Supporting Information

I.   Materials and Methods

All manipulations were carried out using break-and-seal[1] and glove-box techniques under an atmosphere of argon. Tetrahydrofuran (THF, Sigma Aldrich) was dried over Na/K alloy and distilled prior to use. Potassium metal (98%) was purchased from Sigma Aldrich and used as received. [8]CPP ($C_{48}H_{32}$, **1**) was synthesized according to the previously reported procedures and used as received.[2] The UV-Vis spectra were recorded on a Thermo Scientific Evolution 201 UV-Visible Spectrophotometers. The extreme air- and moisture-sensitivity of crystals **2** prevented obtaining of elemental analysis data.

[{K$^+$(THF)$_2$}$_4$(1^{4-})] (2)

THF (0.7 mL) was added to an NMR ampule (O.D. 5 mm) containing excess K metal (4 mg, 0.103 mmol) and **1** (2.0 mg, 0.0033 mmol). The ampule was sealed under reduced pressure and placed at 5 ˚C. The initial yellow color of the mixture (neutral ligand) changed to brown after 6 hours, purple after 12 hours, deepened to purple-violet after 2 days, and turned pale blue after 5 days. Multiple black blocks were deposited in moderate yield (*ca*. 65 %) after 15 days. UV-Vis (THF, nm): λ_{max} 431, 580, 800.

Notes: This polymeric product is nearly insoluble in THF after crystallization.
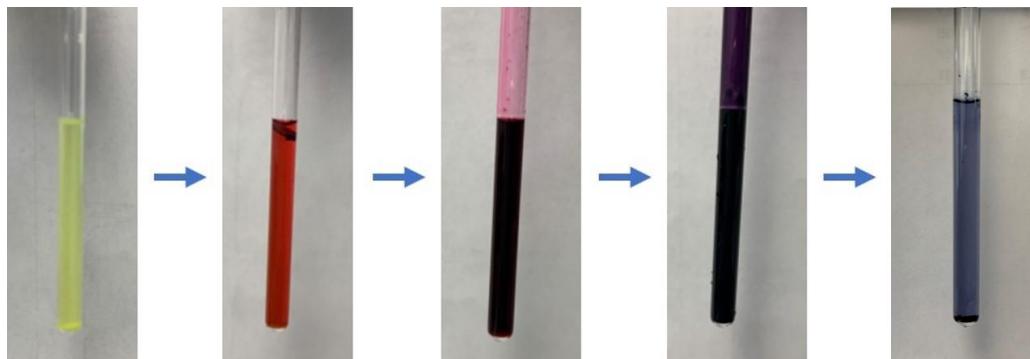

Figure S1. Color changes of stepwise chemical reduction of **1** with K metal in THF.

II.   UV-Vis Spectroscopic Investigation

Sample preparation: THF (2 mL) was added to a glass ampule (O.D. 10 mm) containing excess K (1 mg, 0.026 mmol) and **1** (0.2 mg, 1.6×10^{-4} mmol). The ampule was sealed under argon and UV-Vis spectra were monitored at different reaction times (total 24 hours) at room temperature.

| Label	Time (min)
1	1
2	5
3	15
4	30
5	45
6	55
7	65
8	80
9	100
10	600
11	1440
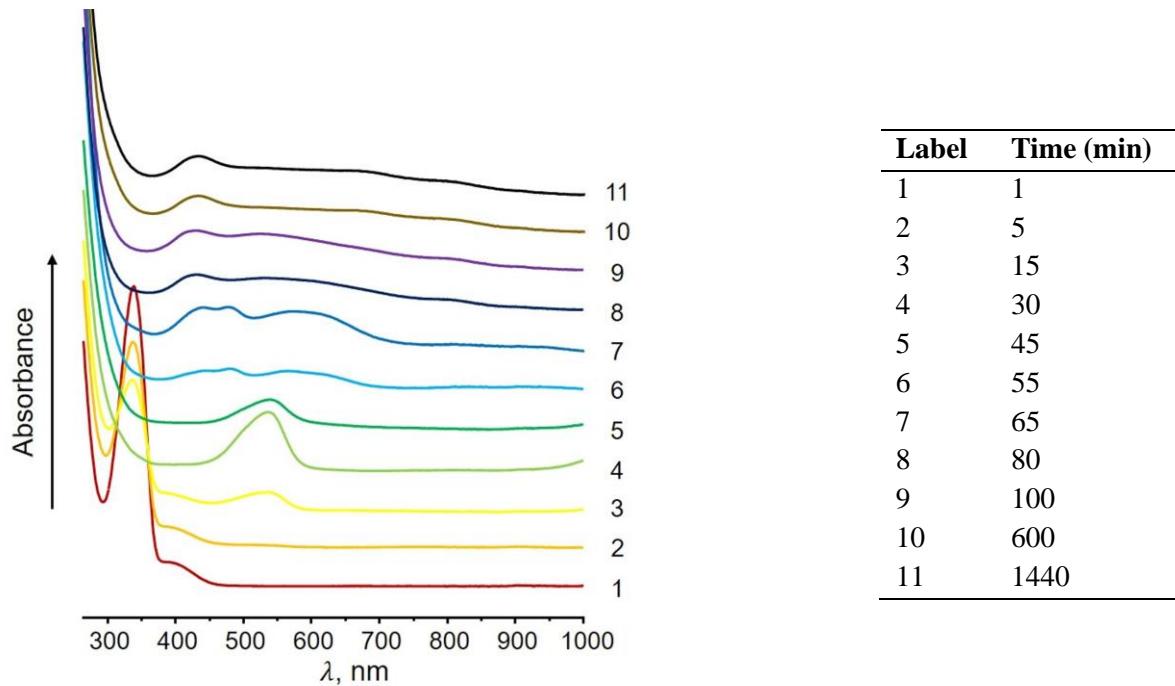
**Figure S2.** UV-Vis spectra of **1**/K in THF.
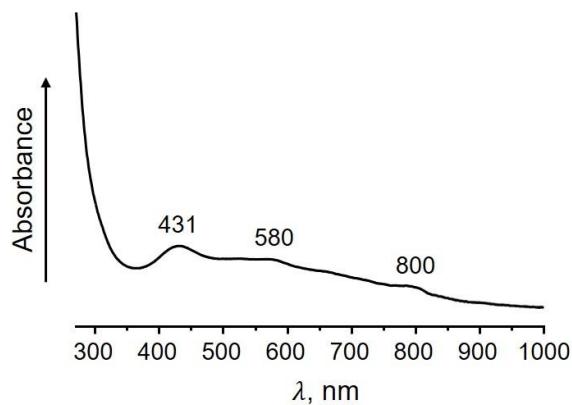
Figure S3. UV-Vis spectrum of crystals of **2** dissolved in THF.

III. Crystal Structure Solution and Refinement Details

Data collection of **2** was performed on a Bruker D8 VENTURE single crystal X-ray diffractometer equipped with a PHOTON 100 CMOS detector and a Mo-target X-ray tube ($\lambda = 0.71073$ Å) at 100(2) K. The data were collected at 50 kV and 30 mA with an appropriate 0.5° ω scan strategy. Data reduction and integration were performed with the Bruker software package SAINT (version 8.37A).[3] Data were corrected for absorption effects using the empirical methods as implemented in SADABS (version 2016/2).[4] The structure was solved by SHELXT (version 2018/2)[5] and refined by full-matrix least-squares procedures using the Bruker SHELXTL (version 2018/3)[6] software package through the OLEX2[7] graphical interface. All non-hydrogen atoms (including those in disordered parts) were refined anisotropically. The H-atoms were included at calculated positions and refined as riders, with $U_{iso}(H) = 1.2\ U_{eq}(C)$. The structure of **2** was refined as a two-component inversion twin with twin law [-1 0 0 0 -1 0 0.5 0 1] with BASF parameter refined to 0.1138(26). In **2**, all four THF molecules bound to K^+ ions were found to be disordered and were modeled with two orientations with their relative occupancies refined. The geometries of the disordered parts were restrained to be similar. The anisotropic displacement parameters of the disordered molecules in the direction of the bonds were restrained to be equal using RIGU command with default standard uncertainty. They were also restrained to have the same U_{ij} components using SIMU with standard uncertainty of 0.01. Crystallographic data and details of the data collection and structure refinement are listed in Table S1.

Table S1. Crystal data and structure refinement parameters for **2**.

Compound	**2**
Empirical formula	$C_{80}H_{96}O_8K_4$
Formula weight	1341.96
Temperature (K)	100(2)
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	$C2/c$
a (Å)	22.330(7)
b (Å)	10.120(3)
c (Å)	31.991(8)
α (°)	90.00
β (°)	99.196(6)
γ (°)	90.00
V (Å^3)	7136(3)
Z	4
ρ_{calcd} (g·cm^{-3})	1.249
μ (mm^{-1})	0.305
$F(000)$	2864
Crystal size (mm)	0.02×0.11×0.15
θ range for data collection (°)	2.84-25.10
Reflections collected	39344
Independent reflections	6517
	[R_{int} = 0.1743]
Transmission factors (min/max)	0.5580/0.6885
Data/restraints/params.	6517/1175/561
$R1$,[a] $wR2$[b] $(I > 2\sigma(I))$	0.1508, 0.3157
$R1$,[a] $wR2$[b] (all data)	0.2049, 0.3469
Quality-of-fit[c]	1.088

[a]$R1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$. [b]$wR2 = [\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]]$.
[c]Quality-of-fit $= [\Sigma[w(F_o^2-F_c^2)^2]/(N_{obs}-N_{params})]^{1/2}$, based on all data.
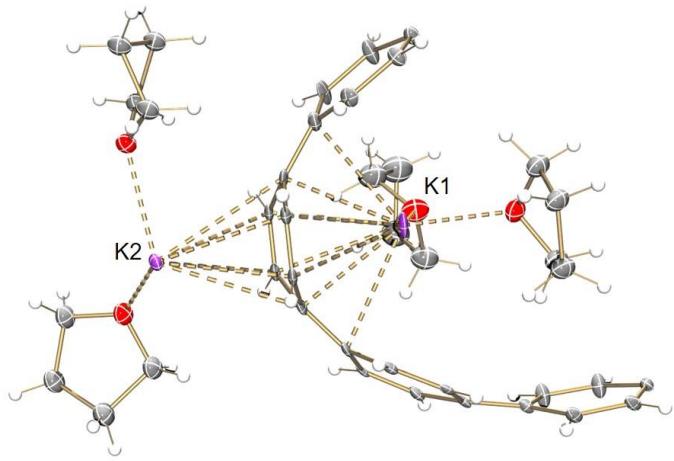
Figure S4. ORTEP drawing of the asymmetric unit of **2** with thermal ellipsoids at the 40% probability level. Color scheme used: K dark orchid, C gray, O red, H white.
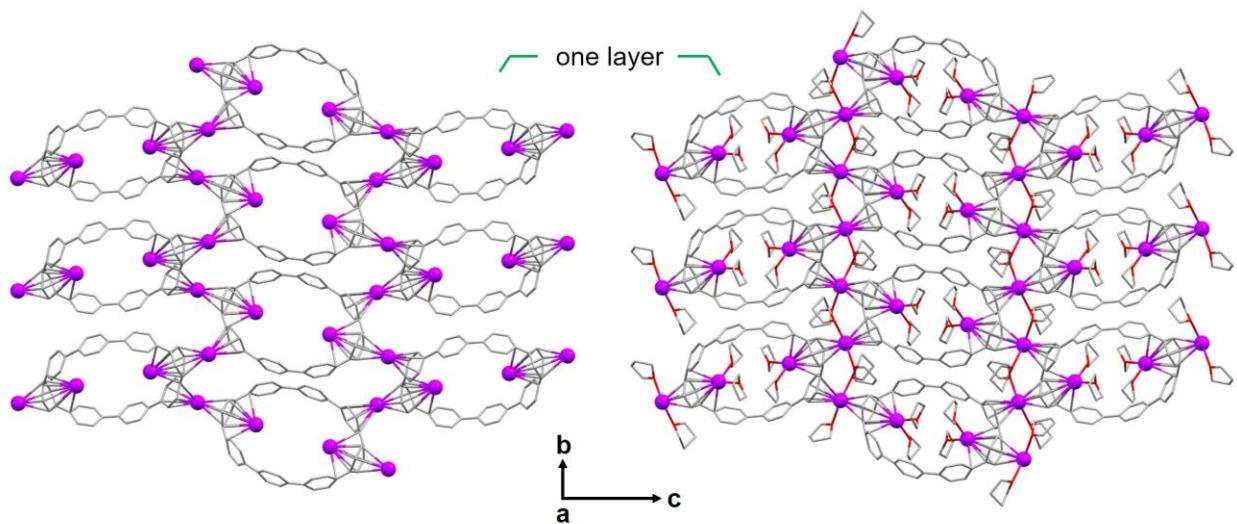
Figure S5. Solid-state packing of **2** along *a* axis, mixed models. H-atoms are omitted for clarity.
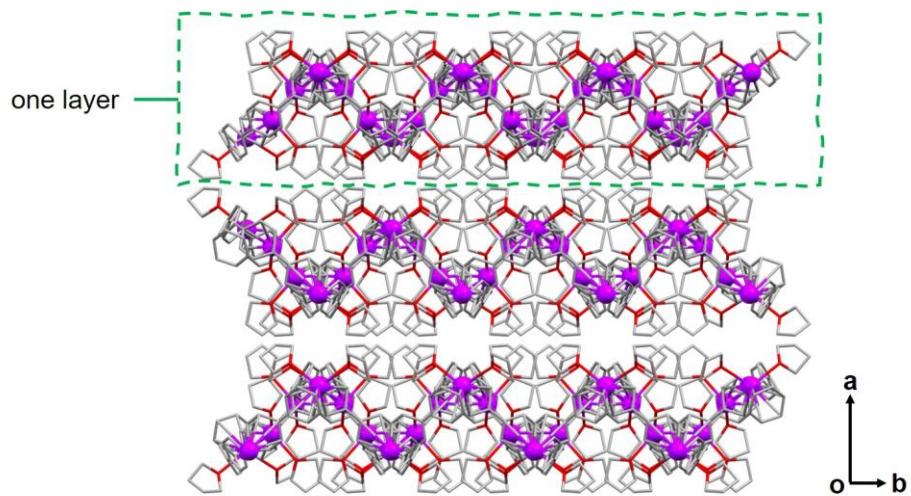
Figure S6. Solid-state packing of **2** along *c* axis, mixed models. H-atoms are omitted for clarity.
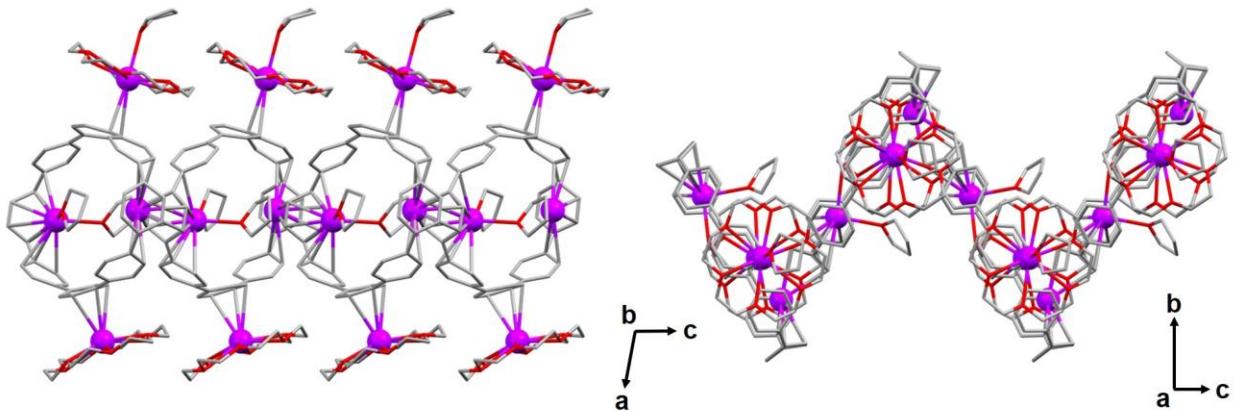
Figure S7. 1D chain of [{K$^+$(18-crown-6)(THF)}{K$^+$(18-crown-6)}{K$^+_2$(THF)$_2$(**1**$^{4-}$)}][8] along *a* and *b* axis, mixed models. H-atoms are omitted for clarity.
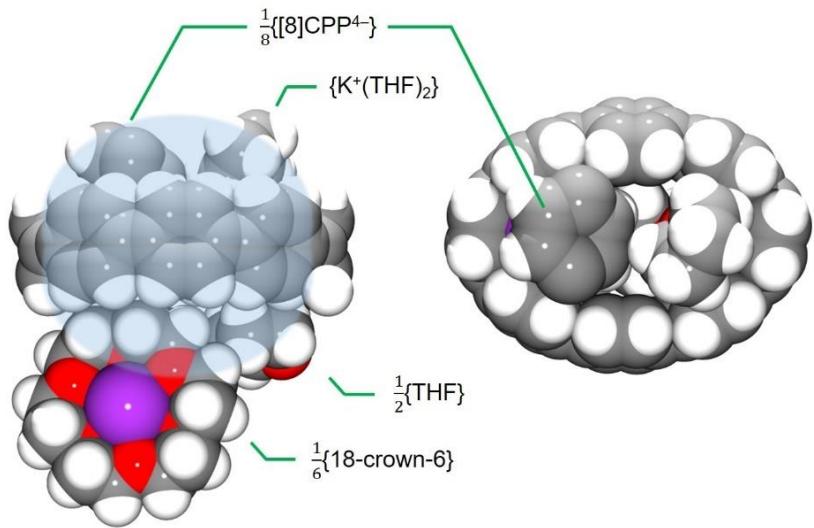
Figure S8. Host-guest interactions of **1**[4−] reported previsouly,[8] side and face views, space-filling models. The internal space is shown as the blue sphere.
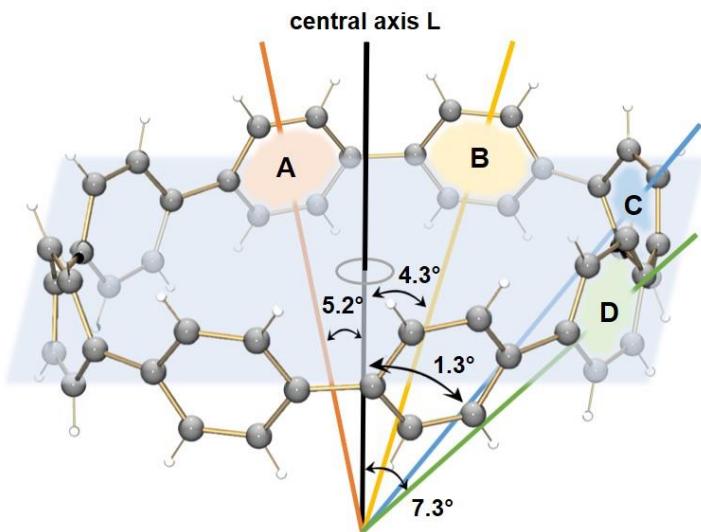
Figure S9. Calculation of the selected angles between the plane of six-membered rings and the macrocycle central axis of **1**[4−] in **2**.

Table S2. Selected C–C distances (Å) of **1** and **1**[4–] in **2**, along with a labeling scheme.
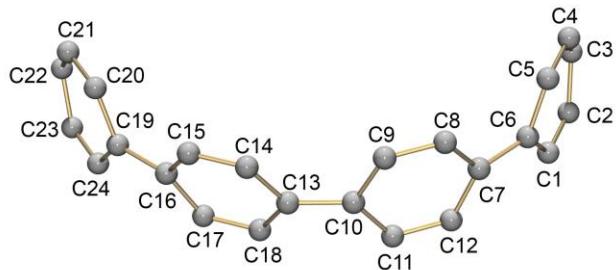
Distance	**1**[2]	**1**[4–]	Distance	**1**[2]	**1**[4–]
C1–C2	1.383(2)	1.397(15)	C11–C12	1.386(2)	1.382(15)
C1–C6	1.399(2)	1.395(14)	C13–C14	1.399(2)	1.503(14)
C2–C3	1.400(2)	1.397(15)	C13–C18	1.402(2)	1.457(16)
C3–C4	1.401(2)	1.409(15)	C14–C15	1.382(2)	1.353(15)
C3–C22	1.490(2)	1.477(15)	C15–C16	1.406(2)	1.454(15)
C4–C5	1.384(2)	1.357(16)	C16–C17	1.400(2)	1.471(15)
C5–C6	1.403(2)	1.418(15)	C16–C19	1.486(2)	1.420(15)
C6–C7	1.486(2)	1.475(15)	C17–C18	1.385(2)	1.341(15)
C7–C8	1.402(2)	1.436(14)	C19–C20	1.401(2)	1.415(16)
C7–C12	1.403(2)	1.408(15)	C19–C24	1.401(2)	1.413(16)
C8–C9	1.377(2)	1.363(15)	C20–C21	1.383(2)	1.389(16)
C9–C10	1.402(2)	1.468(15)	C21–C22	1.402(2)	1.383(16)
C10–C11	1.400(2)	1.444(14)	C22–C23	1.402(2)	1.415(15)
C10–C13	1.481(2)	1.396(15)	C23–C24	1.383(2)	1.374(15)

IV.   Computational Details

All geometry optimizations were performed at the density functional theory level with the help of hybrid correlation-exchange functional PBE0.[9] All light atoms (C, H, O) were described by correlation-consistent basis sets of triple-ζ quality (cc-pVTZ), whereas a triple-ζ def2-TZVP one was used for potassium. No symmetry restrictions were applied. Calculated structures were found to be local minima (no imaginary frequencies) on the corresponding potential energy surfaces, as determined by calculation of the full Hessian matrix, followed by estimation of frequencies in the harmonic approximation. All calculations were performed with help of ORCA package (version 4.2.1).[10]

Converged wavefunctions were then used to get insights into the electronic structure of target systems in terms of natural bond orbitals (NBO).[11] Bond orders quoted are those from the Wiberg formulation[12] (Wiberg bond indices) incorporated in the NBO analysis. All computations were performed with the NBO[13] (version 6.0) program.

Aromaticity descriptors. Using PBE0/cc-pVDZ geometries and PBE0/cc-pVDZ//cc-pVTZ converged wavefunctions, a set of theoretical descriptors/indexes of aromaticity was calculated. This set includes: (*i*) structure-based Harmonic Oscillator Model of Aromaticity (HOMA, as defined by Kruszewski and Krygowski[14]), (*ii*) Nuclear Independent Chemical Shift (NICS, introduced by von Rague Schleyer *et al.*[15]), and (*iii*) descriptors based on topological Quantum Theory of Atom in Molecule (QTAIM[16]) approach such as Para-Delocalized Index (PDI[17]) and Aromatic Fluctuation Index (FLU[18]). In the latter, two types of atomic spaces were tested, namely, AIM, using Bader's atomic basin definition[19] and Fuzzy atomic space[20], using Becke atomic space definition. The correlation between the results calculated in fuzzy atomic space and in AIM atomic space was previously reported to be excellent.[21] All QTAIM calculations were carried out by Multiwfn 3.3.7 program.[22] Calculations of NICS values were performed using Gauge Independent Atomic Orbitals (GIAO) approach with help of Gaussian 09 program[23] at the PBE0/cc-pVTZ level of theory. The set of descriptors was augmented by detailed consideration of magnetically induced ring current on target systems using Anisotropy of the Induced Current Density (ACID) approach.[24] The applied magnetic field is perpendicular to the five-membered ring. To obtain the induced current vectors and plot map, ACID 2.0.0 program uses the current density tensors, calculated by Continuous Set of Gauge Transformations (CSGT) method[25] implemented in the Gaussian 09 package.

Molecular Electrostatic Potential (MEP) maps. Maps of MEP were prepared in two forms: (*i*) 3D distribution mapped on the fast solvent surface of the target species and (*ii*) 2D cross-section maps (the plane of the cross-section along with mapped MEP are visualized in Figures S10-S12 for all systems under consideration). Scales for 3D and 2D maps were taken exactly the same for specific charge state. All computations and visualizations were performed with help of the Molekel (version 4.3) program.[26]

Solvent. Series of calculations were performed taking into account the influence of the solvent. Conductor-like Polarizable Continuum Model[27] approach was used with tetrahydrofuran (THF) utilized as a solvent with default parameters (!CPCM(THF) keyword in ORCA terminology). It was found that the solvent media makes only minimal influence on energetics and aromaticity of the target systems (see Tables S11-S12).
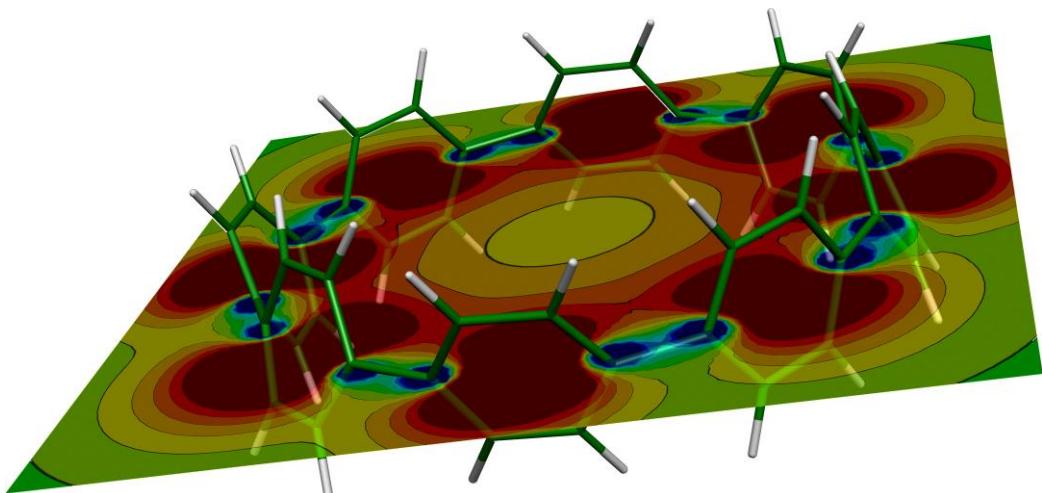
Figure S10. 2D cross-section of the MEP for the neutral [8]CPP molecule.
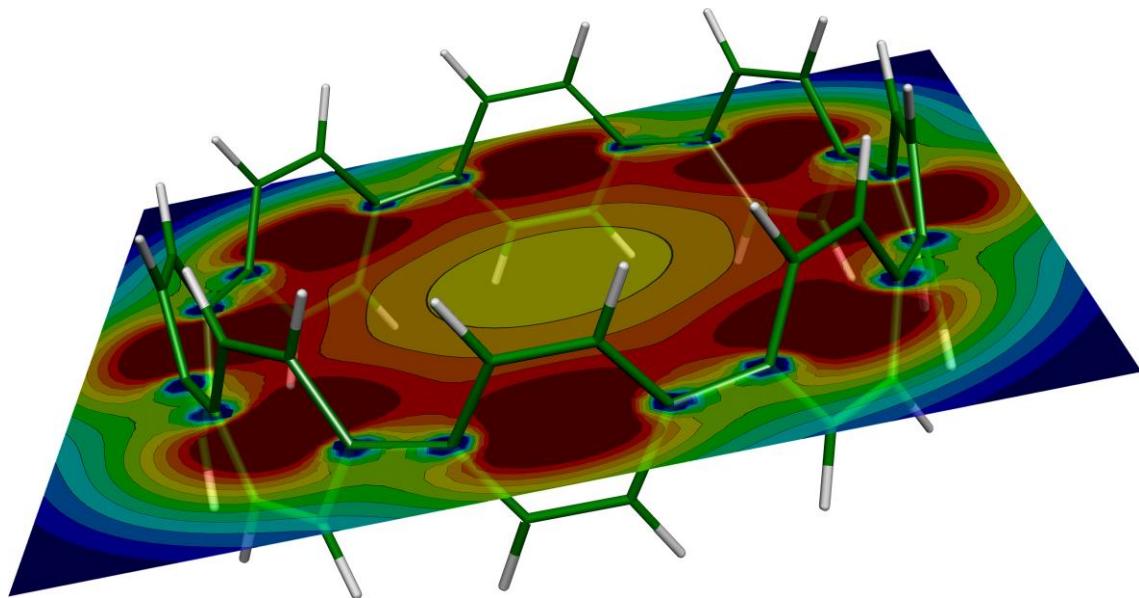
Figure S11. 2D cross-section of the MEP for the di-anionic [8]CPP^{2-} species.
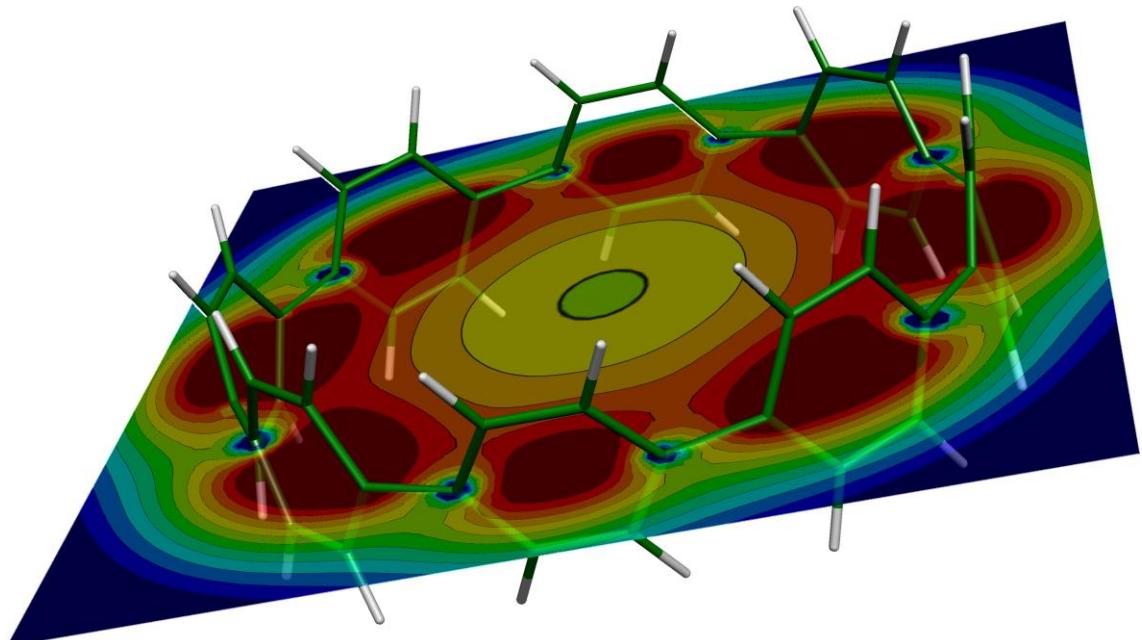
Figure S12. 2D cross-section of the MEP for the tetra-anionic [8]CPP^{4-} species.
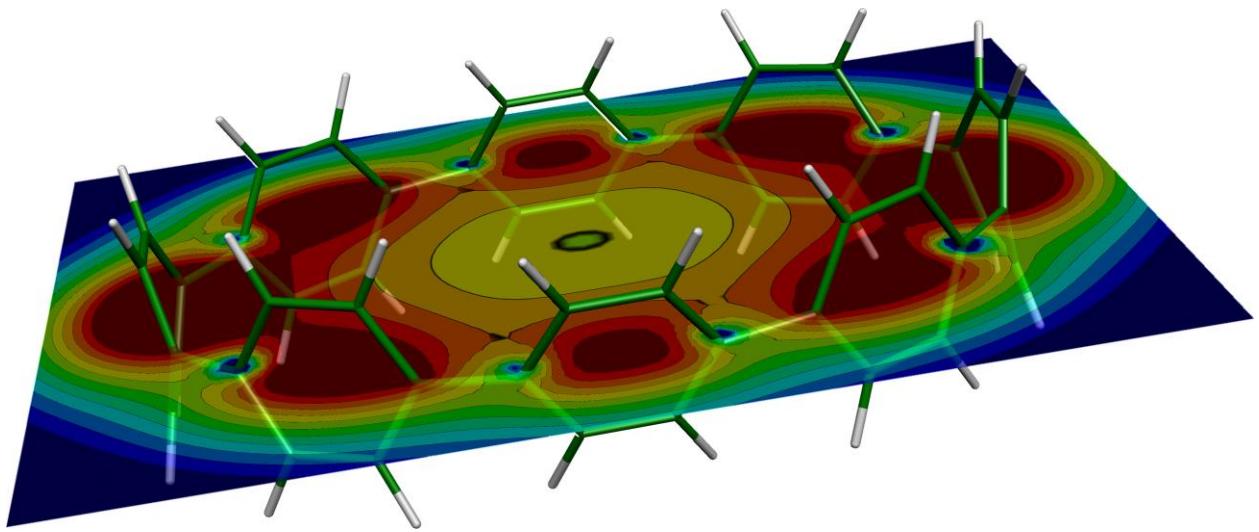
Figure S13. 2D cross-section of the MEP for the tetra-anionic *noK*-[8]CPP^{4-} model.

Table S3. Cartesian coordinates of [8]CPP (q = 0, S = 0).

Symbol	X	Y	Z
C	-5.109458854	0.691936719	-1.245726314
H	-4.78024086	1.161910559	-2.162686278
C	-4.665433099	-3.60631654	-0.937881876
H	-5.279117906	-3.464129549	-1.820002887
C	-5.777854827	0.782934867	1.033044929
H	-6.054410933	1.334988589	1.922999194
C	-5.32406089	1.466286969	-0.10196233
C	-5.344066887	-1.366766243	0.003376066
C	-3.098103567	-4.021144128	1.288745888
H	-2.448908761	-4.117693827	2.150279136
C	-4.791925731	-2.727512768	0.143463529
C	-4.381826642	3.392670448	1.180391186
H	-4.749064265	2.972398573	2.107992001
C	1.370702626	-5.347862141	-0.155024378
C	-5.122385945	-0.687162527	-1.195879516
H	-4.800880348	-1.240437762	-2.069597677
C	-0.693849747	-5.776826545	1.047066661
H	-1.180028398	-6.047787178	1.977271752
C	-1.461334	-5.316706827	-0.027261603
C	-5.780950177	-0.59954533	1.087546148
H	-6.052827342	-1.08803768	2.016271435
C	-3.410344211	4.372390399	1.24959719
H	-3.087911555	4.706104066	2.227715814

C	-4.773020081	2.835984764	-0.041654494
C	-4.067148613	-3.035863354	1.296432345
H	-4.146126293	-2.391960792	2.163695521
C	-2.750548774	4.822052428	0.101013645
C	-2.811067622	-4.742096083	0.127906569
C	0.687995181	-5.798837714	0.981518553
H	1.241808608	-6.093433667	1.864578948
C	-3.695861471	-4.592296654	-0.945535927
H	-3.571061711	-5.201515856	-1.833362714
C	-0.787160752	-5.097046372	-1.229932269
H	-1.341230808	-4.757822396	-2.096430644
C	0.591508802	-5.109098072	-1.29069785
H	1.060209407	-4.780484005	-2.208516561
C	-4.320612744	3.49669804	-1.188618881
H	-4.667570268	3.187801132	-2.166504816
C	-3.323500915	4.4503875	-1.119609998
H	-2.903964785	4.81752336	-2.04759726
C	5.109477483	-0.691934276	1.245705276
H	4.780274556	-1.161905279	2.162671838
C	4.66544163	3.606313726	0.937869163
H	5.279133361	3.464121229	1.819984476
C	5.777833027	-0.782936727	-1.033077044
H	6.054372565	-1.33499182	-1.923035535
C	5.32406108	-1.466287775	0.101939993
C	5.344062803	1.366766931	-0.00340504
C	3.098096123	4.021158388	-1.288744399
H	2.448895422	4.117715447	-2.15027255
C	4.791924822	2.727516188	-0.143482666
C	4.381828042	-3.3926897	-1.18039206
H	4.749068105	-2.972431926	-2.107997872
C	-1.370701659	5.347858368	0.155051615
C	5.122400278	0.68716462	1.195854693
H	4.800910394	1.240440885	2.069577853
C	0.693848479	5.776851644	-1.047033479
H	1.180025804	6.047834349	-1.977232694
C	1.461334907	5.316709216	0.027284037
C	5.780927616	0.599543734	-1.087580822
H	6.052788847	1.088033211	-2.016312288
C	3.410345921	-4.372411178	-1.249584593
H	3.087913714	-4.706138944	-2.227698628
C	4.773022095	-2.835987403	0.041646507
C	4.067139077	3.035875369	-1.296443978
H	4.146110048	2.391979404	-2.163712477

C	2.750549469	-4.822055517	-0.100994872
C	2.811067912	4.74210086	-0.127897369
C	-0.687996217	5.798859834	-0.981482122
H	-1.241812014	6.093475571	-1.864534369
C	3.695868831	4.592292801	0.945538115
H	3.571074423	5.201505571	1.833370191
C	0.787163765	5.097022635	1.229950857
H	1.341235304	4.757779123	2.096440519
C	-0.591505879	5.109070199	1.290718357
H	-1.060205399	4.780436562	2.208530473
C	4.320616219	-3.496686604	1.188619528
H	4.667574729	-3.18777811	2.166501438
C	3.323503141	-4.450375278	1.119623328
H	2.903968264	-4.817499937	2.047615518

Table S4. Cartesian coordinates of [8]CPP (q = −1, S = 1/2).

Symbol	X	Y	Z
C	-5.312106131	0.753717805	-1.234059719
H	-5.126581601	1.235822871	-2.185079328
C	-4.545863297	-3.484457217	-1.037377662
H	-5.098854646	-3.291589486	-1.949758198
C	-5.689242223	0.803956589	1.110605116
H	-5.866726573	1.3336975	2.038871975
C	-5.37675431	1.523956414	-0.058694422
C	-5.338756617	-1.335086596	0.007424383
C	-3.153807891	-4.070705553	1.259752928
H	-2.580750452	-4.231712431	2.164534498
C	-4.765218154	-2.675047289	0.092709544
C	-4.445309797	3.483932387	1.187161635
H	-4.826369397	3.105395538	2.12761136
C	1.42595625	-5.388474084	-0.11250388
C	-5.29228931	-0.622593848	-1.202001161
H	-5.082503542	-1.150295203	-2.124409992
C	-0.670426099	-5.672155495	1.091465379
H	-1.168014445	-5.854569656	2.037260072
C	-1.430663375	-5.30047855	-0.032346967
C	-5.667658128	-0.572945399	1.143348996
H	-5.832873512	-1.07022731	2.092363416
C	-3.467218848	4.451955085	1.232504179
H	-3.146223271	4.806143814	2.204503843
C	-4.837745898	2.880964506	-0.022437192
C	-4.120541025	-3.089370921	1.269842933
H	-4.263232241	-2.524042628	2.182419079
C	-2.794374289	4.879806112	0.072257639
C	-2.761492359	-4.708868518	0.071806826
C	0.705809458	-5.718886818	1.051674755
H	1.237502813	-5.935049359	1.970737479
C	-3.578484432	-4.465634083	-1.047664136
H	-3.402549879	-5.012023951	-1.967486118
C	-0.722785361	-5.230631808	-1.243140835
H	-1.251089924	-4.981687055	-2.155461723
C	0.652933441	-5.273118685	-1.281771334
H	1.135980817	-5.061288982	-2.226892893
C	-4.382884314	3.532355717	-1.184627425
H	-4.730005396	3.207269928	-2.157584291
C	-3.393218666	4.488511848	-1.139235989
H	-2.991657564	4.846347429	-2.079277968

C	5.31212549	-0.753704574	1.23403612
H	5.126628001	-1.235799092	2.185066173
C	4.545897672	3.484474269	1.037334383
H	5.098911797	3.291612721	1.949702422
C	5.689198488	-0.803968299	-1.110637873
H	5.866654768	-1.333718542	-2.038904414
C	5.376743984	-1.523956086	0.058677629
C	5.338749086	1.335087349	-0.007470443
C	3.153780006	4.070702172	-1.25976429
H	2.580696883	4.231700417	-2.164531196
C	4.765217039	2.675051443	-0.092751136
C	4.445319709	-3.483967511	-1.187139426
H	4.8263884	-3.105454721	-2.12759507
C	-1.42594959	5.388464161	0.112545327
C	5.292305601	0.622606838	1.201962669
H	5.082546146	1.150318922	2.124371295
C	0.670423017	5.67217762	-1.091435517
H	1.168003073	5.85460881	-2.037231291
C	1.430671315	5.300487572	0.032364726
C	5.667617338	0.572933535	-1.143396106
H	5.832806942	1.070204922	-2.092420778
C	3.467234451	-4.45199634	-1.232466017
H	3.146249132	-4.806213382	-2.204458924
C	4.837742717	-2.880967994	0.022447811
C	4.120510493	3.089365386	-1.26987131
H	4.263175763	2.524027269	-2.182445485
C	2.794380228	-4.879819411	-0.07221501
C	2.76149914	4.708878146	-0.071814145
C	-0.705812675	5.718900565	-1.051632682
H	-1.237514018	5.935070512	-1.970688625
C	3.578519139	4.465651494	1.047638363
H	3.402611793	5.012053509	1.967458344
C	0.72280367	5.230620816	1.2431636
H	1.251116644	4.981663625	2.155476121
C	-0.652915726	5.273098287	1.281804847
H	-1.135952953	5.061255793	2.226928422
C	4.382875303	-3.532332822	1.184650059
H	4.729985562	-3.207221153	2.157602237
C	3.393209918	-4.488489704	1.139274232
H	2.99163837	-4.846299343	2.07932131

Table S5. Cartesian coordinates of [8]CPP (q = –2, S = 0).

Symbol	X	Y	Z
C	-5.523880398	0.728808361	-1.173106513
H	-5.527558063	1.223224293	-2.137502863
C	-4.491796751	-3.416872582	-1.143275297
H	-4.917942253	-3.108374315	-2.091286127
C	-5.524330379	0.750801959	1.200986981
H	-5.521615138	1.262210267	2.156559618
C	-5.36977966	1.496067257	0.007143883
C	-5.391845435	-1.391403903	0.033122067
C	-3.399113231	-4.310461054	1.209558307
H	-2.985652543	-4.626493709	2.16011611
C	-4.851399108	-2.730738932	0.042823436
C	-4.422866955	3.500092198	1.182171464
H	-4.841520669	3.192866216	2.133876688
C	1.397796519	-5.365722558	-0.050007175
C	-5.533531302	-0.643930155	-1.160822703
H	-5.534535183	-1.155138885	-2.116480778
C	-0.728998466	-5.592676674	1.130891613
H	-1.233114916	-5.697924349	2.085049505
C	-1.488728993	-5.334616415	-0.036198922
C	-5.535299655	-0.621897115	1.213293556
H	-5.55015497	-1.116557718	2.177511058
C	-3.439587133	4.458175066	1.193192794
H	-3.135606253	4.863123961	2.151959522
C	-4.808355453	2.826735263	-0.003109057
C	-4.366597557	-3.336294782	1.227168864
H	-4.667664569	-2.943900673	2.191282868
C	-2.742247735	4.838927404	0.020300088
C	-2.821623715	-4.779764481	0.005754856
C	0.643854417	-5.607634653	1.124296223
H	1.154472334	-5.723376983	2.073751127
C	-3.525788323	-4.392318779	-1.160819988
H	-3.241530399	-4.808854999	-2.120707899
C	-0.738118318	-5.380333695	-1.234948774
H	-1.24321128	-5.264957251	-2.186597484
C	0.634792998	-5.394938622	-1.241535515
H	1.132989092	-5.290150675	-2.198018487
C	-4.328469868	3.431472169	-1.190050094
H	-4.650773244	3.0523854	-2.152658066
C	-3.344079191	4.388623107	-1.178982252
H	-2.939010001	4.705525459	-2.132901073

C	5.523108736	-0.728823663	1.173579313
H	5.526014826	-1.22321352	2.137987255
C	4.491819652	3.417134183	1.14329434
H	4.91809354	3.108903143	2.091336287
C	5.52508705	-0.750807055	-1.200514479
H	5.523147514	-1.262225913	-2.156085563
C	5.369792377	-1.496084401	-0.006769342
C	5.391792648	1.391385422	-0.032719745
C	3.399001433	4.310179958	-1.209681079
H	2.98544037	4.625937456	-2.160285614
C	4.851331215	2.730711637	-0.04266543
C	4.422817052	-3.499806362	-1.182217809
H	4.841305047	-3.19226083	-2.133890922
C	-1.397781028	5.36577485	0.049701479
C	5.532714353	0.643913581	1.16130903
H	5.532936117	1.155110338	2.116971983
C	0.729019081	5.592576256	-1.131210902
H	1.233142847	5.697691215	-2.085379618
C	1.488740043	5.334702471	0.035925874
C	5.536017457	0.621893771	-1.212807625
H	5.551621141	1.116588401	-2.177000179
C	3.439534714	-4.457884536	-1.193409034
H	3.135439649	-4.862538639	-2.152262424
C	4.808414298	-2.826775665	0.003209784
C	4.366445997	3.33596978	-1.227121939
H	4.667318629	2.943229871	-2.191154775
C	2.742286133	-4.838933058	-0.020558091
C	2.821614708	4.77979968	-0.005955533
C	-0.643831338	5.607525081	-1.12463046
H	-1.154438892	5.723117911	-2.074108805
C	3.525825232	4.392597002	1.160671935
H	3.24164921	4.809385806	2.120475874
C	0.738121185	5.380617838	1.23466121
H	1.243205452	5.265399188	2.186334645
C	-0.634793481	5.395214603	1.241233621
H	-1.132996115	5.2905633	2.197729336
C	4.328669987	-3.431870916	1.19003066
H	4.651209102	-3.053179491	2.152716486
C	3.344259423	-4.388998861	1.178794436
H	2.939328307	-4.706224464	2.132665417

Table S6. Cartesian coordinates of [8]CPP (q = –3, S = 1/2).

Symbol	X	Y	Z
C	-5.694273503	0.731433845	-1.183378022
H	-5.73898892	1.225029225	-2.149289064
C	-4.568973922	-3.395061336	-1.127462938
H	-5.022949392	-3.118009879	-2.073296732
C	-5.697336793	0.766830134	1.202830339
H	-5.735964709	1.286010741	2.155452681
C	-5.513652557	1.516964323	-0.001094818
C	-5.524251922	-1.38611617	0.039398484
C	-3.40346176	-4.214671679	1.217291416
H	-2.95440354	-4.494007661	2.164885638
C	-4.927944897	-2.685018745	0.055757811
C	-4.526784207	3.505877473	1.168738012
H	-4.974369836	3.230085046	2.118020516
C	1.418514818	-5.263373735	-0.056385104
C	-5.699786717	-0.635609781	-1.163987688
H	-5.736769553	-1.154621679	-2.116853856
C	-0.721132497	-5.529600634	1.107611066
H	-1.226703292	-5.67410027	2.057307107
C	-1.483304004	-5.220460291	-0.042598912
C	-5.696764283	-0.600076378	1.221059346
H	-5.747140189	-1.094013816	2.186691861
C	-3.511909791	4.429432971	1.179686771
H	-3.214387643	4.844407636	2.138450097
C	-4.912145404	2.809905272	-0.016937084
C	-4.40370682	-3.2732108	1.242754207
H	-4.688873571	-2.867442933	2.206893328
C	-2.787978889	4.787174144	0.013541335
C	-2.838982589	-4.700199284	0.013607115
C	0.657491559	-5.551622819	1.101288931
H	1.16688904	-5.711342408	2.046346817
C	-3.570673353	-4.338650571	-1.144252157
H	-3.293057274	-4.765973147	-2.103485439
C	-0.726451261	-5.19131714	-1.235318261
H	-1.228658294	-4.995025996	-2.176085605
C	0.650631139	-5.213116011	-1.242521775
H	1.149055141	-5.031997731	-2.18819543
C	-4.401655897	3.408094893	-1.2076053
H	-4.717544367	3.025821825	-2.171972272
C	-3.385550399	4.330870501	-1.187867269
H	-2.953326817	4.621398547	-2.14011168

C	5.694206347	-0.731387714	1.183313614
H	5.73877369	-1.224972519	2.149235246
C	4.569224387	3.395288457	1.127303191
H	5.023471402	3.118437604	2.073066526
C	5.697413255	-0.766791114	-1.202895459
H	5.73617793	-1.285981497	-2.155506712
C	5.513648745	-1.516920373	0.001022996
C	5.524264277	1.386156647	-0.039482231
C	3.403111824	4.214429909	-1.217319616
H	2.953687383	4.493471683	-2.164826306
C	4.927917829	2.685037746	-0.055881856
C	4.526577709	-3.505679715	-1.168855934
H	4.973928833	-3.229715805	-2.118197624
C	-1.418493496	5.263394919	0.056569641
C	5.699723769	0.635658199	1.163918446
H	5.736567836	1.154670053	2.116789875
C	0.721140964	5.530091761	-1.107314803
H	1.22676269	5.675045637	-2.05691732
C	1.483279496	5.220469968	0.04276982
C	5.696837115	0.600111802	-1.221131832
H	5.747349514	1.094054031	-2.186756734
C	3.511705338	-4.429234461	-1.17973553
H	3.213988411	-4.844023518	-2.138514415
C	4.912174482	-2.809879708	0.016837885
C	4.403368204	3.272983717	-1.242861484
H	4.688182373	2.866932147	-2.206982204
C	2.78797674	-4.78713059	-0.013500745
C	2.838981291	4.700220364	-0.013593511
C	-0.657493698	5.552132741	-1.100984025
H	-1.166932365	5.712316664	-2.045944011
C	3.570910949	4.338869415	1.144160727
H	3.293507899	4.766399702	2.103367189
C	0.726450209	5.190786612	1.235472017
H	1.22869071	4.993976542	2.176113476
C	-0.650637159	5.212596196	1.242684827
H	-1.149098752	5.030945714	2.188236844
C	4.401954606	-3.408276519	1.207517667
H	4.718171897	-3.026266257	2.171884394
C	3.385851667	-4.331057844	1.18785741
H	2.953954792	-4.621856487	2.140168242

Table S7. Cartesian coordinates of [8]CPP (q = –4, S = 0).

Symbol	X	Y	Z
C	-5.872946885	0.702179399	-1.186026247
H	-5.977659689	1.200331	-2.148271202
C	-4.679017134	-3.397779461	-1.122489373
H	-5.146080983	-3.139977396	-2.068768694
C	-5.870611181	0.747525881	1.211013511
H	-5.962273263	1.276178228	2.157898465
C	-5.639772709	1.495941901	-0.002067057
C	-5.683088883	-1.414724058	0.048473019
C	-3.489070833	-4.183942345	1.224236654
H	-3.035146767	-4.458380924	2.173241629
C	-5.052921365	-2.675326081	0.065007176
C	-4.575358443	3.457338348	1.15562306
H	-5.04041833	3.210832569	2.105793981
C	1.3961964	-5.125820699	-0.053069867
C	-5.903214264	-0.658973647	-1.163218606
H	-6.021026301	-1.18406227	-2.109096768
C	-0.752850676	-5.464009569	1.089843962
H	-1.25756042	-5.653963386	2.033369739
C	-1.522672267	-5.112046237	-0.042047601
C	-5.885334987	-0.614054079	1.234745793
H	-5.997651839	-1.108450035	2.197963092
C	-3.528833047	4.346350398	1.161120905
H	-3.230260339	4.76927378	2.118629567
C	-4.970310109	2.738593736	-0.025457233
C	-4.520911028	-3.279051817	1.257178987
H	-4.820905633	-2.888369518	2.224440754
C	-2.786086327	4.681392135	0.000334877
C	-2.906531168	-4.658096199	0.020110487
C	0.632592893	-5.469531797	1.084333017
H	1.143237858	-5.664339396	2.023782319
C	-3.649230778	-4.304196979	-1.136969964
H	-3.363730994	-4.729309976	-2.097584738
C	-0.75732039	-5.000359903	-1.224178959
H	-1.259525207	-4.739257691	-2.149760889
C	0.6239098	-5.005316627	-1.228695614
H	1.121996295	-4.748198672	-2.157734373
C	-4.424054258	3.317452179	-1.221495352
H	-4.726167489	2.918412071	-2.18447041
C	-3.375358705	4.204261379	-1.197444663
H	-2.913562198	4.456943813	-2.148525953

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C	5.872925639	-0.702157066	1.186045154
H	5.977626452	-1.200290187	2.148301068
C	4.679061942	3.397837059	1.122426608
H	5.146145423	3.140057213	2.068702574
C	5.870594183	-0.747549662	-1.210993476
H	5.962256247	-1.276218515	-2.157868975
C	5.639758906	-1.495943745	0.002101448
C	5.68308107	1.414725913	-0.048494696
C	3.489038135	4.183908108	-1.224289319
H	3.035073322	4.458296656	-2.173288548
C	5.052921967	2.675332253	-0.065053306
C	4.575399728	-3.457386451	-1.155560241
H	5.040500024	-3.210918054	-2.105721057
C	-1.396189356	5.125816879	0.053087716
C	5.903197842	0.658995787	1.163211767
H	6.021009807	1.184100539	2.109080882
C	0.752836151	5.464003963	-1.089867333
H	1.257529969	5.653955576	-2.033402265
C	1.522679495	5.112062849	0.04201653
C	5.885322289	0.614029889	-1.234750556
H	5.997626715	1.108405534	-2.197979759
C	3.528878998	-4.346403748	-1.161063463
H	3.230334852	-4.769356355	-2.118569018
C	4.970310401	-2.738602788	0.025511179
C	4.520872909	3.279011799	-1.257231082
H	4.820834603	2.8882925	-2.224488073
C	2.786095707	-4.681408623	-0.000290723
C	2.906535409	4.658106984	-0.020162338
C	-0.632607687	5.469523864	-1.0843317
H	-1.143266783	5.664316497	-2.023776045
C	3.64926801	4.304246651	1.136909191
H	3.363799374	4.729394033	2.097518482
C	0.757348554	5.000397186	1.224162943
H	1.259570667	4.739320033	2.149742376
C	-0.623881752	5.005343279	1.228703599
H	-1.121948933	4.748247195	2.157758561
C	4.424026941	-3.317434082	1.221550382
H	4.726119459	-2.918374859	2.184524164
C	3.37533532	-4.204247508	1.197492906
H	2.913511577	-4.456904852	2.148568168

Table S8. Cartesian coordinates of $\{K^+\}_2([8]CPP^{2-})$ ($q = -2$, $S = 0$).

Symbol	X	Y	Z
K	-3.878751311	-0.051921972	-0.034860457
C	-6.707987019	-0.70532015	1.167492238
H	-6.918444294	-1.21010201	2.10828826
C	-4.897246512	2.969558538	1.095506107
H	-5.413543405	2.820035665	2.036901076
C	-6.691039924	-0.76869318	-1.253264747
H	-6.886385439	-1.317360962	-2.1721189
C	-6.389761997	-1.479633305	-0.021096595
C	-6.39556891	1.365794393	-0.092874419
C	-3.539390313	3.452854975	-1.251097742
H	-3.022635792	3.614223061	-2.192209615
C	-5.458352283	2.419036806	-0.105253816
C	-4.854398106	-3.068044117	-1.181771016
H	-5.357149798	-2.928648178	-2.132003468
C	1.423753275	4.134475688	0.039211585
C	-6.715786566	0.653393304	1.133249447
H	-6.93079239	1.201388838	2.048152095
C	-0.707930187	4.499612552	-1.101402628
H	-1.216868413	4.778543948	-2.018168846
C	-1.467668051	4.103655246	0.014208564
C	-6.686573706	0.590072283	-1.287071466
H	-6.880706073	1.094191018	-2.231750777
C	-3.622932866	-3.677790799	-1.177044271
H	-3.218459875	-4.008962076	-2.128812785
C	-5.444349049	-2.524373539	0.008791236
C	-4.763765215	2.823001341	-1.294661413
H	-5.154993403	2.525691759	-2.261067508
C	-2.857676051	-3.862212316	-0.004346417
C	-2.894797928	3.800471745	-0.045998305
C	0.675060515	4.514274193	-1.089537088
H	1.193648723	4.803815886	-1.997553353
C	-3.676830221	3.601244442	1.112778019
H	-3.295054131	3.938412256	2.071761105
C	-0.719413119	3.854966775	1.178069349
H	-1.231812605	3.543371517	2.081236254
C	0.660763879	3.869741598	1.190067631
H	1.163999703	3.568718688	2.101945824
C	-4.767040184	-2.921175882	1.210999416
H	-5.181547473	-2.632723964	2.170351437
C	-3.531289913	-3.529353256	1.18932305

H	-3.029995459	-3.684620435	2.139797546
C	6.708053159	0.705225809	-1.167456184
H	6.91830619	1.209839999	-2.108376143
C	4.897646894	-2.970049313	-1.095177722
H	5.414261611	-2.821405948	-2.036539281
C	6.690973131	0.768949139	1.253263378
H	6.885846591	1.317677033	2.172167055
C	6.389607796	1.479583795	0.020999086
C	6.395164095	-1.365519861	0.093146399
C	3.53934535	-3.452685517	1.25134633
H	3.022605611	-3.614170132	2.192448266
C	5.458581118	-2.419279214	0.105592668
C	4.854812038	3.068694366	1.181378618
H	5.357751449	2.929942904	2.131607881
C	-1.423827297	-4.134828866	-0.039445437
C	6.715846895	-0.653511571	-1.133003936
H	6.930345412	-1.201702145	-2.047886959
C	0.707841656	-4.499474144	1.101348791
H	1.216764007	-4.778408791	2.018123399
C	1.467600344	-4.103220772	-0.014149517
C	6.686394244	-0.589844123	1.287263158
H	6.880196401	-1.093895889	2.232029454
C	3.623043089	3.677843352	1.176645351
H	3.218537278	4.009098106	2.12836949
C	5.444669586	2.524721614	-0.009088427
C	4.763891111	-2.823181507	1.294987524
H	5.155061817	-2.525969362	2.261449688
C	2.857525523	3.861643253	0.004010055
C	2.894689951	-3.799999421	0.046189223
C	-0.675136177	-4.514552164	1.089325953
H	-1.193730551	-4.804483182	1.997216907
C	3.676994935	-3.6012544	-1.11250713
H	3.2951549	-3.938382209	-2.071483067
C	0.71939343	-3.85442252	-1.178014185
H	1.231825	-3.542470441	-2.081042512
C	-0.660785178	-3.869536935	-1.19013189
H	-1.163994073	-3.568446303	-2.102000234
C	4.767083537	2.921021094	-1.21134594
H	5.181620564	2.632585822	-2.170689583
C	3.531124843	3.528755452	-1.189657527
H	3.029613868	3.683519665	-2.140102583
K	3.879013862	0.051984323	0.035022292

Table S9. Cartesian coordinates of $(K^+)_2[\{K^+\}_2([8]CPP^{4-})]$ (q = 0, S = 0).

Symbol	X	Y	Z
K	3.829237458	0.010007219	-0.034615683
C	6.720938283	-0.651180429	-1.294358398
H	6.902032759	-1.164327705	-2.2386582
C	4.868080266	2.981565779	-1.218294064
H	5.374789139	2.838528477	-2.16522601
C	6.752587069	-0.68874739	1.13777161
H	6.957943783	-1.226008867	2.063127483
C	6.432622376	-1.408324711	-0.086284717
C	6.429965807	1.433079784	-0.044164444
C	3.526051655	3.441119921	1.141374446
H	3.015307998	3.595275048	2.085842047
C	5.451757193	2.466589865	-0.024191082
C	4.897655454	-2.958209063	1.121170276
H	5.422627601	-2.812309888	2.057659436
C	-1.440220233	4.034999103	-0.071690349
C	6.725313779	0.714445718	-1.27458401
H	6.909853004	1.25237373	-2.203854882
C	0.695899224	4.487104929	1.008652198
H	1.222596059	4.831981767	1.891286471
C	1.427947464	4.035423311	-0.099398023
C	6.746500541	0.67690215	1.157009182
H	6.947905192	1.190678473	2.096829036
C	3.661264243	-3.562057311	1.153911043
H	3.275860239	-3.884037023	2.115255282
C	5.456136509	-2.443606035	-0.085241964
C	4.770004544	2.844017313	1.169432395
H	5.181405869	2.562292285	2.131632327
C	2.873833059	-3.74094644	0.001533495
C	2.865100509	3.757827521	-0.057338028
C	-0.686824919	4.486841949	1.022057352
H	-1.196370591	4.830869769	1.915002739
C	3.629668191	3.582164086	-1.225472563
H	3.224412669	3.904860801	-2.178359739
C	0.672618149	3.701418211	-1.232479333
H	1.176988582	3.348345439	-2.1242012
C	-0.706722553	3.701500986	-1.219279999
H	-1.227984676	3.3479582	-2.101037058
C	4.751424748	-2.824174474	-1.264434075
H	5.142665417	-2.54268815	-2.235047404
C	3.509914881	-3.424302103	-1.210625959

H	2.98081217	-3.581060861	-2.14447972
C	-6.727033189	0.674754799	1.293136421
H	-6.911086739	1.18733463	2.237043476
C	-4.867760291	-2.961265339	1.216811995
H	-5.37474727	-2.817642365	2.16351343
C	-6.758770608	0.712458318	-1.137878468
H	-6.967716033	1.249281907	-2.062577544
C	-6.438199784	1.432161453	0.085636973
C	-6.427133758	-1.408954466	0.043237798
C	-3.524114629	-3.420269569	-1.141893244
H	-3.012215837	-3.573251999	-2.085913321
C	-5.448690799	-2.443224601	0.023094026
C	-4.901368569	2.979075104	-1.122101395
H	-5.426308168	2.833760405	-2.058704889
C	1.438263073	-4.020752528	0.072277103
C	-6.722666597	-0.690900837	1.274239123
H	-6.903312855	-1.229372777	2.204063914
C	-0.697432506	-4.47408582	-1.007960457
H	-1.224164683	-4.819194035	-1.890483552
C	-1.429374508	-4.022063203	0.099936337
C	-6.74385586	-0.653115962	-1.15833994
H	-6.941914746	-1.167414983	-2.098721022
C	-3.663290162	3.579357121	-1.154496113
H	-3.276641732	3.899842927	-2.115839868
C	-5.461996172	2.466674147	0.084568543
C	-4.766338829	-2.81945772	-1.170183361
H	-5.175245677	-2.533715103	-2.132265722
C	-2.876266455	3.758025869	-0.001617985
C	-2.866079743	-3.741782146	0.056961825
C	0.685297447	-4.473790745	-1.021183749
H	1.195110732	-4.819349943	-1.913383646
C	-3.631147569	-3.565717407	1.224507856
H	-3.227764999	-3.890945243	2.177322968
C	-0.674451203	-3.688463869	1.23330365
H	-1.179038767	-3.334581601	2.124572418
C	0.704899568	-3.68778171	1.219992975
H	1.226204991	-3.335342681	2.102152691
C	-4.75766581	2.848105223	1.26409505
H	-5.150989871	2.569839267	2.234801347
C	-3.514559134	3.44478648	1.21047537
H	-2.98618087	3.602003772	2.144673794
K	-3.830944788	0.021983834	0.034164071
K	-9.315126466	-0.076659341	0.094210345

K	9.31409343	-0.009438048	-0.097069263

Table S10. Cartesian coordinates of $\{K^+(THF)_2\}_2([8]CPP^{2-})$ (q = –2, S = 0).

Symbol	X	Y	Z
K	3.544322968	-0.202562518	-0.219909074
O	1.142693446	-0.295199127	-1.419207564
O	3.028557285	-0.02606411	2.621967444
C	6.40358304	0.806912173	0.226602428
H	6.686813564	1.415262609	1.083922351
C	5.109452917	-3.145988035	0.712873095
H	5.749661354	-2.885391712	1.549479709
C	6.02617115	0.621613205	-2.14869352
H	6.01681134	1.084039752	-3.132950866
C	5.872885558	1.439719933	-0.962800039
C	6.122466825	-1.407604244	-0.780884021
C	3.517550148	-3.980433748	-1.371214174
H	2.920035427	-4.303269211	-2.218349926
C	5.387012794	-2.590464986	-0.583842583
C	4.282000732	3.008717229	-2.081900511
H	4.614881786	2.699999087	-3.066341081
C	-1.176777357	-4.571713025	0.636711675
C	6.537544623	-0.547723501	0.313534366
H	6.92052826	-0.978091609	1.236653815
C	0.774499291	-5.049423243	-0.764845758
H	1.139431646	-5.346649615	-1.742363899
C	1.695241896	-4.644425821	0.2235861
C	6.149053955	-0.728388787	-2.064555947
H	6.236760673	-1.305193715	-2.982434134
C	3.13692676	3.762195663	-1.991156995
H	2.633931916	4.022300228	-2.917600758
C	4.989112369	2.542575977	-0.926074626
C	4.622645176	-3.208231564	-1.632979883
H	4.841444234	-2.959063456	-2.664952036
C	2.572207554	4.166119126	-0.761132467
C	3.077862648	-4.281814285	-0.060329716
C	-0.594785938	-5.011513342	-0.567778912
H	-1.234693526	-5.283185779	-1.400792137
C	3.999342072	-3.920134267	0.950588197
H	3.815398992	-4.238193992	1.973220885
C	1.112837147	-4.406184649	1.484491466
H	1.749756388	-4.136790876	2.319703964
C	0.351747173	-1.47209651	-1.543745391

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H	-0.668749403	-1.258219334	-1.209785728
H	0.774739618	-2.244465366	-0.903884176
C	-0.252969	-4.369007033	1.679695477
H	-0.611704938	-4.069984067	2.657817523
C	4.548547619	3.161831308	0.288112819
H	5.089649178	2.964022382	1.207050977
C	3.390448916	3.9047021	0.358421873
H	3.070445531	4.243612541	1.339476733
C	0.382400465	-1.822242892	-3.03308544
H	-0.586324084	-2.194336306	-3.367378356
H	1.123111146	-2.597515447	-3.228445342
C	0.775643675	-0.496485945	-3.714102983
H	1.755851334	-0.581020034	-4.186021224
H	0.061823029	-0.184565848	-4.478221167
C	0.832448274	0.495074637	-2.554083957
H	1.598541949	1.264878722	-2.654189082
H	-0.13747814	0.984798004	-2.403806062
C	3.723015512	1.014205066	3.287926393
H	3.380162477	1.963070467	2.877664372
H	4.799691955	0.920679816	3.092313621
C	3.221604341	-1.182344439	3.420656517
H	4.203342382	-1.618327898	3.200797302
H	2.457989285	-1.909374889	3.146989628
C	3.140617261	-0.700259164	4.873139834
H	3.872269239	-1.212477516	5.499455714
H	2.154038292	-0.892396309	5.295834163
C	3.411117872	0.812827984	4.769197021
H	4.235280531	1.140599744	5.404246673
H	2.525558407	1.383334118	5.052493827
C	-6.406618747	-0.807896956	-0.228780647
H	-6.689438337	-1.415898843	-1.086463625
C	-5.111026982	3.145957436	-0.713938563
H	-5.751308858	2.886067403	-1.550696832
C	-6.030968504	-0.622648005	2.146818251
H	-6.022446787	-1.084747679	3.131243327
C	-5.87739637	-1.441131567	0.961175421
C	-6.124538373	1.40667988	0.778666232
C	-3.519140236	3.978974049	1.370693022
H	-2.921529662	4.300813269	2.218129542
C	-5.388507386	2.589357776	0.58229433
C	-4.285653071	-3.008553462	2.081053264
H	-4.618730282	-2.699488147	3.065323692
C	1.17440677	4.573397587	-0.63660289

C	-6.53924362	0.546911885	-0.315974336
H	-6.9207442	0.977438633	-1.239618168
C	-0.776742651	5.04928646	0.765629327
H	-1.141669204	5.344959577	1.743614686
C	-1.697453405	4.645883093	-0.223507084
C	-6.152409416	0.727473028	2.062339486
H	-6.240304816	1.304463236	2.980098178
C	-3.13988788	-3.761079258	1.990706041
H	-2.636619677	-4.020139717	2.917290368
C	-4.993372998	-2.54380931	0.925007196
C	-4.623935304	3.206085377	1.631846054
H	-4.842151415	2.955545999	2.663622266
C	-2.574773895	-4.165132408	0.76084201
C	-3.079873153	4.282043733	0.06003366
C	0.592524737	5.011593044	0.568508
H	1.232413625	5.282111688	1.401901319
C	-4.001290413	3.920893186	-0.951033028
H	-3.817740269	4.240174355	-1.97335177
C	-1.115135881	4.410233298	-1.484897319
H	-1.751877601	4.142610691	-2.320800537
C	0.250715633	4.372963856	-1.680068112
H	0.609449131	4.075625064	-2.658696309
C	-4.552034253	-3.163055941	-0.288968566
H	-5.093006276	-2.96598901	-1.208135568
C	-3.393162068	-3.904775283	-0.358849967
H	-3.072617021	-4.243521069	-1.339792154
K	-3.547059158	0.196908654	0.223693732
O	-1.144420038	0.296301798	1.42023706
O	-3.026378974	0.023391117	-2.618285043
C	-0.351335718	1.471815154	1.543023668
H	0.667909705	1.256488138	1.206132167
H	-0.774838735	2.245108259	0.904649791
C	-0.377590444	1.821329951	3.032547247
H	0.591999088	2.193455791	3.364277332
H	-1.117921251	2.596378837	3.230221574
C	-0.768622548	0.495207657	3.71412732
H	-1.746449839	0.579859172	4.190910718
H	-0.051301342	0.181999555	4.474419252
C	-0.831261076	-0.49527887	2.553352395
H	-1.598199257	-1.263959131	2.655618311
H	0.137409618	-0.986330102	2.399325729
C	-3.719950349	-1.015025802	-3.287973009
H	-3.378161126	-1.965004819	-2.879382229

H	-4.79695992	-0.921683029	-3.094126441
C	-3.217672159	1.181626665	-3.414631181
H	-4.199832263	1.61714307	-3.195853457
H	-2.454570379	1.907897415	-3.137560662
C	-3.133596854	0.702912922	-4.868014868
H	-3.86338982	1.217160508	-5.494853163
H	-2.14592441	0.895159448	-5.288107355
C	-3.405402763	-0.810261727	-4.76823366
H	-4.228862476	-1.135912865	-5.405299147
H	-2.519811227	-1.380639932	-5.05166552

Table S11. Cartesian coordinates of $[(K^+)_2\{K^+(THF)\}_2([8]CPP^{4-})]$ (q = 0, S = 0).

Symbol	X	Y	Z
K	8.833854888	-0.318696673	0.947738527
K	3.431006289	0.269556879	-0.155862844
O	1.302199747	0.360112127	1.465266765
O	2.947297327	0.020989403	-2.902006439
C	6.337044781	-0.806571609	-0.530729313
H	6.568229127	-1.425475601	-1.397481791
C	5.028624501	3.127904407	-1.004789598
H	5.631505547	2.849887939	-1.862271911
C	6.062578813	-0.59533826	1.862879643
H	6.068791531	-1.042621079	2.855068806
C	5.858394031	-1.416504637	0.689195692
C	6.113482779	1.418826867	0.466257607
C	3.507698481	3.978112733	1.124623969
H	2.928393637	4.293862794	1.985455013
C	5.348523358	2.599158806	0.282826953
C	4.397066007	-3.050462024	1.894365315
H	4.812042591	-2.768828231	2.855062555
C	-1.214738939	4.607650131	-0.667591544
C	6.486153178	0.553172075	-0.637687864
H	6.823336301	0.968991806	-1.585982637
C	0.796900962	5.139596193	0.60472577
H	1.220946333	5.501071545	1.534652069
C	1.64858623	4.658566816	-0.405783639
C	6.198117184	0.760020112	1.757860463
H	6.309064423	1.345562471	2.668627072
C	3.262727099	-3.829425447	1.880743239
H	2.846245574	-4.137835607	2.833660826
C	4.980424235	-2.543241338	0.700817674
C	4.618108433	3.199141948	1.351778078

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H	4.859643488	2.940282735	2.375535659
C	2.606370306	-4.190940331	0.689651266
C	3.040364037	4.279276617	-0.169803825
C	-0.580044576	5.112123735	0.479103647
H	-1.17893222	5.454532936	1.315616629
C	3.917152154	3.914166082	-1.210697242
H	3.698935924	4.234208037	-2.224589343
C	1.013006432	4.344574936	-1.618265892
H	1.605883464	4.003922497	-2.458780111
C	0.498931355	1.492372228	1.774889383
H	-0.551458966	1.260248754	1.561303573
H	0.810175364	2.323104791	1.143480455
C	-0.360473604	4.319817615	-1.743029549
H	-0.778901756	3.961249984	-2.675676028
C	4.450905689	-3.109651357	-0.49015499
H	4.89295049	-2.852496629	-1.445729152
C	3.305308872	-3.877869857	-0.488066664
H	2.892554291	-4.175451084	-1.446034866
C	0.712514913	1.728933046	3.267219569
H	-0.181469558	2.132939849	3.742587679
H	1.522516485	2.441081563	3.42492098
C	1.097571011	0.336042474	3.803578767
H	2.078189224	0.360031598	4.279074032
H	0.385704125	-0.041662563	4.538649674
C	1.122648682	-0.540094834	2.549859842
H	1.934090551	-1.26793685	2.526890007
H	0.174924817	-1.076458286	2.420189485
C	3.422669697	-1.115413787	-3.626803217
H	2.835692299	-1.985873911	-3.328523891
H	4.46943451	-1.297480673	-3.358135127
C	2.843483216	1.146997104	-3.779274492
H	3.298119352	2.009124879	-3.289096709
H	1.783327292	1.364528797	-3.951002425
C	3.537949954	0.743254856	-5.068186493
H	4.608884871	0.950455913	-5.00574374
H	3.140539224	1.267686448	-5.936923862
C	3.289640266	-0.759938336	-5.096083407
H	3.993700589	-1.307273037	-5.722627094
H	2.278765396	-0.973995848	-5.45210664
C	-6.350582152	0.813837947	0.531411675
H	-6.5802996	1.432556746	1.398642838
C	-5.038220184	-3.122257202	1.004718591
H	-5.640244268	-2.844440087	1.862862111

C	-6.081185181	0.601106329	-1.862772882
H	-6.092853616	1.047624898	-2.855307687
C	-5.87639301	1.424039936	-0.690308996
C	-6.124863614	-1.412106906	-0.464217536
C	-3.519100913	-3.971156828	-1.126420521
H	-2.940271042	-4.285995074	-1.987895893
C	-5.358470925	-2.591861838	-0.28197268
C	-4.409734423	3.050087282	-1.898983892
H	-4.823089697	2.764960803	-2.859324471
C	1.20252987	-4.607626407	0.66218032
C	-6.495829121	-0.546149432	0.639926799
H	-6.828287111	-0.961824457	1.58994364
C	-0.810088183	-5.137712729	-0.609284175
H	-1.234907392	-5.49790894	-1.539359834
C	-1.660907668	-4.657322796	0.40228305
C	-6.213532674	-0.754400229	-1.756195802
H	-6.327415517	-1.34073916	-2.666146758
C	-3.273499248	3.826234969	-1.886449638
H	-2.85455422	4.129322496	-2.83996971
C	-4.996948456	2.549522126	-0.704427716
C	-4.628587689	-3.190406481	-1.351997391
H	-4.87012356	-2.929593443	-2.37525818
C	-2.618803146	4.191819295	-0.69564681
C	-3.05220047	-4.275623411	0.167337961
C	0.566970002	-5.110821325	-0.484591222
H	1.165311702	-5.45234664	-1.321867547
C	-3.927980641	-3.910595945	1.209071546
H	-3.709650777	-4.232092865	2.22248787
C	-1.024441327	-4.345508411	1.614850212
H	-1.616660851	-4.005846093	2.456211275
C	0.349128832	-4.32122656	1.738686956
H	0.768439962	-3.963748027	2.671367236
C	-4.467940933	3.119378586	0.48520588
H	-4.912219483	2.867489364	1.441143178
C	-3.320584309	3.884993892	0.481995978
H	-2.909159834	4.185558429	1.439568194
K	-8.850274375	0.31434075	-0.938265942
K	-3.444086351	-0.246394188	0.138815629
O	-1.288220341	-0.359051726	-1.451648397
O	-2.943216234	-0.005522519	2.882174736
C	-0.48322001	-1.497875219	-1.731662688
H	0.563507372	-1.267390829	-1.499294489
H	-0.809796898	-2.319712617	-1.096474593

C	-0.667118015	-1.75356083	-3.225415036
H	0.240456443	-2.152374484	-3.678700382
H	-1.465290936	-2.477113297	-3.390856621
C	-1.056676968	-0.371326	-3.785743693
H	-2.036264462	-0.407757954	-4.262653873
H	-0.344901383	-0.002163938	-4.525183699
C	-1.090380455	0.524076689	-2.546664181
H	-1.89738592	1.257214926	-2.543818949
H	-0.140611661	1.056380655	-2.414342487
C	-3.409886741	1.128292867	3.616914848
H	-2.815448896	1.996850035	3.327722905
H	-4.454528389	1.321169938	3.347990167
C	-2.835635152	-1.136600454	3.752128048
H	-3.286074832	-1.997137772	3.255434435
H	-1.774870579	-1.35105955	3.924561967
C	-3.533356764	-0.743285234	5.04217098
H	-4.604485835	-0.947852627	4.974184953
H	-3.139763435	-1.275897135	5.907677334
C	-3.281748138	0.759039762	5.083499797
H	-3.986008386	1.302738577	5.71297511
H	-2.27133616	0.967146606	5.444345551

Table S12. Aromaticity descriptors calculated for $[\{K^+\}_2([8]CPP^{4-})]$ system in the gas phase (PBE0/cc-pVTZ(C,H)//def2-TZVP(K)).

	HOMA	NICS	AIM		Fuzzy Atomic Space	
			PDI	FLU	PDI	FLU
A	0.939	-2.198	0.080	0.004	0.082	0.006
B	0.749	2.158	0.060	0.011	0.062	0.016
C	0.185	6.205	0.036	0.032	0.039	0.036

Table S13. Aromaticity descriptors calculated for $[\{K^+\}_2([8]CPP^{4-})]$ system in THF (PBE0/cc-pVTZ(C,H)//def2-TZVP(K), CPCM(THF)).

	HOMA	NICS	AIM		Fuzzy Atomic Space	
			PDI	FLU	PDI	FLU
A	0.939	-2.350	0.080	0.004	0.082	0.006
B	0.749	1.950	0.060	0.011	0.062	0.016

| C | 0.185 | 6.220 | 0.036 | 0.032 | 0.040 | 0.036 |

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