Electronic Supplementary Material (ESI) for Chemical Science

Photophysical and Theoretical Investigations of the [8]Cycloparaphenylene Radical Cation and its Charge-Resonance Dimer

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1) General Experimental Considerations

All glassware was oven dried and cooled under an inert atmosphere of N_2 before usage. Triethoxonium hexachloroantimonate was purchased from Sigma-Aldrich and stored at -30 ^oC in an MBraun glovebox filled with N_2. All other manipulations were performed under standard Schlenk technique under an N_2 atmosphere. [8]Cycloparaphenylene (**1**) and [12]Cycloparaphenylene were synthesized as described in the literature.[1,2] Dichloromethane and toluene were dried by filtration through alumina according to the methods described by Grubbs.[3] Anhydrous pentane was purchased from Sigma-Aldrich.

Optical spectra were recorded in screw-top quartz cuvettes using a Shimadzu UV-3600 UV-vis-NIR spectrophotometer under ambient conditions. Spectroelectrochemistry experiments were performed using a honeycomb spectroelectrochemical cell (Pine Instruments) connected to an AUTOLAB PGSTAT 10 potentiostat (Eco Chemie), using 0.1 M *n*-Bu_4NPF_6 in dichloromethane as solvent. UV-Vis spectra were recorded on a Cary 4000 spectrophotometer (Agilent) under ambient conditions with the electrochemical cell inserted into a quartz cuvette. Differential potential voltammetry experiments were performed on a Princeton Applied Research Potentiostat/Galvanastat Model 273 running M270/250 Electrochemical Software (Princeton Applied Research) with a glassy carbon working electrode, platinum counter electrode and silver wire reference electrode. Measurements were conducted in 0.1 M *n*-Bu_4NPF_6 in dichloromethane in an MBraun glovebox filled with N_2. Cyclic voltammetry experiments were performed using an CH Instruments 1200B potentiostat running CH Instruments software. Measurements were conducted in degassed 0.1 M *n*-Bu_4NPF_6 in dichloromethane under an N_2 atmosphere with a glassy carbon working electrode, platinum counter electrode and Ag/AgCl reference electrode. The ferrocene/ferrocenium couple was used as an internal reference for all electrochemical experiments. *n*-Bu_4NPF_6 was recrystallized from EtOH before use. X-band EPR spectra were recorded on a Bruker ELEXSYS-II E500 CW-EPR equipped with a cryo-cooled cavity using a flame-sealed capillary tube containing a dichloromethane solution of sample placed inside a quartz EPR tube. Spectra were collected with a 100 kHz modulation frequency and 1 G modulation amplitude.

Synthesis of $\mathbf{1}^{\cdot+}$

To a 20 mL glass vial with a septum screwcap and stirbar was added triethyloxonium hexachloroantimonate (24 mg, 0.054 mmol) in a glovebox. The vial was sealed, removed from the glovebox and placed under a stream of N_2. To the vial was then added dichloromethane (1 mL) and the gold solution was cooled to 0 ^oC. Then, a bright yellow dichloromethane solution (6 mL) of **1** (21 mg, 0.034 mmol) was added via cannula and the reaction mixture immediately darkened to brown/orange. The solution was stirred at 0 ^oC for 3 h, then cooled to – 50 ^oC whereupon anhydrous pentane (10 mL) was added to precipitate out a dark purple solid. The

solvent was removed via cannula under N_2 pressure and the solid was washed with an additional aliquot of pentane (10 mL). The solid was redissolved in dichloromethane (5 mL) and the process (precipitation then washing) was repeated two additional times (three times total). The dark purple solid was then washed with toluene (10 mL) and pentane (3 x 10 mL), then dried under vacuum to afford highly pure $\mathbf{1}^{\cdot+}$ (22 mg, 69%). UV-vis-NIR (CH_2Cl_2): 535 (ε = 0.81 (± 0.03) x 10^4 M^{-1} cm^{-1}), 1115 (ε = 1.03 (± 0.03) x 10^4 M^{-1} cm^{-1}) nm

2) Optoelectronic Characterization:

The binding constant, K_{dimer}, for $(\mathbf{1})_2^{\cdot+}$ was determined by gradually titrating a dichloromethane solution (8.2 x 10^{-3} M) of **1** into a cuvette containing a dichloromethane solution of $\mathbf{1}^{\cdot+}$ (1.0 x 10^{-4} M). After each aliquot of **1** was added, a spectrum was recorded, carefully noting the absorption at 1747 nm. From these data, a Benesi-Hildebrand plot was constructed (Figure 4 in main text). The data extracted from the plot is summarized below in Table S1 based on the Benesi-Hildebrand equation (Eq 1 in main text).

Table S1. Data extracted from UV-vis-NIR spectrum (Figure 3 in main text) used to construct a Benesi-Hildebrand plot (Figure 4 in main text)

Total Volume of **1** Added (μL)	1/[**1**]	$[\mathbf{1}^{\cdot+}]/A_{1747}$
39	18503.58423	8.5153E-5
44	16487.4552	8.14598E-5
49	13554.90388	7.2748E-5
54	12455.19713	7.07127E-5
59	11524.67604	6.72664E-5
69	10035.84229	6.25136E-5
74	9431.00358	5.96417E-5
79	8897.32237	5.79812E-5
89	7998.49085	5.65055E-5
99	7270.86534	5.40988E-5
109	6669.78339	5.2892E-5
119	6164.87455	5.10385E-5
129	5734.76703	4.99444E-5
149	5041.04521	4.82196E-5
169	4505.88838	4.71776E-5

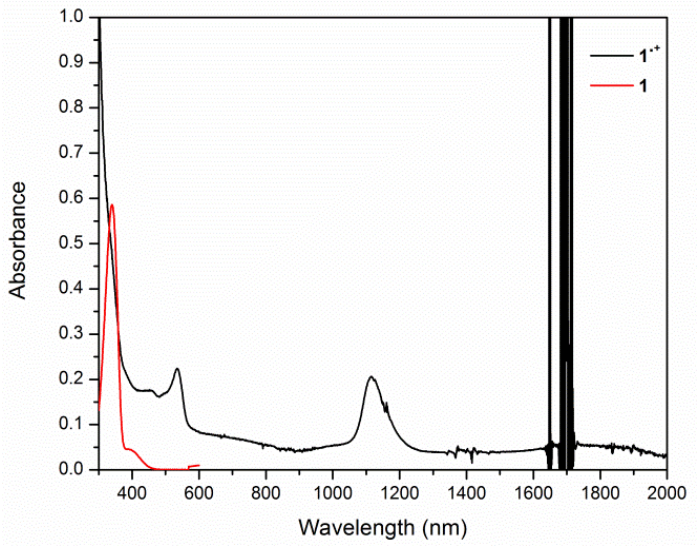

Figure S1. UV-vis-NIR spectrum of $\mathbf{1}^{\cdot+}$ (2.7×10^{-4} M) and **1** (6.4×10^{-6} M). The absence of an absorption at 340 nm and a CR band in the NIR confirms the purity of $\mathbf{1}^{\cdot+}$.

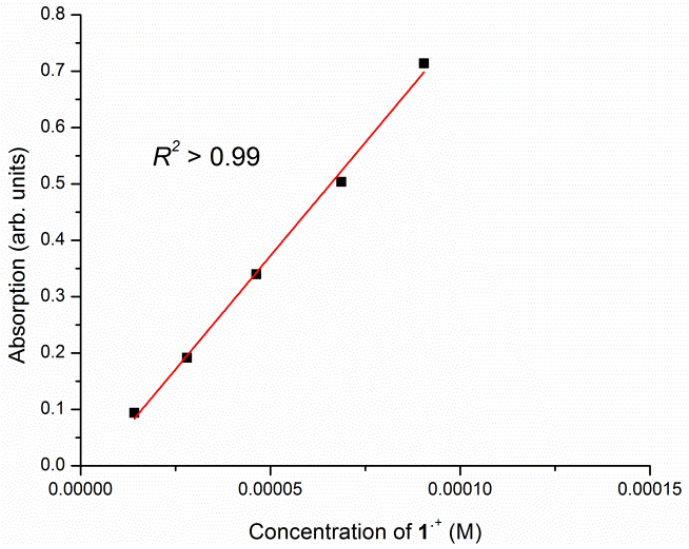

Figure S2. Beer-Lambert plot of $\mathbf{1}^{\cdot+}$ at 535 nm ($\varepsilon = 0.81\ (\pm 0.03) \times 10^4\ M^{-1}\ cm^{-1}$)

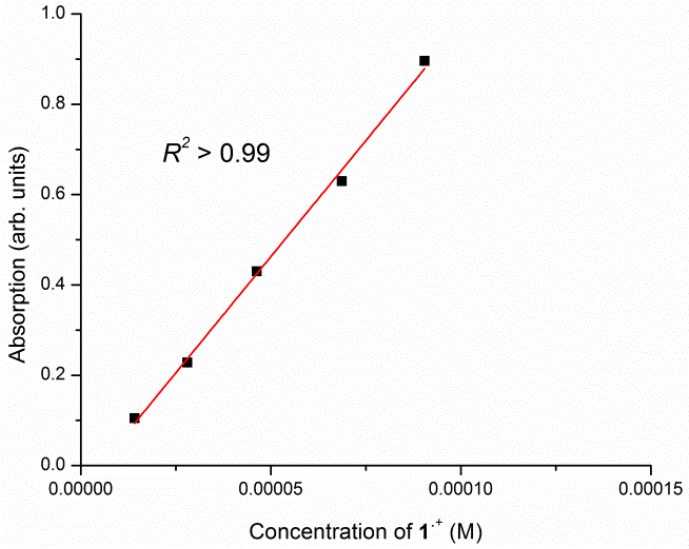

Figure S3. Beer-Lambert plot of $\mathbf{1}^{\cdot+}$ at 1115 nm (ε = 1.03 (± 0.03) x 10^4 M^{-1} cm^{-1}).

Cyclic voltammetry of **1** (1 x 10^{-3} M) was performed at increasing scan rates (25 mV/s → 700 mV/s). At a scan rate of 50 mV/s, $E^{ox}_{1/2}$ = 0.68 V (vs. Fc/Fc^+). The addition of 1 equivalent of ferrocene revealed nearly identical integrated oxidation peak areas for the two species, confirming that **1** is oxidized to $\mathbf{1}^{\cdot+}$ via a one-electron process.

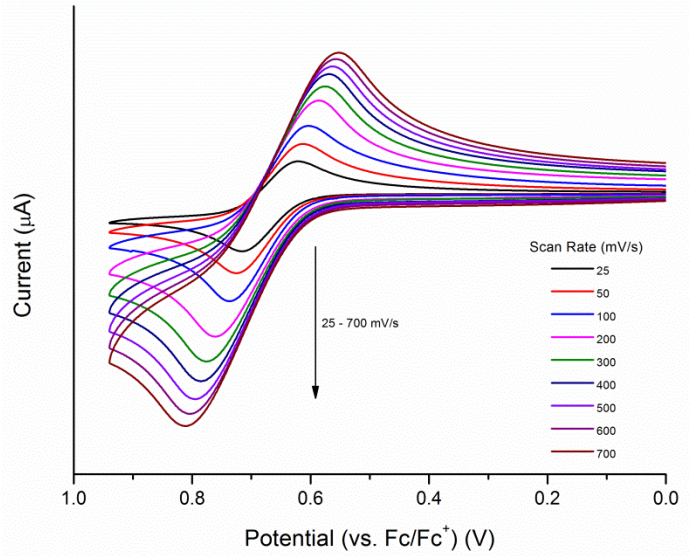

Figure S4. Cyclic voltammograms of **1** (1 x 10^{-3} M) at increasing scan rates (25 mV/s → 700 mV/s) (0.1 M *n*-Bu_4PF_6 in CH_2Cl_2)

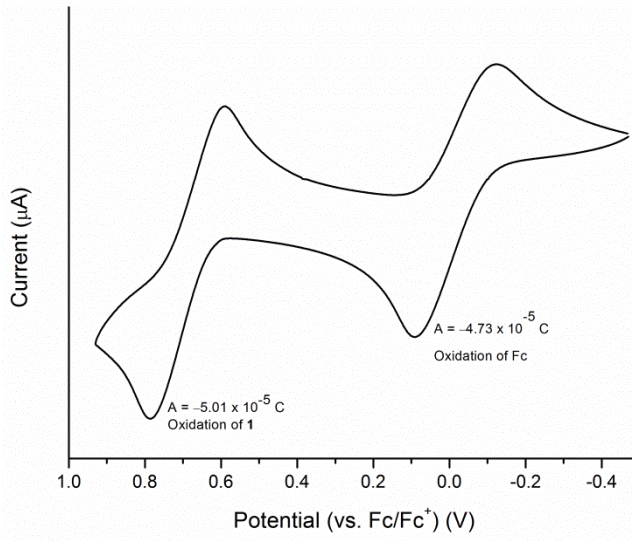

Figure S5. Cyclic voltammogram of **1** (1 x 10^{-3} M) containing 1 equivalent of ferrocene (0.1 M *n*-Bu_4PF_6 in CH_2Cl_2, scan rate = 50 mV/s). $A_{\mathbf{1}}$ / A_{Fc} = 1.06.

Differential potential voltammetry was used to achieve maximum sensitivity in current changes and confirmed that the single wave in the cyclic voltammogram corresponds to a single electron oxidation process.

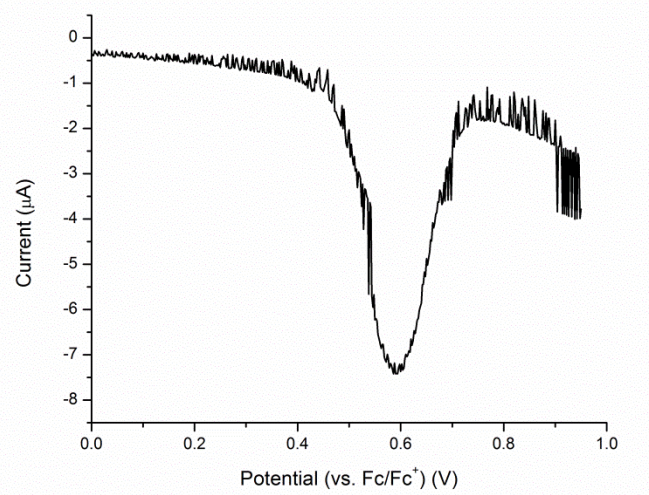

Figure S6. Differential pulse voltammogram of radical cation $\mathbf{1}^{\bullet+}$ (0.1 M *n*-Bu_4PF_6 in CH_2Cl_2) (pulse height = 25 mV, scan increment = 2 mV)

Spectroelectrochemistry experiments were performed in order to probe the behavior of neutral **1** close to its oxidation potential. Thus, based on the cyclic voltammogram (Figure S4), a constant potential of 0.8 V was applied for minutes 0 – 8. The potential was then increased to 0.9 V for another two minutes (minutes 8 – 10). At each time point, a UV-vis spectrum was recorded, showing a gradual increase in absorption at 535 nm (radical cation $\mathbf{1}^{\bullet+}$) and a gradual decrease in absorption at 340 nm (neutral **1**). An isosbestic point was also observed at 368 nm, suggesting direct oxidation from **1** to radical cation $\mathbf{1}^{\bullet+}$.

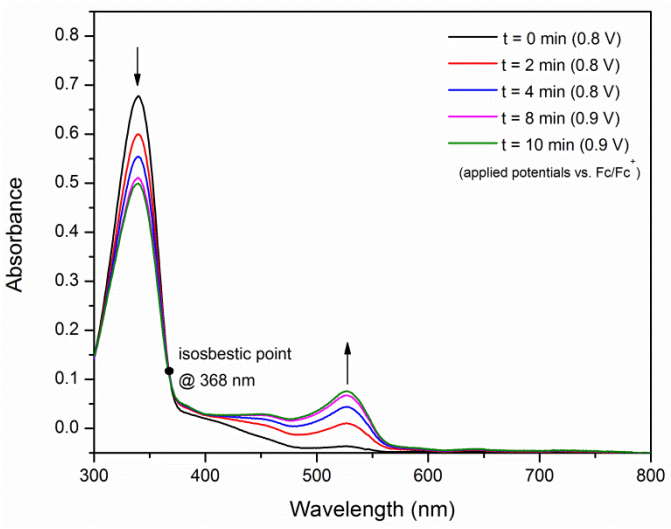

Figure S7. UV-vis spectrum (in CH_2Cl_2) depicting the gradual oxidation over time of neutral **1** to radical cation $\mathbf{1}^{\bullet+}$ with an applied potential. Applied potentials are all relative to the Fc/Fc^+ couple for consistency when referring to cyclic voltammogram (Figure S4)

3) EPR Spectra:

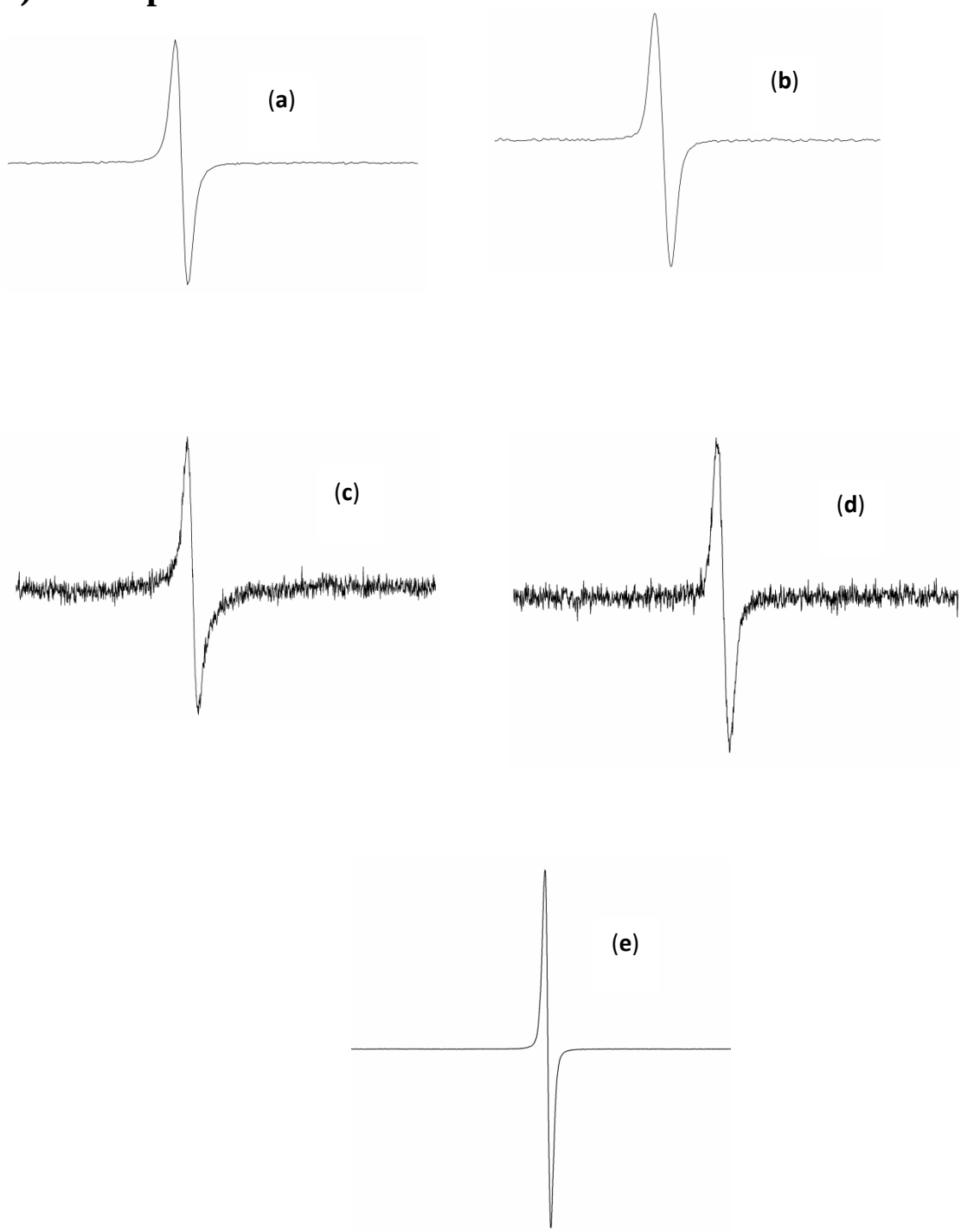

Figure S8. X-band EPR spectra of $\mathbf{1}^{\cdot+}$ (10^{-3} M) recorded at: (a) 293 K. (b) 167 K. (c) 8 K. (d) 8 K (10^{-5} M) (e) 293 K (after 5 equiv oxidant)

Table S2. Parameters associated with the five EPR spectra of $\mathbf{1}^{\cdot+}$ shown in Figure S4

	a	**b**	**c**	**d**	**e**
Frequency (GHz)	9.389310	9.388179	9.389615	9.389778	9.867088
g	2.007	2.006	2.007	2.008	2.007

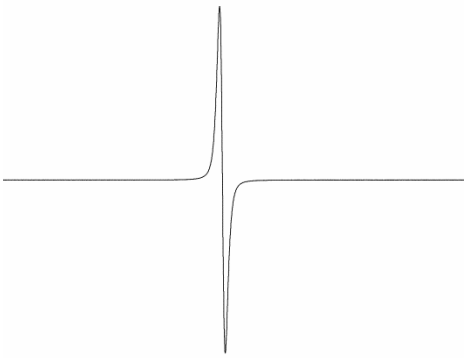

Figure S9. X-band EPR spectrum of charge-resonance dimer $(\mathbf{1})_2^{\cdot+}$ in CH_2Cl_2 after the completion of titration experiments (Frequency = 9.389929 GHz, g = 2.007 G)

Figure S10. Control X-band EPR spectra (CH_2Cl_2) of (a) triethyloxonium hexachloroantimonate and (b) [8]Cycloparaphenylene **1** from 3000 – 4000 G. The absence of signal confirms that the experimentally observed signals come from $\mathbf{1}^{\cdot+}$ and $(\mathbf{1})_2^{\cdot+}$.

4) Oxidation of [12]CPP

To a 20 mL glass vial with a septum screwcap and stirbar was added triethyloxonium hexachloroantimonate (240 mg, 0.55 mmol) in a glovebox. The vial was sealed, removed from the glovebox and placed under a stream of N_2. To the vial was then added dichloromethane (2 mL) and the gold solution was cooled to 0 ^{o}C. Then, a dichloromethane solution (5 mL) of [12]CPP (25 mg, 0.027 mmol) was added via cannula and the reaction mixture immediately darkened to dark blue. The solution was stirred at 0 ^{o}C for 3 h, then warmed to room temperature for another 14 h. The solution was then cooled to –50 ^{o}C whereupon anhydrous pentane (10 mL) was added to precipitate out a dark blue solid. The solvent was removed via cannula under N_2 pressure and the solid was washed with an addition aliquot of pentane (10 mL). The solid was redissolved in dichloromethane (5 mL) and the process (precipitation then washing) was repeated two additional times (three times total). The dark purple solid was then washed with toluene (2 x 10 mL) and pentane (3 x 10 mL), then dried under vacuum to afford 33 mg of a dark blue solid. The compound is EPR active (g = 2.006) and has a broad absorption in the near-IR region, which is reminiscent of a charge-resonance dimer.

The dark blue solid was dissolved to a final concentration of 0.78 mg/mL in CH_2Cl_2. To 2.4 mL of this solution was added 0.15 mL of neutral [12]CPP (1.9 mM in CH_2Cl_2) in three separate aliquots (3 x 0.05 mL). A UV-vis-NIR spectrum was recorded after each increment. Figure S11 shows bands increasing in intensity at 585 nm and beyond 2000 nm in the NIR.

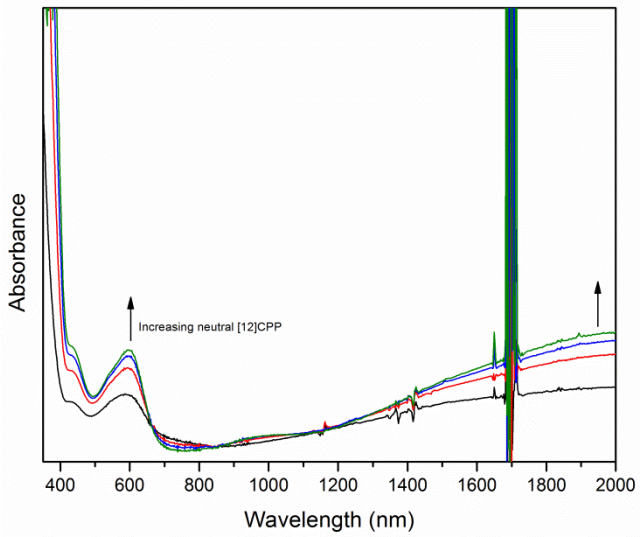

Figure S11. UV-vis-NIR spectra after the oxidation of [12]CPP (with increasing concentrations of neutral [12]CPP added)

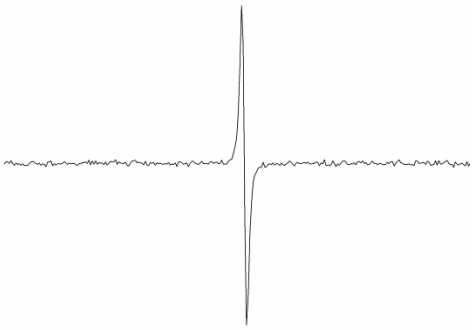

Figure S12. X-band EPR spectrum of $([12]CPP)_2^{\bullet+}$ after optical titration experiments (CH_2Cl_2) (Frequency = 9.857404 GHz, g = 2.006)

5) Computational Details:

All calculations were carried out with the Gaussian 09 package.[4] Calculations performed on **1** and $\mathbf{1}^{\cdot+}$ used the B3LYP exchange-correlation functional[5] and a polarized 6-31G(d,p) basis set[6] using default SCF convergence criteria (density matrix converged to at least 10^{-8}) and the default DFT integration grid (75 radial and 302 angular quadrature points). Calculations performed on the four [*n*]CPP charge-resonance dimers used the long-range corrected hybrid ωB97x functional[7] with an empirical dispersion term (ωB97xD).[8] Calculations performed on the hypothetical $\mathbf{1}^{2+}$ dication species were performed at the RB3LYP/6-31G(d) level of theory (closed-shell singlet) or UB3LYP/6-31G(d) level of theory (open-shell singlet and triplet). All excited state calculations (TD-DFT) were performed on fully optimized structures. The fully optimized structures were confirmed to be true minima by vibrational analysis.

Figure S13. Spin density distribution of $\mathbf{1}^{\cdot+}$ calculated at the UB3LYP/6-31G(d,p) level of theory showing complete delocalization of positive spin (blue).

Table S3. Predicted absorptions of radical cation $\mathbf{1}^{\cdot+}$ via TD-DFT calculations (UB3LYP/6-31G(d,p))

Energy (cm^{-1})	Wavelength (nm)	Osc. Strength	Major contributions
7071.11152	1414.204821	0.2601	H (B)→L (B) (100%)
7071.11152	1414.204821	0.2601	H-1(B)→L (B) (100%)
14679.392	681.2271244	0	H-2(B)→L (B) (97%)
14681.81168	681.1148527	0	H-3(B)→L (B) (97%)
15085.89824	662.8707049	0	H-4(B)→L (B) (99%)
15508.53568	644.8062026	0.0021	H-5(B)→L (B) (99%)
15508.53568	644.8062026	0.0021	H-6(B)→L (B) (99%)
16478.82736	606.8392964	0	H-7(B)→ L (B) (98%)
16480.44048	606.7798984	0	H-8(B)→L (B) (98%)
17091.81296	585.0754407	0	H-9(B)→L (B) (99%)
17091.81296	585.0754407	0	H-10(B)→L (B) (99%)
17423.30912	573.9437859	0	H-11(B)→L (B) (99%)

Table S4. Predicted absorptions of charge-resonance dimer $(\mathbf{1})_2^{\cdot+}$ via TD-DFT calculations (UωB97xD /6-31G(d,p))

Energy (cm^{-1})	Wavelength (nm)	Osc. Strength	Major contributions
6035.48848	1656.86672	0.3842	H-3(B)→L (B) (29%), H-1(B) →L(B) (24%), H(B) →L(B) (39%)
8745.53008	1143.441268	0.2844	H-14(B) →L(B) (10%), H-4(B) →L(B) (75%)
11524.93584	867.6837892	0.1009	H-1(B) →L(B) (63%), H(B) →L(B) (18%)
11925.79616	838.5184407	0.009	H-2(B) →L(B) (79%)
12743.648	784.7046623	0.0113	H-3(B) →L(B) (47%), H(B) →L(B) (42%)
16678.85424	599.561568	0.002	H-22(B) →L(B) (12%), H-20(B) →L(B) (68%)
18579.1096	538.2389262	0.0003	H-27(B) →L(B) (82%)
19057.39968	524.7305597	0.0156	H-15(B) →L(B) (11%), H-13(B) →L(B) (14%), H-9(B) →L(B) (10%), H-6(B) →L(B) (22%), H-1(B) →L(B) (11%)
19346.95472	516.8772112	0.0002	H-14(B) →L(B) (28%), H-4(B) →L(B) (11%)
19914.77296	502.1397944	0.1406	H-5(A) →L(A) (20%), H-1(A) →L(A) (21%)
20626.15888	484.8212437	0.0029	H-13(B) →L(B) (11%), H-6(B) →L(B) (14%)

Theoretical Study of [n]CPP Charge-Resonance Dimer Binding Energies

For each value of "*n*", the geometries of the neutral monomer ([*n*]CPP) and radical cation monomer $([n]CPP)^{\cdot+}$ were minimized. The energy of the charge-resonance complex was then minimized using the same level of theory. The binding energy was calculated by subtracting the sum of the energies of the two monomers from the energy of the charge-resonance dimer.

Table S5. Energies (in Hartress) of the components making up four charge-resonance [*n*]cycloparaphenylene dimers ($([n]CPP)_2^{\cdot+}$) (*n* = 6, 8, 10, 12). Calculations were done at the UωB97xD/6-31G(d,p) level of theory.

n	Neutral Monomer	Radical Cation Monomer	Charge-Resonance Dimer	Binding Energy
6	-1385.75873228	-1385.51883903	-2771.29690059	-0.01932928
8	-1847.76942719	-1847.52228711	-3695.31447870	-0.0227644
10	-2309.76555675	-2309.50991553	-4619.30549827	-0.03002599
12	-2771.75393372	-2771.49492278	-5543.28222063	-0.03336413

Theoretical Investigations of a $\mathbf{1}^{2+}$ Dication

In order to probe the predicted absorption spectrum of the $\mathbf{1}^{2+}$ dication (arising from an oxidation of the radical cation $\mathbf{1}^{\cdot+}$ or over-oxidation of neutral **1**), the ground-state energies of the closed-shell singlet (R), open-shell singlet (U) and triplet (T) were calculated. It was found that the ground-state energies of the closed-shell singlet and the open-shell singlet are nearly equal and have predicted absorptions at 922 nm, which are inconsistent with the experimentally determined values from the oxidation of **1** (H = HOMO, L = LUMO).

Table S6. Difference in ground-state energies between the three configurations of $\mathbf{1}^{2+}$

	Energy (kcal/mol)
ΔU-R	0.01
ΔT-R	7.49
ΔT-U	7.50

Table S7. Predicted absorptions for $\mathbf{1}^{2+}$ (closed-shell singlet) via TD-DFT calculations (RB3LYP/6-31G(d))

Energy (cm^{-1})	**Wavelength (nm)**	**Osc. Strength**	**Major contributions**
10839.35984	922.5637074	0.4944	H→L (100%)
10840.1664	922.4950643	0.4943	H-1→L (100%)
16681.27392	599.4745994	0	H-4→L (100%)
17183.7608	581.9447859	0.0009	H-5→L (100%)
17184.56736	581.9174723	0.0009	H-6→L (100%)
18024.19632	554.8097581	0	H-7→L (53%), H-3→L (43%)
18024.19632	554.8097581	0	H-8→L (53%), H-2→L (43%)
18629.11632	536.7941146	0	H-8→L (40%), H-2→L (48%)
18630.72944	536.7476369	0	H-7→L (40%), H-3→L (48%)
19192.0952	521.0478531	0	H-9→L (100%)
19192.90176	521.0259566	0	H-10→L (100%)
19568.75872	511.0186161	0	H-11→L (100%)

Table S8. Predicted absorptions for $\mathbf{1}^{2+}$ (open-shell singlet) via TD-DFT calculations (UB3LYP/6-31G(d))

Energy (cm-1)	Wavelength (nm)	Osc. Strength	Major contributions
1829.27808	5466.637418	0	H (A)→L (A) (70%), H (B)→L (B) (70%)
1835.73056	5447.422524	0	H-1(A)→L (A) (70%), H-1(B)→L (B) (70%)
10840.1664	922.4950643	0.4941	H (A)→L (A) (50%), H (B)→L (B) (50%)
10840.97296	922.4264314	0.4938	H-1(A)→L (A) (50%), H-1(B)→L (B) (50%)
13816.3728	723.7789646	0	H-2(A)→L (A) (49%), H-2(B)→L (B) (49%)
13817.98592	723.6944702	0	H-3(A)→L (A) (49%), H-3(B)→L (B) (49%)
15164.13456	659.450756	0	H-4(A)→L (A) (49%), H-4(B)→L (B) (49%)
15681.13952	637.7087575	0	H-5(A)→L (A) (49%), H-5(B)→L (B) (49%)
15681.94608	637.6759586	0	H-6(A)→L (A) (49%), H-6(B)→L (B) (49%)
16683.6936	599.387656	0	H-4(A)→L (A) (50%), H-4(B)→L (B) (50%)
16811.13008	594.8440083	0	H-7(A)→L (A) (49%), H-7(B)→L (B) (49%)
16815.96944	594.6728219	0	H-8(A)→L (A) (49%), H-8(B)→L (B) (49%)

Table S9. Predicted absorptions for $\mathbf{1}^{2+}$ (triplet) via TD-DFT calculations (UB3LYP/6-31G(d))

Energy (cm-1)	Wavelength (nm)	Osc. Strength	Major contributions
2467.26704	4053.067559	0	H (B)→L (B) (99%)
9318.18768	1073.170057	0.1331	H (B)→L+1(B) (91%)
12169.37728	821.7347338	0.2469	H-2(B)→L (B) (13%), H-1(B)→L (B) (71%)
12183.89536	820.7555716	0.2184	H-2(B)→L (B) (80%), H-1(B)→L (B) (11%)
12465.3848	802.2215247	0.0133	H-7(B)→L (B) (11%), H-3(B)→L (B) (77%)
12757.35952	783.8612672	0	H-4(B)→L (B) (94%)
12876.7304	776.5946548	0.0001	H-8(B)→L (B) (22%), H-5(B)→L (B) (64%)
13574.4048	736.6805504	0.018	H-6(B)→L (B) (86%)
13900.25504	719.4112605	0.0088	H-8(B)→L+1(B) (11%), H-7(B)→L (B) (73%), H-3(B)→L (B) (14%)
14180.13136	705.2120849	0.0025	H-8(B)→L (B) (62%), H-5(B)→L (B) (26%)
15097.99664	662.3395301	0	H-10(B)→L+1(B) (14%), H-9(B)→L (B) (81%)
15194.78384	658.120583	0.0003	H-10(B)→L (B) (81%), H-9(B)→L+1(B) (14%)

Coordinates of $1^{\bullet+}$: UB3LYP/6-31G(d,p)

C	-2.63949	5.1527	1.10742
C	1.67892	5.00211	1.24213
C	5.15281	2.63945	1.10742
C	5.00228	-1.67894	1.24206
C	2.63948	-5.15266	1.1074
C	-1.67894	-5.00223	1.24215
C	-5.15273	-2.6394	1.10747
C	-5.0024	1.67897	1.24204
C	-3.78768	4.37931	1.10736
C	0.31936	5.2659	1.24202
C	4.37938	3.78761	1.1074
C	5.26606	-0.31937	1.24197
C	3.78768	-4.37929	1.10736
C	-0.31937	-5.26599	1.24202
C	-4.37932	-3.78756	1.10747
C	-5.2662	0.31941	1.24195
C	-0.37467	5.53157	0.04052
C	3.64735	4.17756	-0.04061
C	5.53172	0.37468	0.04048
C	4.17767	-3.64732	-0.04068
C	0.37468	-5.53155	0.0405
C	-3.64736	-4.17759	-0.04057
C	-5.5317	-0.37468	0.04045
C	-4.17763	3.64732	-0.04068
C	-1.81467	5.23916	-0.04063
C	2.42206	4.98856	0.0406
C	5.2393	1.81467	-0.04065
C	4.98869	-2.42206	0.04051
C	1.81468	-5.23913	-0.04066
C	-2.42208	-4.98857	0.04062
C	-5.23927	-1.81466	-0.04064
C	-4.98866	2.42206	0.04049
C	-2.35104	4.72512	-1.2423
C	1.7777	5.51172	-1.10693
C	4.72518	2.35104	-1.24229
C	5.51181	-1.77768	-1.10703
C	2.35107	-4.7251	-1.24232
C	-1.7777	-5.51164	-1.10696
C	-4.72529	-2.35113	-1.24229
C	-5.5117	1.77766	-1.1071
C	-3.49974	3.95138	-1.24235
C	0.41866	5.77552	-1.10699
C	3.95141	3.49972	-1.2423
C	3.49979	-3.95138	-1.24236
C	-0.41867	-5.77543	-1.10704
C	-3.95152	-3.49982	-1.24228
C	-5.77551	0.41863	-1.10713
H	-2.34094	5.64703	2.02684
H	2.13532	4.65633	2.16337
H	5.64717	2.3409	2.02683
H	4.65654	-2.13536	2.16331
H	2.34094	-5.64699	2.02683
H	-2.13533	-4.65654	2.16342
H	-5.64704	-2.34079	2.02689
H	-4.65675	2.13539	2.16332
H	-4.35804	4.28825	2.02672
H	-0.23354	5.11564	2.16302
H	4.28834	4.35795	2.02679
H	5.11587	0.23351	2.16298
H	4.35801	-4.28822	2.02674
H	0.2335	-5.11582	2.16303

H	-4.28822	-4.35784	2.02689
H	-5.11608	-0.23344	2.163
H	-1.78439	4.80368	-2.16385
H	2.33854	5.65181	-2.026
H	4.80373	1.78443	-2.16386
H	5.65189	-2.33849	-2.0261
H	1.78446	-4.80367	-2.16388
H	-2.33853	-5.65167	-2.02603
H	-4.80393	-1.78459	-2.1639
H	-5.65168	2.33847	-2.02619
H	-3.78531	3.45568	-2.16389
H	-0.04905	6.11536	-2.02602
H	3.45566	3.7853	-2.16381
H	3.78538	-3.45567	-2.16389
H	0.04905	-6.11519	-2.02609
H	-3.45588	-3.78547	-2.16383
H	-6.11525	-0.04911	-2.02618
C	5.77562	-0.41864	-1.10706
H	6.11546	0.04906	-2.02609

Coordinates of 1: RB3LYP/6-31G(d,p)

C	-6.75839	-1.44631	-1.08319
C	-4.67859	-3.67239	2.02036
C	-0.49033	-4.30774	3.07342
C	3.34601	-3.01144	1.44092
C	4.5658	-0.43411	-1.87238
C	2.46779	1.75016	-5.02648
C	-1.72175	2.41486	-6.0155
C	-5.49695	1.03655	-4.46379
C	-6.74075	-0.66843	-2.23767
C	-5.66764	-3.09752	1.18228
C	-1.906	-4.33088	3.03272
C	2.32955	-3.60687	2.21839
C	4.53638	-1.2643	-0.74547
C	3.46172	1.15493	-4.20431
C	-0.27794	2.44069	-5.96868
C	-4.49276	1.67392	-5.17605
C	-6.00955	-1.73511	1.39039
C	-2.61052	-3.20895	3.5439
C	1.63795	-2.79005	3.16675
C	4.28088	-0.67691	0.52277
C	3.74887	1.74863	-2.96937
C	0.32733	3.24438	-5.09884
C	-3.90279	2.85866	-4.68981
C	-6.53653	0.8431	-2.02036
C	-6.60093	-0.87012	0.17192
C	-4.08528	-2.8734	3.00505
C	0.15002	-3.1747	3.61589
C	3.63504	-1.63526	1.63838
C	4.34063	0.95948	-1.69209
C	1.82142	2.91173	-4.5563
C	-2.40299	3.23113	-5.15148
C	-5.91186	1.69907	-3.13777
C	-6.8524	0.5207	0.36046
C	-4.73874	-1.6917	3.45306
C	-0.55506	-2.30394	4.47923
C	3.23902	-1.0026	2.84522
C	4.52533	1.54135	-0.43221
C	2.43191	3.69747	-3.54057
C	-1.7632	4.36041	-4.55538
C	-5.59864	3.03935	-2.95962
C	-6.8246	1.35631	-0.76248
C	-5.71813	-1.11878	2.63296
C	-1.97444	-2.32379	4.44235
C	2.23332	-1.5827	3.60952
C	4.49252	0.70433	0.71121
C	3.40495	3.11229	-2.7388
C	-0.35369	4.37276	-4.52012
C	-4.58005	3.6452	-3.72351
H	-6.86041	-2.50598	-1.19195
H	-4.36885	-4.68606	1.87586
H	0.0788	-5.11751	2.66821
H	3.86171	-3.57808	0.69487
H	4.73413	-0.83907	-2.84789
H	2.19121	1.30869	-5.96112
H	-2.24578	1.75635	-6.67551
H	-5.94439	0.11758	-4.78066
H	-6.82373	-1.07528	-3.22415
H	-6.11804	-3.66161	0.39252
H	-2.42995	-5.15541	2.59588
H	2.05934	-4.63233	2.07793
H	4.68151	-2.32038	-0.83742

H	3.9513	0.25363	-4.50812
H	0.29005	1.79305	-6.60295
H	-4.15188	1.22572	-6.08556
H	-7.03889	0.91901	1.33597
H	-4.47345	-1.24059	4.38629
H	-0.0335	-1.63288	5.12892
H	3.69484	-0.08226	3.14556
H	4.65183	2.59902	-0.32933
H	2.13105	4.71242	-3.38587
H	-2.32925	5.1647	-4.1335
H	-6.12204	3.59209	-2.20716
H	-6.98945	2.40945	-0.6674
H	-6.222	-0.22123	2.92548
H	-2.5477	-1.66808	5.06389
H	4.58975	1.11449	1.69434
H	3.87237	3.66646	-1.95161
H	0.176	5.18538	-4.06894
H	-4.30999	4.66804	-3.56445
H	1.89096	-1.11671	4.50982

Coordinates of [6]CPP: UωB97xD/6-31G(d,p)

C	3.51611	1.13415	-1.26581
C	4.10051	1.43878	1.03308
C	2.87595	2.36804	-1.26753
H	3.45786	0.52741	-2.16341
C	3.45905	2.67505	1.03139
H	4.58089	1.10068	1.94704
C	2.69204	3.09374	-0.0757
H	2.34745	2.6681	-2.16635
H	3.45798	3.26426	1.94426
C	3.95438	-1.78869	-1.03544
C	3.3972	-1.43187	1.26278
C	3.20424	-2.96221	-1.03406
H	4.46373	-1.49537	-1.9492
C	2.64894	-2.60317	1.26426
H	3.39255	-0.82155	2.15986
C	2.40248	-3.31061	0.07276
H	3.15029	-3.54876	-1.94705
H	2.09475	-2.8542	2.16263
C	1.08565	-3.99345	-0.06749
C	0.33843	-4.44705	1.03937
C	0.36605	-3.78858	-1.25955
C	-1.05291	-4.38385	1.04002
H	0.8484	-4.74023	1.95285
C	-1.02246	-3.7255	-1.25885
H	0.89092	-3.48078	-2.15787
C	-1.75679	-3.86458	-0.06632
H	-1.58655	-4.63	1.95387
H	-1.51812	-3.37094	-2.15647
C	-3.0073	-3.067	0.07398
C	-3.77441	-2.64837	-1.03304
C	-3.19104	-2.34125	1.26581
C	-4.41589	-1.4121	-1.0347
H	-3.77344	-3.23761	-1.94589
C	-3.83117	-1.10735	1.2641
H	-2.66242	-2.6413	2.16456
C	-4.31783	-0.54165	0.07079
H	-4.89638	-1.07401	-1.94863
H	-3.77281	-0.50055	2.16165
C	-4.2499	0.93974	-0.07166
C	-4.26973	1.81547	1.0337
C	-3.7123	1.45848	-1.26445
C	-3.51957	2.98899	1.0323
H	-4.77916	1.52219	1.94743
C	-2.96406	2.62979	-1.26595
H	-3.70759	0.84807	-2.16147
C	-2.71775	3.33732	-0.07447
H	-3.46568	3.5756	1.94525
H	-2.40977	2.88078	-2.16427
C	-1.40092	4.02019	0.06575
C	-0.65372	4.47376	-1.04112
C	-0.68131	3.81529	1.2578
C	0.73763	4.41054	-1.04177
H	-1.16369	4.76693	-1.95461
C	0.70719	3.75222	1.25711
H	-1.2062	3.50749	2.15613
C	1.44151	3.89128	0.06457
H	1.27127	4.65668	-1.95563
H	1.20285	3.39768	2.15474
C	3.93465	-0.91301	0.06998
C	4.00258	0.56837	-0.07247

Coordinates of $([6]CPP)^{\cdot+}$: UωB97xD/6-31G(d,p)

C	3.51611	1.13415	-1.26581
C	4.10051	1.43878	1.03308
C	2.87595	2.36804	-1.26753
H	3.45786	0.52741	-2.16341
C	3.45905	2.67505	1.03139
H	4.58089	1.10068	1.94704
C	2.69204	3.09374	-0.0757
H	2.34745	2.6681	-2.16635
H	3.45798	3.26426	1.94426
C	3.95438	-1.78869	-1.03544
C	3.3972	-1.43187	1.26278
C	3.20424	-2.96221	-1.03406
H	4.46373	-1.49537	-1.9492
C	2.64894	-2.60317	1.26426
H	3.39255	-0.82155	2.15986
C	2.40248	-3.31061	0.07276
H	3.15029	-3.54876	-1.94705
H	2.09475	-2.8542	2.16263
C	1.08565	-3.99345	-0.06749
C	0.33843	-4.44705	1.03937
C	0.36605	-3.78858	-1.25955
C	-1.05291	-4.38385	1.04002
H	0.8484	-4.74023	1.95285
C	-1.02246	-3.7255	-1.25885
H	0.89092	-3.48078	-2.15787
C	-1.75679	-3.86458	-0.06632
H	-1.58655	-4.63	1.95387
H	-1.51812	-3.37094	-2.15647
C	-3.0073	-3.067	0.07398
C	-3.77441	-2.64837	-1.03304
C	-3.19104	-2.34125	1.26581
C	-4.41589	-1.4121	-1.0347
H	-3.77344	-3.23761	-1.94589
C	-3.83117	-1.10735	1.2641
H	-2.66242	-2.6413	2.16456
C	-4.31783	-0.54165	0.07079
H	-4.89638	-1.07401	-1.94863
H	-3.77281	-0.50055	2.16165
C	-4.2499	0.93974	-0.07166
C	-4.26973	1.81547	1.0337
C	-3.7123	1.45848	-1.26445
C	-3.51957	2.98899	1.0323
H	-4.77916	1.52219	1.94743
C	-2.96406	2.62979	-1.26595
H	-3.70759	0.84807	-2.16147
C	-2.71775	3.33732	-0.07447
H	-3.46568	3.5756	1.94525
H	-2.40977	2.88078	-2.16427
C	-1.40092	4.02019	0.06575
C	-0.65372	4.47376	-1.04112
C	-0.68131	3.81529	1.2578
C	0.73763	4.41054	-1.04177
H	-1.16369	4.76693	-1.95461
C	0.70719	3.75222	1.25711
H	-1.2062	3.50749	2.15613
C	1.44151	3.89128	0.06457
H	1.27127	4.65668	-1.95563
H	1.20285	3.39768	2.15474
C	3.93465	-0.91301	0.06998
C	4.00258	0.56837	-0.07247

Coordinates of $([6]CPP)_2^{\cdot+}$: UωB97xD/6-31G(d,p)

C	2.54687	2.48139	0.67907
C	1.33576	3.8924	2.18289
C	2.09226	3.23579	-0.39634
H	3.1411	1.59836	0.46846
C	0.8802	4.64824	1.10539
H	1.03084	4.1763	3.1863
C	1.11852	4.23706	-0.22254
H	2.35251	2.90728	-1.39713
H	0.23324	5.49905	1.3005
C	2.70081	0.34977	2.73349
C	0.68209	1.34215	3.54561
C	2.17152	-0.91689	2.96859
H	3.70618	0.42904	2.32929
C	0.15406	0.07811	3.7806
H	0.0437	2.20251	3.71743
C	0.82293	-1.08191	3.34717
H	2.77962	-1.78779	2.74001
H	-0.87227	0.00929	4.12574
C	-0.00848	-2.23136	2.89166
C	-1.31826	-2.46075	3.36184
C	0.32389	-2.83324	1.66362
C	-2.3036	-2.97072	2.51989
H	-1.602	-2.12818	4.3565
C	-0.65947	-3.34213	0.82341
H	1.32932	-2.72959	1.26914
C	-2.02135	-3.27346	1.17165
H	-3.32633	-3.02101	2.88317
H	-0.37694	-3.61212	-0.18872
C	-3.0073	-3.067	0.07398
C	-2.7691	-3.47824	-1.25394
C	-3.98092	-2.06563	0.24785
C	-3.2247	-2.7224	-2.33144
H	-2.12223	-4.3291	-1.44907
C	-4.43552	-1.3112	-0.82754
H	-4.24105	-1.73708	1.24866
C	-3.9382	-1.52301	-2.12702
H	-2.91988	-3.00634	-3.33487
H	-5.02963	-0.42809	-0.61693
C	-3.79278	-0.33578	-3.01514
C	-4.58964	0.82027	-2.88214
C	-2.57079	-0.17212	-3.69398
C	-4.06032	2.08694	-3.11724
H	-5.59504	0.741	-2.47803
C	-2.04276	1.09191	-3.92899
H	-1.9324	-1.0325	-3.86567
C	-2.71172	2.25194	-3.49571
H	-4.66844	2.95785	-2.88875
H	-1.01639	1.16077	-4.27403
C	-1.8803	3.40141	-3.04024
C	-0.57052	3.63076	-3.51042
C	-2.21266	4.00326	-1.81218
C	0.41482	4.14071	-2.66845
H	-0.28678	3.29818	-4.50508
C	-1.22931	4.51216	-0.97198
H	-3.21809	3.89961	-1.41772
C	0.13258	4.44346	-1.32021
H	1.43755	4.19099	-3.03173
H	-1.51183	4.78217	0.04015
C	1.90398	1.50584	2.86662
C	2.04939	2.69307	1.97851

C	-4.25881	-4.72226	0.5969
C	-5.24475	-4.51581	-0.50077
C	-3.2423	-5.69814	0.53693
C	-4.60449	-4.26511	1.88238
C	-6.18621	-3.46571	-0.49542
C	-5.54851	-5.61692	-1.32297
C	-2.84436	-6.39024	1.6782
H	-2.84245	-6.00446	-0.42576
C	-4.20741	-4.95595	3.02139
H	-5.34872	-3.48331	1.99253
C	-7.46742	-3.64858	-1.01008
H	-5.95806	-2.53699	0.02023
C	-6.82709	-5.79943	-1.83662
H	-4.84399	-6.43814	-1.40266
C	-3.44585	-6.13587	2.92836
H	-2.14581	-7.21555	1.57177
H	-4.66002	-4.68187	3.96862
C	-7.86229	-4.88943	-1.55193
H	-8.20038	-2.85715	-0.88013
H	-7.06219	-6.75471	-2.29424
C	-3.69848	-7.20458	3.93507
C	-9.24117	-5.43365	-1.40187
C	-4.19134	-6.93481	5.22868
C	-3.88037	-8.51809	3.46341
C	-9.66983	-6.61567	-2.04086
C	-9.98315	-5.03391	-0.27468
C	-5.07527	-7.80943	5.85605
H	-3.97808	-5.97979	5.70081
C	-4.76213	-9.39106	4.08971
H	-3.48591	-8.79956	2.49261
C	-10.55375	-7.49028	-1.41349
H	-9.21938	-6.91502	-2.98319
C	-10.86494	-5.90687	0.35161
H	-9.72996	-4.11037	0.23539
C	-5.50399	-8.99138	5.217
H	-5.52566	-7.51013	6.79842
H	-5.01543	-10.31457	3.57961
H	-10.76693	-8.44533	-1.88556
C	-11.04671	-7.22044	-0.11991
H	-11.25947	-5.62531	1.32236
C	-6.88286	-9.53564	5.36707
C	-11.29934	-8.28914	0.88679
C	-7.27771	-10.77648	4.82521
C	-7.91806	-8.62562	5.65173
C	-10.53796	-9.46917	0.79374
C	-11.90072	-8.03469	2.13701
C	-8.55892	-10.95933	4.31052
H	-6.54474	-11.56789	4.69524
C	-9.19664	-8.80814	5.1381
H	-7.68295	-7.67035	6.10937
C	-10.14084	-10.16	1.93275
H	-10.08544	-9.74334	-0.1535
C	-11.50279	-8.72682	3.27826
H	-12.59918	-7.20932	2.24348
C	-9.50039	-9.90924	4.31588
H	-8.78706	-11.88805	3.79487
H	-9.90117	-7.98692	5.21781
C	-10.48637	-9.70279	3.21825
H	-9.3967	-10.94188	1.82253
H	-11.90256	-8.42044	4.24097

Coordinates of 1: UωB97xD/6-31G(d,p)

C	4.5198	2.54743	1.23447
C	5.03371	1.25606	1.2347
C	5.52039	0.66485	0.05515
C	5.68159	1.51251	-1.05798
C	5.16645	2.80598	-1.05834
C	4.46706	3.31133	0.05483
H	4.01129	2.90225	2.12506
H	4.9077	0.64894	2.12529
H	6.14329	1.1297	-1.96378
H	5.23885	3.40088	-1.96446
C	5.49993	-0.81721	-0.05657
C	5.63732	-1.66908	1.05656
C	4.99753	-1.39467	-1.23635
C	5.0867	-2.94784	1.05656
H	6.10925	-1.29936	1.96252
C	4.44815	-2.67139	-1.23646
H	4.88869	-0.78418	-2.12691
C	4.37385	-3.43352	-0.05683
H	5.14245	-3.54467	1.96258
H	3.93041	-3.01199	-2.12728
C	3.43352	4.37385	-0.05683
C	2.67139	4.44815	-1.23646
C	2.94784	5.0867	1.05656
C	1.39467	4.99753	-1.23635
H	3.01199	3.93041	-2.12728
C	1.66908	5.63732	1.05656
H	3.54467	5.14245	1.96258
C	0.81721	5.49993	-0.05657
H	0.78418	4.88869	-2.12691
H	1.29936	6.10925	1.96252
C	3.31133	-4.46706	0.05483
C	2.80598	-5.16645	-1.05834
C	2.54743	-4.5198	1.23447
C	1.51251	-5.68159	-1.05798
H	3.40088	-5.23885	-1.96446
C	1.25606	-5.03371	1.2347
H	2.90225	-4.01129	2.12506
C	0.66485	-5.52039	0.05515
H	1.1297	-6.14329	-1.96378
H	0.64894	-4.9077	2.12529
C	-0.81721	-5.49993	-0.05657
C	-1.66908	-5.63732	1.05656
C	-1.39467	-4.99753	-1.23635
C	-2.94784	-5.0867	1.05656
H	-1.29936	-6.10925	1.96252
C	-2.67139	-4.44815	-1.23646
H	-0.78418	-4.88869	-2.12691
C	-3.43352	-4.37385	-0.05683
H	-3.54467	-5.14245	1.96258
H	-3.01199	-3.93041	-2.12728
C	-4.46706	-3.31133	0.05483
C	-5.16645	-2.80598	-1.05834
C	-4.5198	-2.54743	1.23447
C	-5.68159	-1.51251	-1.05798
H	-5.23885	-3.40088	-1.96446
C	-5.03371	-1.25606	1.2347
H	-4.01129	-2.90225	2.12506
C	-5.52039	-0.66485	0.05515
H	-6.14329	-1.1297	-1.96378
H	-4.9077	-0.64894	2.12529
C	-5.49993	0.81721	-0.05657

C	-5.63732	1.66908	1.05656
C	-4.99753	1.39467	-1.23635
C	-5.0867	2.94784	1.05656
H	-6.10925	1.29936	1.96252
C	-4.44815	2.67139	-1.23646
H	-4.88869	0.78418	-2.12691
C	-4.37385	3.43352	-0.05683
H	-5.14245	3.54467	1.96258
H	-3.93041	3.01199	-2.12728
C	-3.31133	4.46706	0.05483
C	-2.80598	5.16645	-1.05834
C	-2.54743	4.5198	1.23447
C	-1.51251	5.68159	-1.05798
H	-3.40088	5.23885	-1.96446
C	-1.25606	5.03371	1.2347
H	-2.90225	4.01129	2.12506
C	-0.66485	5.52039	0.05515
H	-1.1297	6.14329	-1.96378
H	-0.64894	4.9077	2.12529

Coordinates of $1^{\cdot+}$: UωB97xD/6-31G(d,p)

C	4.48695	2.52124	1.24391
C	5.00157	1.23534	1.23506
C	5.45411	0.64807	0.04802
C	5.59378	1.48767	-1.07381
C	5.07029	2.7683	-1.07096
C	4.40263	3.27188	0.06322
H	4.00982	2.87046	2.15341
H	4.90126	0.63855	2.13516
H	6.0468	1.10837	-1.98412
H	5.1301	3.3587	-1.97993
C	5.45213	-0.82829	-0.0632
C	5.59076	-1.66647	1.05761
C	4.96624	-1.40463	-1.24092
C	5.05805	-2.94538	1.05675
H	6.05716	-1.29558	1.96513
C	4.42766	-2.68263	-1.23888
H	4.85403	-0.80777	-2.14018
C	4.35546	-3.43122	-0.06026
H	5.12051	-3.53718	1.96467
H	3.92076	-3.02278	-2.1358
C	3.37615	4.32102	-0.02902
C	2.66518	4.48026	-1.23085
C	2.87271	4.98997	1.11055
C	1.40343	5.03918	-1.24154
H	3.03289	4.02465	-2.1434
C	1.60709	5.53606	1.10676
H	3.45382	5.01559	2.02618
C	0.78867	5.46282	-0.04684
H	0.83615	4.99826	-2.16477
H	1.22481	5.98153	2.01914
C	3.30146	-4.46962	0.05588
C	2.80104	-5.16103	-1.06114
C	2.55121	-4.52468	1.23416
C	1.51282	-5.67219	-1.05968
H	3.38916	-5.23352	-1.97085
C	1.2618	-5.03595	1.23555
H	2.899	-4.02277	2.13105
C	0.67645	-5.51256	0.05887
H	1.13179	-6.1291	-1.96789
H	0.6658	-4.90708	2.133
C	-0.80231	-5.47955	-0.05718
C	-1.64791	-5.60622	1.05952
C	-1.36789	-4.98858	-1.23751
C	-2.91388	-5.04381	1.05828
H	-1.2868	-6.07932	1.96723
C	-2.63663	-4.42881	-1.24146
H	-0.76479	-4.89011	-2.13402
C	-3.38768	-4.34183	-0.06462
H	-3.50719	-5.09312	1.96625
H	-2.96437	-3.92053	-2.14236
C	-4.40426	-3.27171	0.04363
C	-5.08146	-2.75701	-1.07928
C	-4.48686	-2.53802	1.23309
C	-5.58331	-1.46824	-1.07479
H	-5.14754	-3.34171	-1.99106
C	-4.99857	-1.25148	1.24357
H	-4.00839	-2.90529	2.13448
C	-5.45044	-0.64554	0.06239
H	-6.03169	-1.07838	-1.98324
H	-4.89615	-0.67187	2.15477
C	-5.42762	0.81997	-0.02727

C	-5.51517	1.65016	1.11543
C	-5.02974	1.42811	-1.23117
C	-4.97285	2.91654	1.11141
H	-5.95225	1.26644	2.03096
C	-4.4961	2.69991	-1.24132
H	-4.99025	0.84722	-2.14581
C	-4.3317	3.42736	-0.04461
H	-4.99736	3.50006	2.02571
H	-4.06194	3.06333	-2.16599
C	-3.29349	4.44252	0.02466
C	-2.75708	5.06271	-1.135
C	-2.58368	4.62483	1.23261
C	-1.48015	5.57088	-1.13451
H	-3.33271	5.08741	-2.05383
C	-1.30493	5.1322	1.2324
H	-2.9732	4.21872	2.15902
C	-0.66428	5.48769	0.02478
H	-1.07686	5.98468	-2.05233
H	-0.742	5.10292	2.15823

Coordinates of $(1)_2^{\cdot+}$: UωB97xD/6-31G(d,p)

C	1.89358	5.37722	0.78398
C	2.34181	4.61962	1.85956
C	3.45033	3.76304	1.73635
C	4.21837	3.88649	0.56228
C	3.76917	4.64509	-0.51529
C	2.53152	5.31565	-0.46786
H	0.94577	5.89751	0.87667
H	1.72775	4.57536	2.7532
H	5.13837	3.31813	0.45857
H	4.34971	4.65016	-1.43352
C	3.54089	2.58531	2.63867
C	3.01292	2.58106	3.94436
C	3.85429	1.33361	2.07942
C	2.60544	1.39656	4.5521
H	2.84351	3.52227	4.45972
C	3.4478	0.15109	2.68626
H	4.2795	1.28418	1.08223
C	2.70772	0.16193	3.88211
H	2.12799	1.44251	5.52684
H	3.57061	-0.7792	2.14118
C	1.73818	5.63084	-1.68478
C	1.8249	4.76148	-2.78687
C	0.66648	6.54467	-1.68217
C	0.78375	4.65031	-3.70091
H	2.64237	4.0501	-2.84446
C	-0.37629	6.43353	-2.59797
H	0.606	7.30168	-0.90532
C	-0.39543	5.40322	-3.55802
H	0.82551	3.85593	-4.43905
H	-1.2249	7.10649	-2.51337
C	1.81575	-0.99046	4.17538
C	2.09052	-2.30021	3.73635
C	0.50203	-0.73029	4.60471
C	1.0649	-3.21633	3.51894
H	3.10924	-2.58139	3.48472
C	-0.52185	-1.6447	4.38732
H	0.24383	0.25902	4.96834
C	-0.28245	-2.86461	3.72988
H	1.30836	-4.18992	3.10295
H	-1.54264	-1.33639	4.58871
C	-1.40767	-3.51463	3.00823
C	-2.75023	-3.38852	3.41473
C	-1.18418	-3.98738	1.70274
C	-3.79299	-3.49967	2.49892
H	-2.97874	-3.12029	4.44235
C	-2.2252	-4.09866	0.78856
H	-0.16712	-4.11819	1.34757
C	-3.54097	-3.74251	1.13467
H	-4.80971	-3.31542	2.83437
H	-1.98354	-4.31275	-0.24748
C	-4.46706	-3.31133	0.05483
C	-4.38123	-3.79723	-1.26434
C	-5.23162	-2.14739	0.25119
C	-4.83087	-3.03825	-2.34147
H	-3.88448	-4.74365	-1.45853
C	-5.68013	-1.38954	-0.8241
H	-5.34266	-1.74245	1.25185
C	-5.38625	-1.75838	-2.14898
H	-4.67394	-3.41092	-3.34977
H	-6.12492	-0.42006	-0.62439
C	-5.34399	-0.69672	-3.18846

C	-6.13944	0.46394	-3.1276
C	-4.25471	-0.67068	-4.07759
C	-5.73196	1.64844	-3.73534
H	-7.04715	0.46392	-2.53074
C	-3.8481	0.51172	-4.68456
H	-3.62111	-1.54644	-4.17371
C	-4.51051	1.72639	-4.43222
H	-6.3317	2.54375	-3.59779
H	-2.91178	0.51654	-5.23312
C	-3.75129	2.99478	-4.58841
C	-2.70258	3.14807	-5.51598
C	-3.84007	3.96012	-3.56953
C	-1.6774	4.06457	-5.29813
H	-2.64401	2.4879	-6.37676
C	-2.81646	4.87478	-3.35186
H	-4.64072	3.89604	-2.83982
C	-1.65347	4.86926	-4.14251
H	-0.84393	4.09713	-5.99416
H	-2.85452	5.4917	-2.4599
C	-6.02265	-4.66331	0.63091
C	-6.94874	-4.23213	-0.44894
C	-5.21378	-5.81189	0.53013
C	-6.1923	-4.12059	1.9172
C	-7.53124	-2.95042	-0.48874
C	-7.53066	-5.21662	-1.2675
C	-4.80111	-6.50335	1.66592
H	-4.97138	-6.21582	-0.44879
C	-5.78066	-4.81107	3.05102
H	-6.79271	-3.22581	2.04566
C	-8.75303	-2.73451	-1.12041
H	-7.06459	-2.12977	0.04881
C	-8.75055	-5.00115	-1.89781
H	-7.10809	-6.21598	-1.28564
C	-5.1789	-6.07845	2.95444
H	-4.24686	-7.42991	1.54553
H	-6.07473	-4.43078	4.02392
C	-9.44856	-3.79043	-1.74079
H	-9.20987	-1.75071	-1.06034
H	-9.23678	-5.84007	-2.38509
C	-5.29336	-7.00821	4.10851
C	-10.92604	-3.79692	-1.90338
C	-5.37664	-6.56355	5.44227
C	-5.66713	-8.34137	3.86208
C	-11.59528	-4.68403	-2.76867
C	-11.71094	-3.14558	-0.93518
C	-6.01513	-7.32603	6.41662
H	-5.01003	-5.57502	5.70417
C	-6.30424	-9.1027	4.83486
H	-5.60471	-8.73714	2.85356
C	-12.91057	-5.07095	-2.52633
H	-11.0563	-5.13984	-3.59446
C	-13.02409	-3.53154	-0.69348
H	-11.24546	-2.43942	-0.25526
C	-6.59919	-8.56841	6.10192
H	-6.13113	-6.91378	7.41501
H	-6.71604	-10.06574	4.55097
C	-13.61718	-4.58786	-1.40785
H	-13.36579	-5.81921	-3.16903
H	-13.53676	-3.11257	0.16632
C	-7.74056	-9.13866	6.86462
C	-14.7273	-5.34172	-0.76836
C	-8.13562	-10.48608	6.75479
C	-8.66381	-8.25516	7.45191

C	-15.62298	-4.75323	0.14549
C	-14.69209	-6.74722	-0.80295
C	-9.45101	-10.8724	6.99753
H	-7.42679	-11.22784	6.39765
C	-9.97703	-8.64074	7.69386
H	-8.4004	-7.20962	7.57482
C	-16.26146	-5.51571	1.11984
H	-15.76055	-3.67561	0.14683
C	-15.32923	-7.50837	0.16995
H	-14.03097	-7.24906	-1.50203
C	-10.43179	-9.92906	7.3605
H	-9.73647	-11.9061	6.82383
H	-10.69177	-7.8824	7.99666
C	-16.0332	-6.90148	1.22535
H	-16.88163	-5.01447	1.85762
H	-15.1424	-8.57705	0.1958
C	-11.878	-10.11927	7.07464
C	-16.17893	-7.64753	2.50268
C	-12.24582	-10.84859	5.92985
C	-12.88507	-9.34475	7.68252
C	-15.9073	-6.97525	3.70766
C	-16.24518	-9.05307	2.56294
C	-13.46567	-10.63331	5.29942
H	-11.51033	-11.47412	5.43445
C	-14.10687	-9.12884	7.05085
H	-12.6818	-8.83878	8.62212
C	-15.4956	-7.66611	4.84123
H	-15.8625	-5.89104	3.71747
C	-15.8324	-9.74513	3.69833
H	-16.54591	-9.61603	1.68383
C	-14.37775	-9.67799	5.7825
H	-13.63892	-11.09883	4.33458
H	-14.82709	-8.45962	7.51304
C	-15.33509	-9.06321	4.82586
H	-15.14445	-7.09639	5.69548
H	-15.8212	-10.83124	3.6774

Coordinates of [10]CPP: UωB97xD/6-31G(d,p)

C	5.5928	-4.63674	1.07216
C	6.37561	-3.48567	1.07167
C	6.4153	-2.63231	-0.04672
C	5.78423	-3.08588	-1.21823
C	5.00281	-4.23524	-1.21784
C	4.81336	-4.98806	-0.04578
H	5.54045	-5.23975	1.9742
H	6.91775	-3.21494	1.97321
H	5.79305	-2.4617	-2.10605
H	4.42537	-4.47347	-2.10537
C	6.82888	-1.20903	0.04441
C	6.54022	-0.4881	1.21641
C	7.25155	-0.4668	-1.07413
C	6.49566	0.90105	1.21608
H	6.21513	-1.02006	2.10488
C	7.20676	0.92446	-1.07451
H	7.56401	-0.98536	-1.97603
C	6.73755	1.63853	0.04379
H	6.13716	1.41145	2.10433
H	7.48521	1.46158	-1.9767
C	3.64141	-5.89546	0.04589
C	3.10766	-6.56342	-1.07201
C	2.86346	-5.88911	1.21683
C	1.79749	-7.03361	-1.07253
H	3.70562	-6.66506	-1.97317
C	1.55525	-6.35868	1.21635
H	3.23758	-5.38854	2.10419
H	1.40123	-7.49211	-1.97406
H	0.94753	-6.21082	2.10335
C	6.23377	3.03242	-0.04763
C	5.57437	3.44453	-1.21886
C	6.14022	3.88175	1.07062
C	4.72117	4.54169	-1.21812
H	5.62264	2.82208	-2.10664
C	5.28563	4.98053	1.07145
H	6.69894	3.64628	1.97197
C	4.48501	5.28144	-0.04624
H	4.12908	4.74245	-2.10529
H	5.19564	5.57911	1.97346
C	3.25807	6.11292	0.04587
C	2.4824	6.05716	1.21695
C	2.68308	6.74625	-1.07173
C	1.14722	6.44339	1.21692
H	2.88754	5.58067	2.10391
C	1.34591	7.13296	-1.07181
H	3.27329	6.8853	-1.97301
C	0.52139	6.90454	0.04559
H	0.55032	6.25694	2.10396
H	0.92108	7.56563	-1.97313
C	-0.95995	6.85777	-0.04673
C	-1.55525	6.35865	-1.2184
C	-1.79749	7.03362	1.07047
C	-2.86346	5.88908	-1.21887
H	-0.94753	6.21077	-2.1054
C	-3.10765	6.56342	1.06996
H	-1.40122	7.49213	1.972
C	-3.64141	5.89545	-0.04792
H	-3.23758	5.38849	-2.10621
H	-3.70561	6.66508	1.97113
C	-4.81337	4.98807	0.04375
C	-5.00283	4.23525	1.21582

C	-5.59281	4.63674	-1.07418
C	-5.78424	3.08589	1.21621
H	-4.4254	4.47349	2.10335
C	-6.37562	3.48567	-1.0737
H	-5.54046	5.23975	-1.97622
C	-6.4153	2.63231	0.04469
H	-5.79307	2.46172	2.10403
H	-6.91775	3.21493	-1.97523
C	-6.82887	1.20903	-0.04644
C	-6.54019	0.48811	-1.21844
C	-7.25155	0.4668	1.0721
C	-6.49564	-0.90104	-1.21812
H	-6.21509	1.02008	-2.1069
C	-7.20676	-0.92447	1.07246
H	-7.56401	0.98534	1.974
C	-6.73754	-1.63853	-0.04584
H	-6.13712	-1.41144	-2.10636
H	-7.48522	-1.46159	1.97465
C	-6.23378	-3.03243	0.04557
C	-5.5744	-3.44455	1.21681
C	-6.14021	-3.88174	-1.0727
C	-4.72119	-4.54171	1.21606
H	-5.62269	-2.82213	2.1046
C	-5.28562	-4.98052	-1.07353
H	-6.69892	-3.64626	-1.97404
C	-4.48502	-5.28144	0.04416
H	-4.12913	-4.7425	2.10324
H	-5.19561	-5.57908	-1.97555
C	-3.25806	-6.11292	-0.04795
C	-2.48238	-6.05712	-1.21902
C	-2.68308	-6.74626	1.06964
C	-1.1472	-6.44335	-1.21898
H	-2.88752	-5.5806	-2.10596
C	-1.34592	-7.13298	1.06973
H	-3.2733	-6.88533	1.97091
C	-0.52139	-6.90454	-0.04766
H	-0.55029	-6.25688	-2.10601
H	-0.9211	-7.56566	1.97104
C	0.95995	-6.85778	0.04467

Coordinates of $([10]CPP)^{\cdot+}$: UωB97xD/6-31G(d,p)

C	5.5928	-4.63674	1.07216
C	6.37561	-3.48567	1.07167
C	6.4153	-2.63231	-0.04672
C	5.78423	-3.08588	-1.21823
C	5.00281	-4.23524	-1.21784
C	4.81336	-4.98806	-0.04578
H	5.54045	-5.23975	1.9742
H	6.91775	-3.21494	1.97321
H	5.79305	-2.4617	-2.10605
H	4.42537	-4.47347	-2.10537
C	6.82888	-1.20903	0.04441
C	6.54022	-0.4881	1.21641
C	7.25155	-0.4668	-1.07413
C	6.49566	0.90105	1.21608
H	6.21513	-1.02006	2.10488
C	7.20676	0.92446	-1.07451
H	7.56401	-0.98536	-1.97603
C	6.73755	1.63853	0.04379
H	6.13716	1.41145	2.10433
H	7.48521	1.46158	-1.9767
C	3.64141	-5.89546	0.04589
C	3.10766	-6.56342	-1.07201
C	2.86346	-5.88911	1.21683
C	1.79749	-7.03361	-1.07253
H	3.70562	-6.66506	-1.97317
C	1.55525	-6.35868	1.21635
H	3.23758	-5.38854	2.10419
H	1.40123	-7.49211	-1.97406
H	0.94753	-6.21082	2.10335
C	6.23377	3.03242	-0.04763
C	5.57437	3.44453	-1.21886
C	6.14022	3.88175	1.07062
C	4.72117	4.54169	-1.21812
H	5.62264	2.82208	-2.10664
C	5.28563	4.98053	1.07145
H	6.69894	3.64628	1.97197
C	4.48501	5.28144	-0.04624
H	4.12908	4.74245	-2.10529
H	5.19564	5.57911	1.97346
C	3.25807	6.11292	0.04587
C	2.4824	6.05716	1.21695
C	2.68308	6.74625	-1.07173
C	1.14722	6.44339	1.21692
H	2.88754	5.58067	2.10391
C	1.34591	7.13296	-1.07181
H	3.27329	6.8853	-1.97301
C	0.52139	6.90454	0.04559
H	0.55032	6.25694	2.10396
H	0.92108	7.56563	-1.97313
C	-0.95995	6.85777	-0.04673
C	-1.55525	6.35865	-1.2184
C	-1.79749	7.03362	1.07047
C	-2.86346	5.88908	-1.21887
H	-0.94753	6.21077	-2.1054
C	-3.10765	6.56342	1.06996
H	-1.40122	7.49213	1.972
C	-3.64141	5.89545	-0.04792
H	-3.23758	5.38849	-2.10621
H	-3.70561	6.66508	1.97113
C	-4.81337	4.98807	0.04375
C	-5.00283	4.23525	1.21582

C	-5.59281	4.63674	-1.07418
C	-5.78424	3.08589	1.21621
H	-4.4254	4.47349	2.10335
C	-6.37562	3.48567	-1.0737
H	-5.54046	5.23975	-1.97622
C	-6.4153	2.63231	0.04469
H	-5.79307	2.46172	2.10403
H	-6.91775	3.21493	-1.97523
C	-6.82887	1.20903	-0.04644
C	-6.54019	0.48811	-1.21844
C	-7.25155	0.4668	1.0721
C	-6.49564	-0.90104	-1.21812
H	-6.21509	1.02008	-2.1069
C	-7.20676	-0.92447	1.07246
H	-7.56401	0.98534	1.974
C	-6.73754	-1.63853	-0.04584
H	-6.13712	-1.41144	-2.10636
H	-7.48522	-1.46159	1.97465
C	-6.23378	-3.03243	0.04557
C	-5.5744	-3.44455	1.21681
C	-6.14021	-3.88174	-1.0727
C	-4.72119	-4.54171	1.21606
H	-5.62269	-2.82213	2.1046
C	-5.28562	-4.98052	-1.07353
H	-6.69892	-3.64626	-1.97404
C	-4.48502	-5.28144	0.04416
H	-4.12913	-4.7425	2.10324
H	-5.19561	-5.57908	-1.97555
C	-3.25806	-6.11292	-0.04795
C	-2.48238	-6.05712	-1.21902
C	-2.68308	-6.74626	1.06964
C	-1.1472	-6.44335	-1.21898
H	-2.88752	-5.5806	-2.10596
C	-1.34592	-7.13298	1.06973
H	-3.2733	-6.88533	1.97091
C	-0.52139	-6.90454	-0.04766
H	-0.55029	-6.25688	-2.10601
H	-0.9211	-7.56566	1.97104
C	0.95995	-6.85778	0.04467

Coordinates of $([10]CPP)_2^{\cdot+}$: UωB97xD/6-31G(d,p)

C	0.35513	6.96059	-0.42505
C	1.21232	7.08568	-1.51469
C	2.26634	6.1761	-1.72043
C	2.52762	5.25804	-0.68829
C	1.67192	5.13326	0.39975
C	0.51216	5.92018	0.50963
H	-0.48301	7.64518	-0.3308
H	1.02513	7.86536	-2.24752
H	3.33359	4.54026	-0.80275
H	1.83587	4.3219	1.10169
C	2.89823	5.96728	-3.0479
C	2.11131	6.09462	-4.206
C	4.17114	5.38691	-3.20137
C	2.49513	5.50922	-5.4067
H	1.12434	6.54065	-4.13532
C	4.55547	4.80047	-4.40387
H	4.84687	5.34176	-2.35207
C	3.68497	4.76732	-5.50921
H	1.79616	5.51601	-6.23701
H	5.5228	4.31031	-4.467
C	-0.59162	5.45746	1.38873
C	-0.36718	4.72582	2.56986
C	-1.91192	5.50395	0.90811
C	-1.36807	3.937	3.12987
H	0.61968	4.72792	3.02383
C	-2.91136	4.71637	1.46734
H	-2.13147	6.05959	0.00203
H	-1.14076	3.34054	4.00884
H	-3.88109	4.68102	0.98122
C	3.83131	3.78927	-6.61695
C	4.33108	2.50625	-6.33323
C	3.24806	3.98201	-7.88316
C	4.09565	1.43542	-7.18742
H	4.79242	2.31327	-5.36999
C	3.01214	2.90957	-8.73864
H	2.92144	4.9751	-8.17834
C	3.34893	1.59432	-8.36788
H	4.3802	0.43889	-6.86509
H	2.50641	3.0886	-9.6832
C	2.72553	0.39985	-8.99228
C	1.38817	0.47279	-9.41929
C	3.30942	-0.87947	-8.93626
C	0.62505	-0.67473	-9.60014
H	0.8989	1.43962	-9.48052
C	2.54518	-2.02871	-9.11727
H	4.3628	-0.97885	-8.6903
C	1.16154	-1.95231	-9.36284
H	-0.43695	-0.56914	-9.79731
H	3.01843	-3.00046	-9.00879
C	0.23751	-3.08609	-9.10633
C	0.50888	-3.9595	-8.03871
C	-1.03439	-3.18015	-9.70126
C	-0.49056	-4.74708	-7.47948
H	1.47861	-3.92415	-7.55257
C	-2.03528	-3.96896	-9.14126
H	-1.26169	-2.5837	-10.58024
C	-1.81086	-4.7006	-7.96012
H	-0.27103	-5.30271	-6.57339
H	-3.02213	-3.97107	-9.59524
C	-2.91464	-5.16333	-7.08103
C	-4.07441	-4.37642	-6.97117

C	-2.75762	-6.20374	-6.14635
C	-4.93011	-4.5012	-5.88313
H	-4.23836	-3.56506	-7.67311
C	-3.61481	-6.32882	-5.05671
H	-1.91947	-6.88833	-6.24061
C	-4.66882	-5.41924	-4.85098
H	-5.73609	-3.78342	-5.76867
H	-3.42761	-7.1085	-4.32387
C	-5.3007	-5.21041	-3.5235
C	-4.51377	-5.33775	-2.36541
C	-6.57362	-4.63005	-3.37002
C	-4.89759	-4.75235	-1.1647
H	-3.52679	-5.78376	-2.4361
C	-6.95794	-4.04361	-2.16752
H	-7.24935	-4.5849	-4.21932
C	-6.08743	-4.01046	-1.06218
H	-4.19861	-4.75913	-0.3344
H	-7.92528	-3.55346	-2.10438
C	-6.23378	-3.03243	0.04557
C	-6.73357	-1.74941	-0.23813
C	-5.6505	-3.22518	1.31177
C	-6.49813	-0.67859	0.61606
H	-7.19494	-1.55643	-1.20136
C	-5.41458	-2.15273	2.16725
H	-5.32387	-4.21826	1.60694
C	-5.75138	-0.83748	1.7965
H	-6.7827	0.31794	0.29375
H	-4.90882	-2.33176	3.1118
C	-5.12798	0.35698	2.42089
C	-3.79061	0.28404	2.84787
C	-5.71187	1.6363	2.36489
C	-3.02749	1.43157	3.02872
H	-3.30132	-0.68278	2.90907
C	-4.94763	2.78554	2.54591
H	-6.76526	1.73568	2.11896
C	-3.56399	2.70915	2.79146
H	-1.96548	1.32599	3.22586
H	-5.42089	3.75729	2.43745
C	-2.63997	3.84294	2.53495
C	-8.13279	-3.81201	0.65024
C	-8.27913	-2.83397	1.758
C	-8.75253	-3.54446	-0.58294
C	-7.63664	-5.11427	0.84659
C	-8.59458	-3.30313	3.04525
C	-8.38557	-1.44774	1.53965
C	-9.02595	-4.56267	-1.4886
H	-9.14674	-2.55245	-0.77896
C	-7.91055	-6.1341	-0.06037
H	-7.07897	-5.34594	1.74957
C	-9.16025	-2.46586	3.99957
H	-8.52228	-4.36458	3.25998
C	-8.95195	-0.60916	2.49547
H	-8.07479	-1.02856	0.58693
C	-8.69311	-5.89902	-1.20628
H	-9.62546	-4.33474	-2.36414
H	-7.56082	-7.13992	0.15419
C	-9.43869	-1.11765	3.71416
H	-9.51243	-2.89905	4.93036
H	-9.07091	0.44634	2.26803
C	-9.39432	-6.98573	-1.93608
C	-10.43973	-0.39753	4.54145
C	-9.88319	-8.08797	-1.2134
C	-9.8334	-6.84822	-3.26613

C	-11.41161	0.39237	3.90275
C	-10.63762	-0.67368	5.90717
C	-10.8908	-8.89687	-1.72553
H	-9.56842	-8.23477	-0.18517
C	-10.84256	-7.65823	-3.77901
H	-9.42125	-6.05948	-3.88903
C	-12.60022	0.72867	4.53973
H	-11.29768	0.63309	2.85062
C	-11.82819	-0.33705	6.54512
H	-9.87406	-1.21082	6.46254
C	-11.45965	-8.64354	-2.98592
H	-11.33215	-9.65091	-1.08171
H	-11.19642	-7.48442	-4.79124
C	-12.8762	0.29153	5.84706
H	-13.3781	1.22176	3.96556
H	-11.96857	-0.61886	7.58478
C	-12.80176	-9.19825	-3.29591
C	-14.28633	0.2531	6.31107
C	-13.25428	-10.42717	-2.78062
C	-13.762	-8.36587	-3.89706
C	-14.75014	-0.88666	6.99091
C	-15.25588	1.17512	5.87447
C	-14.61293	-10.72049	-2.70535
H	-12.53741	-11.13841	-2.3803
C	-15.11864	-8.65872	-3.82182
H	-13.45673	-7.41024	-4.31123
C	-16.10678	-1.17952	7.06616
H	-14.03709	-1.62266	7.34839
C	-16.61452	0.88179	5.94975
H	-14.94173	2.10893	5.41699
C	-15.58246	-9.79847	-3.14196
H	-14.92709	-11.65429	-2.24786
H	-15.83169	-7.92272	-4.17932
C	-17.06703	-0.34713	6.46503
H	-16.41205	-2.13516	7.48031
H	-17.33139	1.59303	5.54944
C	-16.99259	-9.83688	-2.67795
C	-18.40915	-0.90185	6.15506
C	-18.04061	-9.2083	-3.37601
C	-17.26857	-10.27401	-1.37062
C	-18.97802	-0.6485	4.89469
C	-19.02622	-1.88716	6.94814
C	-19.23117	-8.87167	-2.73806
H	-17.90022	-8.92649	-4.41568
C	-18.45718	-9.93771	-0.73364
H	-16.49069	-10.76709	-0.79645
C	-19.98563	-1.4574	4.38256
H	-18.5367	0.10556	4.25086
C	-20.03538	-2.69718	6.43527
H	-18.67233	-2.061	7.96036
C	-19.42906	-9.14783	-1.37235
H	-19.99474	-8.33454	-3.29344
H	-18.57111	-10.17842	0.31849
C	-20.47448	-2.55966	5.10523
H	-20.30042	-1.31058	3.35434
H	-20.44751	-3.48593	7.05816
C	-20.43012	-8.42771	-0.54506
C	-21.17568	-3.64637	4.37541
C	-20.70857	-7.07951	-0.83046
C	-20.91685	-8.93621	0.67363
C	-20.8428	-4.98272	4.65772
C	-21.95825	-3.41129	3.22952
C	-21.27424	-6.24224	0.12386

H	-20.35641	-6.64631	-1.76126
C	-21.48323	-8.09763	1.62946
H	-20.79788	-9.99171	0.90107
C	-21.11622	-6.00092	3.75205
H	-20.24327	-5.21064	5.53324
C	-22.23216	-4.43111	2.32255
H	-22.308	-2.40547	3.01497
C	-21.58967	-6.7114	1.41111
H	-21.34656	-5.18079	-0.09088
H	-21.79399	-8.51682	2.58219
C	-21.736	-5.73337	2.51888
H	-20.72199	-6.99293	3.94805
H	-22.78984	-4.19944	1.41958

Coordinates of [12]CPP: UωB97xD/6-31G(d,p)

C	-0.69304	7.89067	1.21811
C	0.697	7.89069	1.21792
C	1.42637	8.18295	0.05237
C	0.69753	8.62401	-1.06721
C	-0.69424	8.62399	-1.06701
C	2.85789	7.79923	-0.02737
C	3.70774	7.8072	1.09372
C	4.91303	7.11121	1.08939
C	5.32509	6.37422	-0.03591
C	4.54855	6.49539	-1.2013
C	3.34489	7.19056	-1.19703
C	6.37342	5.32592	0.03609
C	6.49469	4.54947	1.20153
C	7.18989	3.34582	1.1973
C	7.79852	2.85876	0.02765
C	7.80639	3.70853	-1.0935
C	7.11037	4.9138	-1.08922
C	8.18229	1.42725	-0.05201
C	8.62338	0.6985	1.06762
C	8.6234	-0.69327	1.06751
C	8.18234	-1.42186	-0.05222
C	7.89006	-0.69224	-1.21761
C	7.89004	0.69779	-1.2175
C	7.79862	-2.85339	0.02721
C	7.18999	-3.34063	1.1968
C	6.49482	-4.54428	1.20085
C	6.37358	-5.32058	0.03531
C	7.11049	-4.90828	-1.08996
C	7.80649	-3.70298	-1.09407
C	5.32528	-6.36889	-0.03685
C	4.91322	-7.10606	1.08835
C	3.70796	-7.80208	1.09256
C	2.85813	-7.794	-0.02856
C	3.34514	-7.18517	-1.19813
C	4.54878	-6.48995	-1.20227
C	1.42663	-8.1778	0.05108
C	0.69721	-7.88583	1.21667
C	-0.69282	-7.88586	1.21682
C	-1.42249	-8.17785	0.0514
C	-0.69393	-8.61862	-1.06847
C	0.69784	-8.6186	-1.06863
C	-2.85401	-7.79411	-0.0279
C	-3.70355	-7.80216	1.09342
C	-4.90884	-7.10615	1.08949
C	-5.32119	-6.36905	-0.03563
C	-4.54496	-6.49011	-1.20124
C	-3.34131	-7.18529	-1.19737
C	-6.3695	-5.32075	0.03672
C	-6.49045	-4.54441	1.20227
C	-7.18568	-3.34079	1.19836
C	-7.79461	-2.85362	0.0289
C	-7.80275	-3.70325	-1.09235
C	-7.10671	-4.90853	-1.08837
C	-8.17843	-1.42211	-0.05044
C	-8.61928	-0.69357	1.0694
C	-8.6193	0.69821	1.06954
C	-8.17847	1.427	-0.05016
C	-7.88639	0.69758	-1.21572
C	-7.88635	-0.69245	-1.21585
C	-7.79473	2.85852	0.02947
C	-7.18587	3.34554	1.19901

C	-6.49069	4.54921	1.20313
C	-6.3697	5.32571	0.0377
C	-7.10689	4.91363	-1.08747
C	-7.80288	3.70834	-1.09165
C	-5.32142	6.37404	-0.03451
C	-4.90905	7.11094	1.09075
C	-3.70378	7.80697	1.09479
C	-3.34159	7.19058	-1.19614
C	-4.54524	6.49537	-1.20011
H	-1.2168	7.54432	2.10354
H	1.22102	7.54437	2.10319
H	1.22671	8.93049	-1.9649
H	-1.22368	8.93046	-1.96455
H	3.4012	8.32981	1.99522
H	5.52348	7.10434	1.9878
H	4.82941	5.94028	-2.09072
H	2.71882	7.15908	-2.08312
H	5.93963	4.83038	2.09096
H	7.15849	2.71981	2.08344
H	8.32895	3.40194	-1.99502
H	7.10343	5.52417	-1.98768
H	8.92985	1.22775	1.96527
H	8.92989	-1.22264	1.96509
H	7.54374	-1.21608	-2.10299
H	7.5437	1.22175	-2.10281
H	7.15859	-2.71474	2.08302
H	5.93977	-4.82534	2.09024
H	7.10355	-5.51851	-1.98851
H	8.32902	-3.39624	-1.99555
H	5.52365	-7.09929	1.98677
H	3.40141	-8.32484	1.99398
H	2.7191	-7.15361	-2.08424
H	4.82965	-5.93474	-2.09162
H	1.22118	-7.5397	2.10205
H	-1.21662	-7.53975	2.10232
H	-1.22334	-8.92488	-1.96611
H	1.22705	-8.92484	-1.96638
H	-3.39678	-8.32484	1.9948
H	-5.51903	-7.09935	1.98807
H	-4.82608	-5.93493	-2.09054
H	-2.71547	-7.15374	-2.08362
H	-5.93516	-4.82544	2.09153
H	-7.1541	-2.71486	2.08455
H	-8.32552	-3.39656	-1.9937
H	-7.09997	-5.51879	-1.9869
H	-8.92554	-1.22297	1.96703
H	-8.9256	1.22743	1.96727
H	-7.54021	1.22158	-2.10107
H	-7.54016	-1.21627	-2.1013
H	-7.15426	2.71951	2.08512
H	-5.93544	4.83009	2.09246
H	-7.10018	5.52405	-1.98589
H	-8.32565	3.40177	-1.99305
H	-5.51923	7.10396	1.98933
H	-3.39699	8.3295	1.99625
H	-2.7158	7.15922	-2.08243
H	-4.82634	5.94035	-2.08952
C	-2.85427	7.79915	-0.02657
C	-1.42274	8.18292	0.05278

Coordinates of $([12]CPP)^{\cdot+}$: UωB97xD/6-31G(d,p)

C	-0.69304	7.89067	1.21811
C	0.697	7.89069	1.21792
C	1.42637	8.18295	0.05237
C	0.69753	8.62401	-1.06721
C	-0.69424	8.62399	-1.06701
C	2.85789	7.79923	-0.02737
C	3.70774	7.8072	1.09372
C	4.91303	7.11121	1.08939
C	5.32509	6.37422	-0.03591
C	4.54855	6.49539	-1.2013
C	3.34489	7.19056	-1.19703
C	6.37342	5.32592	0.03609
C	6.49469	4.54947	1.20153
C	7.18989	3.34582	1.1973
C	7.79852	2.85876	0.02765
C	7.80639	3.70853	-1.0935
C	7.11037	4.9138	-1.08922
C	8.18229	1.42725	-0.05201
C	8.62338	0.6985	1.06762
C	8.6234	-0.69327	1.06751
C	8.18234	-1.42186	-0.05222
C	7.89006	-0.69224	-1.21761
C	7.89004	0.69779	-1.2175
C	7.79862	-2.85339	0.02721
C	7.18999	-3.34063	1.1968
C	6.49482	-4.54428	1.20085
C	6.37358	-5.32058	0.03531
C	7.11049	-4.90828	-1.08996
C	7.80649	-3.70298	-1.09407
C	5.32528	-6.36889	-0.03685
C	4.91322	-7.10606	1.08835
C	3.70796	-7.80208	1.09256
C	2.85813	-7.794	-0.02856
C	3.34514	-7.18517	-1.19813
C	4.54878	-6.48995	-1.20227
C	1.42663	-8.1778	0.05108
C	0.69721	-7.88583	1.21667
C	-0.69282	-7.88586	1.21682
C	-1.42249	-8.17785	0.0514
C	-0.69393	-8.61862	-1.06847
C	0.69784	-8.6186	-1.06863
C	-2.85401	-7.79411	-0.0279
C	-3.70355	-7.80216	1.09342
C	-4.90884	-7.10615	1.08949
C	-5.32119	-6.36905	-0.03563
C	-4.54496	-6.49011	-1.20124
C	-3.34131	-7.18529	-1.19737
C	-6.3695	-5.32075	0.03672
C	-6.49045	-4.54441	1.20227
C	-7.18568	-3.34079	1.19836
C	-7.79461	-2.85362	0.0289
C	-7.80275	-3.70325	-1.09235
C	-7.10671	-4.90853	-1.08837
C	-8.17843	-1.42211	-0.05044
C	-8.61928	-0.69357	1.0694
C	-8.6193	0.69821	1.06954
C	-8.17847	1.427	-0.05016
C	-7.88639	0.69758	-1.21572
C	-7.88635	-0.69245	-1.21585
C	-7.79473	2.85852	0.02947
C	-7.18587	3.34554	1.19901

C	-6.49069	4.54921	1.20313
C	-6.3697	5.32571	0.0377
C	-7.10689	4.91363	-1.08747
C	-7.80288	3.70834	-1.09165
C	-5.32142	6.37404	-0.03451
C	-4.90905	7.11094	1.09075
C	-3.70378	7.80697	1.09479
C	-3.34159	7.19058	-1.19614
C	-4.54524	6.49537	-1.20011
H	-1.2168	7.54432	2.10354
H	1.22102	7.54437	2.10319
H	1.22671	8.93049	-1.9649
H	-1.22368	8.93046	-1.96455
H	3.4012	8.32981	1.99522
H	5.52348	7.10434	1.9878
H	4.82941	5.94028	-2.09072
H	2.71882	7.15908	-2.08312
H	5.93963	4.83038	2.09096
H	7.15849	2.71981	2.08344
H	8.32895	3.40194	-1.99502
H	7.10343	5.52417	-1.98768
H	8.92985	1.22775	1.96527
H	8.92989	-1.22264	1.96509
H	7.54374	-1.21608	-2.10299
H	7.5437	1.22175	-2.10281
H	7.15859	-2.71474	2.08302
H	5.93977	-4.82534	2.09024
H	7.10355	-5.51851	-1.98851
H	8.32902	-3.39624	-1.99555
H	5.52365	-7.09929	1.98677
H	3.40141	-8.32484	1.99398
H	2.7191	-7.15361	-2.08424
H	4.82965	-5.93474	-2.09162
H	1.22118	-7.5397	2.10205
H	-1.21662	-7.53975	2.10232
H	-1.22334	-8.92488	-1.96611
H	1.22705	-8.92484	-1.96638
H	-3.39678	-8.32484	1.9948
H	-5.51903	-7.09935	1.98807
H	-4.82608	-5.93493	-2.09054
H	-2.71547	-7.15374	-2.08362
H	-5.93516	-4.82544	2.09153
H	-7.1541	-2.71486	2.08455
H	-8.32552	-3.39656	-1.9937
H	-7.09997	-5.51879	-1.9869
H	-8.92554	-1.22297	1.96703
H	-8.9256	1.22743	1.96727
H	-7.54021	1.22158	-2.10107
H	-7.54016	-1.21627	-2.1013
H	-7.15426	2.71951	2.08512
H	-5.93544	4.83009	2.09246
H	-7.10018	5.52405	-1.98589
H	-8.32565	3.40177	-1.99305
H	-5.51923	7.10396	1.98933
H	-3.39699	8.3295	1.99625
H	-2.7158	7.15922	-2.08243
H	-4.82634	5.94035	-2.08952
C	-2.85427	7.79915	-0.02657
C	-1.42274	8.18292	0.05278

Coordinates of $([12]CPP)_2^{\cdot+}$: UωB97xD/6-31G(d,p)

C	3.25709	-5.78434	1.90277
C	4.2864	-4.89647	2.19331
C	4.13409	-3.89749	3.17042
C	2.96046	-3.93131	3.94542
C	1.92988	-4.82029	3.65453
C	5.0681	-2.74413	3.18575
C	6.41993	-2.85926	2.81363
C	7.17397	-1.73765	2.48114
C	6.61174	-0.44823	2.50468
C	5.31092	-0.32525	3.02291
C	4.55789	-1.44538	3.35509
C	7.22989	0.70544	1.80464
C	7.91763	0.4928	0.59731
C	8.19493	1.54337	-0.26958
C	7.79852	2.85876	0.02765
C	7.24921	3.09124	1.30176
C	6.97164	2.0393	2.16982
C	7.75222	3.86878	-1.05889
C	8.65666	3.86318	-2.13646
C	8.38507	4.56177	-3.30917
C	7.19627	5.29887	-3.45955
C	6.37279	5.42576	-2.32744
C	6.64403	4.72804	-1.1562
C	6.68389	5.72594	-4.78541
C	6.89017	4.89957	-5.90359
C	6.14312	5.05733	-7.0651
C	5.1524	6.04935	-7.16612
C	5.055	6.9694	-6.10628
C	5.80295	6.81138	-4.94319
C	4.12513	5.94805	-8.23269
C	4.39969	5.39855	-9.49837
C	3.37401	4.97567	-10.33878
C	2.02532	5.08278	-9.95312
C	1.7527	5.77043	-8.75791
C	2.77706	6.19266	-7.91855
C	0.94152	4.3147	-10.61514
C	1.20779	3.02245	-11.09998
C	0.17846	2.1346	-11.3905
C	-1.16828	2.4949	-11.21062
C	-1.43483	3.83462	-10.87403
C	-0.40421	4.72357	-10.58314
C	-2.20456	1.43429	-11.14699
C	-2.11423	0.24172	-11.88777
C	-2.87358	-0.87508	-11.55115
C	-3.75863	-0.85212	-10.45781
C	-3.95691	0.38426	-9.81916
C	-3.19865	1.49964	-10.15539
C	-4.28394	-2.08997	-9.82941
C	-3.47257	-3.2367	-9.77895
C	-3.75513	-4.28251	-8.90804
C	-4.86304	-4.2338	-8.04437
C	-5.75582	-3.15859	-8.20554
C	-5.47294	-2.11145	-9.07771
C	-4.91902	-5.15112	-6.87893
C	-4.38328	-6.4515	-6.9129
C	-4.11168	-7.15011	-5.74021
C	-4.36302	-6.58125	-4.47831
C	-5.0385	-5.34876	-4.45347
C	-5.30975	-4.65103	-5.62469
C	-3.74834	-7.10107	-3.23139
C	-2.45037	-7.63881	-3.27422

C	-1.69805	-7.80133	-2.11676
C	-2.20636	-7.434	-0.85878
C	-3.55622	-7.04172	-0.80164
C	-4.30949	-6.87886	-1.9606
C	-1.27194	-7.24853	0.27944
C	-0.0992	-8.01134	0.42809
C	0.93178	-7.59326	1.26441
C	-0.39338	-5.71634	1.95764
C	-1.42296	-6.13383	1.12232
H	3.37099	-6.46147	1.06207
H	5.17617	-4.90434	1.57162
H	2.83491	-3.22356	4.75976
H	1.02043	-4.78873	4.24759
H	6.87456	-3.84316	2.74255
H	8.20241	-1.86835	2.15702
H	4.8387	0.65151	3.05525
H	3.51831	-1.3126	3.63751
H	8.1333	-0.52147	0.27663
H	8.61935	1.32063	-1.24343
H	6.99669	4.10469	1.6
H	6.50786	2.25258	3.12859
H	9.5641	3.26972	-2.07196
H	9.08594	4.49967	-4.13666
H	5.44478	5.98391	-2.4018
H	5.92048	4.76026	-0.34768
H	7.55889	4.04848	-5.82258
H	6.24913	4.32513	-7.85929
H	4.35301	7.79534	-6.176
H	5.67009	7.51697	-4.12815
H	5.43079	5.26099	-9.811
H	3.62464	4.51647	-11.29068
H	0.72544	5.87162	-8.42234
H	2.52151	6.61212	-6.95064
H	2.23269	2.66695	-11.13825
H	0.42747	1.10987	-11.64776
H	-2.46385	4.17379	-10.79722
H	-0.64932	5.73891	-10.28508
H	-1.40941	0.17422	-12.71145
H	-2.74633	-1.79232	-12.11887
H	-4.62863	0.44479	-8.96874
H	-3.29891	2.40044	-9.55822
H	-2.54435	-3.25969	-10.34107
H	-3.03978	-5.09338	-8.81382
H	-6.66274	-3.12064	-7.609
H	-6.16479	-1.27677	-9.1446
H	-4.13617	-6.90496	-7.86848
H	-3.65799	-8.13497	-5.8038
H	-5.2492	-4.87426	-3.50021
H	-5.72493	-3.65056	-5.55431
H	-1.97931	-7.82127	-4.23491
H	-0.66019	-8.1064	-2.20544
H	-4.00986	-6.81976	0.16001
H	-5.33607	-6.53311	-1.88079
H	0.02537	-8.92166	-0.15123
H	1.84059	-8.18537	1.32143
H	-0.50595	-4.78397	2.50182
H	-2.31133	-5.51603	1.03731
C	0.83832	-6.39272	1.99183
C	2.02437	-5.71734	2.57491
C	9.76071	3.45611	0.63804
C	10.33652	3.15539	-0.60846
C	9.36839	4.78892	0.8591
C	9.80701	2.4461	1.72458

C	10.64328	4.15698	-1.52213
H	10.6571	2.1397	-0.81756
C	9.67547	5.7918	-0.05583
H	8.85371	5.0508	1.77905
C	9.73788	1.06316	1.47581
C	10.15714	2.84697	3.02558
C	10.38958	5.50931	-1.2346
H	11.19486	3.89585	-2.41972
H	9.39435	6.81679	0.16821
C	10.14606	0.1375	2.43162
H	9.40059	0.70887	0.50601
C	10.5648	1.92247	3.98019
H	10.22482	3.90501	3.25847
C	11.06757	6.5635	-2.02966
C	10.64259	0.55118	3.68123
H	10.11924	-0.92087	2.18883
H	10.93978	2.28363	4.93268
C	11.37829	6.40182	-3.39222
C	11.62748	7.67214	-1.37145
C	11.43597	-0.34299	4.56091
C	12.3177	7.21529	-4.01905
H	10.91007	5.60126	-3.95765
C	12.56558	8.48463	-1.99748
H	11.41636	7.8313	-0.31874
C	12.29753	-1.29172	3.98352
C	11.54207	-0.14041	5.94902
C	12.99037	8.22912	-3.31277
H	12.56416	7.03375	-5.0612
H	13.06136	9.2558	-1.41644
C	13.31032	-1.89121	4.72308
H	12.25094	-1.47478	2.91467
C	12.55612	-0.74079	6.68957
H	10.84753	0.5294	6.44777
C	14.24503	8.84945	-3.80659
C	13.51201	-1.57161	6.07697
H	14.02671	-2.5261	4.21142
H	12.63301	-0.5276	7.75186
C	15.16343	8.06861	-4.52959
C	14.67143	10.12541	-3.3951
C	14.8049	-1.91186	6.72177
C	16.48167	8.47616	-4.69785
H	14.87513	7.07663	-4.86295
C	15.99132	10.53347	-3.56358
H	13.97111	10.7905	-2.89809
C	15.54799	-3.054	6.37159
C	15.43581	-0.96433	7.54635
H	17.18706	7.79139	-5.15804
C	16.94701	9.68481	-4.15149
H	16.29496	11.50895	-3.19471
C	16.89564	-3.16633	6.70075
H	15.07578	-3.84548	5.79679
C	16.78169	-1.07656	7.8752
H	14.89903	-0.0667	7.83655
C	18.40753	9.90392	-4.00423
C	17.56358	-2.14182	7.39602
H	17.4487	-4.04313	6.37651
H	17.25894	-0.26345	8.41297
C	19.34651	9.38824	-4.91614
C	18.90671	10.44521	-2.80692
C	19.04332	-2.03192	7.42934
C	20.69316	9.28157	-4.58107
H	19.01134	9.02678	-5.88403
C	20.2516	10.33856	-2.47225

H	18.21524	10.84942	-2.07439
C	19.79041	-2.42419	6.30512
C	19.72831	-1.34245	8.4465
C	21.16425	9.6851	-3.31833
H	21.38255	8.83884	-5.2942
H	20.57339	10.66261	-1.4876
C	21.10866	-2.01661	6.13689
H	19.29908	-2.95565	5.49616
C	21.0482	-0.93436	8.27806
H	19.20767	-1.08488	9.36432
C	22.47459	9.24569	-2.777
C	21.7453	-1.19652	7.08452
H	21.61099	-2.24085	5.20113
H	21.53151	-0.36638	9.06776
C	22.95805	7.96439	-3.09379
C	23.15847	9.96048	-1.77667
C	22.98072	-0.46694	6.70469
C	23.96986	7.37052	-2.34837
H	22.45668	7.37765	-3.85698
C	24.17151	9.3658	-1.03018
H	22.86439	10.98148	-1.55104
C	23.92436	-0.99314	5.80369
C	23.12281	0.88401	7.06595
C	24.54865	8.02828	-1.24924
H	24.23069	6.33635	-2.54981
H	24.64815	9.93422	-0.23677
C	24.86276	-0.17398	5.18277
H	23.89577	-2.04975	5.55362
C	24.05991	1.7021	6.44575
H	22.41286	1.33002	7.75526
C	25.3228	7.24336	-0.25556
C	24.90152	1.20987	5.43322
H	25.54812	-0.60754	4.46019
H	24.0561	2.76451	6.66795
C	26.09005	6.11901	-0.61102
C	25.11876	7.47291	1.11615
C	25.59695	2.16492	4.53469
C	26.49823	5.19337	0.34482
H	26.33389	5.94438	-1.65498
C	25.52642	6.54843	2.07078
H	24.52969	8.32788	1.43281
C	25.62493	1.91638	3.15146
C	26.03907	3.42794	4.9689
C	26.15838	5.34848	1.70114
H	27.05252	4.31466	0.02789
H	25.24465	6.70652	3.10706
C	25.93074	2.92356	2.24365
H	25.28832	0.95594	2.77419
C	26.34516	4.4365	4.05989
H	26.10299	3.63708	6.03286
C	26.22387	4.22927	2.67372
H	25.82439	2.72208	1.18242
H	26.64194	5.41279	4.43215

Coordinates of R ([8]CPP)$^{2+}$ ($\mathbf{1}^{2+}$): RB3LYP/6-31G(d)
Closed-shell Singlet (R)

C	3.22739	5.43218	-0.98437
C	-1.01898	4.74006	-1.74981
C	-4.42877	2.25458	-2.02178
C	-3.56185	-1.99614	-2.16618
C	-1.12343	-5.38266	-1.67395
C	3.15481	-4.72227	-1.18038
C	6.4573	-2.21208	-0.50069
C	5.78336	2.09124	-0.79285
C	4.43746	4.76442	-0.81316
C	0.30578	5.12153	-1.56781
C	-3.73756	3.46152	-1.92694
C	-3.97753	-0.67131	-2.1765
C	-2.3262	-4.70647	-1.85955
C	1.83212	-5.09708	-1.38464
C	5.78636	-3.42827	-0.59925
C	6.168	0.75672	-0.73263
C	0.77711	5.54552	-0.31212
C	-3.10314	3.84252	-0.7299
C	-4.67446	-0.10042	-1.09725
C	-2.91703	-3.97312	-0.8128
C	1.0195	-5.5199	-0.31719
C	4.8673	-3.83488	0.38783
C	6.42231	0.12552	0.49836
C	4.69762	4.01485	0.35073
C	2.22118	5.38075	-0.00008
C	-1.93646	4.76237	-0.68423
C	-4.515	1.37442	-0.92606
C	-3.81517	-2.81357	-1.05275
C	-0.45282	-5.34999	-0.4355
C	3.73142	-4.75028	0.10212
C	6.24065	-1.3471	0.58963
C	5.63418	2.86062	0.37499
C	2.58142	4.83015	1.24299
C	-1.51945	5.40445	0.49788
C	-4.07304	1.86464	0.31648
C	-4.70451	-2.31257	-0.08708
C	-1.16231	-4.81277	0.6539
C	2.99097	-5.39101	1.11462
C	5.51093	-1.86732	1.67369
C	6.11756	2.29498	1.57125
C	3.78937	4.164	1.4141
C	-0.19336	5.78799	0.67947
C	-3.38426	3.06737	0.41005
C	-2.3665	-4.14188	0.46983
C	1.66594	-5.7675	0.90958
C	4.84051	-3.08125	1.57499
C	6.50174	0.95791	1.63184
H	3.03126	5.93235	-1.9293
H	-1.30034	4.27135	-2.68817
H	-4.83367	1.95395	-2.98502
H	-2.89979	-2.34457	-2.95289
H	-0.65885	-5.87344	-2.52521
H	3.69237	-4.25384	-1.99917
H	7.09438	-1.89387	-1.32195
H	5.44207	2.48893	-1.74375
H	5.15593	4.75976	-1.62884
H	1.01288	4.93717	-2.37105
H	-3.62447	4.07586	-2.81668
H	-3.61187	-0.02253	-2.96643

H	-2.77088	-4.68196	-2.8512
H	1.38558	-4.90762	-2.35591
H	5.91666	-4.03024	-1.4949
H	6.11339	0.16078	-1.63864
H	1.84656	4.78166	2.04068
H	-2.2222	5.53199	1.31729
H	-4.14775	1.23693	1.19765
H	-5.27274	-3.03418	0.52355
H	-0.69559	-4.77961	1.63368
H	3.42931	-5.52432	2.10034
H	5.33132	-1.24597	2.54579
H	6.1151	2.88366	2.48502
H	3.95362	3.61963	2.33905
H	0.10684	6.20735	1.63629
H	-2.92955	3.3303	1.3604
H	-2.80047	-3.60935	1.31109
H	1.1039	-6.18649	1.74025
H	4.16114	-3.36394	2.37343
H	6.78931	0.53567	2.59132
C	-5.15725	-0.98384	-0.09227
H	-5.8454	-0.59446	0.62866

Coordinates of ([8]CPP)$^{2+}$ ($\mathbf{1}^{2+}$): UB3LYP/6-31G(d)
Open-shell Singlet (U)

C	3.22739	5.43218	-0.98437
C	-1.01898	4.74006	-1.74981
C	-4.42877	2.25458	-2.02178
C	-3.56185	-1.99614	-2.16618
C	-1.12343	-5.38266	-1.67395
C	3.15481	-4.72227	-1.18038
C	6.4573	-2.21208	-0.50069
C	5.78336	2.09124	-0.79285
C	4.43746	4.76442	-0.81316
C	0.30578	5.12153	-1.56781
C	-3.73756	3.46152	-1.92694
C	-3.97753	-0.67131	-2.1765
C	-2.3262	-4.70647	-1.85955
C	1.83212	-5.09708	-1.38464
C	5.78636	-3.42827	-0.59925
C	6.168	0.75672	-0.73263
C	0.77711	5.54552	-0.31212
C	-3.10314	3.84252	-0.7299
C	-4.67446	-0.10042	-1.09725
C	-2.91703	-3.97312	-0.8128
C	1.0195	-5.5199	-0.31719
C	4.8673	-3.83488	0.38783
C	6.42231	0.12552	0.49836
C	4.69762	4.01485	0.35073
C	2.22118	5.38075	-0.00008
C	-1.93646	4.76237	-0.68423
C	-4.515	1.37442	-0.92606
C	-3.81517	-2.81357	-1.05275
C	-0.45282	-5.34999	-0.4355
C	3.73142	-4.75028	0.10212
C	6.24065	-1.3471	0.58963
C	5.63418	2.86062	0.37499
C	2.58142	4.83015	1.24299
C	-1.51945	5.40445	0.49788
C	-4.07304	1.86464	0.31648
C	-4.70451	-2.31257	-0.08708
C	-1.16231	-4.81277	0.6539
C	2.99097	-5.39101	1.11462
C	5.51093	-1.86732	1.67369
C	6.11756	2.29498	1.57125
C	3.78937	4.164	1.4141
C	-0.19336	5.78799	0.67947
C	-3.38426	3.06737	0.41005
C	-2.3665	-4.14188	0.46983
C	1.66594	-5.7675	0.90958
C	4.84051	-3.08125	1.57499
C	6.50174	0.95791	1.63184
H	3.03126	5.93235	-1.9293
H	-1.30034	4.27135	-2.68817
H	-4.83367	1.95395	-2.98502
H	-2.89979	-2.34457	-2.95289
H	-0.65885	-5.87344	-2.52521
H	3.69237	-4.25384	-1.99917
H	7.09438	-1.89387	-1.32195
H	5.44207	2.48893	-1.74375
H	5.15593	4.75976	-1.62884
H	1.01288	4.93717	-2.37105
H	-3.62447	4.07586	-2.81668
H	-3.61187	-0.02253	-2.96643

H	-2.77088	-4.68196	-2.8512
H	1.38558	-4.90762	-2.35591
H	5.91666	-4.03024	-1.4949
H	6.11339	0.16078	-1.63864
H	1.84656	4.78166	2.04068
H	-2.2222	5.53199	1.31729
H	-4.14775	1.23693	1.19765
H	-5.27274	-3.03418	0.52355
H	-0.69559	-4.77961	1.63368
H	3.42931	-5.52432	2.10034
H	5.33132	-1.24597	2.54579
H	6.1151	2.88366	2.48502
H	3.95362	3.61963	2.33905
H	0.10684	6.20735	1.63629
H	-2.92955	3.3303	1.3604
H	-2.80047	-3.60935	1.31109
H	1.1039	-6.18649	1.74025
H	4.16114	-3.36394	2.37343
H	6.78931	0.53567	2.59132
C	-5.15725	-0.98384	-0.09227
H	-5.8454	-0.59446	0.62866

Coordinates of ([8]CPP)$^{2+}$ ($\mathbf{1}^{2+}$): UB3LYP/6-31G(d)
Triplet (T)

C	3.22739	5.43218	-0.98437
C	-1.01898	4.74006	-1.74981
C	-4.42877	2.25458	-2.02178
C	-3.56185	-1.99614	-2.16618
C	-1.12343	-5.38266	-1.67395
C	3.15481	-4.72227	-1.18038
C	6.4573	-2.21208	-0.50069
C	5.78336	2.09124	-0.79285
C	4.43746	4.76442	-0.81316
C	0.30578	5.12153	-1.56781
C	-3.73756	3.46152	-1.92694
C	-3.97753	-0.67131	-2.1765
C	-2.3262	-4.70647	-1.85955
C	1.83212	-5.09708	-1.38464
C	5.78636	-3.42827	-0.59925
C	6.168	0.75672	-0.73263
C	0.77711	5.54552	-0.31212
C	-3.10314	3.84252	-0.7299
C	-4.67446	-0.10042	-1.09725
C	-2.91703	-3.97312	-0.8128
C	1.0195	-5.5199	-0.31719
C	4.8673	-3.83488	0.38783
C	6.42231	0.12552	0.49836
C	4.69762	4.01485	0.35073
C	2.22118	5.38075	-0.00008
C	-1.93646	4.76237	-0.68423
C	-4.515	1.37442	-0.92606
C	-3.81517	-2.81357	-1.05275
C	-0.45282	-5.34999	-0.4355
C	3.73142	-4.75028	0.10212
C	6.24065	-1.3471	0.58963
C	5.63418	2.86062	0.37499
C	2.58142	4.83015	1.24299
C	-1.51945	5.40445	0.49788
C	-4.07304	1.86464	0.31648
C	-4.70451	-2.31257	-0.08708
C	-1.16231	-4.81277	0.6539
C	2.99097	-5.39101	1.11462
C	5.51093	-1.86732	1.67369
C	6.11756	2.29498	1.57125
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C	-0.19336	5.78799	0.67947
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C	-2.3665	-4.14188	0.46983
C	1.66594	-5.7675	0.90958
C	4.84051	-3.08125	1.57499
C	6.50174	0.95791	1.63184
H	3.03126	5.93235	-1.9293
H	-1.30034	4.27135	-2.68817
H	-4.83367	1.95395	-2.98502
H	-2.89979	-2.34457	-2.95289
H	-0.65885	-5.87344	-2.52521
H	3.69237	-4.25384	-1.99917
H	7.09438	-1.89387	-1.32195
H	5.44207	2.48893	-1.74375
H	5.15593	4.75976	-1.62884
H	1.01288	4.93717	-2.37105
H	-3.62447	4.07586	-2.81668
H	-3.61187	-0.02253	-2.96643

H	-2.77088	-4.68196	-2.8512
H	1.38558	-4.90762	-2.35591
H	5.91666	-4.03024	-1.4949
H	6.11339	0.16078	-1.63864
H	1.84656	4.78166	2.04068
H	-2.2222	5.53199	1.31729
H	-4.14775	1.23693	1.19765
H	-5.27274	-3.03418	0.52355
H	-0.69559	-4.77961	1.63368
H	3.42931	-5.52432	2.10034
H	5.33132	-1.24597	2.54579
H	6.1151	2.88366	2.48502
H	3.95362	3.61963	2.33905
H	0.10684	6.20735	1.63629
H	-2.92955	3.3303	1.3604
H	-2.80047	-3.60935	1.31109
H	1.1039	-6.18649	1.74025
H	4.16114	-3.36394	2.37343
H	6.78931	0.53567	2.59132
C	-5.15725	-0.98384	-0.09227
H	-5.8454	-0.59446	0.62866

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