# Electronic Supplementary Information for

# Significant Structural Relaxations of Excited [*n*]Cycloparaphenylene Dications (*n* = 5 - 9)

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**Fluorescence decay of [6]CPP$^{2+}$.**

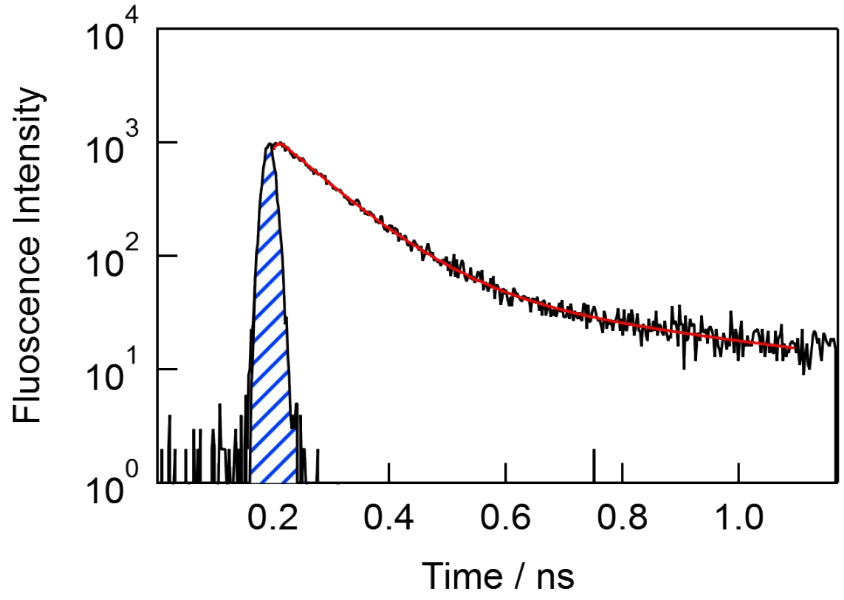
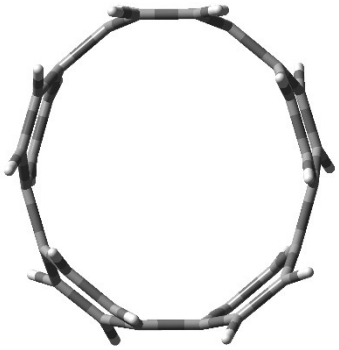
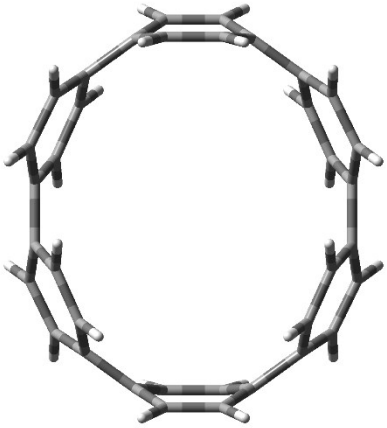



**Figure S1.** Fluorescence decay profile of [6]CPP$^{2+}$ around 800 nm in $CH_2Cl_2$ upon excitation at 460 nm. Red line is a fitted curve assuming two exponential function with 91 ps (96%) and 640 ps (4%) of lifetimes. Hatched part indicates IRF.

**Structures of [n]CPP$^{2+}$ in the $S_1$ state estimated at UB3LYP/6-31G(d) level**

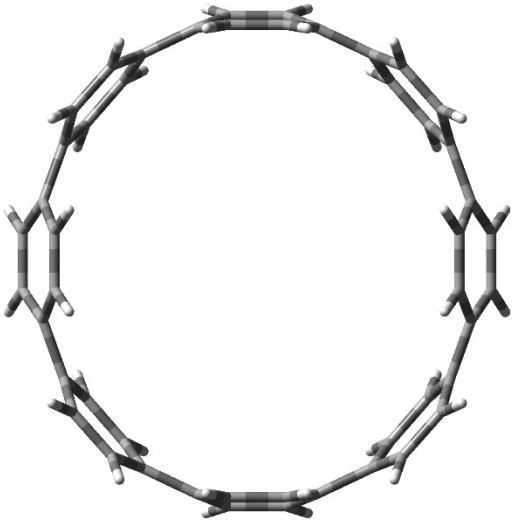


[5]CPP



[6]CPP

[7]CPP



[8]CPP

[9]CPP

**Figure S2.** Structures of [n]CPP$^{2+}$ in the S1 state estimated at UB3LYP/6-31G(d) level

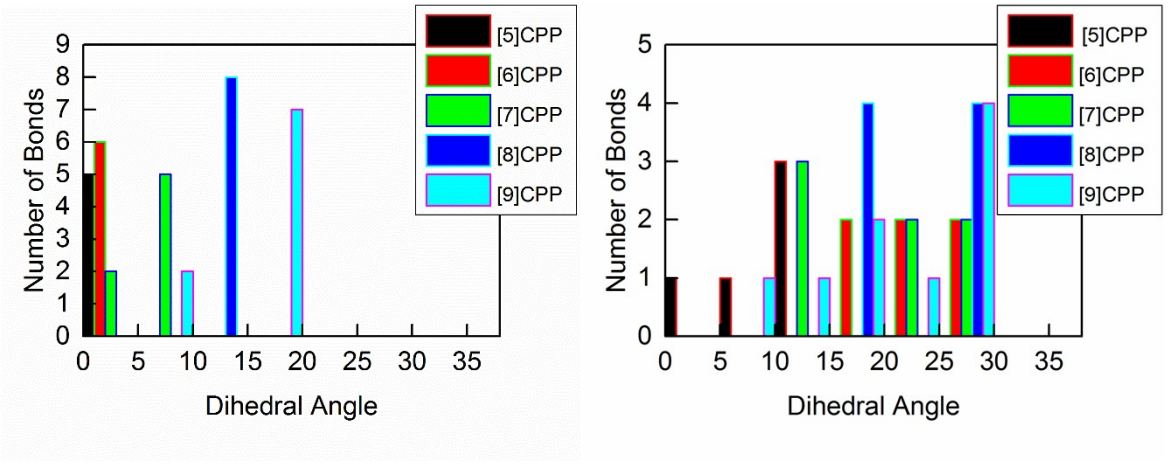



**Figure S3.** Distribution of dihedral angles of [*n*]CPP$^{2+}$ in (left) $S_0$ and (right) $S_1$ states estimated at UB3LYP/6-31G(d) level.

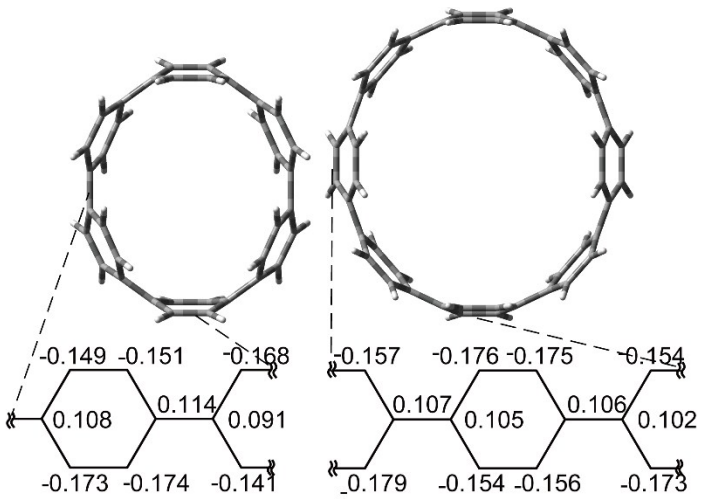



**Figure S4.** Charge distribution of [6]CPP$^{2+}$ (left) and (right) [8]CPP$^{2+}$.

**Optimized structures of [*n*]CPP$^{2+}$.**

Table S1. XYZ coordinate of [5]CPP$^{2+}$($D_0$) by B3LYP/6-31G(d).

| | X | Y | Z |
|---|---|---|---|
| C | 1.98682600 | 2.86315900 | -1.21315400 |
| C | 2.93789500 | 1.87459400 | -1.21320500 |
| C | 3.25507900 | 1.17800700 | 0.00017500 |
| C | 2.93787100 | 1.87444700 | 1.21362700 |
| C | 1.98680100 | 2.86302000 | 1.21368100 |
| C | 1.30309400 | 3.20700300 | 0.00028300 |
| C | 3.45296200 | -0.24832900 | 0.00008200 |
| C | 3.33736900 | -1.00481600 | -1.21338000 |
| C | 3.33736800 | -1.00498500 | 1.21344800 |
| C | 2.69085300 | -2.21470800 | -1.21345700 |
| C | 2.69085300 | -2.21487300 | 1.21336000 |
| C | 2.12633800 | -2.73162600 | -0.00008800 |

| | | | |
|---|---|---|---|
| C | 0.83086200 | -3.36033200 | -0.00016400 |
| C | 0.07564000 | -3.48386700 | -1.21365000 |
| C | 0.07551600 | -3.48388000 | 1.21323900 |
| C | -1.27485900 | -3.24306100 | -1.21373300 |
| C | -1.27498200 | -3.24307800 | 1.21317900 |
| C | -1.94092200 | -2.86611600 | -0.00030500 |
| C | -2.93947100 | -1.82856500 | -0.00030500 |
| C | -3.29086000 | -1.14871100 | 1.21312200 |
| C | -3.29055300 | -1.14846900 | -1.21368000 |
| C | -3.47918600 | 0.21010800 | 1.21324200 |
| C | -3.47888800 | 0.21034900 | -1.21356300 |
| C | -3.32602100 | 0.96010600 | -0.00006700 |
| C | -0.11454500 | 3.45969700 | 0.00028600 |
| C | -0.87495800 | 3.37309900 | 1.21371400 |
| C | -0.87495700 | 3.37344700 | -1.21316300 |
| C | -2.10897100 | 2.77391400 | 1.21363800 |
| C | -2.10897400 | 2.77427000 | -1.21326400 |
| C | -2.64727300 | 2.23010700 | 0.00010300 |
| H | 0.57931200 | -3.63801300 | 2.16096700 |
| H | -1.80096000 | -3.21349600 | -2.16143500 |
| H | -1.80116200 | -3.21345700 | 2.16083400 |
| H | -3.28195100 | -1.67573900 | 2.16070300 |
| H | -3.28137300 | -1.67529300 | -2.16137100 |
| H | 1.66989000 | 3.28419900 | -2.16078500 |
| H | 3.34643100 | 1.54171300 | -2.16085900 |
| H | 3.34636800 | 1.54145400 | 2.16125700 |
| H | 1.66983800 | 3.28392300 | 2.16136600 |

| | | | |
|---|---|---|---|
| H | 3.63987100 | -0.57325600 | -2.16100700 |
| H | 3.63990700 | -0.57355800 | 2.16112400 |
| H | 2.50035500 | -2.70593400 | -2.16115700 |
| H | 2.50039500 | -2.70625900 | 2.16098300 |
| H | 0.57954300 | -3.63803500 | -2.16131900 |
| H | -3.61389600 | 0.71950500 | 2.16092500 |
| H | -3.61332400 | 0.71994400 | -2.16117700 |
| H | -0.43205300 | 3.65849900 | 2.16141500 |
| H | -0.43207600 | 3.65913600 | -2.16078800 |
| H | -2.60728600 | 2.60228700 | 2.16127400 |
| H | -2.60728600 | 2.60293600 | -2.16095600 |

Sum of electronic and zero-point Energies = -1154.151475 Hartree

Table S2. XYZ coordinate of [6]CPP$^{2+}$($D_0$) by B3LYP/6-31G(d).

| | X | Y | Z |
|---|---|---|---|
| C | -2.67077000 | 3.17993700 | -0.00001600 |
| C | -3.21948600 | 2.65187400 | -1.21040200 |
| C | -3.90622400 | 1.46205600 | -1.21040300 |
| C | -4.08906400 | 0.72284900 | -0.00002100 |
| C | -3.90649200 | 1.46220900 | 1.21030300 |
| C | -3.21976300 | 2.65203300 | 1.21031000 |
| C | -4.08906400 | -0.72284900 | 0.00002700 |
| C | -1.41855900 | 3.90252000 | 0.00002700 |
| C | -3.90622100 | -1.46205800 | 1.21040700 |
| C | -3.21948300 | -2.65187600 | 1.21040300 |
| C | -2.67077000 | -3.17993800 | 0.00001400 |
| C | -3.21976600 | -2.65203100 | -1.21031000 |

| | | | |
|---|---|---|---|
| C | -3.90649500 | -1.46220700 | -1.21029800 |
| C | -0.68688200 | 4.11339100 | 1.21042500 |
| C | 0.68688700 | 4.11339200 | 1.21042200 |
| C | 1.41855900 | 3.90252000 | 0.00002100 |
| C | 0.68688300 | 4.11372500 | -1.21031500 |
| C | -0.68688900 | 4.11372600 | -1.21031200 |
| C | -1.41855900 | -3.90252000 | -0.00003100 |
| C | -0.68688200 | -4.11338900 | -1.21043000 |
| C | 0.68688700 | -4.11338900 | -1.21042700 |
| C | 1.41855900 | -3.90252000 | -0.00002500 |
| C | 0.68688300 | -4.11372800 | 1.21031000 |
| C | -0.68688900 | -4.11372800 | 1.21030700 |
| C | 2.67077000 | -3.17993700 | 0.00002200 |
| C | 3.21948200 | -2.65187300 | 1.21041000 |
| C | 3.90622000 | -1.46205500 | 1.21041100 |
| C | 4.08906400 | -0.72284900 | 0.00002900 |
| C | 3.90649600 | -1.46221100 | -1.21029400 |
| C | 3.21976700 | -2.65203500 | -1.21030300 |
| C | 4.08906400 | 0.72284900 | -0.00002300 |
| C | 3.90622300 | 1.46205200 | -1.21040700 |
| C | 3.21948500 | 2.65187000 | -1.21040900 |
| C | 2.67077000 | 3.17993700 | -0.00002400 |
| C | 3.21976400 | 2.65203700 | 1.21030300 |
| C | 3.90649200 | 1.46221300 | 1.21029800 |
| H | -3.00563000 | 3.12488100 | -2.16190800 |
| H | -4.20888300 | 1.04030400 | -2.16190500 |
| H | -4.20941500 | 1.04060100 | 2.16178600 |

| | | | |
|---|---|---|---|
| H | -3.00620100 | 3.12520900 | 2.16179900 |
| H | -4.20887800 | -1.04030800 | 2.16191100 |
| H | -3.00562500 | -3.12488500 | 2.16190700 |
| H | -3.00620600 | -3.12520400 | -2.16180000 |
| H | -4.20942000 | -1.04059700 | -2.16178000 |
| H | -1.20343700 | 4.16455400 | 2.16193800 |
| H | 1.20344600 | 4.16455400 | 2.16193300 |
| H | 1.20344300 | 4.16523300 | -2.16180900 |
| H | -1.20345300 | 4.16523400 | -2.16180400 |
| H | -1.20343600 | -4.16455000 | -2.16194300 |
| H | 1.20344600 | -4.16455100 | -2.16193800 |
| H | 1.20344300 | -4.16523700 | 2.16180400 |
| H | -1.20345300 | -4.16523700 | 2.16179900 |
| H | 3.00562400 | -3.12487900 | 2.16191600 |
| H | 4.20887700 | -1.04030200 | 2.16191400 |
| H | 4.20942100 | -1.04060300 | -2.16177700 |
| H | 3.00620700 | -3.12521100 | -2.16179200 |
| H | 4.20888200 | 1.04029800 | -2.16190800 |
| H | 3.00562800 | 3.12487400 | -2.16191700 |
| H | 3.00620200 | 3.12521500 | 2.16179100 |
| H | 4.20941600 | 1.04060700 | 2.16178300 |

Sum of electronic and zero-point Energies= -1385.165117 Hartree

Table S3. XYZ coordinate of [7]CPP$^{2+}$($D_0$) by B3LYP/6-31G(d).

| | X | Y | Z |
|---|---|---|---|
| C | -1.41573700 | 4.61514200 | -0.02321000 |

| | | | |
|---|---|---|---|
| C | -0.68049600 | 4.89260000 | 1.16847700 |
| C | 0.69480100 | 4.88813900 | 1.17105000 |
| C | 1.43229500 | 4.60663200 | -0.01798700 |
| C | 0.69916300 | 4.68309200 | -1.23725100 |
| C | -0.67732800 | 4.68665300 | -1.23977400 |
| C | 2.73788300 | 3.97376900 | 0.01883600 |
| C | 3.24977700 | 3.44157400 | 1.23708000 |
| C | 4.10549400 | 2.36306200 | 1.23746500 |
| C | 4.50758700 | 1.74296300 | 0.01963200 |
| C | 4.27189400 | 2.49510400 | -1.17026100 |
| C | 3.41705600 | 3.57251500 | -1.17067200 |
| C | 4.82615700 | 0.32729800 | -0.01630800 |
| C | 4.93295400 | -0.45391500 | 1.17339600 |
| C | 4.62218400 | -1.79367600 | 1.17245100 |
| C | 4.18275400 | -2.44660300 | -0.01827100 |
| C | 4.41986000 | -1.74577200 | -1.23568300 |
| C | 4.73110700 | -0.40468100 | -1.23472600 |
| C | 3.27400200 | -3.57766100 | 0.01636300 |
| C | 2.64372700 | -3.96314400 | 1.23466000 |
| C | 1.40145100 | -4.55593900 | 1.23555500 |
| C | 0.70398700 | -4.80527400 | 0.01819700 |
| C | 1.48792800 | -4.73903700 | -1.17294800 |
| C | 2.72873900 | -4.14591100 | -1.17389400 |
| C | -0.74649400 | -4.80165400 | -0.01791500 |
| C | -1.52966600 | -4.69918200 | 1.17060200 |
| C | -2.76748900 | -4.10000000 | 1.15572400 |

| | | | |
|---|---|---|---|
| C | -3.31011500 | -3.55848900 | -0.04838400 |
| C | -2.68188400 | -3.98165200 | -1.25631600 |
| C | -1.44431200 | -4.58285100 | -1.24160200 |
| C | -4.21231900 | -2.42255700 | -0.03209300 |
| C | -4.54939300 | -1.76471700 | 1.18822500 |
| C | -4.85066900 | -0.42284500 | 1.21262700 |
| C | -4.83830800 | 0.35720800 | 0.01825700 |
| C | -4.85359100 | -0.37991200 | -1.20310400 |
| C | -4.55063100 | -1.72142000 | -1.22749500 |
| C | -4.50985500 | 1.77013400 | 0.03746200 |
| C | -4.12225600 | 2.41805600 | 1.24686500 |
| C | -3.26100800 | 3.49113200 | 1.23439500 |
| C | -2.72507200 | 3.99085900 | 0.01167700 |
| C | -3.38995900 | 3.56644000 | -1.17753100 |
| C | -4.25230100 | 2.49515200 | -1.16490800 |
| H | -1.19864100 | 5.03731400 | 2.10975800 |
| H | 1.21114200 | 5.03070800 | 2.11373400 |
| H | 1.21199100 | 4.61211200 | -2.18912100 |
| H | -1.18654400 | 4.62035500 | -2.19385400 |
| H | 2.87381600 | 3.79601700 | 2.18949800 |
| H | 4.36480000 | 1.91665600 | 2.19012900 |
| H | 4.70968100 | 2.18104600 | -2.11119100 |
| H | 3.21117300 | 4.06969900 | -2.11197700 |
| H | 5.19203400 | 0.01687100 | 2.11513000 |
| H | 4.64710200 | -2.33154800 | 2.11356000 |
| H | 4.23424800 | -2.22666600 | -2.18876400 |

| | | | |
|---|---|---|---|
| H | 4.77635000 | 0.11021100 | -2.18706200 |
| H | 3.07655800 | -3.68163400 | 2.18729300 |
| H | 0.91287200 | -4.71660100 | 2.18920300 |
| H | 1.08213200 | -5.08964600 | -2.11517100 |
| H | 3.25662800 | -4.05170200 | -2.11624100 |
| H | -1.12442900 | -5.02277500 | 2.12258700 |
| H | -3.28735600 | -3.97002000 | 2.09789300 |
| H | -3.11970500 | -3.73724600 | -2.21679600 |
| H | -0.95968500 | -4.77909500 | -2.19069900 |
| H | -4.47344600 | -2.29000800 | 2.13303800 |
| H | -5.00808600 | 0.05035700 | 2.17481400 |
| H | -5.00308600 | 0.12871700 | -2.14824100 |
| H | -4.48311100 | -2.21462000 | -2.19012100 |
| H | -4.41152800 | 2.00636500 | 2.20643600 |
| H | -2.90539700 | 3.87261400 | 2.18421700 |
| H | -3.16343200 | 4.03558000 | -2.12824200 |
| H | -4.66823000 | 2.15828200 | -2.10746300 |

Sum of electronic and zero-point Energies = -1616.169565 Hartree

Table S4. XYZ coordinate of [8]CPP$^{2+}$($D_0$) by B3LYP/6-31G(d).

| | X | Y | Z |
|---|---|---|---|
| C | 5.34311700 | 1.42584100 | -0.02451100 |
| C | 5.65469300 | 0.68856200 | 1.15395500 |
| C | 5.65469300 | -0.68856300 | 1.15395600 |
| C | 5.34311700 | -1.42584200 | -0.02451000 |

| | | | |
|---|---|---|---|
| C | 5.33035200 | -0.68937400 | -1.23987200 |
| C | 5.33035200 | 0.68937200 | -1.23987300 |
| C | 4.78646200 | -2.77005200 | 0.02450800 |
| C | 4.25683900 | -3.28191800 | 1.23988600 |
| C | 3.28191800 | -4.25683800 | 1.23988600 |
| C | 2.77005300 | -4.78646200 | 0.02450800 |
| C | 3.51170400 | -4.48547300 | -1.15396600 |
| C | 4.48547300 | -3.51170300 | -1.15396600 |
| C | 1.42584200 | -5.34311700 | -0.02451000 |
| C | 0.68856300 | -5.65469200 | 1.15395600 |
| C | -0.68856200 | -5.65469200 | 1.15395600 |
| C | -1.42584100 | -5.34311700 | -0.02451100 |
| C | -0.68937100 | -5.33035300 | -1.23987300 |
| C | 0.68937500 | -5.33035300 | -1.23987200 |
| C | -2.77005200 | -4.78646200 | 0.02450500 |
| C | -3.28192000 | -4.25684100 | 1.23988400 |
| C | -4.25684100 | -3.28192000 | 1.23988400 |
| C | -4.78646200 | -2.77005200 | 0.02450500 |
| C | -4.48547100 | -3.51170100 | -1.15396900 |
| C | -3.51170100 | -4.48547100 | -1.15396900 |
| C | -5.34311700 | -1.42584100 | -0.02451100 |
| C | -5.65469200 | -0.68856200 | 1.15395600 |
| C | -5.65469200 | 0.68856300 | 1.15395600 |
| C | -5.34311700 | 1.42584200 | -0.02451000 |
| C | -5.33035300 | 0.68937500 | -1.23987200 |
| C | -5.33035300 | -0.68937100 | -1.23987300 |

| | | | |
|---|---|---|---|
| C | -4.78646200 | 2.77005300 | 0.02450800 |
| C | -4.25683900 | 3.28191800 | 1.23988600 |
| C | -3.28191800 | 4.25683900 | 1.23988600 |
| C | -2.77005200 | 4.78646200 | 0.02450800 |
| C | -3.51170300 | 4.48547300 | -1.15396600 |
| C | -4.48547300 | 3.51170400 | -1.15396600 |
| C | -1.42584200 | 5.34311700 | -0.02451000 |
| C | -0.68856300 | 5.65469300 | 1.15395600 |
| C | 0.68856200 | 5.65469200 | 1.15395600 |
| C | 1.42584100 | 5.34311700 | -0.02451100 |
| C | 0.68937200 | 5.33035200 | -1.23987300 |
| C | -0.68937400 | 5.33035200 | -1.23987200 |
| C | 2.77005200 | 4.78646100 | 0.02450600 |
| C | 3.28191900 | 4.25684000 | 1.23988400 |
| C | 4.25684000 | 3.28191900 | 1.23988400 |
| C | 4.78646100 | 2.77005200 | 0.02450600 |
| C | 4.48547100 | 3.51170100 | -1.15396900 |
| C | 3.51170100 | 4.48547100 | -1.15396900 |
| H | 5.84549100 | 1.20812000 | 2.08668300 |
| H | 5.84549100 | -1.20812000 | 2.08668400 |
| H | 5.18824200 | -1.20031200 | -2.18492000 |
| H | 5.18824200 | 1.20030800 | -2.18492100 |
| H | 4.51774500 | -2.82019700 | 2.18493100 |
| H | 2.82019800 | -4.51774500 | 2.18493100 |
| H | 3.27920500 | -4.98776200 | -2.08668800 |
| H | 4.98776200 | -3.27920500 | -2.08668800 |

| | | | |
|---|---|---|---|
| H | 1.20812000 | -5.84549000 | 2.08668400 |
| H | -1.20812000 | -5.84549000 | 2.08668300 |
| H | -1.20030800 | -5.18824400 | -2.18492100 |
| H | 1.20031200 | -5.18824300 | -2.18491900 |
| H | -2.82020100 | -4.51774900 | 2.18492900 |
| H | -4.51774900 | -2.82020100 | 2.18492900 |
| H | -4.98775800 | -3.27920100 | -2.08669300 |
| H | -3.27920100 | -4.98775800 | -2.08669300 |
| H | -5.84549000 | -1.20812000 | 2.08668300 |
| H | -5.84549000 | 1.20812000 | 2.08668400 |
| H | -5.18824400 | 1.20031200 | -2.18492000 |
| H | -5.18824400 | -1.20030800 | -2.18492100 |
| H | -4.51774500 | 2.82019800 | 2.18493100 |
| H | -2.82019700 | 4.51774500 | 2.18493100 |
| H | -3.27920500 | 4.98776200 | -2.08668900 |
| H | -4.98776200 | 3.27920500 | -2.08668800 |
| H | -1.20812000 | 5.84549000 | 2.08668400 |
| H | 1.20812000 | 5.84549000 | 2.08668300 |
| H | 1.20030800 | 5.18824200 | -2.18492100 |
| H | -1.20031200 | 5.18824200 | -2.18492000 |
| H | 2.82020000 | 4.51774800 | 2.18492900 |
| H | 4.51774800 | 2.82020000 | 2.18492900 |
| H | 4.98775900 | 3.27920100 | -2.08669200 |
| H | 3.27920100 | 4.98775900 | -2.08669200 |

Sum of electronic and zero-point Energies = -1847.168436 Hartree

Table S5. XYZ coordinate of [9]CPP$^{2+}$($D_0$) by B3LYP/6-31G(d).

| | X | Y | Z |
|---|---|---|---|
| C | -0.51093000 | 6.18950800 | 0.04862400 |
| C | 0.25419600 | 6.41862000 | -1.12786800 |
| C | 1.61737500 | 6.21264100 | -1.14527800 |
| C | 2.31011300 | 5.76536400 | 0.01326900 |
| C | 1.58453700 | 5.78966100 | 1.23210800 |
| C | 0.21956400 | 5.99460700 | 1.24904200 |
| C | 3.59013500 | 5.07037700 | -0.06337900 |
| C | 4.00707600 | 4.47929000 | -1.28420300 |
| C | 4.91979300 | 3.44552700 | -1.30472400 |
| C | 5.48625800 | 2.93345600 | -0.10725400 |
| C | 5.26372300 | 3.70217400 | 1.06963900 |
| C | 4.34530500 | 4.73036100 | 1.09203000 |
| C | 6.02838500 | 1.57985100 | -0.05947000 |
| C | 6.18941900 | 0.79273500 | -1.23210300 |
| C | 6.22380300 | -0.58416500 | -1.17366400 |
| C | 6.10030900 | -1.27682700 | 0.06172300 |
| C | 6.21739600 | -0.48262600 | 1.23480000 |
| C | 6.18242000 | 0.89426800 | 1.17637000 |
| C | 5.08797800 | -3.19798800 | 1.30524800 |
| C | 4.22804600 | -4.27602500 | 1.28370500 |
| C | 3.83991800 | -4.88511600 | 0.06220300 |
| C | 4.57626900 | -4.50594200 | -1.09315200 |
| C | 5.44217700 | -3.43318800 | -1.06974100 |
| C | 2.59607300 | -5.64288000 | -0.01481100 |

| | | | |
|---|---|---|---|
| C | 1.87238800 | -5.70241100 | -1.23357600 |
| C | 0.51935300 | -5.97518300 | -1.25052300 |
| C | -0.20035700 | -6.20711500 | -0.05016500 |
| C | 0.57542200 | -6.39862900 | 1.12607500 |
| C | 1.92665500 | -6.12503500 | 1.14347200 |
| C | -1.64331800 | -5.99182500 | -0.00652900 |
| C | -2.26773600 | -5.59575900 | 1.20399300 |
| C | -3.48092000 | -4.93726100 | 1.20265000 |
| C | -4.15132700 | -4.63088800 | -0.00926400 |
| C | -3.64911200 | -5.25364900 | -1.18472500 |
| C | -2.43670400 | -5.91077300 | -1.18359700 |
| C | 5.62692800 | -2.65605200 | 0.10817600 |
| C | -5.11812700 | -3.53803000 | -0.05673000 |
| C | -5.31699100 | -2.81432100 | -1.26033700 |
| C | -5.82298600 | -1.52998200 | -1.24916800 |
| C | -6.16298200 | -0.88330000 | -0.03344900 |
| C | -6.20243200 | -1.70086700 | 1.12897000 |
| C | -5.69794500 | -2.98430400 | 1.11755500 |
| C | -6.19960100 | 0.57442600 | 0.03496100 |
| C | -5.89186400 | 1.23748900 | 1.25045900 |
| C | -5.45093200 | 2.54560500 | 1.26126200 |
| C | -5.28916500 | 3.27820000 | 0.05747300 |
| C | -5.84104200 | 2.69594700 | -1.11646900 |
| C | -6.28059400 | 1.38885600 | -1.12750700 |
| C | -4.37829800 | 4.41806100 | 0.00933100 |
| C | -3.90756700 | 5.06572600 | 1.18436200 |

| | | | |
|---|---|---|---|
| C | -2.72949800 | 5.78260900 | 1.18259500 |
| C | -1.94137100 | 5.90251900 | 0.00532100 |
| C | -2.54549400 | 5.47514200 | -1.20485100 |
| C | -3.72431200 | 4.75695300 | -1.20289100 |
| H | -0.23867700 | 6.72141700 | -2.04555900 |
| H | 2.15490000 | 6.35979300 | -2.07604100 |
| H | 2.07397300 | 5.51831900 | 2.16046600 |
| H | -0.30476600 | 5.87571400 | 2.19021500 |
| H | 3.51775600 | 4.74923800 | -2.21296000 |
| H | 5.11071500 | 2.95680300 | -2.25242500 |
| H | 5.78073400 | 3.45396700 | 1.98975300 |
| H | 4.17452000 | 5.25550800 | 2.02581300 |
| H | 6.22057400 | 1.26445200 | -2.20743300 |
| H | 6.25274400 | -1.13312900 | -2.10757100 |
| H | 6.26837300 | -0.95204900 | 2.21037500 |
| H | 6.17966000 | 1.44394200 | 2.11031200 |
| H | 5.25558000 | -2.70243900 | 2.25380200 |
| H | 3.75396700 | -4.57182200 | 2.21249200 |
| H | 4.43113200 | -5.03731200 | -2.02774300 |
| H | 5.94493900 | -3.15785600 | -1.99001300 |
| H | 2.34752800 | -5.40639800 | -2.16181400 |
| H | -0.01037100 | -5.88198200 | -2.19156800 |
| H | 0.09837300 | -6.72622400 | 2.04361300 |
| H | 2.47094500 | -6.24591000 | 2.07408200 |
| H | -1.73796300 | -5.69108300 | 2.14479000 |
| H | -3.85114500 | -4.54415900 | 2.14243600 |

| | | | |
|---|---|---|---|
| H | -4.20118200 | -5.18125600 | -2.11572300 |
| H | -2.07315700 | -6.33460200 | -2.11369200 |
| H | -4.95332900 | -3.21317300 | -2.20028500 |
| H | -5.83443700 | -0.97546700 | -2.18047800 |
| H | -6.59688000 | -1.30402600 | 2.05841900 |
| H | -5.71147400 | -3.55724400 | 2.03862200 |
| H | -5.87503000 | 0.68320800 | 2.18183100 |
| H | -5.10726400 | 2.96231100 | 2.20098800 |
| H | -5.88368300 | 3.26735600 | -2.03759700 |
| H | -6.65501700 | 0.97259400 | -2.05674800 |
| H | -4.45510800 | 4.96629400 | 2.11554200 |
| H | -2.38736700 | 6.22452500 | 2.11239500 |
| H | -2.02136800 | 5.59631600 | -2.14583700 |
| H | -4.07464700 | 4.34539000 | -2.14239800 |

Sum of electronic and zero-point Energies = -2078.163583 Hartree

Table S6. XYZ coordinate of [5]CPP$^{2+}$($D_0$) by UB3LYP/6-31G(d).

| | X | Y | Z |
|---|---|---|---|
| C | 1.90925600 | 2.91543900 | -1.21315300 |
| C | 2.88652300 | 1.95276600 | -1.21320400 |
| C | 3.22229200 | 1.26494600 | 0.00017500 |
| C | 2.88650000 | 1.95261500 | 1.21362900 |
| C | 1.90923200 | 2.91529700 | 1.21368200 |
| C | 1.21653900 | 3.24080900 | 0.00028400 |
| C | 3.45838800 | -0.15556800 | 0.00008100 |

| | | | |
|---|---|---|---|
| C | 3.36313500 | -0.91488200 | -1.21338100 |
| C | 3.36314000 | -0.91505200 | 1.21344700 |
| C | 2.74933000 | -2.14169200 | -1.21345800 |
| C | 2.74933700 | -2.14185900 | 1.21335900 |
| C | 2.19890000 | -2.67358300 | -0.00008900 |
| C | 0.92076300 | -3.33682900 | -0.00016400 |
| C | 0.16912800 | -3.48058700 | -1.21365000 |
| C | 0.16900500 | -3.48060200 | 1.21323800 |
| C | -1.18734500 | -3.27610400 | -1.21373200 |
| C | -1.18746700 | -3.27612400 | 1.21318000 |
| C | -1.86328600 | -2.91716800 | -0.00030500 |
| C | -2.88932300 | -1.90679300 | -0.00030400 |
| C | -3.25883500 | -1.23661800 | 1.21312200 |
| C | -3.25853700 | -1.23637000 | -1.21368000 |
| C | -3.48357200 | 0.11665700 | 1.21324300 |
| C | -3.48328300 | 0.11690500 | -1.21356300 |
| C | -3.35059700 | 0.87049800 | -0.00006700 |
| C | -0.20736800 | 3.45536900 | 0.00028500 |
| C | -0.96518700 | 3.34840800 | 1.21371200 |
| C | -0.96519300 | 3.34875300 | -1.21316200 |
| C | -2.18267900 | 2.71632800 | 1.21363600 |
| C | -2.18268900 | 2.71668100 | -1.21326400 |
| C | -2.70619000 | 2.15826200 | 0.00010200 |
| H | 0.67675500 | -3.62116300 | 2.16096600 |
| H | -1.71405000 | -3.26066600 | -2.16143300 |
| H | -1.71425200 | -3.26063200 | 2.16083400 |

| | | | |
|---|---|---|---|
| H | -3.23578200 | -1.76321600 | 2.16070400 |
| H | -3.23521900 | -1.76275700 | -2.16137000 |
| H | 1.58113400 | 3.32782200 | -2.16078500 |
| H | 3.30384500 | 1.63096600 | -2.16085700 |
| H | 3.30378300 | 1.63069900 | 2.16125800 |
| H | 1.58108400 | 3.32753800 | 2.16136800 |
| H | 3.65394000 | -0.47535600 | -2.16100900 |
| H | 3.65398900 | -0.47566100 | 2.16112400 |
| H | 2.57207900 | -2.63785200 | -2.16115800 |
| H | 2.57213300 | -2.63817900 | 2.16098300 |
| H | 0.67698500 | -3.62117900 | -2.16131800 |
| H | -3.63190400 | 0.62225500 | 2.16092700 |
| H | -3.63134700 | 0.62270700 | -2.16117800 |
| H | -0.53010100 | 3.64559400 | 2.16141300 |
| H | -0.53013600 | 3.64622400 | -2.16078700 |
| H | -2.67621200 | 2.53140200 | 2.16127200 |
| H | -2.67622500 | 2.53204500 | -2.16095700 |

Sum of electronic and zero-point Energies = -1154.151483 Hartree

Table S7. XYZ coordinate of [6]CPP$^{2+}$($D_0$) by UB3LYP/6-31G(d).

| | X | Y | Z |
|---|---|---|---|
| C | -2.67077000 | 3.17993700 | -0.00001600 |
| C | -3.21948600 | 2.65187400 | -1.21040200 |
| C | -3.90622400 | 1.46205600 | -1.21040300 |
| C | -4.08906400 | 0.72284900 | -0.00002100 |

| | | | |
|---|---|---|---|
| C | -3.90649200 | 1.46220900 | 1.21030300 |
| C | -3.21976300 | 2.65203300 | 1.21031000 |
| C | -4.08906400 | -0.72284900 | 0.00002700 |
| C | -1.41855900 | 3.90252000 | 0.00002700 |
| C | -3.90622100 | -1.46205800 | 1.21040700 |
| C | -3.21948300 | -2.65187600 | 1.21040300 |
| C | -2.67077000 | -3.17993800 | 0.00001400 |
| C | -3.21976600 | -2.65203100 | -1.21031000 |
| C | -3.90649500 | -1.46220700 | -1.21029800 |
| C | -0.68688200 | 4.11339100 | 1.21042500 |
| C | 0.68688700 | 4.11339200 | 1.21042200 |
| C | 1.41855900 | 3.90252000 | 0.00002100 |
| C | 0.68688300 | 4.11372500 | -1.21031500 |
| C | -0.68688900 | 4.11372600 | -1.21031200 |
| C | -1.41855900 | -3.90252000 | -0.00003100 |
| C | -0.68688200 | -4.11338900 | -1.21043000 |
| C | 0.68688800 | -4.11338900 | -1.21042700 |
| C | 1.41855900 | -3.90252000 | -0.00002500 |
| C | 0.68688300 | -4.11372800 | 1.21031000 |
| C | -0.68688900 | -4.11372800 | 1.21030700 |
| C | 2.67077000 | -3.17993700 | 0.00002200 |
| C | 3.21948200 | -2.65187300 | 1.21041000 |
| C | 3.90622000 | -1.46205500 | 1.21041100 |
| C | 4.08906400 | -0.72284900 | 0.00002900 |
| C | 3.90649600 | -1.46221100 | -1.21029400 |
| C | 3.21976700 | -2.65203500 | -1.21030300 |

| | | | |
|---|---|---|---|
| C | 4.08906400 | 0.72284900 | -0.00002300 |
| C | 3.90622300 | 1.46205200 | -1.21040700 |
| C | 3.21948500 | 2.65187000 | -1.21040900 |
| C | 2.67077000 | 3.17993700 | -0.00002400 |
| C | 3.21976400 | 2.65203700 | 1.21030300 |
| C | 3.90649200 | 1.46221300 | 1.21029800 |
| H | -3.00563000 | 3.12488100 | -2.16190800 |
| H | -4.20888300 | 1.04030400 | -2.16190500 |
| H | -4.20941500 | 1.04060100 | 2.16178600 |
| H | -3.00620100 | 3.12520900 | 2.16180000 |
| H | -4.20887800 | -1.04030800 | 2.16191100 |
| H | -3.00562500 | -3.12488500 | 2.16190700 |
| H | -3.00620600 | -3.12520400 | -2.16180100 |
| H | -4.20942000 | -1.04059700 | -2.16178000 |
| H | -1.20343700 | 4.16455400 | 2.16193800 |
| H | 1.20344600 | 4.16455400 | 2.16193300 |
| H | 1.20344300 | 4.16523300 | -2.16180900 |
| H | -1.20345300 | 4.16523400 | -2.16180400 |
| H | -1.20343600 | -4.16455000 | -2.16194300 |
| H | 1.20344600 | -4.16455100 | -2.16193800 |
| H | 1.20344300 | -4.16523700 | 2.16180400 |
| H | -1.20345300 | -4.16523700 | 2.16179900 |
| H | 3.00562400 | -3.12487900 | 2.16191600 |
| H | 4.20887700 | -1.04030200 | 2.16191400 |
| H | 4.20942100 | -1.04060300 | -2.16177700 |
| H | 3.00620700 | -3.12521100 | -2.16179200 |

| | | | |
|---|---|---|---|
| H | 4.20888200 | 1.04029800 | -2.16190800 |
| H | 3.00562800 | 3.12487400 | -2.16191700 |
| H | 3.00620200 | 3.12521500 | 2.16179100 |
| H | 4.20941600 | 1.04060700 | 2.16178300 |

Sum of electronic and zero-point Energies = -1385.165117 Hartree

Table S8. XYZ coordinate of [7]CPP$^{2+}$($D_0$) by UB3LYP/6-31G(d).

| | X | Y | Z |
|---|---|---|---|
| C | -1.41651600 | 4.61490800 | -0.02307300 |
| C | -0.68128600 | 4.89244700 | 1.16860200 |
| C | 0.69401200 | 4.88821600 | 1.17113400 |
| C | 1.43151800 | 4.60687400 | -0.01793500 |
| C | 0.69833700 | 4.68325800 | -1.23717400 |
| C | -0.67815500 | 4.68658800 | -1.23965600 |
| C | 2.73721300 | 3.97422900 | 0.01882800 |
| C | 3.24924000 | 3.44209000 | 1.23704200 |
| C | 4.10513700 | 2.36372100 | 1.23737000 |
| C | 4.50729000 | 1.74371800 | 0.01950800 |
| C | 4.27142900 | 2.49584800 | -1.17035900 |
| C | 3.41641100 | 3.57311600 | -1.17071300 |
| C | 4.82609700 | 0.32810700 | -0.01647600 |
| C | 4.93307300 | -0.45311400 | 1.17320600 |
| C | 4.62253000 | -1.79292700 | 1.17224400 |
| C | 4.18316100 | -2.44590200 | -0.01847500 |
| C | 4.42009900 | -1.74500400 | -1.23588000 |

| | | | |
|---|---|---|---|
| C | 4.73112000 | -0.40386000 | -1.23490600 |
| C | 3.27460100 | -3.57711400 | 0.01616900 |
| C | 2.64442800 | -3.96271800 | 1.23448000 |
| C | 1.40225100 | -4.55572200 | 1.23540400 |
| C | 0.70479300 | -4.80515800 | 0.01806300 |
| C | 1.48868600 | -4.73877200 | -1.17310500 |
| C | 2.72939800 | -4.14543700 | -1.17407900 |
| C | -0.74569000 | -4.80177900 | -0.01800100 |
| C | -1.52884300 | -4.69949600 | 1.17054500 |
| C | -2.76676700 | -4.10052100 | 1.15573300 |
| C | -3.30951900 | -3.55904200 | -0.04833300 |
| C | -2.68125400 | -3.98204000 | -1.25630400 |
| C | -1.44358000 | -4.58303300 | -1.24165700 |
| C | -4.21191300 | -2.42326200 | -0.03196800 |
| C | -4.54899700 | -1.76548900 | 1.18838200 |
| C | -4.85049900 | -0.42366700 | 1.21281900 |
| C | -4.83836800 | 0.35639600 | 0.01845500 |
| C | -4.85362600 | -0.38071700 | -1.20291100 |
| C | -4.55044200 | -1.72217300 | -1.22733700 |
| C | -4.51015400 | 1.76937700 | 0.03765400 |
| C | -4.12265700 | 2.41737800 | 1.24704900 |
| C | -3.26159000 | 3.49059800 | 1.23456300 |
| C | -2.72574500 | 3.99040400 | 0.01183600 |
| C | -3.39057000 | 3.56586200 | -1.17736200 |
| C | -4.25273100 | 2.49442900 | -1.16472400 |
| H | -1.19942500 | 5.03703500 | 2.10990500 |

| | | | |
|---|---|---|---|
| H | 1.21035700 | 5.03083400 | 2.11380900 |
| H | 1.21114800 | 4.61240400 | -2.18906300 |
| H | -1.18738700 | 4.62024800 | -2.19372400 |
| H | 2.87325500 | 3.79644800 | 2.18948200 |
| H | 4.36455200 | 1.91733600 | 2.19001400 |
| H | 4.70923500 | 2.18188500 | -2.11131100 |
| H | 3.21041200 | 4.07028800 | -2.11199900 |
| H | 5.19211400 | 0.01769400 | 2.11494000 |
| H | 4.64757700 | -2.33081700 | 2.11334000 |
| H | 4.23452700 | -2.22590600 | -2.18896500 |
| H | 4.77623400 | 0.11106100 | -2.18723200 |
| H | 3.07723800 | -3.68114500 | 2.18710300 |
| H | 0.91372500 | -4.71647300 | 2.18906400 |
| H | 1.08292100 | -5.08943800 | -2.11531900 |
| H | 3.25724400 | -4.05112800 | -2.11644000 |
| H | -1.12352600 | -5.02307300 | 2.12250000 |
| H | -3.28663400 | -3.97068100 | 2.09792200 |
| H | -3.11913900 | -3.73765000 | -2.21675900 |
| H | -0.95894500 | -4.77914100 | -2.19077700 |
| H | -4.47287100 | -2.29077000 | 2.13318600 |
| H | -5.00790200 | 0.04950100 | 2.17502400 |
| H | -5.00329900 | 0.12789200 | -2.14803000 |
| H | -4.48292800 | -2.21535900 | -2.18997100 |
| H | -4.41186700 | 2.00565600 | 2.20662500 |
| H | -2.90604700 | 3.87215700 | 2.18437900 |
| H | -3.16412300 | 4.03502400 | -2.12808100 |

| | | | |
|---|---|---|---|
| H | -4.66860000 | 2.15747500 | -2.10727500 |

Sum of electronic and zero-point Energies = -1616.169565 Hartree

Table S9. XYZ coordinate of [8]CPP$^{2+}$($D_0$) by UB3LYP/6-31G(d).

| | X | Y | Z |
|---|---|---|---|
| C | 5.34311700 | 1.42584100 | -0.02451100 |
| C | 5.65469200 | 0.68856200 | 1.15395600 |
| C | 5.65469300 | -0.68856200 | 1.15395600 |
| C | 5.34311700 | -1.42584200 | -0.02451000 |
| C | 5.33035200 | -0.68937400 | -1.23987200 |
| C | 5.33035200 | 0.68937200 | -1.23987300 |
| C | 4.78646200 | -2.77005200 | 0.02450800 |
| C | 4.25683900 | -3.28191800 | 1.23988600 |
| C | 3.28191900 | -4.25683900 | 1.23988600 |
| C | 2.77005300 | -4.78646200 | 0.02450800 |
| C | 3.51170300 | -4.48547300 | -1.15396600 |
| C | 4.48547300 | -3.51170300 | -1.15396600 |
| C | 1.42584200 | -5.34311700 | -0.02451000 |
| C | 0.68856300 | -5.65469200 | 1.15395700 |
| C | -0.68856200 | -5.65469200 | 1.15395600 |
| C | -1.42584100 | -5.34311700 | -0.02451100 |
| C | -0.68937200 | -5.33035300 | -1.23987300 |
| C | 0.68937500 | -5.33035300 | -1.23987200 |
| C | -2.77005200 | -4.78646200 | 0.02450600 |
| C | -3.28192000 | -4.25684100 | 1.23988400 |

| | | | |
|---|---|---|---|
| C | -4.25684100 | -3.28192000 | 1.23988400 |
| C | -4.78646200 | -2.77005200 | 0.02450500 |
| C | -4.48547100 | -3.51170100 | -1.15397000 |
| C | -3.51170100 | -4.48547100 | -1.15396900 |
| C | -5.34311700 | -1.42584000 | -0.02451100 |
| C | -5.65469200 | -0.68856200 | 1.15395600 |
| C | -5.65469200 | 0.68856300 | 1.15395600 |
| C | -5.34311700 | 1.42584300 | -0.02451000 |
| C | -5.33035200 | 0.68937500 | -1.23987200 |
| C | -5.33035200 | -0.68937100 | -1.23987300 |
| C | -4.78646200 | 2.77005300 | 0.02450800 |
| C | -4.25683800 | 3.28191800 | 1.23988600 |
| C | -3.28191700 | 4.25683900 | 1.23988600 |
| C | -2.77005200 | 4.78646200 | 0.02450800 |
| C | -3.51170300 | 4.48547300 | -1.15396600 |
| C | -4.48547300 | 3.51170400 | -1.15396600 |
| C | -1.42584200 | 5.34311700 | -0.02451000 |
| C | -0.68856300 | 5.65469300 | 1.15395600 |
| C | 0.68856200 | 5.65469300 | 1.15395500 |
| C | 1.42584100 | 5.34311700 | -0.02451100 |
| C | 0.68937200 | 5.33035100 | -1.23987300 |
| C | -0.68937400 | 5.33035100 | -1.23987300 |
| C | 2.77005100 | 4.78646100 | 0.02450600 |
| C | 3.28191900 | 4.25684000 | 1.23988400 |
| C | 4.25684000 | 3.28191900 | 1.23988400 |
| C | 4.78646100 | 2.77005200 | 0.02450600 |

| | | | |
|---|---|---|---|
| C | 4.48547100 | 3.51170100 | -1.15396900 |
| C | 3.51170100 | 4.48547100 | -1.15396900 |
| H | 5.84549000 | 1.20812000 | 2.08668300 |
| H | 5.84549000 | -1.20812000 | 2.08668400 |
| H | 5.18824300 | -1.20031100 | -2.18492000 |
| H | 5.18824300 | 1.20030900 | -2.18492100 |
| H | 4.51774600 | -2.82019800 | 2.18493100 |
| H | 2.82019800 | -4.51774500 | 2.18493100 |
| H | 3.27920500 | -4.98776200 | -2.08668900 |
| H | 4.98776200 | -3.27920400 | -2.08668900 |
| H | 1.20812000 | -5.84548900 | 2.08668500 |
| H | -1.20812000 | -5.84549000 | 2.08668400 |
| H | -1.20030800 | -5.18824400 | -2.18492100 |
| H | 1.20031200 | -5.18824400 | -2.18492000 |
| H | -2.82020200 | -4.51774900 | 2.18492900 |
| H | -4.51774900 | -2.82020100 | 2.18492900 |
| H | -4.98775800 | -3.27920000 | -2.08669300 |
| H | -3.27920100 | -4.98775800 | -2.08669300 |
| H | -5.84549000 | -1.20812000 | 2.08668300 |
| H | -5.84549000 | 1.20812000 | 2.08668400 |
| H | -5.18824300 | 1.20031200 | -2.18491900 |
| H | -5.18824300 | -1.20030800 | -2.18492100 |
| H | -4.51774400 | 2.82019700 | 2.18493100 |
| H | -2.82019700 | 4.51774500 | 2.18493100 |
| H | -3.27920500 | 4.98776200 | -2.08668800 |
| H | -4.98776200 | 3.27920500 | -2.08668800 |

| | | | |
|---|---|---|---|
| H | -1.20812000 | 5.84549100 | 2.08668300 |
| H | 1.20812000 | 5.84549100 | 2.08668200 |
| H | 1.20030800 | 5.18824100 | -2.18492100 |
| H | -1.20031200 | 5.18824200 | -2.18492000 |
| H | 2.82019900 | 4.51774800 | 2.18492900 |
| H | 4.51774700 | 2.82020000 | 2.18492900 |
| H | 4.98775900 | 3.27920200 | -2.08669200 |
| H | 3.27920100 | 4.98775900 | -2.08669200 |

Sum of electronic and zero-point Energies = -1847.168436 Hartree

Table S10. XYZ coordinate of [9]CPP$^{2+}$($D_0$) by UB3LYP/6-31G(d).

| | X | Y | Z |
|---|---|---|---|
| C | -0.51035600 | 6.18955400 | 0.04863000 |
| C | 0.25479100 | 6.41860100 | -1.12786100 |
| C | 1.61795200 | 6.21249600 | -1.14527200 |
| C | 2.31064800 | 5.76514900 | 0.01327300 |
| C | 1.58507400 | 5.78950800 | 1.23211200 |
| C | 0.22012000 | 5.99458000 | 1.24904700 |
| C | 3.59060600 | 5.07004400 | -0.06337800 |
| C | 4.00749000 | 4.47892000 | -1.28420300 |
| C | 4.92011200 | 3.44507300 | -1.30472700 |
| C | 5.48653200 | 2.93294900 | -0.10725900 |
| C | 5.26407100 | 3.70168700 | 1.06963600 |
| C | 4.34574700 | 4.72995800 | 1.09202900 |
| C | 6.02853400 | 1.57929400 | -0.05947500 |

| | | | |
|---|---|---|---|
| C | 6.18948900 | 0.79216200 | -1.23210900 |
| C | 6.22374400 | -0.58474100 | -1.17367000 |
| C | 6.10019100 | -1.27739100 | 0.06171800 |
| C | 6.21735800 | -0.48320000 | 1.23479400 |
| C | 6.18250900 | 0.89369600 | 1.17636400 |
| C | 5.08767800 | -3.19845200 | 1.30524700 |
| C | 4.22764700 | -4.27640900 | 1.28370700 |
| C | 3.83946500 | -4.88547000 | 0.06220600 |
| C | 4.57585400 | -4.50636900 | -1.09314800 |
| C | 5.44186100 | -3.43369500 | -1.06974000 |
| C | 2.59555000 | -5.64311900 | -0.01480800 |
| C | 1.87185900 | -5.70258200 | -1.23357200 |
| C | 0.51879900 | -5.97522800 | -1.25051800 |
| C | -0.20093200 | -6.20709500 | -0.05016100 |
| C | 0.57483000 | -6.39868200 | 1.12607900 |
| C | 1.92608800 | -6.12521300 | 1.14347600 |
| C | -1.64387400 | -5.99167200 | -0.00652500 |
| C | -2.26825400 | -5.59554300 | 1.20399600 |
| C | -3.48137700 | -4.93693400 | 1.20265200 |
| C | -4.15175800 | -4.63050500 | -0.00926300 |
| C | -3.64960100 | -5.25331700 | -1.18472100 |
| C | -2.43725300 | -5.91055300 | -1.18359200 |
| C | 5.62668200 | -2.65657200 | 0.10817400 |
| C | -5.11845700 | -3.53755800 | -0.05673300 |
| C | -5.31724900 | -2.81383100 | -1.26034000 |
| C | -5.82312500 | -1.52944400 | -1.24917300 |

| | | | |
|---|---|---|---|
| C | -6.16306600 | -0.88273100 | -0.03345500 |
| C | -6.20259700 | -1.70029500 | 1.12896300 |
| C | -5.69822800 | -2.98377800 | 1.11755000 |
| C | -6.19954900 | 0.57499900 | 0.03495500 |
| C | -5.89175200 | 1.23803300 | 1.25045500 |
| C | -5.45069800 | 2.54610700 | 1.26125900 |
| C | -5.28886200 | 3.27868900 | 0.05747100 |
| C | -5.84079200 | 2.69648800 | -1.11647200 |
| C | -6.28046500 | 1.38943800 | -1.12751200 |
| C | -4.37788900 | 4.41846500 | 0.00933100 |
| C | -3.90709800 | 5.06608500 | 1.18436500 |
| C | -2.72896200 | 5.78285800 | 1.18260000 |
| C | -1.94082400 | 5.90269800 | 0.00532600 |
| C | -2.54498600 | 5.47538000 | -1.20484700 |
| C | -3.72387000 | 4.75730000 | -1.20288900 |
| H | -0.23805400 | 6.72144800 | -2.04555000 |
| H | 2.15549000 | 6.35960300 | -2.07603400 |
| H | 2.07448500 | 5.51811600 | 2.16046800 |
| H | -0.30422000 | 5.87573000 | 2.19021900 |
| H | 3.51819300 | 4.74891300 | -2.21295900 |
| H | 5.11098700 | 2.95633200 | -2.25242800 |
| H | 5.78106000 | 3.45343200 | 1.98974900 |
| H | 4.17501300 | 5.25512100 | 2.02581300 |
| H | 6.22068400 | 1.26387600 | -2.20744000 |
| H | 6.25262900 | -1.13370800 | -2.10757600 |
| H | 6.26829600 | -0.95262900 | 2.21036900 |

| | | | |
|---|---|---|---|
| H | 6.17980500 | 1.44337100 | 2.11030500 |
| H | 5.25532300 | -2.70291300 | 2.25379800 |
| H | 3.75353600 | -4.57215700 | 2.21249300 |
| H | 4.43066900 | -5.03773000 | -2.02773800 |
| H | 5.94465100 | -3.15841400 | -1.99001200 |
| H | 2.34702700 | -5.40661100 | -2.16181000 |
| H | -0.01091700 | -5.88197600 | -2.19156300 |
| H | 0.09775000 | -6.72623400 | 2.04361600 |
| H | 2.47036700 | -6.24614000 | 2.07408500 |
| H | -1.73848800 | -5.69091100 | 2.14479300 |
| H | -3.85156400 | -4.54379200 | 2.14243600 |
| H | -4.20166500 | -5.18087800 | -2.11572000 |
| H | -2.07374600 | -6.33442000 | -2.11368600 |
| H | -4.95361900 | -3.21271500 | -2.20028600 |
| H | -5.83451900 | -0.97492700 | -2.18048300 |
| H | -6.59701300 | -1.30341700 | 2.05841100 |
| H | -5.71181500 | -3.55671800 | 2.03861600 |
| H | -5.87497000 | 0.68374900 | 2.18182600 |
| H | -5.10699100 | 2.96278000 | 2.20098700 |
| H | -5.88338000 | 3.26790200 | -2.03760000 |
| H | -6.65492600 | 0.97321200 | -2.05675300 |
| H | -4.45464900 | 4.96670200 | 2.11554400 |
| H | -2.38679100 | 6.22474100 | 2.11240000 |
| H | -2.02084900 | 5.59650700 | -2.14583300 |
| H | -4.07424400 | 4.34577100 | -2.14239800 |

Sum of electronic and zero-point Energies = -2078.163583 Hartree

Table S11. XYZ coordinate of [5]CPP$^{2+}$($D_1$) by B3LYP/6-31G(d).

| | X | Y | Z |
|---|---|---|---|
| C | -2.90015300 | 1.96104300 | -1.21578500 |
| C | -1.91040600 | 2.91305500 | -1.21475600 |
| C | -1.21471900 | 3.22896700 | 0.00016200 |
| C | -1.91044400 | 2.91318500 | 1.21509600 |
| C | -2.90019500 | 1.96118100 | 1.21621900 |
| C | -3.24367200 | 1.27483700 | 0.00026400 |
| C | 0.21787800 | 3.43758700 | 0.00018700 |
| C | 0.97288000 | 3.32981400 | -1.21423500 |
| C | 0.97279400 | 3.32957900 | 1.21462800 |
| C | 2.19569900 | 2.70187500 | -1.21505100 |
| C | 2.19561500 | 2.70161200 | 1.21538800 |
| C | 2.72470800 | 2.14901700 | 0.00011300 |
| C | 3.37457500 | 0.86178400 | -0.00002400 |
| C | 3.51301900 | 0.10596800 | -1.21645500 |
| C | 3.51291900 | 0.10566300 | 1.21625300 |
| C | 3.28246200 | -1.24616000 | -1.21636800 |
| C | 3.28239300 | -1.24647500 | 1.21584500 |
| C | 2.90190100 | -1.91310600 | -0.00034500 |
| C | 1.86416500 | -2.91675200 | -0.00045200 |
| C | 1.18457800 | -3.26553000 | 1.21434900 |
| C | 1.18426100 | -3.26485800 | -1.21527700 |
| C | -0.17640100 | -3.46206400 | 1.21406900 |
| C | -0.17673200 | -3.46140500 | -1.21473600 |
| C | -0.92590100 | -3.32015300 | -0.00019600 |

| | | | |
|---|---|---|---|
| C | -3.48498000 | -0.14499800 | 0.00030900 |
| C | -3.38898400 | -0.90735600 | 1.21661700 |
| C | -3.38951700 | -0.90738000 | -1.21600200 |
| C | -2.76752800 | -2.13109100 | 1.21555300 |
| C | -2.76806400 | -2.13112100 | -1.21517900 |
| C | -2.21137000 | -2.65664900 | 0.00007000 |
| H | 3.67937200 | 0.61080300 | 2.16138300 |
| H | 3.27175100 | -1.77799300 | -2.16143500 |
| H | 3.27157000 | -1.77852700 | 2.16078400 |
| H | 1.71134400 | -3.25431400 | 2.16202300 |
| H | 1.71076200 | -3.25311500 | -2.16308700 |
| H | -3.32825400 | 1.64973600 | -2.16225400 |
| H | -1.58119100 | 3.32790100 | -2.16098600 |
| H | -1.58123400 | 3.32813100 | 2.16128800 |
| H | -3.32831100 | 1.65000300 | 2.16272300 |
| H | 0.53679900 | 3.62689600 | -2.16147000 |
| H | 0.53665100 | 3.62649000 | 2.16188900 |
| H | 2.69138300 | 2.52194500 | -2.16252100 |
| H | 2.69127900 | 2.52155300 | 2.16284100 |
| H | 3.67955400 | 0.61134800 | -2.16144300 |
| H | -0.68496500 | -3.59966500 | 2.16173500 |
| H | -0.68556700 | -3.59842900 | -2.16234000 |
| H | -3.69409700 | -0.47350000 | 2.16253100 |
| H | -3.69505000 | -0.47356700 | -2.16180200 |
| H | -2.59566900 | -2.63337500 | 2.16113100 |
| H | -2.59665300 | -2.63345600 | -2.16081500 |

Sum of electronic and zero-point Energies = -1154.080229 Hartree

Table S12. XYZ coordinate of [6]CPP$^{2+}$($D_1$) by B3LYP/6-31G(d).

| | X | Y | A |
|---|---|---|---|
| C | -2.66464200 | 3.20001100 | -0.01512300 |
| C | -3.11792600 | 2.61643200 | -1.23855900 |
| C | -3.79218100 | 1.41487400 | -1.23861600 |
| C | -4.05930500 | 0.72828200 | -0.01781000 |
| C | -3.96274500 | 1.51011000 | 1.17428100 |
| C | -3.28436400 | 2.70749800 | 1.17688900 |
| C | -4.05931400 | -0.72830800 | 0.01781300 |
| C | -1.41780700 | 3.93371900 | 0.02038300 |
| C | -3.79221600 | -1.41491300 | 1.23862000 |
| C | -3.11797400 | -2.61647400 | 1.23856500 |
| C | -2.66467300 | -3.20004700 | 0.01512600 |
| C | -3.28439400 | -2.70752800 | -1.17689000 |
| C | -3.96276400 | -1.51013800 | -1.17428000 |
| C | -0.68697800 | 4.06631300 | 1.24469600 |
| C | 0.68700800 | 4.06632700 | 1.24469600 |
| C | 1.41784000 | 3.93374200 | 0.02038000 |
| C | 0.68627900 | 4.23815000 | -1.17506100 |
| C | -0.68625600 | 4.23814000 | -1.17505800 |
| C | -1.41784000 | -3.93374100 | -0.02037900 |
| C | -0.68700800 | -4.06632800 | -1.24469400 |
| C | 0.68697700 | -4.06631400 | -1.24469500 |
| C | 1.41780600 | -3.93371800 | -0.02038200 |

| | | | |
|---|---|---|---|
| C | 0.68625500 | -4.23813800 | 1.17505900 |
| C | -0.68627900 | -4.23814800 | 1.17506200 |
| C | 2.66464100 | -3.20001200 | 0.01512400 |
| C | 3.11792700 | -2.61643200 | 1.23855900 |
| C | 3.79218300 | -1.41487500 | 1.23861500 |
| C | 4.05930500 | -0.72828200 | 0.01780900 |
| C | 3.96274300 | -1.51011100 | -1.17428200 |
| C | 3.28436300 | -2.70749900 | -1.17688900 |
| C | 4.05931500 | 0.72830800 | -0.01781500 |
| C | 3.79221600 | 1.41491300 | -1.23862100 |
| C | 3.11797400 | 2.61647500 | -1.23856500 |
| C | 2.66467300 | 3.20004800 | -0.01512600 |
| C | 3.28439500 | 2.70752900 | 1.17688900 |
| C | 3.96276600 | 1.51013800 | 1.17427900 |
| H | -2.82333700 | 3.04112900 | -2.19106000 |
| H | -3.99756100 | 0.94081900 | -2.19125900 |
| H | -4.34517200 | 1.12671300 | 2.11381100 |
| H | -3.15247200 | 3.22898500 | 2.11851400 |
| H | -3.99760700 | -0.94086100 | 2.19126300 |
| H | -2.82340700 | -3.04118600 | 2.19106500 |
| H | -3.15250700 | -3.22901800 | -2.11851400 |
| H | -4.34519400 | -1.12673800 | -2.11380800 |
| H | -1.20423500 | 4.03565900 | 2.19674200 |
| H | 1.20426600 | 4.03568700 | 2.19674200 |
| H | 1.20925000 | 4.38667900 | -2.11346000 |
| H | -1.20923200 | 4.38666300 | -2.11345500 |

| | | | |
|---|---|---|---|
| H | -1.20426600 | -4.03568900 | -2.19674000 |
| H | 1.20423500 | -4.03566200 | -2.19674100 |
| H | 1.20923100 | -4.38665900 | 2.11345700 |
| H | -1.20925000 | -4.38667500 | 2.11346100 |
| H | 2.82334000 | -3.04112900 | 2.19106000 |
| H | 3.99756400 | -0.94081900 | 2.19125800 |
| H | 4.34517000 | -1.12671400 | -2.11381300 |
| H | 3.15246900 | -3.22898500 | -2.11851400 |
| H | 3.99760600 | 0.94086100 | -2.19126400 |
| H | 2.82340500 | 3.04118600 | -2.19106600 |
| H | 3.15250800 | 3.22901800 | 2.11851400 |
| H | 4.34519600 | 1.12673700 | 2.11380700 |

Table S13. XYZ coordinate of [7]CPP$^{2+}$($D_1$) by B3LYP/6-31G(d).

| | X | Y | Z |
|---|---|---|---|
| C | -1.39846700 | 4.56643600 | -0.03796000 |
| C | -0.65420800 | 4.95461000 | 1.11162000 |
| C | 0.72558900 | 4.95902600 | 1.09492900 |
| C | 1.44546400 | 4.57865400 | -0.07381200 |
| C | 0.69806100 | 4.50825800 | -1.28062400 |
| C | -0.68367800 | 4.49977300 | -1.26232100 |
| C | 2.76585800 | 3.96314700 | -0.01388300 |
| C | 3.24757800 | 3.42877200 | 1.21471900 |
| C | 4.11842800 | 2.36153400 | 1.23029800 |
| C | 4.55905600 | 1.75508400 | 0.01587900 |

| | | | |
|---|---|---|---|
| C | 4.34926500 | 2.51676700 | -1.17575000 |
| C | 3.48378400 | 3.58583000 | -1.18906100 |
| C | 4.87597000 | 0.34104800 | -0.01684300 |
| C | 5.01316900 | -0.43706600 | 1.17452300 |
| C | 4.68781200 | -1.77373800 | 1.18826600 |
| C | 4.19856100 | -2.42154900 | 0.01402800 |
| C | 4.40193400 | -1.73246400 | -1.21467000 |
| C | 4.73343700 | -0.39527600 | -1.23088200 |
| C | 3.26886300 | -3.54400200 | 0.07504800 |
| C | 2.56139600 | -3.79703300 | 1.28107000 |
| C | 1.31010000 | -4.38339900 | 1.26235200 |
| C | 0.69548700 | -4.75467800 | 0.03798200 |
| C | 1.53638900 | -4.78836000 | -1.11001600 |
| C | 2.78449700 | -4.19984800 | -1.09259300 |
| C | -0.76369900 | -4.76072400 | -0.05795000 |
| C | -1.60376500 | -4.76671600 | 1.09289800 |
| C | -2.85105100 | -4.18251200 | 1.06206700 |
| C | -3.34190500 | -3.55584400 | -0.12381000 |
| C | -2.63978100 | -3.86160300 | -1.32703700 |
| C | -1.38979700 | -4.44261100 | -1.29360800 |
| C | -4.25811600 | -2.43246100 | -0.07662400 |
| C | -4.59924500 | -1.81377400 | 1.16586100 |
| C | -4.89886300 | -0.47378600 | 1.23102400 |
| C | -4.88056900 | 0.34338200 | 0.05790400 |
| C | -4.91111800 | -0.35821700 | -1.18663800 |
| C | -4.60994800 | -1.69788100 | -1.25188300 |

| | | | |
|---|---|---|---|
| C | -4.53224500 | 1.75087800 | 0.11113600 |
| C | -4.02542400 | 2.31906800 | 1.31661100 |
| C | -3.14464600 | 3.37996600 | 1.28813000 |
| C | -2.71909300 | 3.94447200 | 0.05555300 |
| C | -3.48196100 | 3.59662300 | -1.09614800 |
| C | -4.35864100 | 2.53383000 | -1.07031600 |
| H | -1.16667400 | 5.19069700 | 2.03838900 |
| H | 1.25786000 | 5.19746500 | 2.00973200 |
| H | 1.19878700 | 4.31900800 | -2.22290400 |
| H | -1.20776700 | 4.30127500 | -2.19006600 |
| H | 2.82743700 | 3.76404500 | 2.15604200 |
| H | 4.35227700 | 1.90376600 | 2.18437900 |
| H | 4.82491900 | 2.21863200 | -2.10387500 |
| H | 3.30271700 | 4.10148000 | -2.12622500 |
| H | 5.31683200 | 0.03570900 | 2.10232500 |
| H | 4.74581000 | -2.31738400 | 2.12532600 |
| H | 4.16233700 | -2.21481300 | -2.15540100 |
| H | 4.74672400 | 0.11855900 | -2.18497100 |
| H | 2.93027400 | -3.40727900 | 2.22260600 |
| H | 0.75005200 | -4.42643800 | 2.18929500 |
| H | 1.17686000 | -5.22410100 | -2.03634700 |
| H | 3.36947000 | -4.18921200 | -2.00624600 |
| H | -1.23989800 | -5.17417800 | 2.03024900 |
| H | -3.42709400 | -4.14318700 | 1.97992500 |
| H | -3.02188900 | -3.52834200 | -2.28443200 |
| H | -0.83709300 | -4.52803900 | -2.22220300 |

| | | | |
|---|---|---|---|
| H | -4.52025000 | -2.36963200 | 2.09305300 |
| H | -5.06711000 | -0.02818400 | 2.20488300 |
| H | -5.06401100 | 0.18113700 | -2.11433800 |
| H | -4.55939900 | -2.16920600 | -2.22678400 |
| H | -4.22368100 | 1.84631700 | 2.27101400 |
| H | -2.67854200 | 3.68670900 | 2.21748500 |
| H | -3.32922100 | 4.12634800 | -2.03058200 |
| H | -4.86444000 | 2.25721000 | -1.98878600 |

Sum of electronic and zero-point Energies = -1616.116523 Hartree

Table S14. XYZ coordinate of [8]CPP$^{2+}$($D_1$) by B3LYP/6-31G(d).

| | X | Y | Z |
|---|---|---|---|
| C | 5.34121700 | 1.38568500 | 0.00765900 |
| C | 5.68990600 | 0.63832900 | 1.16791400 |
| C | 5.70887400 | -0.73948800 | 1.14658300 |
| C | 5.38600100 | -1.46259000 | -0.03920500 |
| C | 5.33697500 | -0.70592400 | -1.24373800 |
| C | 5.31201000 | 0.67344700 | -1.21962300 |
| C | 4.83930900 | -2.80883400 | -0.00463000 |
| C | 4.31821300 | -3.34046000 | 1.20963800 |
| C | 3.33712600 | -4.30799200 | 1.20127200 |
| C | 2.81106400 | -4.81184800 | -0.02103000 |
| C | 3.55276000 | -4.50491400 | -1.20027200 |
| C | 4.53137000 | -3.53739100 | -1.19277400 |
| C | 1.45695900 | -5.34735600 | -0.07054600 |

| | | | |
|---|---|---|---|
| C | 0.73464300 | -5.70827600 | 1.10172200 |
| C | -0.64537700 | -5.68904300 | 1.12282900 |
| C | -1.38953700 | -5.30093200 | -0.02380100 |
| C | -0.67817300 | -5.21387100 | -1.24584500 |
| C | 0.70324800 | -5.24045900 | -1.27026000 |
| C | -2.73821400 | -4.72900200 | 0.06909300 |
| C | -3.14313500 | -4.11040100 | 1.27629900 |
| C | -4.12785200 | -3.13807400 | 1.28490800 |
| C | -4.76053000 | -2.72722400 | 0.08525600 |
| C | -4.53502200 | -3.53113700 | -1.06375700 |
| C | -3.55353700 | -4.50458200 | -1.07096300 |
| C | -5.34121100 | -1.38569600 | 0.00747700 |
| C | -5.68987800 | -0.63821000 | 1.16766000 |
| C | -5.70884300 | 0.73960100 | 1.14618400 |
| C | -5.38599000 | 1.46258500 | -0.03968600 |
| C | -5.33701200 | 0.70578400 | -1.24414100 |
| C | -5.31205300 | -0.67358100 | -1.21988200 |
| C | -4.83930300 | 2.80882400 | -0.00524300 |
| C | -4.31836900 | 3.34067000 | 1.20900400 |
| C | -3.33728500 | 4.30819900 | 1.20060300 |
| C | -2.81105000 | 4.81184600 | -0.02171700 |
| C | -3.55260500 | 4.50471500 | -1.20100000 |
| C | -4.53121100 | 3.53719400 | -1.19346700 |
| C | -1.45694900 | 5.34734900 | -0.07116400 |
| C | -0.73472100 | 5.70832700 | 1.10114500 |
| C | 0.64529500 | 5.68909800 | 1.12236300 |

| | | | |
|---|---|---|---|
| C | 1.38955000 | 5.30093000 | -0.02418900 |
| C | 0.67828100 | 5.21382500 | -1.24628800 |
| C | -0.70313500 | 5.24040800 | -1.27081500 |
| C | 2.73821800 | 4.72900500 | 0.06884500 |
| C | 3.14303800 | 4.11047500 | 1.27612200 |
| C | 4.12775300 | 3.13814500 | 1.28486900 |
| C | 4.76052900 | 2.72722900 | 0.08529500 |
| C | 4.53511600 | 3.53106400 | -1.06378800 |
| C | 3.55362800 | 4.50450900 | -1.07113400 |
| H | 5.89323700 | 1.15150300 | 2.10213300 |
| H | 5.92627400 | -1.27198200 | 2.06632300 |
| H | 5.18205200 | -1.20421000 | -2.19359600 |
| H | 5.13310100 | 1.20219600 | -2.14909800 |
| H | 4.59063900 | -2.89462300 | 2.15920700 |
| H | 2.87706100 | -4.58158100 | 2.14385800 |
| H | 3.31397400 | -4.99986700 | -2.13563000 |
| H | 5.03512800 | -3.29769900 | -2.12305200 |
| H | 1.26692500 | -5.95737800 | 2.01371000 |
| H | -1.15997600 | -5.92323600 | 2.04920000 |
| H | -1.20644700 | -4.98997300 | -2.16591100 |
| H | 1.20278400 | -5.04122700 | -2.21124000 |
| H | -2.59257500 | -4.29425300 | 2.19207500 |
| H | -4.31055100 | -2.60005600 | 2.20813000 |
| H | -5.10295000 | -3.35360400 | -1.97129800 |
| H | -3.37694300 | -5.06507100 | -1.98343400 |
| H | -5.89319300 | -1.15127800 | 2.10193900 |

| | | | |
|---|---|---|---|
| H | -5.92622200 | 1.27218200 | 2.06587700 |
| H | -5.18214500 | 1.20396200 | -2.19406400 |
| H | -5.13319900 | -1.20242300 | -2.14931400 |
| H | -4.59093900 | 2.89502200 | 2.15862000 |
| H | -2.87736900 | 4.58196700 | 2.14320900 |
| H | -3.31370700 | 4.99950800 | -2.13641300 |
| H | -5.03484200 | 3.29735300 | -2.12377400 |
| H | -1.26706900 | 5.95747200 | 2.01308200 |
| H | 1.15982000 | 5.92333700 | 2.04876400 |
| H | 1.20663100 | 4.98989900 | -2.16630500 |
| H | -1.20259000 | 5.04115100 | -2.21183300 |
| H | 2.59240100 | 4.29437900 | 2.19184100 |
| H | 4.31037500 | 2.60017100 | 2.20813300 |
| H | 5.10311900 | 3.35346700 | -1.97127000 |
| H | 3.37710600 | 5.06493800 | -1.98365600 |

Sum of electronic and zero-point Energies = -1847.122560 Hartree

Table S15. XYZ coordinate of [9]CPP$^{2+}$($D_1$) by B3LYP/6-31G(d).

| | X | Y | Z |
|---|---|---|---|
| C | -5.34753300 | 3.00597000 | 0.06097800 |
| C | -5.17422400 | 3.82583400 | -1.08119600 |
| C | -4.24201400 | 4.84872100 | -1.09015400 |
| C | -3.43534500 | 5.11289100 | 0.04520000 |
| C | -3.77507600 | 4.44310900 | 1.24411700 |
| C | -4.70428300 | 3.41577600 | 1.25065700 |

| | | | |
|---|---|---|---|
| C | -2.14670600 | 5.80717500 | -0.04685000 |
| C | -1.43077000 | 5.80086700 | -1.26964800 |
| C | -0.06582200 | 6.00397900 | -1.29972700 |
| C | 0.67547600 | 6.22841900 | -0.10757100 |
| C | -0.08634000 | 6.48594600 | 1.06763100 |
| C | -1.45069900 | 6.28062400 | 1.09681400 |
| C | 2.10183200 | 5.93596200 | -0.06023200 |
| C | 2.84958800 | 5.63476200 | -1.23442000 |
| C | 4.00873200 | 4.89338800 | -1.17545000 |
| C | 4.50882000 | 4.39664800 | 0.06213000 |
| C | 3.91948400 | 4.94578300 | 1.23678700 |
| C | 2.76022300 | 5.68701900 | 1.17779700 |
| C | 5.48312900 | 2.45760700 | 1.30012200 |
| C | 5.87091600 | 1.13335700 | 1.26922800 |
| C | 6.17330900 | 0.48560000 | 0.04564400 |
| C | 6.30857400 | 1.31602400 | -1.09844100 |
| C | 5.92309200 | 2.64068000 | -1.06841000 |
| C | 6.08287500 | -0.97516100 | -0.04626800 |
| C | 5.61713600 | -1.56468100 | -1.24513100 |
| C | 5.07365700 | -2.83879500 | -1.25136900 |
| C | 4.97102800 | -3.59428300 | -0.06151400 |
| C | 5.64308500 | -3.09326500 | 1.08048900 |
| C | 6.18114900 | -1.81823800 | 1.08921000 |
| C | 3.98327800 | -4.68294700 | 0.01632700 |
| C | 3.27869900 | -4.89423200 | 1.22350200 |
| C | 2.06239300 | -5.55427300 | 1.23559800 |

| | | | |
|---|---|---|---|
| C | 1.47719000 | -6.03488900 | 0.03801800 |
| C | 2.29468700 | -6.02270800 | -1.12241500 |
| C | 3.51303000 | -5.36842900 | -1.13167800 |
| C | 5.37259900 | 3.22457600 | 0.10806500 |
| C | 0.03128700 | -6.25130900 | -0.02007900 |
| C | -0.67157800 | -6.03675300 | -1.23380800 |
| C | -2.02252600 | -5.75483100 | -1.23754400 |
| C | -2.75989800 | -5.66435000 | -0.02587200 |
| C | -2.10807300 | -6.13862800 | 1.14801000 |
| C | -0.75947300 | -6.42447400 | 1.14980200 |
| C | -3.98617900 | -4.88003000 | 0.02589900 |
| C | -4.37786800 | -4.24889300 | 1.23766400 |
| C | -5.20038900 | -3.14080600 | 1.23408700 |
| C | -5.68962100 | -2.59226300 | 0.02032900 |
| C | -5.51499300 | -3.38259400 | -1.14971600 |
| C | -4.68998200 | -4.48697300 | -1.14803000 |
| C | -6.09925900 | -1.18902900 | -0.03767900 |
| C | -6.42993800 | -0.44150600 | 1.12298700 |
| C | -6.34666700 | 0.93882500 | 1.13197800 |
| C | -5.92221200 | 1.65301300 | -0.01647000 |
| C | -5.82008200 | 0.92459600 | -1.22374300 |
| C | -5.90957000 | -0.45629900 | -1.23561100 |
| H | -5.74581300 | 3.62678000 | -1.98228600 |
| H | -4.10599300 | 5.42719400 | -1.99847500 |
| H | -3.21525800 | 4.63907300 | 2.15199700 |
| H | -4.83772400 | 2.84403100 | 2.16257300 |

| | | | |
|---|---|---|---|
| H | -1.93043300 | 5.50865100 | -2.18664800 |
| H | 0.44640300 | 5.87192700 | -2.24513100 |
| H | 0.40739400 | 6.80358500 | 1.97937400 |
| H | -1.98662800 | 6.44340000 | 2.02639200 |
| H | 2.47799400 | 5.93092000 | -2.20870500 |
| H | 4.48376500 | 4.61198100 | -2.10806300 |
| H | 4.34190600 | 4.72961300 | 2.21136500 |
| H | 2.30326700 | 5.99688100 | 2.11043300 |
| H | 5.15189900 | 2.86757500 | 2.24657900 |
| H | 5.81803000 | 0.55753000 | 2.18659300 |
| H | 6.67870400 | 0.89771700 | -2.02894100 |
| H | 6.00209000 | 3.22178400 | -1.98052800 |
| H | 5.56057900 | -0.97461700 | -2.15322900 |
| H | 4.61043000 | -3.19978600 | -2.16318200 |
| H | 5.70195900 | -3.69553900 | 1.98165900 |
| H | 6.64961500 | -1.45235300 | 1.99740800 |
| H | 3.62397100 | -4.42796300 | 2.13983500 |
| H | 1.50189900 | -5.58206600 | 2.16318500 |
| H | 1.94937100 | -6.49799800 | -2.03484100 |
| H | 4.09144000 | -5.34576700 | -2.04996400 |
| H | -0.12717800 | -5.96264100 | -2.16849100 |
| H | -2.48512400 | -5.47293300 | -2.17641300 |
| H | -2.66469400 | -6.24187300 | 2.07348700 |
| H | -0.29297600 | -6.74450600 | 2.07571500 |
| H | -3.92818000 | -4.55089000 | 2.17655700 |
| H | -5.36167700 | -2.61582800 | 2.16890300 |

| | | | |
|---|---|---|---|
| H | -6.00103600 | -3.09312400 | -2.07563000 |
| H | -4.55019200 | -5.03541900 | -2.07359000 |
| H | -6.71605100 | -0.95411200 | 2.03569000 |
| H | -6.56785800 | 1.47359200 | 2.05035400 |
| H | -5.54247700 | 1.43343200 | -2.14043000 |
| H | -5.70087700 | -0.97693900 | -2.16336400 |

Sum of electronic and zero-point Energies = -2078.122848 Hartree

Table S16. XYZ coordinate of [5]CPP$^{2+}$($D_1$) by UB3LYP/6-31G(d).

| | X | Y | Z |
|---|---|---|---|
| C | -3.10500300 | 2.09861100 | -1.11143400 |
| C | -2.07752000 | 3.01477300 | -1.08670000 |
| C | -1.27696500 | 3.15918400 | 0.08515500 |
| C | -1.86481100 | 2.72835500 | 1.30564000 |
| C | -2.91013800 | 1.82933400 | 1.29555900 |
| C | -3.38396500 | 1.29862300 | 0.04962900 |
| C | 0.20424400 | 3.32251200 | 0.00255900 |
| C | 0.84225300 | 3.06838300 | -1.23123300 |
| C | 1.01834100 | 3.29338000 | 1.16029600 |
| C | 2.09635300 | 2.47239800 | -1.27093600 |
| C | 2.26561000 | 2.68507100 | 1.12798800 |
| C | 2.75029700 | 2.09149000 | -0.07022600 |
| C | 3.48841200 | 0.83031700 | -0.04040200 |
| C | 3.65944100 | 0.04176700 | -1.23297700 |
| C | 3.66419900 | 0.11600900 | 1.19495100 |

| | | | |
|---|---|---|---|
| C | 3.42892700 | -1.30846300 | -1.19312600 |
| C | 3.44069900 | -1.23541200 | 1.23481300 |
| C | 3.02523700 | -1.92546700 | 0.04129600 |
| C | 1.91534200 | -2.87600500 | 0.06884900 |
| C | 1.17292400 | -3.02695600 | 1.26913400 |
| C | 1.26296200 | -3.27386400 | -1.13076000 |
| C | -0.20706100 | -3.17999800 | 1.22901800 |
| C | -0.11468100 | -3.44075100 | -1.16352700 |
| C | -0.89335700 | -3.20650000 | -0.00483700 |
| C | -3.62253600 | -0.12022300 | -0.04684000 |
| C | -3.61830600 | -0.96772600 | 1.11399000 |
| C | -3.35046200 | -0.77637500 | -1.29337800 |
| C | -2.94702300 | -2.16955200 | 1.08769300 |
| C | -2.65671100 | -1.96788900 | -1.30502800 |
| C | -2.23983900 | -2.56763100 | -0.08547300 |
| H | 3.82728100 | 0.65422500 | 2.12239800 |
| H | 3.41111900 | -1.87116500 | -2.12021300 |
| H | 3.44541000 | -1.74686100 | 2.19129000 |
| H | 1.64322900 | -2.88107700 | 2.23462600 |
| H | 1.81366800 | -3.34291800 | -2.06268900 |
| H | -3.62862900 | 1.91267300 | -2.04360000 |
| H | -1.81193300 | 3.53330400 | -2.00203300 |
| H | -1.40384300 | 2.97433900 | 2.25549100 |
| H | -3.24306500 | 1.40311500 | 2.23528700 |
| H | 0.31038600 | 3.19714400 | -2.16679900 |
| H | 0.63825100 | 3.64243800 | 2.11458300 |

| | | | |
|---|---|---|---|
| H | 2.49133200 | 2.17645200 | -2.23584000 |
| H | 2.81027200 | 2.57401600 | 2.05943300 |
| H | 3.83494700 | 0.52319300 | -2.18897100 |
| H | -0.75157100 | -3.13214500 | 2.16495000 |
| H | -0.58803100 | -3.64219500 | -2.11866800 |
| H | -4.05057200 | -0.62105400 | 2.04707300 |
| H | -3.52729200 | -0.26449600 | -2.23268100 |
| H | -2.86401200 | -2.74652100 | 2.00279700 |
| H | -2.30355900 | -2.35092800 | -2.25569100 |

Sum of electronic and zero-point Energies = -1154.116655 Hartree

Table S17. XYZ coordinate of [6]CPP$^{2+}$($D_1$) by UB3LYP/6-31G(d).

| | X | Y | Z |
|---|---|---|---|
| C | -2.58070900 | 3.31368100 | -0.04088500 |
| C | -2.72892300 | 2.58698700 | -1.24838600 |
| C | -3.29792200 | 1.31882100 | -1.24478900 |
| C | -3.78354300 | 0.75092600 | -0.05581800 |
| C | -3.91454000 | 1.59569000 | 1.06686400 |
| C | -3.30442300 | 2.84438700 | 1.08593600 |
| C | -3.78368100 | -0.75119600 | 0.05588800 |
| C | -1.40098400 | 4.16541600 | 0.06995400 |
| C | -3.29832000 | -1.31924800 | 1.24490700 |
| C | -2.72946700 | -2.58746300 | 1.24849200 |
| C | -2.58107700 | -3.31405100 | 0.04091300 |
| C | -3.30470100 | -2.84463500 | -1.08595100 |

| | | | |
|---|---|---|---|
| C | -3.91471600 | -1.59591000 | -1.06684800 |
| C | -0.68555400 | 4.22362700 | 1.31370900 |
| C | 0.68589300 | 4.22376600 | 1.31370100 |
| C | 1.40131700 | 4.16564600 | 0.06991900 |
| C | 0.68428800 | 4.62970300 | -1.08896800 |
| C | -0.68407800 | 4.62960500 | -1.08894100 |
| C | -1.40131600 | -4.16564300 | -0.06993400 |
| C | -0.68588700 | -4.22375000 | -1.31371300 |
| C | 0.68556000 | -4.22360800 | -1.31371600 |
| C | 1.40098600 | -4.16541300 | -0.06995800 |
| C | 0.68407500 | -4.62961400 | 1.08892900 |
| C | -0.68429000 | -4.62970800 | 1.08895200 |
| C | 2.58071200 | -3.31368300 | 0.04089400 |
| C | 2.72892100 | -2.58699100 | 1.24839700 |
| C | 3.29791300 | -1.31882200 | 1.24480200 |
| C | 3.78353600 | -0.75092600 | 0.05583300 |
| C | 3.91455400 | -1.59569500 | -1.06684300 |
| C | 3.30443800 | -2.84439100 | -1.08592000 |
| C | 3.78367100 | 0.75119500 | -0.05588100 |
| C | 3.29830900 | 1.31923800 | -1.24490300 |
| C | 2.72945800 | 2.58745200 | -1.24849700 |
| C | 2.58107700 | 3.31405300 | -0.04092500 |
| C | 3.30470200 | 2.84464400 | 1.08594000 |
| C | 3.91471200 | 1.59591700 | 1.06684700 |
| H | -2.26286300 | 2.93903700 | -2.16173400 |
| H | -3.24395700 | 0.72601700 | -2.15148300 |

| | | | |
|---|---|---|---|
| H | -4.40977400 | 1.23887100 | 1.96484300 |
| H | -3.33666600 | 3.42968800 | 1.99984800 |
| H | -3.24443600 | -0.72651200 | 2.15164900 |
| H | -2.26359200 | -2.93964900 | 2.16188200 |
| H | -3.33692100 | -3.42988900 | -1.99989200 |
| H | -4.40986300 | -1.23898900 | -1.96483400 |
| H | -1.21475200 | 4.08292500 | 2.24981400 |
| H | 1.21513100 | 4.08318900 | 2.24980100 |
| H | 1.22672200 | 4.88654000 | -1.99335700 |
| H | -1.22658600 | 4.88635400 | -1.99331000 |
| H | -1.21512100 | -4.08316400 | -2.24981400 |
| H | 1.21476100 | -4.08289600 | -2.24981700 |
| H | 1.22657900 | -4.88637600 | 1.99329700 |
| H | -1.22672700 | -4.88655200 | 1.99333700 |
| H | 2.26285700 | -2.93904200 | 2.16174300 |
| H | 3.24394100 | -0.72601900 | 2.15149500 |
| H | 4.40979700 | -1.23887600 | -1.96481700 |
| H | 3.33669100 | -3.42969400 | -1.99983000 |
| H | 3.24442100 | 0.72649400 | -2.15164000 |
| H | 2.26358000 | 2.93963000 | -2.16188900 |
| H | 3.33692500 | 3.42990500 | 1.99987700 |
| H | 4.40986100 | 1.23900300 | 1.96483300 |

Sum of electronic and zero-point Energies = -1385.157357 Hartree

Table S18. XYZ coordinate of [7]CPP$^{2+}$($D_1$) by UB3LYP/6-31G(d).

| | X | Y | Z |
|---|---|---|---|
| C | -1.33965300 | 4.34420700 | -0.05072300 |
| C | -0.60447400 | 4.86073900 | 1.03675400 |
| C | 0.78480800 | 4.89770200 | 1.00273800 |
| C | 1.49513000 | 4.43075800 | -0.12690000 |
| C | 0.74580500 | 4.14471800 | -1.28701200 |
| C | -0.64268200 | 4.09680000 | -1.24648600 |
| C | 2.86883300 | 3.90297000 | -0.04657700 |
| C | 3.36818800 | 3.41455400 | 1.19156500 |
| C | 4.29579400 | 2.39743500 | 1.22428800 |
| C | 4.76555000 | 1.79839000 | 0.01297000 |
| C | 4.53801900 | 2.54751800 | -1.18734100 |
| C | 3.62258100 | 3.57305400 | -1.21163000 |
| C | 5.08128600 | 0.38979500 | -0.01004400 |
| C | 5.19421000 | -0.38506600 | 1.19003900 |
| C | 4.80500800 | -1.70366500 | 1.21340900 |
| C | 4.26612800 | -2.32374700 | 0.04772000 |
| C | 4.50864800 | -1.66794100 | -1.18976900 |
| C | 4.91270200 | -0.35186000 | -1.22168100 |
| C | 3.25106000 | -3.38981800 | 0.12657600 |
| C | 2.44945900 | -3.45226900 | 1.28515700 |
| C | 1.17488000 | -4.00510000 | 1.24271100 |
| C | 0.65367900 | -4.52843800 | 0.04634500 |
| C | 1.54124000 | -4.67966300 | -1.03956200 |
| C | 2.81196700 | -4.11686700 | -1.00345200 |
| C | -0.82626600 | -4.57664800 | -0.10713200 |

| | | | |
|---|---|---|---|
| C | -1.69906300 | -4.72392900 | 0.99708200 |
| C | -2.98240900 | -4.20727200 | 0.95820100 |
| C | -3.46451600 | -3.53202200 | -0.19886600 |
| C | -2.68651900 | -3.66630300 | -1.38108000 |
| C | -1.39732000 | -4.16669600 | -1.33059600 |
| C | -4.44658200 | -2.46367100 | -0.11771500 |
| C | -4.80437100 | -1.89553600 | 1.14819300 |
| C | -5.10133700 | -0.56057800 | 1.25549200 |
| C | -5.06436800 | 0.29135900 | 0.10347500 |
| C | -5.14109800 | -0.37404500 | -1.16315400 |
| C | -4.83970900 | -1.70799800 | -1.27051100 |
| C | -4.63307100 | 1.67712600 | 0.18692500 |
| C | -3.98730800 | 2.12838100 | 1.37000500 |
| C | -3.03693600 | 3.13329200 | 1.32206700 |
| C | -2.69726600 | 3.75202400 | 0.10045800 |
| C | -3.54826600 | 3.51318200 | -1.00457900 |
| C | -4.48628600 | 2.49600600 | -0.96827600 |
| H | -1.11640200 | 5.17469900 | 1.94145500 |
| H | 1.31979800 | 5.24166200 | 1.88262100 |
| H | 1.24367600 | 3.82360500 | -2.19511100 |
| H | -1.17319000 | 3.73811100 | -2.12198100 |
| H | 2.91348300 | 3.73466500 | 2.12239800 |
| H | 4.54734400 | 1.95773600 | 2.18234600 |
| H | 5.03885400 | 2.26659000 | -2.10765100 |
| H | 3.41823700 | 4.08010300 | -2.14893200 |
| H | 5.52574900 | 0.08256500 | 2.11098100 |

| | | | |
|---|---|---|---|
| H | 4.83598900 | -2.24966700 | 2.15059500 |
| H | 4.23452400 | -2.15110600 | -2.12094600 |
| H | 4.95248400 | 0.15359000 | -2.17951000 |
| H | 2.75968700 | -2.94798700 | 2.19352100 |
| H | 0.54034600 | -3.90838300 | 2.11712000 |
| H | 1.21527800 | -5.18328300 | -1.94468000 |
| H | 3.44439300 | -4.19825000 | -1.88217200 |
| H | -1.33931800 | -5.17593700 | 1.91615500 |
| H | -3.59485900 | -4.26971700 | 1.85145200 |
| H | -3.03684700 | -3.25169200 | -2.31881600 |
| H | -0.78392800 | -4.11380300 | -2.22361400 |
| H | -4.71989300 | -2.48573100 | 2.05351100 |
| H | -5.27089500 | -0.13772400 | 2.23937500 |
| H | -5.31297500 | 0.19660300 | -2.06862900 |
| H | -4.80902600 | -2.16177400 | -2.25473200 |
| H | -4.12561700 | 1.60076900 | 2.30621800 |
| H | -2.45977600 | 3.34582100 | 2.21551500 |
| H | -3.41669700 | 4.07775600 | -1.92239900 |
| H | -5.06613100 | 2.29187500 | -1.86216700 |

Sum of electronic and zero-point Energies = -1616.172617 Hartree

Table S19. XYZ coordinate of [8]CPP$^{2+}$($D_1$) by UB3LYP/6-31G(d).

| | X | Y | Z |
|---|---|---|---|
| C | 5.43095700 | 1.56202600 | -0.07515900 |
| C | 5.74543300 | 0.83846100 | 1.11008900 |

| | | | |
|---|---|---|---|
| C | 5.66283400 | -0.53980600 | 1.14558800 |
| C | 5.24668500 | -1.27478500 | 0.00661200 |
| C | 5.20010000 | -0.57942700 | -1.22330400 |
| C | 5.29544600 | 0.79892400 | -1.26655900 |
| C | 4.61692300 | -2.60838000 | 0.11394400 |
| C | 3.90533200 | -2.92329100 | 1.28814600 |
| C | 2.92338200 | -3.90525000 | 1.28822000 |
| C | 2.60837800 | -4.61691900 | 0.11408800 |
| C | 3.46419100 | -4.44628200 | -0.99623600 |
| C | 4.44621100 | -3.46427100 | -0.99630500 |
| C | 1.27477600 | -5.24668100 | 0.00688200 |
| C | 0.53979500 | -5.66262600 | 1.14593600 |
| C | -0.83846800 | -5.74526500 | 1.11044600 |
| C | -1.56203800 | -5.43098100 | -0.07484900 |
| C | -0.79893000 | -5.29567100 | -1.26627400 |
| C | 0.57941800 | -5.20034300 | -1.22304500 |
| C | -2.93014300 | -4.94144900 | -0.04314300 |
| C | -3.50035200 | -4.47264200 | 1.17834900 |
| C | -4.47266200 | -3.50027200 | 1.17829900 |
| C | -4.94140800 | -2.93014500 | -0.04325300 |
| C | -4.62535600 | -3.65456400 | -1.23566300 |
| C | -3.65448800 | -4.62544000 | -1.23561400 |
| C | -5.43091700 | -1.56203600 | -0.07507800 |
| C | -5.74547700 | -0.83842200 | 1.11011400 |
| C | -5.66288000 | 0.53985200 | 1.14554700 |
| C | -5.24663700 | 1.27477000 | 0.00656700 |

| | | | |
|---|---|---|---|
| C | -5.19996700 | 0.57935900 | -1.22331300 |
| C | -5.29531600 | -0.79899000 | -1.26650500 |
| C | -4.61689500 | 2.60837700 | 0.11386000 |
| C | -3.90540800 | 2.92336300 | 1.28810000 |
| C | -2.92346000 | 3.90532500 | 1.28818400 |
| C | -2.60838800 | 4.61695400 | 0.11404600 |
| C | -3.46412200 | 4.44624900 | -0.99633100 |
| C | -4.44610700 | 3.46420300 | -0.99642800 |
| C | -1.27479400 | 5.24675400 | 0.00691700 |
| C | -0.53978400 | 5.66240700 | 1.14605700 |
| C | 0.83847800 | 5.74500700 | 1.11057500 |
| C | 1.56203300 | 5.43102100 | -0.07480900 |
| C | 0.79890700 | 5.29601100 | -1.26625600 |
| C | -0.57944300 | 5.20067600 | -1.22302800 |
| C | 2.93012100 | 4.94143800 | -0.04319100 |
| C | 3.50036000 | 4.47258700 | 1.17827500 |
| C | 4.47269700 | 3.50025700 | 1.17818800 |
| C | 4.94141000 | 2.93012200 | -0.04337500 |
| C | 4.62524300 | 3.65448700 | -1.23578500 |
| C | 3.65439300 | 4.62538900 | -1.23569400 |
| H | 6.00848400 | 1.36836400 | 2.01948700 |
| H | 5.86024900 | -1.05638100 | 2.07944900 |
| H | 4.95477600 | -1.11169700 | -2.13581800 |
| H | 5.12729100 | 1.29427800 | -2.21573100 |
| H | 4.02601700 | -2.31402600 | 2.17735000 |
| H | 2.31418300 | -4.02586500 | 2.17747800 |

| | | | |
|---|---|---|---|
| H | 3.32989600 | -5.05400100 | -1.88592200 |
| H | 5.05385800 | -3.33002400 | -1.88604800 |
| H | 1.05636800 | -5.85988100 | 2.07983100 |
| H | -1.36836900 | -6.00814600 | 2.01989500 |
| H | -1.29427700 | -5.12770000 | -2.21548000 |
| H | 1.11168000 | -4.95519000 | -2.13560700 |
| H | -3.07457700 | -4.77633500 | 2.12750000 |
| H | -4.77638900 | -3.07442300 | 2.12740700 |
| H | -5.11241600 | -3.39867600 | -2.17030800 |
| H | -3.39858300 | -5.11256200 | -2.17022000 |
| H | -6.00859800 | -1.36829000 | 2.01951300 |
| H | -5.86035900 | 1.05648100 | 2.07936600 |
| H | -4.95457200 | 1.11158700 | -2.13583300 |
| H | -5.12708700 | -1.29439700 | -2.21563700 |
| H | -4.02616100 | 2.31414500 | 2.17732700 |
| H | -2.31434000 | 4.02600000 | 2.17748700 |
| H | -3.32978300 | 5.05393100 | -1.88603600 |
| H | -5.05369500 | 3.32990000 | -1.88620500 |
| H | -1.05633300 | 5.85943200 | 2.08001400 |
| H | 1.36838700 | 6.00764000 | 2.02008900 |
| H | 1.29423600 | 5.12825800 | -2.21551100 |
| H | -1.11171200 | 4.95573400 | -2.13564200 |
| H | 3.07464200 | 4.77628700 | 2.12744800 |
| H | 4.77648000 | 3.07444300 | 2.12729200 |
| H | 5.11221300 | 3.39856000 | -2.17046700 |
| H | 3.39842600 | 5.11247300 | -2.17030300 |

Sum of electronic and zero-point Energies = -1847.176949 Hartree

Table S20. XYZ coordinate of [9]CPP$^{2+}$($D_1$) by UB3LYP/6-31G(d).

| | X | Y | Z |
|---|---|---|---|
| C | -5.21502100 | 2.92322500 | 0.06477200 |
| C | -5.07026600 | 3.76203400 | -1.06186800 |
| C | -4.14648200 | 4.79721600 | -1.06790000 |
| C | -3.32665900 | 5.04789800 | 0.05558600 |
| C | -3.61790500 | 4.33748700 | 1.23859200 |
| C | -4.53842700 | 3.29892500 | 1.24184600 |
| C | -2.05422700 | 5.78461800 | -0.03977600 |
| C | -1.34268400 | 5.80076500 | -1.26266600 |
| C | 0.01441700 | 6.05373100 | -1.29644000 |
| C | 0.74802300 | 6.30637100 | -0.10569100 |
| C | -0.01903700 | 6.53481200 | 1.07156900 |
| C | -1.37648400 | 6.28323000 | 1.10150100 |
| C | 2.17982700 | 6.05018400 | -0.05938500 |
| C | 2.93420700 | 5.76241400 | -1.23526400 |
| C | 4.09296700 | 5.02403400 | -1.17679800 |
| C | 4.58469200 | 4.51537800 | 0.06201800 |
| C | 4.00282000 | 5.07383300 | 1.23863100 |
| C | 2.84505400 | 5.81381200 | 1.18009000 |
| C | 5.50421300 | 2.55287100 | 1.29707100 |
| C | 5.84358200 | 1.21500500 | 1.26213600 |
| C | 6.12050900 | 0.56141900 | 0.03780900 |
| C | 6.28445700 | 1.38587700 | -1.10436600 |

| | | | |
|---|---|---|---|
| C | 5.94399100 | 2.72352800 | -1.07318400 |
| C | 5.98325800 | -0.90207300 | -0.05717500 |
| C | 5.45944100 | -1.46420000 | -1.24001700 |
| C | 4.90030900 | -2.73430800 | -1.24259300 |
| C | 4.84155300 | -3.50534800 | -0.06511500 |
| C | 5.54361700 | -3.02312900 | 1.06116100 |
| C | 6.09814600 | -1.75140300 | 1.06667000 |
| C | 3.86174400 | -4.61062700 | 0.02175400 |
| C | 3.15450800 | -4.81332300 | 1.22482600 |
| C | 1.95722600 | -5.51004200 | 1.24274800 |
| C | 1.39882600 | -6.03545000 | 0.05366600 |
| C | 2.21662600 | -6.01154300 | -1.10380600 |
| C | 3.41782500 | -5.32231200 | -1.11650800 |
| C | 5.41927800 | 3.32440700 | 0.10617800 |
| C | -0.03958900 | -6.30390300 | -0.00448400 |
| C | -0.74844500 | -6.14237200 | -1.22440600 |
| C | -2.10415500 | -5.89405600 | -1.23411100 |
| C | -2.84234700 | -5.78568400 | -0.02124600 |
| C | -2.18022700 | -6.22899100 | 1.16219300 |
| C | -0.82715200 | -6.48296200 | 1.16816300 |
| C | -4.06531000 | -5.00490800 | 0.02060600 |
| C | -4.47545300 | -4.38212700 | 1.23384200 |
| C | -5.27082100 | -3.25669200 | 1.22464700 |
| C | -5.71404200 | -2.67979400 | 0.00469400 |
| C | -5.54480100 | -3.46907900 | -1.16853800 |
| C | -4.74562200 | -4.58989400 | -1.16292500 |

| | | | |
|---|---|---|---|
| C | -6.07350100 | -1.26189200 | -0.05288600 |
| C | -6.39144800 | -0.50901300 | 1.10550600 |
| C | -6.26822400 | 0.87019600 | 1.11795400 |
| C | -5.80990400 | 1.57139800 | -0.02134600 |
| C | -5.70205500 | 0.84434700 | -1.22505600 |
| C | -5.83397900 | -0.53444700 | -1.24283200 |
| H | -5.65587200 | 3.57401300 | -1.95660300 |
| H | -4.03338700 | 5.39443600 | -1.96751300 |
| H | -3.03255700 | 4.51242100 | 2.13492900 |
| H | -4.64025400 | 2.69873500 | 2.13980400 |
| H | -1.83480900 | 5.48785000 | -2.17695100 |
| H | 0.52967000 | 5.93766600 | -2.24233100 |
| H | 0.46495600 | 6.86672000 | 1.98350900 |
| H | -1.91762500 | 6.42378700 | 2.03164000 |
| H | 2.56280200 | 6.06395900 | -2.20781400 |
| H | 4.57386400 | 4.74874400 | -2.10806000 |
| H | 4.42952200 | 4.85970800 | 2.21163200 |
| H | 2.38967000 | 6.12937800 | 2.11141000 |
| H | 5.18868400 | 2.97251400 | 2.24467300 |
| H | 5.77115900 | 0.63760800 | 2.17720600 |
| H | 6.63503600 | 0.95349200 | -2.03594300 |
| H | 6.03837300 | 3.30169400 | -1.98573800 |
| H | 5.37379500 | -0.85990400 | -2.13673300 |
| H | 4.39746900 | -3.07812200 | -2.14030000 |
| H | 5.61748500 | -3.63346700 | 1.95607700 |
| H | 6.59380000 | -1.39903400 | 1.96605800 |

| | | | |
|---|---|---|---|
| H | 3.48039800 | -4.31722800 | 2.13276200 |
| H | 1.39107500 | -5.53417000 | 2.16709800 |
| H | 1.88966200 | -6.50741000 | -2.01217800 |
| H | 3.99888800 | -5.29267700 | -2.03300900 |
| H | -0.20565100 | -6.08094700 | -2.16069100 |
| H | -2.57444200 | -5.65081500 | -2.17966700 |
| H | -2.73425600 | -6.32922400 | 2.08926900 |
| H | -0.35190700 | -6.77576300 | 2.09832400 |
| H | -4.05800000 | -4.70766800 | 2.17944100 |
| H | -5.44448500 | -2.73970300 | 2.16144000 |
| H | -6.00986100 | -3.16044800 | -2.09870900 |
| H | -4.60318900 | -5.13417600 | -2.09024600 |
| H | -6.70302000 | -1.01342900 | 2.01454700 |
| H | -6.48242800 | 1.41027900 | 2.03494800 |
| H | -5.39065700 | 1.34805100 | -2.13387500 |
| H | -5.62206400 | -1.05848800 | -2.16802300 |

Sum of electronic and zero-point Energies = -2078.173680 Hartree

**Changes in bond lengths of [*n*]CPP$^{2+}$.**

Table S21. Distribution of bond lengths of [*n*]CPP$^{2+}$ in the $S_0$ and $S_1$ states and changes in averaged bond lengths ($\Delta r_{av}$) estimated at UB3LYP/6-31G(d) level.

| *n* | Bond [a] | $S_0$ [b] | $S_1$ [b] | $\Delta r_{av}$ [c] |
|---|---|---|---|---|
| 5 | C(1)-C(1') | 1.4400 (1.4400) | 1.4420 – 1.4925 (1.4700) | 0.0300 |
| | C(1)-C(2) | 1.4346 (1.4346) | 1.4121 – 1.4399 (1.4267) | -0.0079 |
| | C(2)-C(3) | 1.3718 (1.3718) | 1.3704 – 1.3891 (1.3806) | 0.0088 |
| 6 | C(1)-C(1') | 1.4457 (1.4457) | 1.4592 – 1.5063 (1.4749) | 0.0292 |
| | C(1)-C(2) | 1.4300 (1.4300) | 1.4043 – 1.4396 (1.4212) | -0.0088 |
| | C(2)-C(3) | 1.3738 (1.3738) | 1.3684 – 1.3900 (1.3833) | 0.0095 |
| 7 | C(1)-C(1') | 1.4507 – 1.4515 (1.4511) | 1.4437 – 1.4888 (1.4680) | 0.0169 |
| | C(1)-C(2) | 1.4245 – 1.4275 (1.4262) | 1.4060 – 1.4334 (1.4207) | -0.0055 |
| | C(2)-C(3) | 1.3753 – 1.3768 (1.3758) | 1.3718 – 1.3903 (1.3817) | 0.0059 |
| 8 | C(1)-C(1') | 1.4557 (1.4557) | 1.4534 – 1.4787 (1.4661) | 0.0104 |
| | C(1)-C(2) | 1.4211 – 1.4246 (1.4229) | 1.4086 – 1.4306 (1.4194) | -0.0035 |
| | C(2)-C(3) | 1.3771 – 1.3788 (1.3779) | 1.3730 – 1.3888 (1.3816) | 0.0037 |
| 9 | C(1)-C(1') | 1.4593 – 1.4585 (1.4593) | 1.4516 – 1.4796 (1.4662) | 0.0069 |
| | C(1)-C(2) | 1.4184 – 1.4232 (1.4205) | 1.4087 – 1.4268 (1.4182) | -0.0023 |
| | C(2)-C(3) | 1.3786 – 1.3805 (1.3794) | 1.3753 – 1.3878 (1.3819) | 0.0025 |

[a] Numbering of the carbon atoms is indicated below. [b] Numbers in parentheses are averaged values. Unit: Å. [c] Difference between averaged values in the $S_1$ and $S_0$ states. Unit: Å.