**Cob**$^{+}$@**P5**]- II.

Interaction	ρ	$\nabla^2\rho$	λ_1	λ_2	λ_3
C-H···π(1)	0.0053	0.0186	-0.0036	-0.0008	0.0230
C-H···π(2)	0.0051	0.0158	-0.0034	-0.0029	0.0221
C-H···π(3)	0.0051	0.0157	-0.0033	-0.0029	0.0220

C-H···π(4)	0.0053	0.0186	-0.0036	-0.0008	0.0230
C-H···π(5)	0.0063	0.0223	-0.0046	-0.0010	0.0279
C-H···π(6)	0.0063	0.0223	-0.0046	-0.0010	0.0278
π···π(1)	0.0070	0.0224	-0.0030	-0.00023	0.0277
π···π(2)	0.0070	0.0224	-0.0030	-0.0023	0.0277

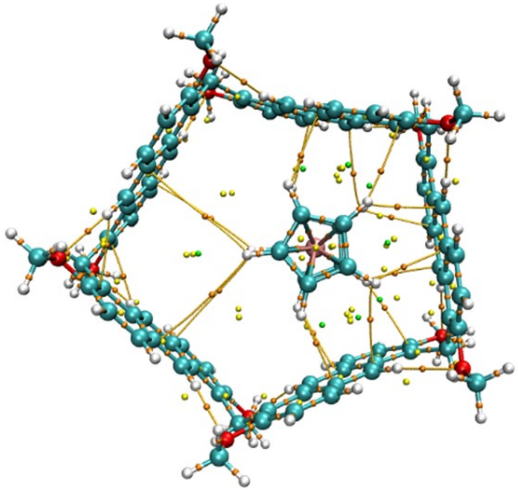


Fig. S19 AIM analysis of [**Fc**$^{+}$@**P5**]-I.

Table S3. The computed electron density values (ρ), the corresponding Laplacian values ($\nabla^2\rho$), and the eigenvalues ($\lambda1 < \lambda2 < \lambda3$, $\nabla^2\rho = \lambda1 + \lambda2 + \lambda3$) for selected bond critical points of [**Fc**$^{+}$@**P5**]-I.

Interaction	ρ	$\nabla^2\rho$	λ_1	λ_2	λ_3
C-H···π(1)	0.0001	0.0007	-0.0001	0.0000	0.0009
C-H···π(2)	0.0002	0.0008	-0.0001	-0.0001	0.0010
C-H···π(3)	0.0003	0.0011	-0.0001	-0.0001	0.0014
C-H···π(4)	0.0002	0.0009	-0.0001	-0.0001	0.0011
C-H···π(5)	0.0077	0.0265	-0.0055	-0.0047	0.0368

C-H···π(6)	0.0070	0.0227	-0.0053	-0.0022	0.0302
C-H···π(7)	0.0036	0.0112	-0.0021	-0.0013	0.0146
C-H···π(8)	0.0051	0.0155	-0.0030	-0.0017	0.0203
C-H···π(9)	0.0070	0.0224	-0.0052	-0.0040	0.0315
C-H···π(10)	0.0071	0.0259	-0.0043	-0.0019	0.0321
C-H···π(11)	0.0075	0.0279	-0.0047	-0.0018	0.0343
C-H···π(12)	0.0073	0.0235	-0.0055	-0.0043	0.0333
C-H···π(13)	0.0055	0.0164	-0.0034	-0.0020	0.0218
C-H···π(14)	0.0033	0.0105	-0.0019	-0.0009	0.0133
C-H···π(15)	0.0075	0.0256	-0.0056	-0.0044	0.0356
C-H···π(16)	0.0356	0.0233	-0.0055	-0.0027	0.0315

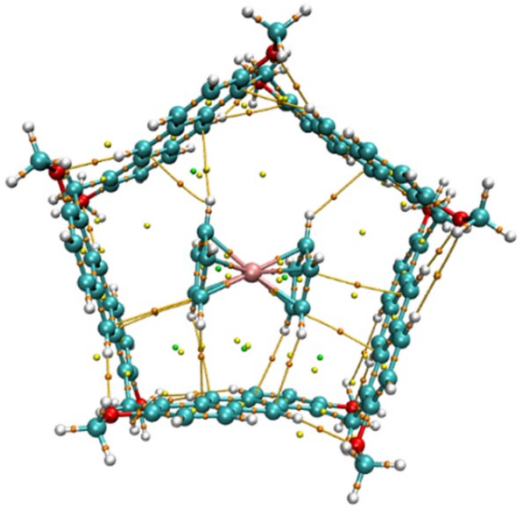


Fig. S20 AIM analysis of [**Fc**$^{+}$@**P5**]-II.

Table S4. The computed electron density values (ρ), the corresponding Laplacian values ($\nabla^2\rho$), and the eigenvalues ($\lambda1 < \lambda2 < \lambda3$, $\nabla^2\rho = \lambda1 + \lambda2 + \lambda3$) for selected bond critical points of [**Fc**$^{+}$@**P5**]-II.

Interaction	ρ	$\nabla^2\rho$	λ_1	λ_2	λ_3
C-H···π(1)	0.0061	0.0212	-0.0033	-0.0009	0.0254
C-H···π(2)	0.0051	0.0179	-0.0028	-0.0001	0.0208
C-H···π(3)	0.0050	0.0171	-0.0031	-0.0019	0.0221
C-H···π(4)	0.0040	0.0123	-0.0024	-0.0020	0.0167
C-H···π(5)	0.0063	0.0227	-0.0041	-0.0010	0.0278
C-H···π(6)	0.0064	0.0201	-0.0047	-0.0036	0.0284
C-H···π(7)	0.0068	0.0226	-0.0053	-0.0025	0.0304
π···π(1)	0.0066	0.0186	-0.0035	-0.0012	0.0233
π···π(2)	0.0081	0.0268	-0.0033	-0.0020	0.0322
π···π(3)	0.0084	0.0269	-0.0045	-0.0024	0.0338
π···π(4)	0.0054	0.0151	-0.0027	-0.0008	-0.0008

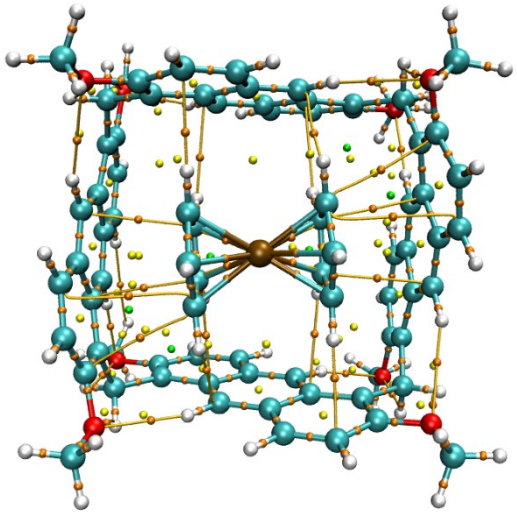


Fig. S21 AIM analysis of **Cob**$^+$**@P4**.

Table S5. The computed electron density values (ρ), the corresponding Laplacian values ($\nabla^2\rho$), and the eigenvalues ($\lambda1 < \lambda2 < \lambda3$, $\nabla^2\rho = \lambda1 + \lambda2 + \lambda3$) for selected

bond critical points of **Cob^{+}@P4.**

Interaction	ρ	$\nabla^2\rho$	λ_1	λ_2	λ_3
C-H···π(1)	0.0077	0.0259	-0.0056	-0.0032	0.0347
C-H···π(2)	0.0128	0.0426	-0.0120	-0.0059	0.0605
C-H···π(3)	0.0093	0.0315	-0.0077	-0.0041	0.0433
C-H···π(4)	0.0085	0.0310	-0.0059	-0.0040	0.0409
C-H···π(5)	0.0128	0.0426	-0.0120	-0.0059	0.0605
C-H···π(6)	0.0077	0.0259	-0.0056	-0.0032	0.0348
C-H···π(7)	0.0085	0.0310	-0.0059	-0.0040	0.0409
C-H···π(8)	0.0093	0.0315	-0.0077	-0.0041	0.0433
π···π(1)	0.0120	0.0384	-0.0067	-0.0047	0.0498
π···π(2)	0.0111	0.0370	-0.0063	-0.0033	0.0466
π···π(3)	0.0079	0.0237	-0.0033	-0.0048	0.0274
π···π(4)	0.0074	0.0232	-0.0036	-0.0008	0.0276
π···π(5)	0.0074	0.0232	-0.0036	-0.0008	0.0276
π···π(6)	0.0111	0.0370	-0.0063	-0.0033	0.0466
π···π(7)	0.0079	0.0237	-0.0033	-0.0005	0.0274
π···π(8)	0.0120	0.0383	-0.0067	-0.0047	0.0498

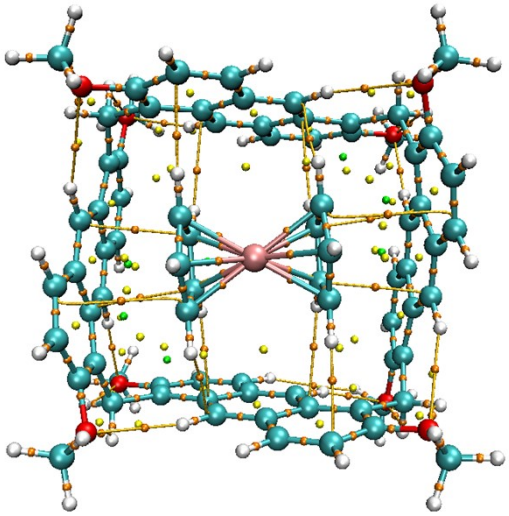


Fig. S22 AIM analysis of **Fc^{+}@P4.**

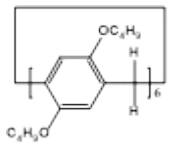
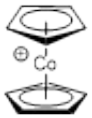
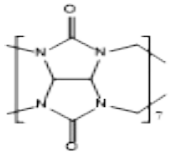
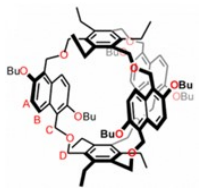
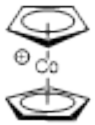
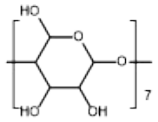
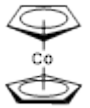
Table S6. The computed electron density values (ρ), the corresponding Laplacian values ($\nabla^2\rho$), and the eigenvalues ($\lambda1 < \lambda2 < \lambda3$, $\nabla^2\rho = \lambda1 + \lambda2 + \lambda3$) for selected bond critical points of **Fc^{+}@P4.**

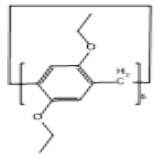
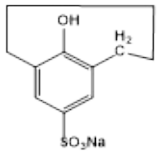
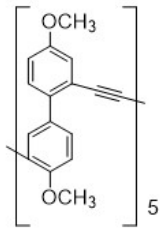
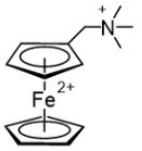
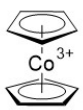
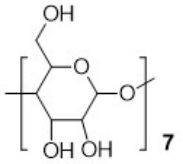
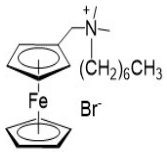
Interaction	ρ	$\nabla^2\rho$	λ_1	λ_2	λ_3
C-H···π(1)	0.0093	0.0314	-0.0078	-0.0034	0.0426
C-H···π(2)	0.0082	0.0298	-0.0055	-0.0035	0.0388
C-H···π(3)	0.0077	0.0262	-0.0056	-0.0036	0.0353
C-H···π(4)	0.0128	0.0425	-0.0120	-0.0058	0.0603
C-H···π(5)	0.0082	0.0298	-0.0055	-0.0035	0.0389
C-H···π(6)	0.0093	0.0314	-0.0078	-0.0034	0.0427
C-H···π(7)	0.0077	0.0262	-0.0056	-0.0036	0.0354
C-H···π(8)	0.0128	0.0426	-0.0120	-0.0058	0.0603
π···π(1)	0.0122	0.0388	-0.0069	-0.0048	0.0505
π···π(2)	0.0109	0.0361	-0.0063	-0.0028	0.0453

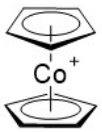
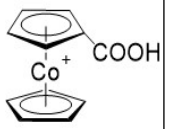
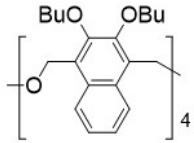
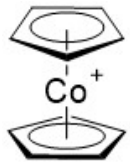
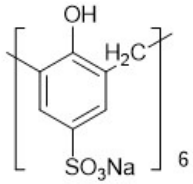
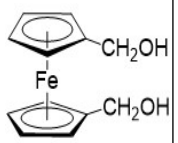
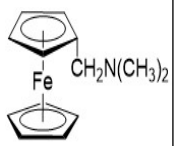
π···π(3)	0.0082	0.0244	-0.0035	-0.0004	0.0283
π···π(4)	0.0122	0.0388	-0.0069	-0.0048	0.0505
π···π(4)	0.0109	0.0362	-0.0063	-0.0028	0.0453
π···π(4)	0.0082	0.0244	-0.0035	-0.0004	0.0284

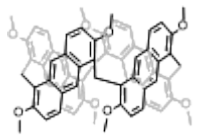
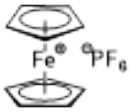
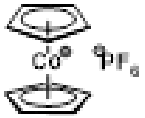
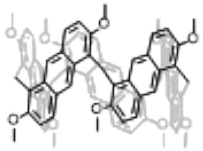
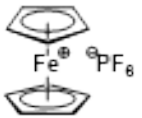
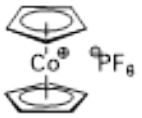
11. Comparison of complexation properties

Table S7. Comparison of complexation properties between Pagoda[n]arenes and other reported hosts.

Host	Guest	FL	*Ka*[M^{-1}]	Solvent	Testing method of *Ka*	Ref.
		NO	$(3.7 \pm 1.0) \times 10^4$	$CDCl_3/CD_3CN$ = 5/1	^{1}H NMR Titration	Chem. Commun., 2013, 49, 5085-5087.
		NO	$(4.0 \pm 1.0) \times 10^{12}$	Water	ITC	J. Am. Chem. Soc. 2005, 127, 12984–12989.
		NO	1.3×10^8	EDC/Acetone =1:1	CV	J. Am. Chem. Soc. 2019, 141, 4468−4473.
		NO	$(6.1 \pm 1.9) \times 10^9$	EDC/Acetone =1:1	ITC	
		NO	$(2.0 \pm 0.2) \times 10^3$	NaCl aqueous solution	CV	Inorg. Chem. 1998, 37, 317-320.

		NO	$(0.9 \pm 0.2) \times 10^2$	$CDCl_3$	^1H NMR	Org. Lett. 2020, 22, 4, 1552–1556.
		NO	5.5×10^4	NaCl aqueous solution	CV	Journal of Electroanalytical Chemistry, 2002, 523, 126–135.
		YES	2.46×10^4	$CHCl_3$	Fl titration	J. Am. Chem. Soc. 2022, 144, 20351–20362.
		YES	4.79×10^7	$CHCl_3$	Fl titration	
		NO	$(1.9 \pm 0.2) \times 10^3$	NaCl aqueous solution	RDV	J. Org. Chem. 1991, 56, 35-41.
		NO	$(1.4 \pm 0.1) \times 10^3$	NaCl aqueous solution	RDV	

		NO	2.2×10^3	NaCl aqueous solution	CV	Inorg. Chem. 1998, 37, 317-320.
		NO	$(1.8 \pm 0.2) \times 10^3$	0.1 M Ph=7 phosphate buffer	CV	
		NO	$(4.3 \pm 1.0) \times 10^4$	CH_2Cl_2/CH_3CN (1/1, v/v)	ITC	Beilstein J. Org. Chem. 2018, 14, 1570–1577.
		NO	4.4×10^2	NaCl aqueous solution	CV	J. Electroanal. Chem. 2002, 523, 126–135.
		NO	5.5×10^4	NaCl aqueous solution	CV	

		YES	(4.3 ± 0.7) × 10^3	$CHCl_3/CH_3CN$ (4/1, v/v)	Fl titration	This Work
		YES	(1.4 ± 0.2) × 10^4	$CHCl_3/CH_3CN$ (4/1, v/v)	Fl titration	
		YES	(1.5 ± 0.7) × 10^3	$CHCl_3/CH_3CN$ (4/1, v/v)	Fl titration	
		YES	(4.3 ± 0.4) × 10^4	$CHCl_3/CH_3CN$ (4/1, v/v)	Fl titration	
		YES	(2.5 ± 0.1) × 10^5	$CHCl_3/CH_3CN$ (4/1, v/v)	Fl titration	

12. The atomic coordinates of optimized structures

The atomic coordinates of **Cob**$^{+}$:

C	1.67815462	-0.52719633	1.09473369
C	1.67779285	-1.20429634	-0.16326791
C	1.67728079	-0.21694155	-1.19575441
C	1.67760458	1.07011104	-0.57601456
C	1.67820936	0.87844516	0.83954037
C	-1.67834353	-0.57030961	1.07290333
C	-1.67832545	0.84435566	0.87360844
C	-1.67747430	-1.19686552	-0.21099725
C	-1.67755935	1.09205851	-0.53328829
C	-1.67704511	-0.16941319	-1.20356978
Co	-0.00007197	-0.00000047	0.00053776
H	1.64651001	-0.99598164	2.06895894
H	1.64574074	-2.27555452	-0.30848214
H	1.64445894	-0.40995428	-2.25944617
H	1.64472336	2.02206064	-1.08825009
H	1.64619088	1.65978939	1.58665575
H	-1.64691490	-1.07751441	2.02771902
H	-1.64680734	1.59555797	1.65107910
H	-1.64501976	-2.26147877	-0.39875400
H	-1.64460758	2.06360318	-1.00733153
H	-1.64409787	-0.32020173	-2.27403013

The atomic coordinates of **Fc**$^{+}$:

C	1.70301500	-0.48831700	-1.11380200
C	1.70215100	0.90871700	-0.80849900
C	1.70197300	1.05021800	0.61428400
C	1.70179700	-0.25938600	1.18839600
C	1.70310600	-1.21045500	0.12041500
C	-1.70271100	-0.44530100	-1.13170200
C	-1.70281000	-1.21427000	0.07391500
C	-1.70203800	0.93902600	-0.77339200
C	-1.70211200	-0.30484600	1.17753600
C	-1.70209100	1.02585000	0.65375600
Fe	-0.00006900	-0.00034200	-0.00024300
H	1.66854900	-0.92248900	-2.10396800
H	1.66710700	1.71631400	-1.52715400
H	1.66703500	1.98327100	1.15991500
H	1.66675800	-0.48988800	2.24474300
H	1.66898800	-2.28616700	0.22723600
H	-1.66820500	-0.84121900	-2.13770300
H	-1.66842500	-2.29332200	0.13944300
H	-1.66668800	1.77351900	-1.46059900

H	-1.66749700	-0.57587500	2.22429300
H	-1.66749300	1.93733400	1.23468300

The atomic coordinates of **P4**:

O	-5.72937345	-0.23276798	2.75532935
O	0.23276798	5.72937345	-2.75532935
O	-0.23276798	5.72937345	2.75532935
O	5.72937345	-0.23276798	-2.75532935
O	5.72937345	0.23276798	2.75532935
O	-0.23276798	-5.72937345	-2.75532935
O	0.23276798	-5.72937345	2.75532935
O	-5.72937345	0.23276798	-2.75532935
C	-4.71461481	0.87859106	0.94823301
C	-4.86236631	0.74384043	2.31683866
C	-4.13258360	1.55387186	3.23482913
H	-4.26895472	1.42366893	4.30157006
C	-3.24900718	2.49024182	2.77449771
H	-2.68067049	3.09844663	3.47365097
C	-3.04436912	2.68063772	1.37956451
C	-2.12180379	3.62306663	0.91175113
H	-1.59860517	4.22524494	1.64205205
C	-1.87716689	3.80832640	-0.45417877
C	-0.87859106	4.71461481	-0.94823301
C	-0.74384043	4.86236631	-2.31683866
C	-1.55387186	4.13258360	-3.23482913
H	-1.42366893	4.26895472	-4.30157006
C	-2.49024182	3.24900718	-2.77449771
H	-3.09844663	2.68067049	-3.47365097
C	-2.68063772	3.04436912	-1.37956451
C	-3.62306663	2.12180379	-0.91175113
H	-4.22524494	1.59860517	-1.64205205
C	-3.80832640	1.87716689	0.45417877
C	-5.81015717	-0.50979854	4.14078623
H	-6.50349203	-1.34763325	4.23525850
H	-6.20156751	0.34579146	4.70651366
H	-4.83494322	-0.79864483	4.55528351
C	0.50979854	5.81015717	-4.14078623
H	0.79864483	4.83494322	-4.55528351
H	1.34763325	6.50349203	-4.23525850
H	-0.34579146	6.20156751	-4.70651366
C	0.00000000	5.51662138	0.00000000
H	-0.63672910	6.17114485	0.60055962
H	0.63672910	6.17114485	-0.60055962
C	0.87859106	4.71461481	0.94823301
C	0.74384043	4.86236631	2.31683866

C	1.55387186	4.13258360	3.23482913
H	1.42366893	4.26895472	4.30157006
C	2.49024182	3.24900718	2.77449771
H	3.09844663	2.68067049	3.47365097
C	2.68063772	3.04436912	1.37956451
C	3.62306663	2.12180379	0.91175113
H	4.22524494	1.59860517	1.64205205
C	3.80832640	1.87716689	-0.45417877
C	4.71461481	0.87859106	-0.94823301
C	4.86236631	0.74384043	-2.31683866
C	4.13258360	1.55387186	-3.23482913
H	4.26895472	1.42366893	-4.30157006
C	3.24900718	2.49024182	-2.77449771
H	2.68067049	3.09844663	-3.47365097
C	3.04436912	2.68063772	-1.37956451
C	2.12180379	3.62306663	-0.91175113
H	1.59860517	4.22524494	-1.64205205
C	1.87716689	3.80832640	0.45417877
C	-0.50979854	5.81015717	4.14078623
H	-0.79864483	4.83494322	4.55528351
H	-1.34763325	6.50349203	4.23525850
H	0.34579146	6.20156751	4.70651366
C	5.81015717	-0.50979854	-4.14078623
H	4.83494322	-0.79864483	-4.55528351
H	6.50349203	-1.34763325	-4.23525850
H	6.20156751	0.34579146	-4.70651366
C	5.51662138	-0.00000000	0.00000000
H	6.17114485	0.63672910	0.60055962
H	6.17114485	-0.63672910	-0.60055962
C	4.71461481	-0.87859106	0.94823301
C	3.80832640	-1.87716689	0.45417877
C	3.62306663	-2.12180379	-0.91175113
H	4.22524494	-1.59860517	-1.64205205
C	2.68063772	-3.04436912	-1.37956451
C	2.49024182	-3.24900718	-2.77449771
H	3.09844663	-2.68067049	-3.47365097
C	1.55387186	-4.13258360	-3.23482913
H	1.42366893	-4.26895472	-4.30157006
C	0.74384043	-4.86236631	-2.31683866
C	0.87859106	-4.71461481	-0.94823301
C	1.87716689	-3.80832640	-0.45417877
C	2.12180379	-3.62306663	0.91175113
H	1.59860517	-4.22524494	1.64205205
C	3.04436912	-2.68063772	1.37956451

C	3.24900718	-2.49024182	2.77449771
H	2.68067049	-3.09844663	3.47365097
C	4.13258360	-1.55387186	3.23482913
H	4.26895472	-1.42366893	4.30157006
C	4.86236631	-0.74384043	2.31683866
C	5.81015717	0.50979854	4.14078623
H	6.20156751	-0.34579146	4.70651366
H	4.83494322	0.79864483	4.55528351
H	6.50349203	1.34763325	4.23525850
C	-0.50979854	-5.81015717	-4.14078623
H	-1.34763325	-6.50349203	-4.23525850
H	0.34579146	-6.20156751	-4.70651366
H	-0.79864483	-4.83494322	-4.55528351
C	-0.00000000	-5.51662138	0.00000000
H	-0.63672910	-6.17114485	-0.60055962
H	0.63672910	-6.17114485	0.60055962
C	-0.87859106	-4.71461481	0.94823301
C	-0.74384043	-4.86236631	2.31683866
C	-1.55387186	-4.13258360	3.23482913
H	-1.42366893	-4.26895472	4.30157006
C	-2.49024182	-3.24900718	2.77449771
H	-3.09844663	-2.68067049	3.47365097
C	-2.68063772	-3.04436912	1.37956451
C	-3.62306663	-2.12180379	0.91175113
H	-4.22524494	-1.59860517	1.64205205
C	-3.80832640	-1.87716689	-0.45417877
C	-4.71461481	-0.87859106	-0.94823301
C	-4.86236631	-0.74384043	-2.31683866
C	-4.13258360	-1.55387186	-3.23482913
H	-4.26895472	-1.42366893	-4.30157006
C	-3.24900718	-2.49024182	-2.77449771
H	-2.68067049	-3.09844663	-3.47365097
C	-3.04436912	-2.68063772	-1.37956451
C	-2.12180379	-3.62306663	-0.91175113
H	-1.59860517	-4.22524494	-1.64205205
C	-1.87716689	-3.80832640	0.45417877
C	0.50979854	-5.81015717	4.14078623
H	-0.34579146	-6.20156751	4.70651366
H	0.79864483	-4.83494322	4.55528351
H	1.34763325	-6.50349203	4.23525850
C	-5.81015717	0.50979854	-4.14078623
H	-6.20156751	-0.34579146	-4.70651366
H	-4.83494322	0.79864483	-4.55528351
H	-6.50349203	1.34763325	-4.23525850

C	-5.51662138	0.00000000	0.00000000
H	-6.17114485	-0.63672910	0.60055962
H	-6.17114485	0.63672910	-0.60055962

The atomic coordinates of **P5**:

O	-6.34474166	-2.34136090	2.74070717
O	0.27007838	-6.83362380	2.75682744
O	6.41927590	-1.84182049	2.85233886
O	3.78072986	5.66024210	2.73979808
O	0.83807375	-6.78927420	-2.75689748
O	6.65048588	-1.29388370	-2.73967775
O	3.28477102	5.93757554	-2.77381343
O	-6.03866448	-2.84742427	-2.85004810
O	-4.65160543	4.97930181	-2.74158391
O	-4.19861694	5.33793167	2.77265408
C	-4.91123770	4.84642301	-4.12653908
C	-3.34656375	5.04744925	-2.30546111
C	-2.26164132	5.10885647	-3.22805702
C	-0.97529484	5.19205963	-2.77347414
C	-3.14257718	5.04655454	-0.93688699
C	-0.69156316	5.21449083	-1.37944117
C	-1.79355473	5.13540920	-0.44952303
C	0.62443656	5.33310467	-0.91815546
C	-1.48387580	5.17352853	0.91488664
C	0.93559531	5.35428229	0.44636165
C	-0.16586673	5.26563118	1.37620194
C	2.28125397	5.48355426	0.93444695
C	0.11660916	5.29539333	2.77031798
C	1.39972211	5.41627446	3.22540785
C	2.48143627	5.52177060	2.30308439
C	4.05551325	5.58115085	4.12585716
C	3.45431511	5.67672354	-0.01642871
C	3.08369621	6.13593085	-4.16071282
C	3.74622648	4.71862398	-2.32942696
C	3.80780106	4.53458566	-0.95851834
C	4.13473986	3.69770001	-3.24441076
C	4.60560307	2.50084245	-2.78022337
C	4.71137825	2.24914717	-1.38497355
C	4.30009338	3.27967996	-0.46260853
C	4.42583440	3.00390640	0.90544976
C	5.22357863	1.03377226	-0.91266565
C	5.33291327	0.75424414	0.45171223
C	4.91072710	1.78023566	1.37713260
C	5.00853425	1.52934263	2.77908580
C	5.50725283	0.34455934	3.23504341

C	5.94990865	-0.65079409	2.31592649
C	5.87527153	-0.48624862	0.95075712
C	7.72760706	-1.75814097	3.40824048
C	6.43807117	-1.54752254	0.01679370
C	6.78573988	-1.04242369	-4.12563392
C	5.64141800	-2.12533170	-2.30300915
C	4.80213946	-2.81754133	-3.22404580
C	5.47915659	-2.24725600	-0.93463210
C	3.81699145	-3.64772833	-2.76655345
C	3.60584740	-3.83642669	-1.37222979
C	4.44892452	-3.12068117	-0.44372773
C	4.22921783	-3.33811865	0.92123032
C	2.61772154	-4.71286693	-0.90919282
C	2.38346878	-4.91441580	0.45617733
C	3.22249048	-4.19312998	1.38381147
C	3.01970737	-4.38313164	2.77925456
C	2.05414453	-5.23575170	3.23665675
C	1.23858123	-5.95776195	2.31678339
C	1.37488078	-5.81255614	0.94741958
C	0.00423230	-6.92893598	4.14338812
C	0.54296716	-6.66522103	-0.00033283
C	1.11683117	-6.84048289	-4.14324208
C	-0.25695241	-6.07799330	-2.31705279
C	-1.17448037	-5.49056787	-3.23675742
C	-2.26149672	-4.79956164	-2.77921255
C	-1.55433912	-5.23239069	-0.45634960
C	-2.49413100	-4.64788740	-1.38375774
C	-0.41548168	-5.95796929	-0.94760583
C	-1.82049967	-5.07597281	0.90901909
C	-3.62370121	-3.96341364	-0.92100940
C	-3.87849201	-3.78973071	0.44413241
C	-2.93529489	-4.36789299	1.37238553
C	-3.17600668	-4.21964742	2.76683313
C	-4.27931866	-3.55474814	3.22467684
C	-5.21588450	-3.00089278	2.30387931
C	-5.03558290	-3.09333847	0.93543574
C	-6.51927130	-2.11512887	4.12666994
C	-6.09770119	-2.56163488	-0.01544794
C	-7.34292648	-2.98362830	-3.40510663
C	-5.77382518	-1.59473044	-2.31418499
C	-5.50593290	-0.53900585	-3.23353820
C	-5.20665187	0.71114663	-2.77752114
C	-5.72284382	-1.42068901	-0.94902818
C	-5.14604208	0.97373991	-1.37569029

C	-5.39165136	-0.10791871	-0.44999988
C	-4.02348622	5.56665213	4.15843684
C	-4.67558492	2.99036241	3.24480424
C	-4.94913353	1.73328017	2.78128137
C	-5.01740023	1.46787961	1.38624380
C	-5.32619383	0.18534033	0.91433276
C	-4.45987837	4.06066505	2.32930475
C	-4.49548189	3.86948911	0.95852440
C	-4.78125906	2.55169181	0.46350546
C	-4.86501161	2.25971145	-0.90433173
C	-4.33033589	5.05300413	0.01497682
H	-5.99496243	4.75111524	-4.21608436
H	-4.57964927	5.72800309	-4.69043719
H	-4.43401059	3.95065253	-4.54590878
H	-2.45455713	5.09579796	-4.29385769
H	-0.14760925	5.24434612	-3.47619379
H	1.41022551	5.43611416	-1.65343035
H	-2.27675856	5.15947996	1.64975497
H	-0.70968329	5.22116171	3.47270445
H	1.59143819	5.43816890	4.29126460
H	5.14066187	5.65709000	4.21667653
H	3.58931600	6.40482973	4.68208299
H	3.72307458	4.62538837	4.55247810
H	4.33686119	5.90670344	0.58575890
H	3.25553392	6.56175841	-0.62600120
H	2.66446733	7.13906105	-4.25797652
H	4.02618421	6.08356591	-4.72109756
H	2.37647493	5.40627459	-4.57715480
H	4.06429584	3.86912808	-4.31162249
H	4.90785649	1.72274813	-3.47646643
H	4.16646411	3.75938594	1.63369942
H	5.56415669	0.31136603	-1.64123440
H	4.66802610	2.29561083	3.47083019
H	5.56577068	0.12450128	4.29689297
H	7.95510761	-2.74354032	3.82117523
H	8.46609037	-1.50247590	2.63676346
H	7.77759955	-1.00742892	4.20789685
H	6.91085966	-2.31075551	0.64135160
H	7.22960836	-1.09040806	-0.58218570
H	7.60349997	-0.32512948	-4.21765201
H	7.04119787	-1.95305993	-4.68303702
H	5.87234947	-0.60542092	-4.55095654
H	4.94582611	-2.69202410	-4.29034859
H	3.17935716	-4.17985856	-3.46791958

H	4.85838759	-2.85959752	1.65869750
H	2.04413756	-5.26126676	-1.64348514
H	3.64991516	-3.83649044	3.47560817
H	1.91613304	-5.36666462	4.30307119
H	-0.82694708	-7.63039583	4.23731088
H	0.86749795	-7.31734346	4.69933223
H	-0.29032760	-5.96014976	4.56873151
H	-0.03421097	-7.36891660	0.60490430
H	1.22709441	-7.26513277	-0.60560918
H	2.04981797	-7.39956596	-4.23652402
H	0.32749953	-7.36238195	-4.69979510
H	1.25267454	-5.83705451	-4.56853888
H	-1.01627179	-5.59589933	-4.30323187
H	-2.96823103	-4.35651764	-3.47568001
H	-1.16941850	-5.53047382	1.64276356
H	-4.31810632	-3.58613633	-1.65869422
H	-2.46406008	-4.64749309	3.46801118
H	-4.44259318	-3.45628428	4.29099885
H	-7.44055714	-1.53666095	4.21802827
H	-6.62780545	-3.05477884	4.68383195
H	-5.68720252	-1.53882053	4.55292238
H	-6.95436824	-2.24506469	0.58488281
H	-6.43525764	-3.39322377	-0.64022535
H	-7.40244035	-3.99299732	-3.81853178
H	-8.11336373	-2.85583130	-2.63310312
H	-7.51839594	-2.25149679	-4.20424430
H	-5.53165780	-0.76457527	-4.29553996
H	-4.99907253	1.52339470	-3.46944320
H	-3.77210422	6.62461366	4.25366800
H	-4.94115746	5.36265721	4.72532229
H	-3.20436419	4.96197120	4.56998460
H	-4.62920048	3.17091657	4.31183685
H	-5.11910282	0.91646673	3.47801679
H	-5.54207687	-0.58335248	1.64325008
H	-4.73375533	3.04749554	-1.63269725
H	-5.23887269	5.13860545	-0.58630866
H	-4.27438247	5.95911252	0.62325761

The atomic coordinates of **Cob**$^{+}$@**P4**:

O	-4.19156789	-3.85459718	2.97931547
O	-3.71978882	4.60051270	-2.34188734
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O	4.59376015	3.80351952	-2.46417341
O	4.19139323	3.85459954	2.97942210
O	3.71991911	-4.60046286	-2.34185852
O	3.77080060	-4.06800911	3.13366668

O	-4.59371559	-3.80357676	-2.46427415
C	-4.31554471	-2.32210021	1.21384966
C	-4.26966017	-2.55314626	2.57356071
C	-4.23294105	-1.48672646	3.52343165
C	-4.21573498	-0.19628783	3.09551486
C	-4.28788286	0.11508320	1.70616411
C	-4.20103142	1.44020894	1.27830401
C	-4.26407939	1.78358070	-0.07556958
C	-3.95526916	3.10849911	-0.54769141
C	-4.08754880	3.36039566	-1.89710789
C	-4.55721035	2.35779732	-2.80204116
C	-4.79492713	1.08685232	-2.36660665
C	-4.60132786	0.73341881	-0.99976858
C	-4.65807664	-0.60280333	-0.57524843
C	-4.42512327	-0.95919245	0.75885289
C	-4.28420120	-4.15313714	4.35743235
C	-4.01845290	4.96565511	-3.67329237
C	-3.54163598	4.23369845	0.39497620
C	-2.32621121	4.03233112	1.29058737
C	-2.49373567	3.98587158	2.66025306
C	-1.39371964	3.81895791	3.55633418
C	-0.12776948	3.71736845	3.07218449
C	0.12808523	3.80266514	1.67257516
C	1.44020250	3.72671982	1.20030819
C	1.75336157	3.83459919	-0.15840626
C	3.10426837	3.71740548	-0.65564438
C	3.31746195	3.94224442	-2.00116192
C	2.24436734	4.28762042	-2.88304147
C	0.95997533	4.35050485	-2.42585879
C	0.65586437	4.10539166	-1.05346371
C	-0.66533153	4.17243870	-0.58045143
C	-0.97928428	3.99569355	0.77328181
C	-3.98884120	4.16150404	4.52715801
C	4.88899851	4.18760485	-3.79121323
C	4.31317911	3.50010408	0.25484420
C	4.31553650	2.32211523	1.21397057
C	4.42518594	0.95921321	0.75896727
C	4.65821939	0.60282639	-0.57512083
C	4.60145267	-0.73339165	-0.99965940
C	4.79508167	-1.08680921	-2.36649622
C	4.55735093	-2.35774224	-2.80196014
C	4.08764042	-3.36034325	-1.89705840
C	3.95532291	-3.10846490	-0.54764134
C	4.26414222	-1.78355976	-0.07548827
C	4.20104726	-1.44019481	1.27838537
C	4.28788509	-0.11507235	1.70625896
C	4.21565661	0.19628327	3.09560836
C	4.23280649	1.48671844	3.52354050
C	4.26953885	2.55314721	2.57368083
C	4.28345300	4.15312349	4.35757867

C	4.01840868	-4.96548827	-3.67333177
C	3.54166977	-4.23368977	0.39499153
C	2.32622159	-4.03234363	1.29057316
C	2.49370366	-3.98592096	2.66024551
C	1.39367569	-3.81896105	3.55630085
C	0.12774377	-3.71731665	3.07211928
C	-0.12807422	-3.80261418	1.67250228
C	-1.44018160	-3.72666183	1.20021689
C	-1.75332750	-3.83456548	-0.15849835
C	-3.10422873	-3.71738553	-0.65575718
C	-3.31741281	-3.94227338	-2.00126826
C	-2.24431811	-4.28772953	-2.88311655
C	-0.95992910	-4.35059732	-2.42591510
C	-0.65582266	-4.10541182	-1.05353084
C	0.66537070	-4.17246528	-0.58050073
C	0.97930761	-3.99567514	0.77323000
C	3.98866327	-4.16210806	4.52720009
C	-4.88890937	-4.18743824	-3.79138667
C	-4.31315910	-3.50007469	0.25470581
H	-4.19031511	-1.70419034	4.58357864
H	-4.14543889	0.62083292	3.80852833
H	-4.09282134	2.21381003	2.02893854
H	-4.70131213	2.59776114	-3.84896750
H	-5.11383986	0.31920722	-3.06734856
H	-4.83988547	-1.37803107	-1.31869126
H	-4.29152873	-5.24058960	4.42552883
H	-5.20834077	-3.75514245	4.79052900
H	-3.42315722	-3.76354501	4.91383785
H	-3.44739876	4.36736172	-4.39425135
H	-3.72915902	6.01217111	-3.76744767
H	-5.08870093	4.86514071	-3.88528993
H	-4.39244589	4.45437494	1.04599274
H	-3.38059468	5.12959725	-0.21011510
H	-1.56762461	3.76570976	4.62397535
H	0.71199337	3.57673733	3.74746829
H	2.23234335	3.63161965	1.93093833
H	2.44927493	4.49471634	-3.92675689
H	0.15143120	4.61407529	-3.10409352
H	-1.46119478	4.39924148	-1.28946130
H	-3.68188124	3.24557446	5.04593994
H	-5.06268695	4.29984987	4.64966409
H	-3.46025982	5.01939019	4.95685721
H	4.37930441	3.54644581	-4.52080736
H	5.96639495	4.06786188	-3.90245841
H	4.62052013	5.23398292	-3.97454341
H	4.43891521	4.40954859	0.85016481
H	5.19566868	3.43290633	-0.38543931
H	4.84006186	1.37805294	-1.31855686
H	5.11404049	-0.31916129	-3.06721419
H	4.70149027	-2.59769425	-3.84888408

H	4.09279457	-2.21379483	2.02901247
H	4.14534095	-0.62084741	3.80860892
H	4.19013202	1.70416071	4.58368877
H	5.20753067	3.75533900	4.79100195
H	3.42230109	3.76330490	4.91365853
H	4.29049239	5.24057549	4.42570207
H	3.72901584	-6.01196992	-3.76756335
H	5.08864219	-4.86504552	-3.88543898
H	3.44732755	-4.36706638	-4.39416385
H	3.38065585	-5.12957430	-0.21012699
H	4.39246337	-4.45437376	1.04602657
H	1.56756494	-3.76570991	4.62394563
H	-0.71203419	-3.57664521	3.74737624
H	-2.23231873	-3.63154449	1.93084184
H	-2.44922015	-4.49494786	-3.92680768
H	-0.15138330	-4.61423797	-3.10412102
H	1.46123326	-4.39936568	-1.28948613
H	3.45988751	-5.02004356	4.95656106
H	3.68183329	-3.24630049	5.04627324
H	5.06247465	-4.30068812	4.64974330
H	-4.62055046	-5.23382362	-3.97484934
H	-4.37908115	-3.54623911	-4.52085240
H	-5.96628345	-4.06754795	-3.90268919
H	-4.43892825	-4.40952880	0.85000548
H	-5.19562708	-3.43285111	-0.38560583
C	1.71871917	0.47076512	-0.85000032
C	1.51497633	-0.93612558	-0.82595334
C	1.50098704	-1.39966781	-2.17097327
C	1.71380928	-0.28144501	-3.02407979
C	1.85138990	0.87360610	-2.20935271
C	-1.51502024	0.93624962	-0.82610956
C	-1.50105430	1.39964687	-2.17118234
C	-1.71859756	-0.47066963	-0.85000686
C	-1.71370405	0.28129298	-3.02416875
C	-1.85116653	-0.87368298	-2.20931008
Co	0.00004915	0.00009019	-1.86885186
H	1.72215469	1.12963565	0.00876752
H	1.33232703	-1.53999937	0.05296453
H	1.30054232	-2.41402229	-2.48530294
H	1.71643301	-0.30083195	-4.10563591
H	1.95185225	1.89074339	-2.55832593
H	-1.33248623	1.54023294	0.05275438
H	-1.30076927	2.41399716	-2.48564681
H	-1.72199725	-1.12944341	0.00883663
H	-1.71628662	0.30054632	-4.10572720
H	-1.95146803	-1.89088184	-2.55815251

The atomic coordinates of **Fc**$^{+}$@**P4**:

O	5.38259300	-1.86555400	-2.75560600
O	1.35791100	5.46959600	2.73795400

O	1.82249600	5.30376900	-2.76557000
O	-5.44245300	1.29510700	2.77430900
O	-5.34876200	1.80084900	-2.72736100
O	-1.30858600	-5.53366500	2.74916600
O	-1.82359400	-5.39061800	-2.75250700
O	5.53660100	-1.36524500	2.74724000
C	4.83162300	-0.47487500	-0.95038200
C	4.92121300	-0.65790300	-2.31578000
C	4.52966500	0.36227900	-3.23758500
C	4.04164000	1.55074600	-2.78548200
C	3.91252400	1.80649400	-1.38937300
C	3.28933100	2.97673600	-0.93399100
C	3.07210900	3.21098900	0.42660300
C	2.23810000	4.28183300	0.91772500
C	2.15510300	4.45854700	2.28498700
C	2.86761300	3.61973600	3.19999900
C	3.61806300	2.57953200	2.74331500
C	3.70705200	2.30156500	1.34694400
C	4.30616700	1.12049400	0.89440700
C	4.35180000	0.79516800	-0.46645000
C	5.63313900	-2.04664400	-4.13501500
C	1.38923100	5.81437600	4.10899100
C	1.55334600	5.27900900	-0.01279900
C	0.43094000	4.81936000	-0.93899900
C	0.59790700	4.90980600	-2.30707800
C	-0.46137300	4.60433600	-3.21856400
C	-1.66664200	4.17013800	-2.75822600
C	-1.89695700	4.00203800	-1.36100100
C	-3.04239300	3.33543800	-0.90477400
C	-3.25106300	3.08694400	0.45575100
C	-4.29548100	2.22159100	0.94900400
C	-4.45716200	2.12255800	2.31708700
C	-3.62774100	2.84695300	3.22989600
C	-2.61708800	3.63453800	2.76999500
C	-2.35557500	3.74508300	1.37219600
C	-1.17841400	4.35398100	0.91594400
C	-0.85948900	4.40129300	-0.44529200
C	1.98075800	5.60661300	-4.13745200
C	-5.78967600	1.32566700	4.14474000
C	-5.28955300	1.52692000	0.02264700
C	-4.82079500	0.41467400	-0.91084500
C	-4.36910500	-0.86678600	-0.42371800
C	-4.28997600	-1.17988800	0.93627400
C	-3.63734100	-2.33502400	1.38861400

C	-3.48978600	-2.58395200	2.78459900
C	-2.74277400	-3.63003800	3.23428200
C	-2.08806200	-4.50236300	2.31017700
C	-2.19555200	-4.32666900	0.94499800
C	-3.01487700	-3.24329800	0.46312700
C	-3.26607200	-3.02743000	-0.89713400
C	-3.94446500	-1.88872300	-1.34661800
C	-4.13235000	-1.66076900	-2.74200500
C	-4.60471600	-0.46697600	-3.19526000
C	-4.92503800	0.58378800	-2.27778700
C	-5.61357300	1.97486000	-4.10504100
C	-1.31953000	-5.86939800	4.12271500
C	-1.53575500	-5.31982000	-0.00207100
C	-0.45191200	-4.81017000	-0.94253600
C	-0.62767800	-4.90433700	-2.30937700
C	0.39074300	-4.49809200	-3.22813700
C	1.56365100	-3.97739100	-2.77202100
C	1.80570100	-3.83132400	-1.37473000
C	2.96801000	-3.20106800	-0.91582300
C	3.20036200	-2.98641700	0.44642900
C	4.30850400	-2.20547700	0.93597800
C	4.48371800	-2.11058200	2.30257700
C	3.59240500	-2.74824200	3.22147600
C	2.52121800	-3.45480000	2.76519100
C	2.26800900	-3.58047800	1.36766600
C	1.11150500	-4.22141200	0.90855700
C	0.80442400	-4.29925400	-0.45352400
C	-2.01118200	-5.60672700	-4.13699500
C	5.85345000	-1.37339100	4.12526000
C	5.31911100	-1.56466000	-0.00576400
H	4.61315100	0.18917200	-4.30353600
H	3.72695900	2.31785100	-3.48887600
H	2.93275700	3.69310600	-1.67111200
H	2.79721600	3.80150800	4.26548600
H	4.12866000	1.92147300	3.44134300
H	4.73630900	0.44589400	1.63022800
H	6.06486300	-3.04256000	-4.22985000
H	6.34585500	-1.30469900	-4.51107900
H	4.70892400	-1.99605700	-4.72311800
H	0.98789600	5.01027100	4.73716300
H	0.75639700	6.69619400	4.20692500
H	2.40570600	6.06012700	4.43468500
H	2.32638200	5.72984100	-0.64111800
H	1.15755600	6.08458100	0.61161500

H	-0.30287600	4.70904200	-4.28493700
H	-2.45904600	3.90829200	-3.45473400
H	-3.75725600	2.97213500	-1.63972300
H	-3.79632100	2.76136100	4.29653300
H	-1.96775900	4.15769300	3.46715300
H	-0.48735100	4.76137400	1.65030700
H	1.86181700	4.71515900	-4.76459600
H	2.99683400	5.98623200	-4.24210700
H	1.27103700	6.37663300	-4.45894000
H	-4.97776800	0.94526900	4.77592600
H	-6.65730400	0.67389600	4.24513700
H	-6.05763400	2.33828300	4.46493000
H	-5.75518400	2.29634500	-0.59914100
H	-6.08527600	1.11804000	0.65132800
H	-4.70322900	-0.49590200	1.67434700
H	-3.97073400	-1.91059400	3.48963200
H	-2.63930300	-3.79542200	4.29993700
H	-2.92378000	-3.74855800	-1.63537800
H	-3.85490300	-2.44448200	-3.44204000
H	-4.72266200	-0.30835700	-4.26013600
H	-6.36656000	1.26243700	-4.45918000
H	-4.70270200	1.87373000	-4.70702500
H	-6.00125800	2.98822000	-4.20637300
H	-0.71772600	-6.77349100	4.21149300
H	-2.33668400	-6.07396600	4.47401200
H	-0.87323500	-5.07761100	4.73616100
H	-1.10954800	-6.12307700	0.60493300
H	-2.31751600	-5.77753000	-0.61405200
H	0.22603800	-4.59229000	-4.29437700
H	2.32787300	-3.64872700	-3.47182100
H	3.69628600	-2.86805900	-1.65086000
H	3.76182000	-2.66060100	4.28779900
H	1.83284700	-3.92156700	3.46503600
H	0.43890100	-4.65733500	1.64280100
H	-1.26744900	-6.30485900	-4.53613200
H	-1.96977900	-4.66692600	-4.70047200
H	-3.00472400	-6.04274900	-4.23697500
H	6.03200100	-2.39193900	4.48660100
H	5.06281100	-0.90609900	4.72421000
H	6.76891100	-0.79027800	4.22213200
H	5.76611300	-2.35551400	-0.61426600
H	6.12638400	-1.15191500	0.60501800
C	-1.18533800	-0.21658100	1.76840700
C	-0.16696900	-1.21092000	1.72922700

C	1.09439400	-0.54031400	1.72973400
C	0.84020100	0.85940500	1.76983300
C	-0.56188700	1.05480300	1.79166100
C	-1.17582000	-0.26118200	-1.76480800
C	-0.60584600	1.03422200	-1.79225800
C	-0.11905800	-1.21310300	-1.73046000
C	0.80375300	0.89668900	-1.77750500
C	1.11442800	-0.49275400	-1.73952400
Fe	-0.00729200	0.02017500	-0.00140900
H	-2.24855100	-0.38335200	1.71253200
H	-0.33060700	-2.27821600	1.64037100
H	2.07270000	-0.99551000	1.64629900
H	1.57078700	1.64829100	1.73196500
H	-1.06148500	2.00634800	1.76331400
H	-2.22967000	-0.47197900	-1.71696400
H	-1.15279400	1.95957300	-1.76116800
H	-0.24765800	-2.28384600	-1.64417000
H	1.50490800	1.71355800	-1.72753700
H	2.10848800	-0.91612200	-1.65891400

The atomic coordinates of [**Fc**$^{+}$@**P5**]-I:

O	-2.37225500	6.04584000	2.77820300
O	-7.33774000	-0.28982500	2.72474100
O	-1.95362200	-6.12358400	2.80043000
O	5.67220800	-3.85366000	2.68366400
O	-7.25083100	-0.75766900	-2.78316100
O	-1.40137900	-6.28823200	-2.72967700
O	5.85698800	-3.29932600	-2.83828700
O	-2.88363300	5.89870900	-2.75084400
O	4.93763300	4.59241600	-2.69186700
O	5.23995300	4.03677600	2.83221200
C	5.05474900	4.89009300	-4.06845800
C	5.09664900	3.30328700	-2.27522300
C	5.23728200	2.23184300	-3.21183700
C	5.37015200	0.94835800	-2.77457900
C	5.08336600	3.07622000	-0.91448700
C	5.37255200	0.64805700	-1.38042700
C	5.24703400	1.72985100	-0.44448100
C	5.49548500	-0.66868600	-0.93147100
C	5.31487500	1.41981800	0.91717700
C	5.47761900	-0.98554000	0.43096000
C	5.41636500	0.10199500	1.36625700
C	5.54934700	-2.33828600	0.90522200
C	5.46153900	-0.19121200	2.76118100
C	5.55428500	-1.47690700	3.20155800

C	5.60490100	-2.55701000	2.26603300
C	5.87683000	-4.12540300	4.05553900
C	5.63232000	-3.49545900	-0.07154200
C	6.13721300	-3.45145700	-4.21584800
C	4.61732000	-3.63500600	-2.37285700
C	4.44902800	-3.68525200	-1.00504800
C	3.53859900	-3.90033500	-3.27358300
C	2.31837300	-4.26711400	-2.79304800
C	2.08709500	-4.37547300	-1.38952300
C	3.15587100	-4.04675500	-0.48819000
C	2.89666600	-4.15644700	0.88174200
C	0.85798900	-4.83234800	-0.90492000
C	0.60359400	-4.95820000	0.46481600
C	1.65729700	-4.58433000	1.36718000
C	1.42372600	-4.69210700	2.76972900
C	0.23923900	-5.16797200	3.24307100
C	-0.78320800	-5.59545700	2.33903500
C	-0.63160900	-5.49189200	0.97193300
C	-2.11258500	-6.34018100	4.18684300
C	-1.67169700	-6.08167900	0.03313200
C	-1.47935000	-6.71900400	-4.07298800
C	-2.28132200	-5.33545600	-2.29031500
C	-3.02735100	-4.54492800	-3.21866400
C	-2.39294100	-5.15493200	-0.92955800
C	-3.90724600	-3.60890100	-2.76937000
C	-4.09601500	-3.39207100	-1.37211600
C	-3.31887300	-4.16608600	-0.44498400
C	-3.54453400	-3.95810300	0.91783800
C	-5.04117800	-2.47140700	-0.91525800
C	-5.25553500	-2.25051700	0.44920300
C	-4.48122600	-3.02714400	1.37577900
C	-4.71369400	-2.85496100	2.77136400
C	-5.65094600	-1.97524300	3.22059300
C	-6.41495800	-1.20216200	2.29387500
C	-6.22888700	-1.31161100	0.93313100
C	-7.65413700	-0.23482600	4.09889000
C	-7.08689800	-0.50701400	-0.02687500
C	-7.55063200	-0.85068600	-4.15901500
C	-6.50423600	0.29731400	-2.33666700
C	-5.87193100	1.19547200	-3.25016900
C	-5.10245100	2.21804500	-2.78471100
C	-5.56166100	1.51490200	-0.47290300
C	-4.91522400	2.41539800	-1.38563900
C	-6.35886700	0.43017400	-0.97329400

C	-5.40389000	1.75944600	0.89487900
C	-4.14442400	3.47988600	-0.91070800
C	-3.96081800	3.70430400	0.45600200
C	-4.61886800	2.81180800	1.36892000
C	-4.47854200	3.04153000	2.76944800
C	-3.74844200	4.09090200	3.23630500
C	-3.11343300	4.98839200	2.32246000
C	-3.19163400	4.81062500	0.95893300
C	-2.50522000	6.43736200	4.12883600
C	-2.59477500	5.83772900	0.01239200
C	-3.07977400	6.09152100	-4.13587500
C	-1.65823500	5.50257700	-2.29996200
C	-0.59678700	5.20968700	-3.21184300
C	0.63635100	4.86689500	-2.74683300
C	-1.49172900	5.39575200	-0.93476400
C	0.88600300	4.77031400	-1.34648300
C	-0.20148500	5.00353800	-0.43683500
C	5.49309600	4.16555500	4.21700900
C	2.86008100	4.28422200	3.27988500
C	1.59891400	4.48666400	2.80816900
C	1.34856500	4.58285700	1.40681300
C	0.06970500	4.88641100	0.93087800
C	3.96192600	4.18665400	2.37343600
C	3.78193400	4.22486800	1.00657700
C	2.44794100	4.40795500	0.49861500
C	2.17055800	4.49299500	-0.86907600
C	4.97579900	4.22922000	0.06655400
H	4.95820100	5.97253800	-4.14704600
H	6.02981000	4.58240600	-4.46187900
H	4.25860000	4.41322900	-4.65275900
H	5.24055300	2.43902200	-4.27509600
H	5.47635500	0.13280600	-3.48538900
H	5.64173800	-1.44669200	-1.67275700
H	5.32731600	2.21119300	1.65822000
H	5.41994000	0.63289500	3.46888900
H	5.58990500	-1.67958600	4.26516400
H	5.98589700	-5.20696100	4.13051400
H	6.78744400	-3.64201300	4.42628600
H	5.02116200	-3.80683000	4.66286900
H	5.76545500	-4.41728700	0.50132300
H	6.53216900	-3.37255000	-0.68108400
H	7.20166100	-3.24627600	-4.32699400
H	5.92528100	-4.47173300	-4.55377700
H	5.56782100	-2.73982300	-4.82566800

H	3.69736900	-3.83240100	-4.34310300
H	1.50458900	-4.50116800	-3.47491300
H	3.68306900	-3.96906800	1.60379100
H	0.11213100	-5.14254100	-1.62739900
H	2.21352600	-4.39672400	3.45588600
H	0.08338300	-5.24754800	4.31212800
H	-3.09080300	-6.80582900	4.30383300
H	-1.34115800	-7.01321400	4.57759900
H	-2.09241600	-5.39748000	4.74685400
H	-2.42599800	-6.58290500	0.64606300
H	-1.17979000	-6.86014500	-0.55713700
H	-0.82227700	-7.58563200	-4.14676000
H	-2.50108300	-7.01218200	-4.33816000
H	-1.13161000	-5.94603400	-4.76895800
H	-2.90230500	-4.70070600	-4.28375400
H	-4.49039500	-3.01813700	-3.47103600
H	-3.02116700	-4.55629000	1.65509500
H	-5.64477100	-1.95364200	-1.65228000
H	-4.13511100	-3.45012300	3.47331000
H	-5.81816600	-1.86541900	4.28540700
H	-8.45029000	0.50353500	4.19225900
H	-8.01204600	-1.20325200	4.46627500
H	-6.79447500	0.08571400	4.70006700
H	-7.79509100	0.08118100	0.56352700
H	-7.68170800	-1.20156200	-0.62644000
H	-8.21568600	-1.70816500	-4.26112400
H	-8.06156500	0.04947900	-4.51940900
H	-6.64891700	-1.02173200	-4.75996800
H	-6.00598700	1.06643300	-4.31756900
H	-4.62624400	2.90736300	-3.47733000
H	-5.92787700	1.14890500	1.62123300
H	-3.72092100	4.16381500	-1.63723100
H	-4.97399500	2.36447600	3.46054200
H	-3.65736600	4.25207400	4.30398400
H	-1.95951900	7.37639300	4.22249800
H	-3.55578600	6.59887800	4.39491200
H	-2.06752700	5.69934500	4.81174500
H	-2.20330400	6.66180700	0.61587600
H	-3.40730800	6.25018100	-0.59217600
H	-4.10426700	6.44700400	-4.24318700
H	-2.39107500	6.84326900	-4.53723600
H	-2.96235600	5.15422500	-4.69327100
H	-0.76400900	5.28635000	-4.27938900
H	1.45294600	4.67661600	-3.43884600

H	6.57547100	4.10483400	4.32765700
H	5.14127500	5.13019600	4.59827000
H	5.02620400	3.35521600	4.78957300
H	3.03175300	4.22608700	4.34792700
H	0.76494500	4.59837300	3.49649300
H	-0.70835300	5.08468700	1.65903000
H	2.97086700	4.40840800	-1.59531300
H	4.95361600	5.16113100	-0.50488800
H	5.88596300	4.25329600	0.67250000
C	2.05785400	-0.55769000	1.75097300
C	1.91036900	0.86284600	1.74046700
C	0.51551200	1.15893600	1.72171000
C	-0.19809400	-0.07501100	1.72209600
C	0.75400500	-1.13566300	1.74073400
C	2.03146200	-0.63428500	-1.76695700
C	0.69689600	-1.13650000	-1.75640800
C	1.96445600	0.79205500	-1.76972500
C	-0.19363300	-0.02346700	-1.75358600
C	0.58859900	1.16842100	-1.76189700
Fe	1.02785200	0.03929500	-0.01328500
H	2.99133400	-1.10865600	1.70716800
H	2.71140300	1.59305500	1.68085300
H	0.08193000	2.14907600	1.64551400
H	-1.27326900	-0.18747800	1.65985500
H	0.53174100	-2.19499500	1.69331700
H	2.93414800	-1.23428000	-1.71011300
H	0.41374600	-2.18024800	-1.69017500
H	2.80575800	1.47451100	-1.71840300
H	-1.27357800	-0.07580000	-1.69632800
H	0.20988200	2.18237700	-1.70889800

The atomic coordinates of [**Cob**$^{+}$@**P5**]-I:

O	5.74797600	4.28385800	-2.63845600
O	5.91574600	-3.72816400	-2.86748100
O	-1.56101700	-5.87178800	-2.66688800
O	-7.41750000	-0.26401000	-2.75148500
O	5.74905400	-4.28328000	2.63834800
O	-2.12555300	-5.51075200	2.86697400
O	-7.41756300	0.26319100	2.75142800
O	5.91527500	3.72874200	2.86736500
O	-1.56176700	5.87149700	2.66711400
O	-2.12634600	5.51081000	-2.86676700
C	-1.41318400	6.12681800	4.05527700
C	-2.43647400	4.90476600	2.24572400
C	-3.17925500	4.11701100	3.17604100

C	-4.07175100	3.18140200	2.73044600
C	-2.55822500	4.72122300	0.87661800
C	-4.26898400	2.96503600	1.33681900
C	-3.48927100	3.73817300	0.39975000
C	-5.21584700	2.04298600	0.87878300
C	-3.71378300	3.51749700	-0.96491500
C	-5.41843600	1.79914900	-0.48687900
C	-4.63573600	2.56959900	-1.42287500
C	-6.36807200	0.83937600	-0.96745600
C	-4.83959700	2.36227900	-2.81678200
C	-5.75816200	1.45249800	-3.26418300
C	-6.52684300	0.69077400	-2.33512800
C	-7.63476400	-0.45671600	-4.14055300
C	-7.18413300	-0.00043900	-0.00001400
C	-7.63487700	0.45591500	4.14048500
C	-6.52676800	-0.69148500	2.33512100
C	-6.36796300	-0.84011900	0.96745600
C	-5.75798600	-1.45306400	3.26421000
C	-4.83928500	-2.36273000	2.81685100
C	-4.63538400	-2.57007900	1.42295600
C	-5.41819000	-1.79977900	0.48692400
C	-5.21557800	-2.04366200	-0.87872700
C	-3.71331000	-3.51788300	0.96504100
C	-3.48877200	-3.73858900	-0.39961500
C	-4.26858600	-2.96559900	-1.33672000
C	-4.07132800	-3.18200500	-2.73033900
C	-3.17871100	-4.11751600	-3.17589400
C	-2.43582400	-4.90513100	-2.24554100
C	-2.55759000	-4.72153400	-0.87644500
C	-1.41242400	-6.12716600	-4.05503600
C	-1.81995800	-5.62766900	0.09544100
C	-2.31369200	-5.64750700	4.26708700
C	-0.93013800	-5.03692100	2.38614500
C	0.10388100	-4.60556400	3.27174400
C	-0.77126600	-5.00820200	1.00960700
C	1.32458200	-4.23836500	2.77737400
C	1.57494600	-4.23894700	1.37467200
C	0.48813500	-4.55888900	0.47927400
C	0.74653600	-4.48085500	-0.89445100
C	2.85941100	-3.99909400	0.87343100
C	3.13840600	-4.00612300	-0.50073300
C	2.02189800	-4.19194000	-1.39798500
C	2.25927300	-4.14004900	-2.80089000
C	3.52464300	-3.96558400	-3.29048600

C	4.63382000	-3.86140000	-2.40021700
C	4.46855800	-3.87733300	-1.02454000
C	6.15291900	-3.71193700	-4.26585500
C	5.68138000	-3.87492400	-0.10584600
C	5.79113800	-4.59510200	4.01997700
C	5.82882300	-2.97068400	2.24232100
C	5.90042600	-1.90632100	3.18933300
C	5.91287100	-0.60632000	2.76373100
C	5.83985600	-1.37013200	0.42162900
C	5.87453900	-0.28865000	1.37624200
C	5.78226300	-2.72613100	0.88077300
C	5.87943300	-1.03888900	-0.93887900
C	5.87937300	1.03948700	0.93875100
C	5.83957200	1.37072400	-0.42175000
C	5.87432000	0.28924700	-1.37636700
C	5.91242500	0.60692300	-2.76386300
C	5.89970200	1.90692000	-3.18946600
C	5.82804300	2.97127100	-2.24244200
C	5.78170500	2.72671500	-0.88089100
C	5.78986200	4.59569400	-4.02008700
C	5.68077900	3.87549100	0.10573800
C	6.15250700	3.71247100	4.26572800
C	4.63332000	3.86187700	2.40015500
C	3.52416400	3.96594300	3.29046800
C	2.25876000	4.14029800	2.80092000
C	4.46800100	3.87780400	1.02448600
C	2.02132900	4.19218700	1.39802200
C	3.13781900	4.00647700	0.50073000
C	-2.31452200	5.64763100	-4.26686900
C	0.10312800	4.60576400	-3.27163500
C	1.32386900	4.23863300	-2.77731200
C	1.57427600	4.23919300	-1.37461700
C	2.85878000	3.99943800	-0.87342500
C	-0.93090400	5.03700100	-2.38599100
C	-0.77199400	5.00821800	-1.00945700
C	0.48746600	4.55901800	-0.47917600
C	0.74592200	4.48099000	0.89454000
C	-1.82073800	5.62751200	-0.09523500
H	-0.68783500	6.93821600	4.12779100
H	-2.35935600	6.44301400	4.51049500
H	-1.02774000	5.24865500	4.58974400
H	-3.04981900	4.27063400	4.24023300
H	-4.65002500	2.59390900	3.43861700
H	-5.83303300	1.54936700	1.61579200

H	-3.20406800	4.12005600	-1.70387400
H	-4.25670700	2.94690100	-3.52353300
H	-5.90092700	1.31375400	-4.32882900
H	-8.38815900	-1.24202900	-4.21453000
H	-8.01240800	0.45451200	-4.61986700
H	-6.71993200	-0.78414900	-4.65188700
H	-7.83836700	-0.65628300	-0.57994600
H	-7.83846600	0.65531700	0.57990500
H	-8.38838500	1.24112400	4.21442400
H	-8.01239900	-0.45534900	4.61982700
H	-6.72010000	0.78349600	4.65182300
H	-5.90078200	-1.31430800	4.32885000
H	-4.25631600	-2.94724000	3.52363000
H	-5.83284400	-1.55017700	-1.61575800
H	-3.20352100	-4.12034300	1.70402900
H	-4.64967900	-2.59461800	-3.43853500
H	-3.04924900	-4.27116600	-4.24007900
H	-0.68701000	-6.93850800	-4.12751800
H	-2.35857100	-6.44346200	-4.51023700
H	-1.02705500	-5.24899500	-4.58954800
H	-1.32959900	-6.41185400	-0.48628600
H	-2.56160700	-6.12399300	0.72674500
H	-3.30582000	-6.08464000	4.38852400
H	-1.56540400	-6.31509400	4.71024300
H	-2.28189600	-4.67573300	4.77700900
H	-0.06228900	-4.60960600	4.34191600
H	2.13010500	-3.96268600	3.45298000
H	-0.03090000	-4.71527400	-1.60691500
H	3.65869500	-3.85515100	1.58525800
H	1.41981100	-4.26421300	-3.48022300
H	3.68544700	-3.93631000	-4.36118400
H	7.23309900	-3.61052000	-4.37949400
H	5.82447500	-4.64385600	-4.74206100
H	5.65722800	-2.86070200	-4.75071600
H	6.57843800	-3.88909400	-0.72986200
H	5.68128600	-4.80995300	0.46014000
H	5.72792400	-5.68275400	4.07948300
H	6.72809200	-4.26139400	4.48288800
H	4.94347000	-4.15457700	4.56213900
H	5.93693500	-2.12481700	4.24963800
H	5.95574100	0.20611400	3.48459700
H	5.95007400	-1.81770300	-1.68593400
H	5.94997700	1.81831200	1.68579800
H	5.95534100	-0.20550700	-3.48473000

H	5.93602600	2.12542400	-4.24977500
H	5.72644200	5.68333500	-4.07958000
H	6.72683000	4.26216300	-4.48309700
H	4.94222000	4.15501800	-4.56216800
H	5.68058000	4.81052300	-0.46024300
H	6.57787000	3.88972700	0.72970600
H	7.23270200	3.61115000	4.37931700
H	5.82399700	4.64433700	4.74199200
H	5.65691700	2.86116600	4.75057000
H	3.68500700	3.93664800	4.36115900
H	1.41930800	4.26436200	3.48028300
H	-3.30666600	6.08473900	-4.38826200
H	-1.56626700	6.31526300	-4.71001100
H	-2.28270400	4.67588100	-4.77683800
H	-0.06307100	4.60983900	-4.34180200
H	2.12939100	3.96303300	-3.45295000
H	3.65805400	3.85557200	-1.58528100
H	-0.03150500	4.71533700	1.60703900
H	-1.33047800	6.41173800	0.48651900
H	-2.56247200	6.12376300	-0.72649700
C	0.22158500	0.68242700	-1.67156100
C	0.20011700	-0.74854300	-1.65655200
C	-1.16652600	-1.16922800	-1.65205500
C	-1.98994500	0.00034400	-1.66166100
C	-1.13159300	1.14466700	-1.67507400
C	0.20039600	0.74844500	1.65623700
C	-1.16624900	1.16913000	1.65198900
C	0.22186800	-0.68252400	1.67115600
C	-1.98966700	-0.00044200	1.66166100
C	-1.13131200	-1.14476400	1.67485200
Co	-0.77098300	-0.00000600	-0.00010000
H	1.09821200	1.31474700	-1.62175300
H	1.05761600	-1.40638700	-1.59767400
H	-1.51315800	-2.19071400	-1.58093200
H	-3.06983600	0.01543200	-1.60116300
H	-1.44713300	2.17748800	-1.61744800
H	1.05788100	1.40629900	1.59727500
H	-1.51289300	2.19062100	1.58102000
H	1.09847500	-1.31485500	1.62114700
H	-3.06956600	-0.01552800	1.60131000
H	-1.44687200	-2.17757600	1.61719100

The atomic coordinates of [**Fc**$^{+}$@**P5**]-II:

O	3.55297297	-5.65690654	2.74861690
O	6.65070480	1.67025736	2.81925687

O	0.45252443	6.66315766	2.76483734
O	-6.40672869	2.62375003	2.71330937
O	6.55901590	2.22443197	-2.70887192
O	-0.03430833	6.67553972	-2.75840441
O	-6.51274877	2.06025085	-2.81453148
O	4.00340853	-5.29219895	-2.77545001
O	-3.90863810	-5.44070043	-2.73227682
O	-4.34064503	-5.04830703	2.79104972
C	-4.06015751	-5.76714956	-4.09850115
C	-4.29820092	-4.20398229	-2.30018001
C	-4.61147041	-3.16249337	-3.22814108
C	-4.97629223	-1.93001088	-2.77725632
C	-4.33551065	-3.99505001	-0.93807097
C	-5.05063076	-1.65409773	-1.38104490
C	-4.73292249	-2.70265920	-0.45406110
C	-5.43282738	-0.39122444	-0.92387962
C	-4.83448961	-2.41268106	0.90952262
C	-5.49855369	-0.08971843	0.43982756
C	-5.19144648	-1.14215387	1.36677833
C	-5.90823181	1.19972545	0.92142305
C	-5.28934049	-0.87196959	2.76268079
C	-5.68297582	0.35211868	3.21072935
C	-6.00800580	1.38952890	2.28263815
C	-6.62331654	2.83113041	4.09274437
C	-6.31367101	2.29641300	-0.04656220
C	-6.82788154	2.13449742	-4.18923887
C	-5.39593013	2.70296011	-2.35712602
C	-5.23820581	2.80075041	-0.99206917
C	-4.41908371	3.21754661	-3.26528853
C	-3.31336344	3.85793538	-2.79459669
C	-3.10873542	4.02728592	-1.39352832
C	-4.07912740	3.48232345	-0.48574691
C	-3.86784368	3.68338645	0.88236772
C	-2.01233712	4.74906600	-0.91495884
C	-1.80405646	4.95526548	0.45253289
C	-2.76012575	4.38655545	1.36192087
C	-2.57384800	4.58814352	2.76136383
C	-1.52588947	5.32150288	3.22711688
C	-0.59990364	5.91692180	2.31469015
C	-0.71358243	5.74642237	0.95217601
C	0.50247910	7.02759510	4.12818504
C	0.20391895	6.49647720	0.00330738
C	-0.06055407	7.04157999	-4.12190219
C	0.97473531	5.87158438	-2.30734186

C	1.86506036	5.22417354	-3.21961914
C	1.07983592	5.69673147	-0.94468897
C	2.87022636	4.43316802	-2.75359717
C	3.04495478	4.22225546	-1.35404185
C	2.12433703	4.84617674	-0.44442025
C	2.32394755	4.63317442	0.92321200
C	4.10975182	3.45540384	-0.87490260
C	4.30925831	3.24242714	0.49310221
C	3.37652824	3.84864510	1.40158470
C	3.57541117	3.67287347	2.80262144
C	4.63980602	2.96593963	3.27297341
C	5.57778284	2.38497186	2.36395617
C	5.42260707	2.48860310	0.99908356
C	6.96456554	1.70943436	4.19548466
C	6.45664502	1.90458392	0.05288591
C	6.84808918	2.39118227	-4.08087840
C	6.07647239	1.02171351	-2.27505492
C	5.67190855	0.01119314	-3.20156427
C	5.19744711	-1.18299209	-2.75187681
C	5.47262448	-0.41817581	-0.42970531
C	5.09152454	-1.44722685	-1.35522555
C	5.96895839	0.83992081	-0.91342666
C	5.39116060	-0.71464374	0.93434659
C	4.65633361	-2.69271685	-0.89683572
C	4.54264660	-2.97684463	0.46706296
C	4.92858386	-1.95019829	1.39287053
C	4.84182082	-2.22150302	2.78936789
C	4.40129338	-3.42827624	3.24132220
C	4.01889204	-4.44754605	2.31470675
C	4.06623953	-4.24196416	0.95238086
C	3.68372876	-5.99025090	4.11525885
C	3.70195064	-5.35580754	-0.01140018
C	4.21978555	-5.55907018	-4.14641130
C	2.72459674	-5.14175085	-2.32223961
C	1.63210411	-5.00519539	-3.23427668
C	0.35675109	-4.89755772	-2.76846325
C	2.53821549	-5.10743008	-0.95634865
C	0.08913370	-4.89628095	-1.36757846
C	1.19711154	-4.96638487	-0.45533769
C	-4.57581761	-5.26769143	4.16714243
C	-1.95623482	-4.90351785	3.25189031
C	-0.67681125	-4.87253088	2.78634556
C	-0.40901112	-4.88496879	1.38554695
C	0.90437725	-4.94743719	0.91259664

C	-3.05480766	-4.97298266	2.33950682
C	-2.86622560	-4.94904636	0.97366295
C	-1.51916273	-4.88639449	0.47301782
C	-1.22557064	-4.88026071	-0.89474154
C	-4.04222935	-5.12759288	0.02808659
H	-3.80161178	-6.82251241	-4.18242391
H	-5.09318053	-5.61744743	-4.43169711
H	-3.38517421	-5.18008187	-4.73295629
H	-4.56550853	-3.35413945	-4.29347006
H	-5.22254590	-1.13683596	-3.47872557
H	-5.72434161	0.34714620	-1.66123451
H	-4.67202043	-3.18944289	1.64748464
H	-5.05741939	-1.66803124	3.46570243
H	-5.76122828	0.53413015	4.27583908
H	-6.99582557	3.85107924	4.18540173
H	-7.37009851	2.13473867	4.49001394
H	-5.69337029	2.73307554	4.66633198
H	-6.68513386	3.14448900	0.53530805
H	-7.15380573	1.93558594	-0.64665866
H	-7.80910571	1.67238424	-4.29599171
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The atomic coordinates of [**Cob**$^{+}$@**P5**]-II:

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O	-3.73562100	-5.58912700	-2.68395600
O	4.16136400	-5.10603400	-2.83043300
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