Electronic Supplementary Material (ESI) for ChemComm.

SUPPORTING INFORMATION

Stepwise reduction of interlocked viologen-based complexes in the gas phase

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Experimental

Materials

Synthetic procedures for preparing cyclobis(paraquat-*p*-phenylene) (**BB**), porphyrin-strapped catenanes (**1-3**), stoppered dumbbell (**DB**) and rotaxanes (**4-5**), all as hexafluorophosphate salts, were based on previously described methods.[1-5]

Mass spectrometry

All experiments were performed with a high-resolution Orbitrap Elite mass spectrometer (Thermo Fisher Scientific, Bremen, Germany) operating at a mass resolution of 60,000 (at *m/z* 400). Mass calibration in positive ion mode was performed prior to use. Target compounds were dissolved in chloroform at approximately 0.1 mg/mL, then diluted into methanol or acetonitrile to achieve a final concentration of *ca.* 2 μM. Diluted samples were infused into the heated electrospray ionisation (HESI) source at 3-5 μL/min with an accompanying make-up flow of methanol from a solvent pump at 0.1 mL/min to improve spray stability. Typical ion source parameters were source voltage 4.8 kV, capillary temperature 300 °C, sheath gas 6 arbitrary units, auxiliary gas 8 arbitrary units, S-lens RF level 50%. Mass-to-charge ratios of precursor ions and reaction products were within 5 ppm of their predicted values (Table S1).

Ion-ion reactions of viologen cations with fluoranthene radical anions (**FL**$^{-\bullet}$) were performed using the electron transfer dissociation (ETD) module of the Orbitrap Elite.[6, 7] Multiply charged analyte cations (from ESI) were mass-selected in the ion trap with an isolation window of 3 - 4 Da and the ion trap stability parameter (*q*) set to 0.25. Fluoranthene ions were generated by chemical ionisation and transferred into the ion trap for a given reaction time before the cationic reaction products were scanned out and analysed in the Orbitrap.

Reaction Kinetics

Ion-ion reaction kinetics in an ion trap have been detailed by McLuckey and co-workers.[8, 9] Primarily, the reaction rate is proportional to the square of the number of charges.[8] As long as the local concentration of **FL**$^{-\bullet}$ greatly exceeds that of the cation and *q* is held constant, the stepwise electrochemical reduction of multiply-charged viologen cations can be described by pseudo-first order kinetics of consecutive reactions.[10-13] To confirm pseudo-first order conditions, rate constants were measured at different **FL**$^{-\bullet}$ number densities. The reaction time was varied from 1 – 300 ms in random order, to account for temporal fluctuations in fluoranthene ion concentration.

The reaction of a viologen ion in the n+ charge state ($\mathbf{V}^{n+}$) with $\mathbf{FL}^{-\bullet}$ forms a radical cation $\mathbf{V}^{(n-1)+\bullet}$ and neutral **FL** (Equation 1). Further reduction with a second $\mathbf{FL}^{-\bullet}$ yields $\mathbf{V}^{(n-2)+}$ and so on (Equation 3), eventually forming $\mathbf{V}^{+\bullet}$. Rate constants were obtained using the raw abundances of the precursor ion and each charge-reduced product ion as a function of reaction time. Plotting the abundance of $\mathbf{V}^{n+}$ against reaction time and fitting to Equation 2 by a non-linear least squares method (MATLAB, R2017b) yields the observed reaction rate k_1. Using this value, plotting radical cation [$\mathbf{V}^{(n-1)+\bullet}$] against trapping time yields k_2 by Equation 4. Similarly, k_3 can be derived from Equation 6 once k_1 and k_2 are known.

$$\mathbf{V}^{n+} + \mathbf{FL}^{-\bullet} \longrightarrow \mathbf{V}^{(n-1)+\bullet} + \mathbf{FL} \quad (1)$$

$$\mathbf{V}^{n+}(t) = \mathbf{V}_0^{n+} e^{-k_1 t} \quad (2)$$

$$\mathbf{V}^{(n-1)+\bullet} + \mathbf{FL}^{-\bullet} \longrightarrow \mathbf{V}^{(n-2)+} + \mathbf{FL} \quad (3)$$

$$\mathbf{V}^{(n-1)+\bullet}(t) = \frac{\mathbf{V}_0^{n+} k_1}{k_2 - k_1}\left(e^{-k_1 t} - e^{-k_2 t}\right) \quad (4)$$

$$\mathbf{V}^{(n-2)+} + \mathbf{FL}^{-\bullet} \longrightarrow \mathbf{V}^{(n-3)+\bullet} + \mathbf{FL} \quad (5)$$

$$\begin{aligned}\mathbf{V}^{(n-2)+}(t) = {} & \frac{\mathbf{V}_0^{n+} k_1 k_2 e^{-k_3 t}}{k_3^2 + (-k_2 - k_1)k_3 + k_1 k_2} \\ & - \frac{\mathbf{V}_0^{n+} k_1 k_2 e^{-k_2 t}}{(k_2 - k_1)k_3 - k_2^2 + k_1 k_2} \\ & + \frac{\mathbf{V}_0^{n+} k_1 k_2 e^{-k_1 t}}{(k_2 - k_1)k_3 - k_1 k_2 + k_1^2}\end{aligned} \quad (6)$$

Computational Methods

Density functional theory calculations were carried out using Gaussian 09, Version B.01.[14] Geometries and frequencies for all species were computed at the (U)M06-2X/6-31G(d,p) level. Symmetry was disabled using the "NOSYMM" keyword. Structures were confirmed to be local minima on the potential energy surface by the absence of negative frequencies. Starting geometries and energies for the 4+ charge state of **BB** were benchmarked against previous DFT calculations.[15] All reported energies include zero point correction.

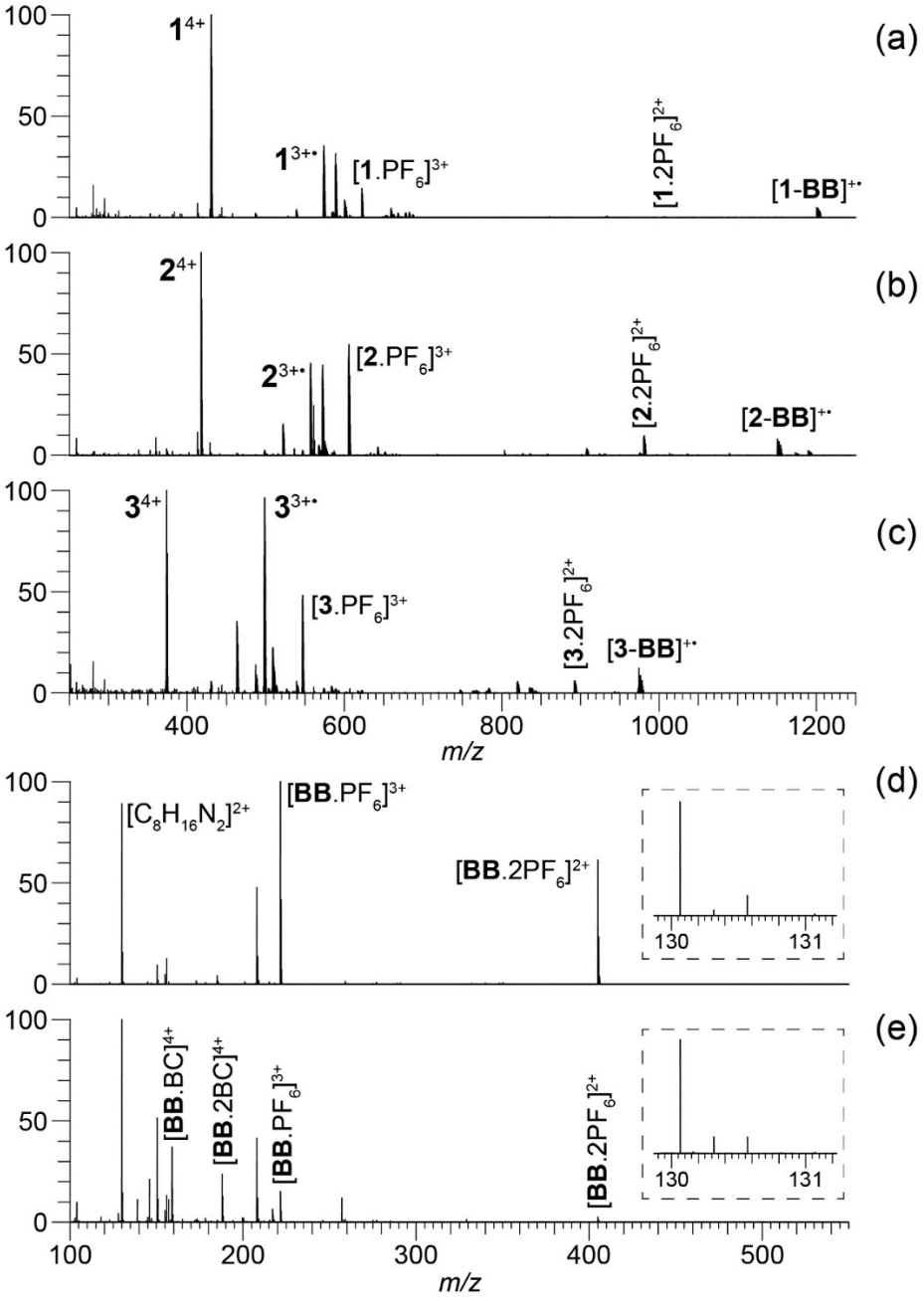
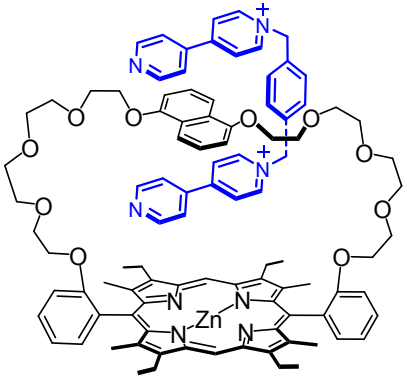


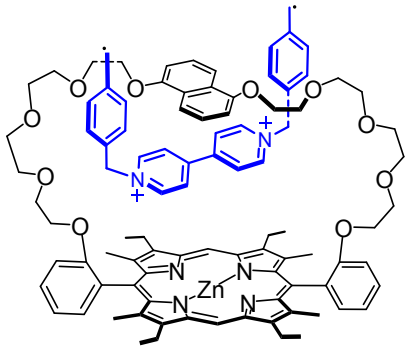
Figure S1: Positive ion ESI mass spectra of: (a) catenane **1**; (b) catenane **2**; (c) catenane **3**; (d) cyclobis(paraquat-*p*-phenylene) (**BB**); (e) **BB** with 1% 1,2-butylene carbonate (BC). Isotopic spacings shown in the inset of spectra (d) and (e) demonstrate that the major species at *m/z* 130 is $C_8H_{16}N_2^{2+}$, rather than $\mathbf{BB}^{4+}$ ($C_{16}H_{32}N_4^{4+}$). Isolation of [**BB**.BC]$^{4+}$ or [**BB**.2BC]$^{4+}$ provides sufficient thermal activation to desolvate these complexes, however, attempts to re-isolate $\mathbf{BB}^{4+}$ resulted in dissociation. Stabilisation of $\mathbf{BB}^{4+}$ by small donors (*e.g.*, *p*-dimethoxybenzene) in solution did not yield ionic complexes by ESI-MS.

Table S1: Experimentally measured mass-to-charge ratios (*m/z*) of monoisotopic product ions resulting from electrochemical reduction of catenane $\mathbf{1}^{4+}$ with $\mathbf{FL}^{-\bullet}$ for 20 ms (see also Figure 1A, main text).

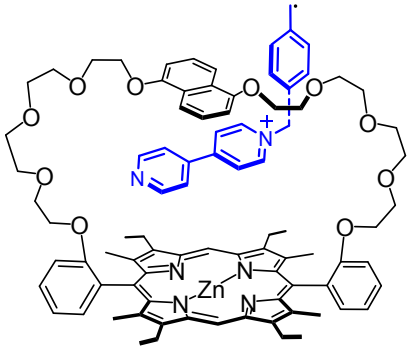
	Assignment	Experimental *m/z*	Elemental Formula	Theoretical *m/z*	Δ (ppm)
Catenane 1	$\mathbf{1}^{4+}$	430.1957	$C_{106}H_{112}N_8O_{10}Zn^{4+}$	430.1943	3.3
	$\mathbf{1}^{3+\bullet}$	573.5946	$C_{106}H_{112}N_8O_{10}Zn^{3+\bullet}$	573.5925	3.5
	$\mathbf{1}^{2(+\bullet)}$	860.3912	$C_{106}H_{112}N_8O_{10}Zn^{2(+\bullet)}$	860.3891	2.4
	$\mathbf{1}^{+\bullet}$	1720.7852	$C_{106}H_{112}N_8O_{10}Zn^{+\bullet}$	1720.7787	3.8
	$[\mathbf{1}\text{-}C_{10}H_8N_2]^{+\bullet}$	1564.7174	$C_{96}H_{104}N_6O_{10}Zn^{+\bullet}$	1564.7100	4.7
	$[\mathbf{1}\text{-}C_{18}H_{16}N_2]^{+\bullet}$	1460.6523	$C_{88}H_{96}N_6O_{10}Zn^{+\bullet}$	1460.6474	3.4
	$[\mathbf{1}\text{-}C_{28}H_{24}N_4]^{+\bullet}$	1304.5832	$C_{78}H_{88}N_4O_{10}Zn^{+\bullet}$	1304.5786	3.5
	$[\mathbf{1}\text{-}\mathbf{BB}]^{+}$	1200.5187	$C_{70}H_{80}N_4O_{10}Zn^{+}$	1200.5160	2.2
	$[\mathbf{1}\text{-}C_8H_8]^{2+}$	808.3592	$C_{98}H_{104}N_8O_{10}Zn^{2+}$	808.3578	1.7
	$[\mathbf{1}\text{-}C_{10}H_8N_2]^{2(+\bullet)}$	782.3564	$C_{96}H_{104}N_6O_{10}Zn^{2+}$	782.3547	2.2
	$[\mathbf{1}\text{-}C_{18}H_{16}N_2]^{2+}$	730.3252	$C_{88}H_{96}N_6O_{10}Zn^{2+}$	730.3234	2.4
	$[\mathbf{1}\text{-}C_{28}H_{24}N_4]^{2+\bullet}$	652.2911	$C_{78}H_{88}N_4O_{10}Zn^{2+\bullet}$	652.2890	3.2
	$[\mathbf{1}\text{-}\mathbf{BB}]^{2+}$	600.2595	$C_{70}H_{80}N_4O_{10}Zn^{2+}$	600.2577	2.9



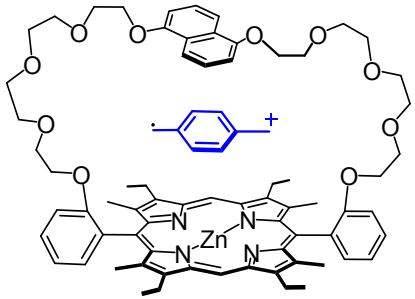
Chemical Formula: $C_{98}H_{104}N_8O_{10}Zn^{2+}$
Exact Mass: 1616.7156



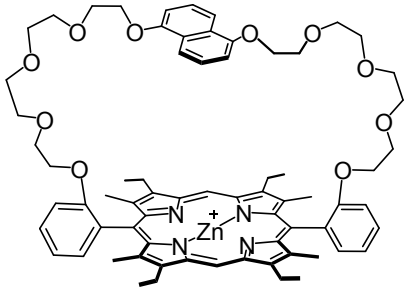
Chemical Formula: $C_{96}H_{104}N_6O_{10}Zn^{2\bullet 2+}$
Exact Mass: 1564.7094



Chemical Formula: $C_{88}H_{96}N_6O_{10}Zn^{\bullet +}$
Exact Mass: 1460.6474



Chemical Formula: $C_{78}H_{88}N_4O_{10}Zn^{\bullet +}$
Exact Mass: 1304.5786



Chemical Formula: $C_{70}H_{80}N_4O_{10}Zn^{+}$
Exact Mass: 1200.5160

Chart S1: Proposed chemical structures for fragment ions of catenane **1** arising from electrochemical reduction with $\mathbf{FL}^{-\bullet}$

Table S2: Experimentally measured mass-to-charge ratios (*m/z*) of monoisotopic product ions resulting from electrochemical reduction of catenane $\mathbf{2}^{4+}$ with $\mathbf{FL}^{-\bullet}$ for 20 ms (see also Figure 1B, main text).

	Assignment	Experimental *m/z*	Elemental Formula	Theoretical *m/z*	Δ (ppm)
Catenane 2	$\mathbf{2}^{4+}$	417.6919	$C_{102}H_{110}N_8O_{10}Zn^{4+}$	417.6904	3.7
	$\mathbf{2}^{3+\bullet}$	556.9223	$C_{102}H_{110}N_8O_{10}Zn^{3+\bullet}$	556.9207	3.0
	$\mathbf{2}^{2(+\bullet)}$	835.3834	$C_{102}H_{110}N_8O_{10}Zn^{2(+\bullet)}$	835.3813	2.5
	$\mathbf{2}^{+\bullet}$	1670.7677	$C_{102}H_{110}N_8O_{10}Zn^{+\bullet}$	1670.7631	2.8
	$[\mathbf{2}\text{-}C_{18}H_{16}N_2]^{+\bullet}$	1410.6376	$C_{84}H_{94}N_6O_{10}Zn^{+\bullet}$	1410.6317	4.2
	$[\mathbf{2}\text{-}\mathbf{BB}]^{+}$	1150.5034	$C_{66}H_{78}N_4O_{10}Zn^{+}$	1150.5004	2.6
	$[\mathbf{2}\text{-}C_8H_8]^{2+}$	783.3511	$C_{94}H_{102}N_8O_{10}Zn^{2+}$	783.3500	1.4
	$[\mathbf{2}\text{-}C_{10}H_8N_2]^{2(+\bullet)}$	757.3487	$C_{92}H_{102}N_6O_{10}Zn^{2+}$	757.3469	2.3
	$[\mathbf{2}\text{-}C_{18}H_{16}N_2]^{2+}$	705.3183	$C_{84}H_{94}N_6O_{10}Zn^{2+}$	705.3156	3.8
	$\mathbf{BB}^{2+\bullet}$	260.1319	$C_{36}H_{32}N_4{}^{2+}$	260.1308	4.1
	$[\mathbf{BB}\text{-}C_8H_8]^{2+}$	208.1002	$C_{28}H_{24}N_4{}^{2+}$	208.0995	3.5

Table S3: Experimentally measured mass-to-charge ratios (*m/z*) of monoisotopic product ions resulting from electrochemical reduction of catenane $\mathbf{3}^{4+}$ with $\mathbf{FL}^{-\bullet}$ for 20 ms (see also Figure 1C, main text).

	Assignment	Experimental *m/z*	Elemental Formula	Theoretical *m/z*	Δ (ppm)
Catenane 3	$\mathbf{3}^{4+}$	373.6655	$C_{94}H_{94}N_8O_6Zn^{4+}$	373.6641	3.6
	$\mathbf{3}^{3+\bullet}$	498.2204	$C_{94}H_{94}N_8O_6Zn^{3+\bullet}$	498.2190	2.6
	$\mathbf{3}^{2(+\bullet)}$	747.3303	$C_{94}H_{94}N_8O_6Zn^{2(+\bullet)}$	747.3288	1.9
	$\mathbf{3}^{+\bullet}$	1494.6615	$C_{94}H_{94}N_8O_6Zn^{+\bullet}$	1494.6582	2.2
	[**3-BB**]$^{+}$	974.3975	$C_{58}H_{62}N_4O_6Zn^{+}$	974.3955	2.0
	[**3**-C_8H_8]$^{2+}$	695.2987	$C_{86}H_{86}N_8O_6Zn^{2+}$	695.2975	1.7
	[**3**-$C_{10}H_8N_2$]$^{2(+\bullet)}$	669.2962	$C_{84}H_{86}N_6O_6Zn^{2+}$	669.2945	2.6
	[**3**-$C_{18}H_{16}N_2$]$^{2+}$	617.2642	$C_{76}H_{78}N_6O_6Zn^{2+}$	617.2632	1.6
	[**3**-$C_{28}H_{24}N_4$]$^{2+\bullet}$	539.2300	$C_{66}H_{70}N_4O_6Zn^{2+\bullet}$	539.2288	2.3
	$\mathbf{BB}^{+\bullet}$	520.2638	$C_{36}H_{32}N_4^{+\bullet}$	520.2621	3.2
	[**3-BB**]$^{2+}$	487.1985	$C_{58}H_{62}N_4O_6Zn^{2+}$	487.1975	2.0
	$\mathbf{BB}^{2+\bullet}$	260.1317	$C_{36}H_{32}N_4^{2+}$	260.1308	3.4
	[**BB**-C_8H_8]$^{2+}$	208.1002	$C_{28}H_{24}N_4^{2+}$	208.0995	3.4

Table S4: Experimentally measured mass-to-charge ratios (*m/z*) of monoisotopic product ions resulting from electrochemical reduction of [**BB**.BC]$^{4+}$ with **FL**$^{-\bullet}$ for 20 ms (see also Figure 1D, main text).

	Assignment	Experimental *m/z*	Elemental Formula	Theoretical *m/z*	Δ (ppm)
Bluebox (BB)	**BB**$^{4+}$	130.0652	$C_{36}H_{32}N_4^{4+}$	130.0651	0.3
	[**BB**-$C_{18}H_{16}N_2$]$^{+\bullet}$	260.1310	$C_{18}H_{16}N_2^{+\bullet}$	260.1308	0.6
	[**BB**-C_8H_8]$^{2+}$	208.0996	$C_{28}H_{24}N_4^{2+}$	208.0995	0.7
	[**BB**-$C_{28}H_{24}N_4$]$^{+\bullet}$	104.0621	$C_8H_8^{+\bullet}$	104.0621	0.5

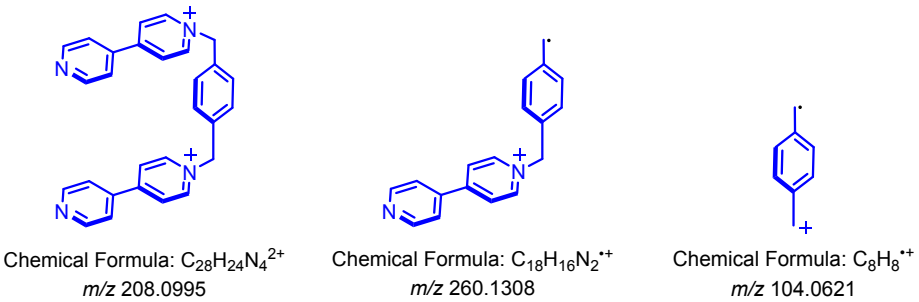


Chart S2: Proposed chemical structures for fragment ions of **BB** arising from electrochemical reduction with **FL**$^{-\bullet}$

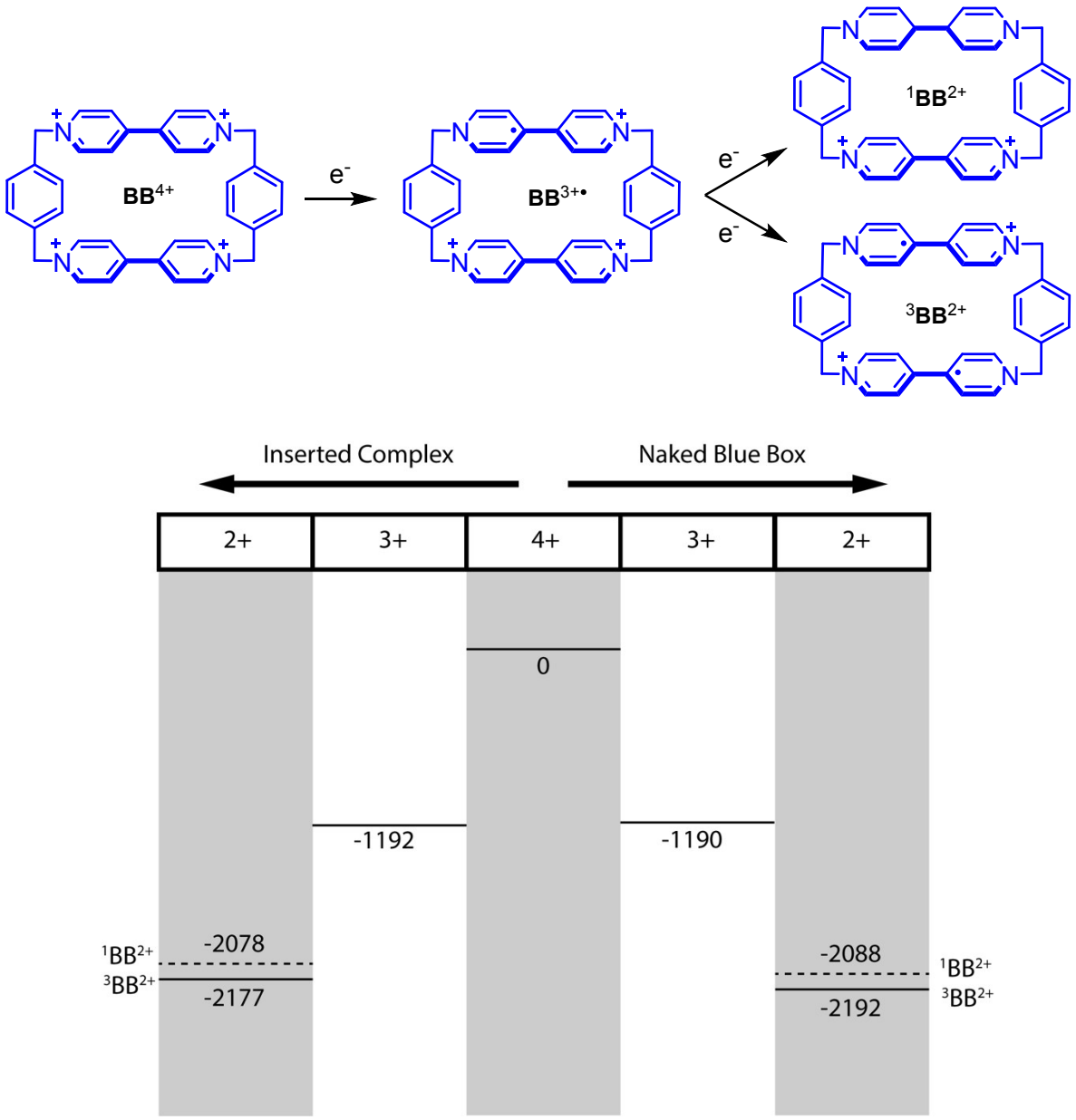


Figure S2: Calculated gas phase energies (in kJ/mol) of **BB**$^{4+}$, **BB**$^{3+\bullet}$, as well as the singlet and triplet states of **BB**$^{2+}$. Calculated energetics of each **BB** charge state as an inserted complex with a *p*-dimethoxybenzene guest are also shown. In both cases, displayed energies are relative to the corresponding 4+ charge state and are zero-point corrected.

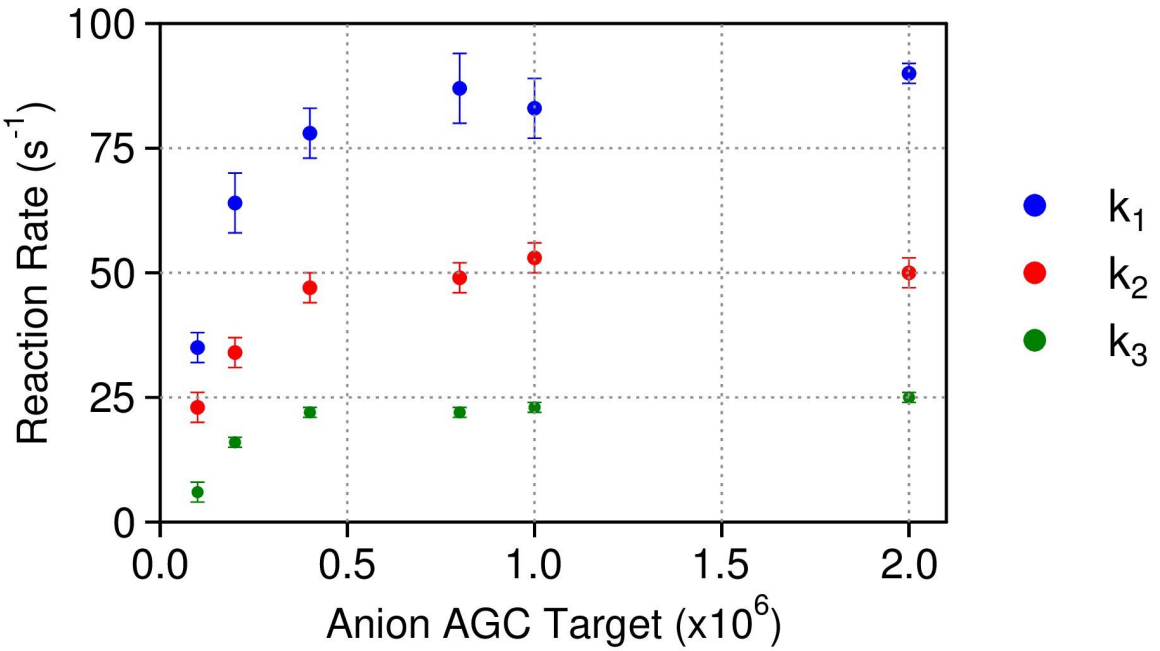


Figure S3: Effect of automatic gain control (AGC) target on the consecutive electrochemical reduction rates (k_1, k_2, k_3) of catenane $\mathbf{1}^{4+}$. The anion AGC target can be considered a proxy for the number density of $\mathbf{FL}^{-\bullet}$ in the ion trap. Reaction rates rise with increasing $\mathbf{FL}^{-\bullet}$ number density, until the ion trap is saturated with negative charges and no further increase is observed.[11]

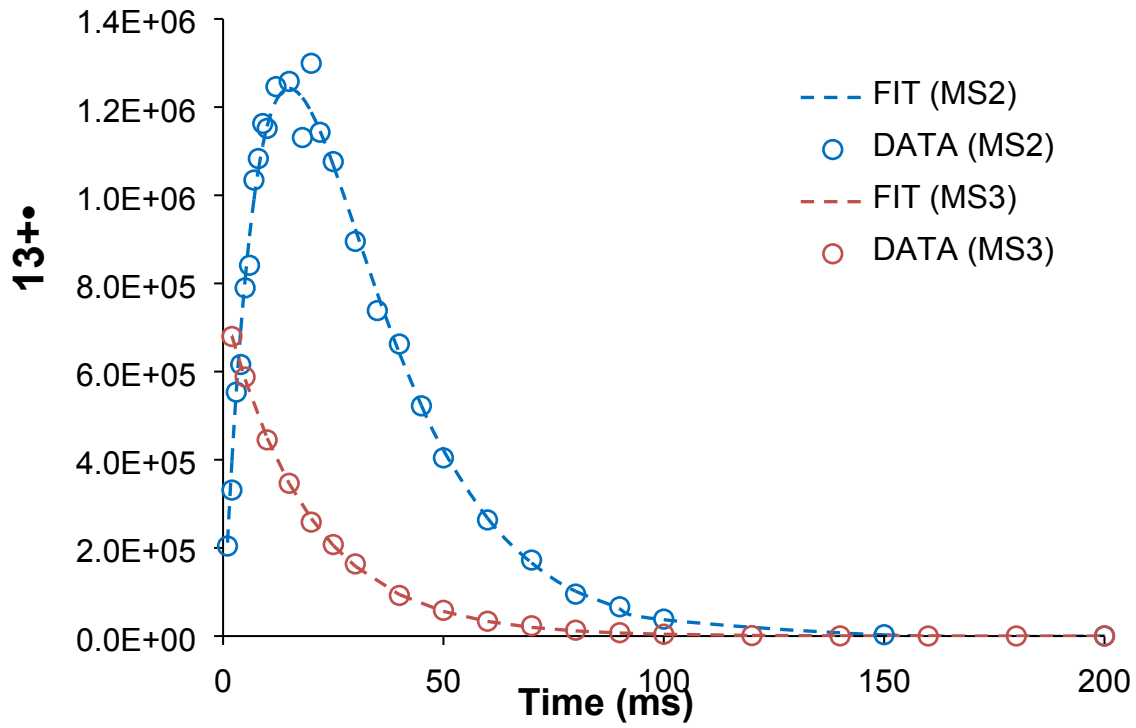


Figure S4: Determination of the second reduction rate for catenane $\mathbf{1}^{4+}$ by Equation 4 (blue, k = 53 ± 3 s^{-1}). Alternately, re-isolating the $\mathbf{1}^{3+\bullet}$ product ion and further reaction with $\mathbf{FL}^{-\bullet}$ in an MS^3 experiment results in a single exponential decay (*i.e.*, Equation 2), which yields the same result within experimental uncertainty (k = 52 ± 1 s^{-1}, red).

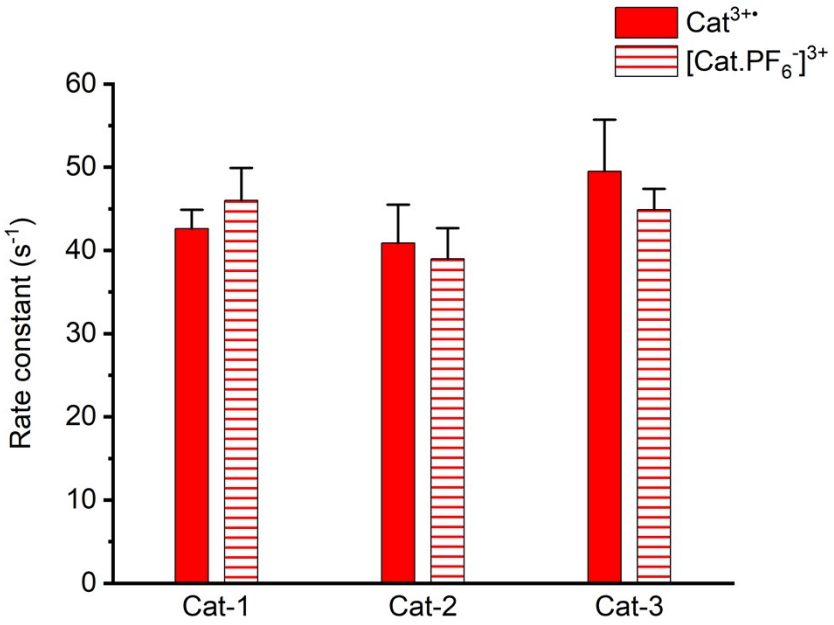
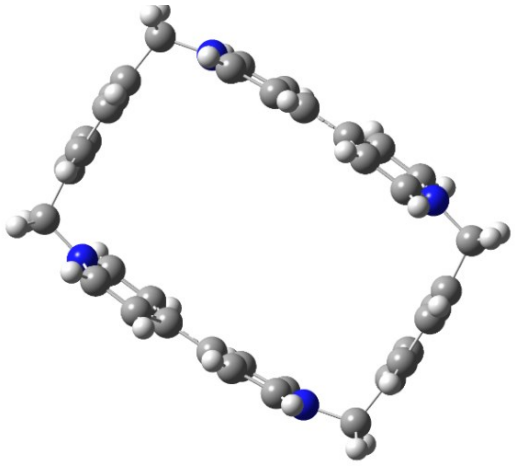


Figure S5: Comparison of the reduction rate constants of trivalent catenanes **1-3** in their radical cation form ($Cat^{3+\bullet}$) and as single anion adducts ($[Cat.PF_6]^{3+}$). The rate constant for each $Cat^{3+\bullet}$ species was determined from an MS^3 experiment and calculated from a single exponential decay. Error bars represent 95% confidence intervals based on the fit of the data to Equation 2.

Computational Results (all energies given in Hartrees)

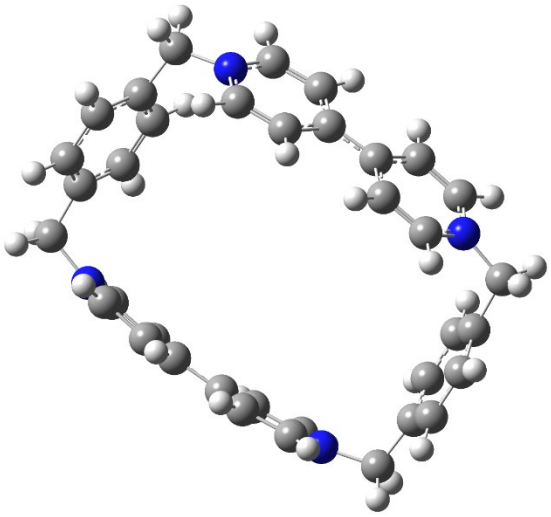
^{1}BB^{2+} (HF = -1608.9283684; Zero Point Energy = 0.6065221)



	X	Y	Z
C	-0.004	-0.0158	-0.1015
C	-0.072	-0.087	1.2554
C	1.1086	-0.2152	2.0538
C	2.3352	-0.1469	1.3227
C	2.3456	-0.0673	-0.0383
N	1.1905	-0.0295	-0.7638
C	1.0585	-0.4551	3.4573
C	-0.1747	-0.5434	4.1772
C	-0.2063	-0.9232	5.4832
N	0.9348	-1.2104	6.1767
C	2.1391	-1.0627	5.5526
C	2.2288	-0.6874	4.2452
C	0.1848	-7.128	-1.3179
C	0.0942	-7.502	-0.0101
C	-0.9578	-7.0204	0.8297
C	-1.9399	-6.2232	0.161
C	-1.7971	-5.8746	-1.1465
N	-0.7313	-6.2945	-1.8908
C	-0.9971	-7.2602	2.2333
C	0.0396	-7.9578	2.928
C	0.0497	-8.0401	4.2887
N	-0.9378	-7.4848	5.0488
C	-1.9889	-6.8773	4.4224
C	-2.0497	-6.7675	3.0677
C	1.3402	-4.2331	6.8345
C	0.9513	-5.5429	6.5995
C	-0.3584	-5.9515	6.8711
C	-1.2593	-5.0363	7.4091

C	-0.8682	-3.7183	7.645
C	0.427	-3.3048	7.3453
C	1.6091	-2.6907	-2.2147
C	1.2065	-3.9952	-2.4488
C	-0.027	-4.2572	-3.0553
C	-0.8327	-3.1926	-3.4475
C	-0.4269	-1.878	-3.2117
C	0.787	-1.6197	-2.5825
C	0.8343	-1.8557	7.5001
C	-0.7975	-7.3545	6.5121
C	-0.4939	-5.6883	-3.2144
C	1.1978	-0.2064	-2.2283
H	-0.8883	0.04	-0.7261
H	-1.0577	-0.0633	1.7006
H	3.2948	-0.1618	1.8224
H	3.2664	-0.0295	-0.6091
H	-1.1225	-0.3192	3.7066
H	-1.1332	-1.0239	6.0365
H	3.0157	-1.2616	6.1584
H	3.2221	-0.5888	3.8277
H	0.9826	-7.4741	-1.965
H	0.8536	-8.176	0.3639
H	-2.8155	-5.8523	0.6767
H	-2.5088	-5.2383	-1.6603
H	0.8586	-8.4285	2.4003
H	0.8382	-8.5493	4.8308
H	-2.7622	-6.4846	5.0727
H	-2.9254	-6.2879	2.6512
H	2.3623	-3.9305	6.6209
H	1.6718	-6.254	6.2033
H	-2.2715	-5.3472	7.6537
H	-1.5796	-3.0155	8.0704
H	2.568	-2.5019	-1.7385
H	1.8526	-4.8185	-2.1543
H	-1.7839	-3.3806	-3.9384
H	-1.0655	-1.0549	-3.5213
H	1.8082	-1.7586	7.985
H	0.1055	-1.2994	8.095
H	-1.7599	-7.5984	6.9692
H	-0.0708	-8.1015	6.839
H	0.2509	-6.3026	-3.7257
H	-1.423	-5.7401	-3.7875
H	0.5149	0.526	-2.6659
H	2.2066	0.0225	-2.5796

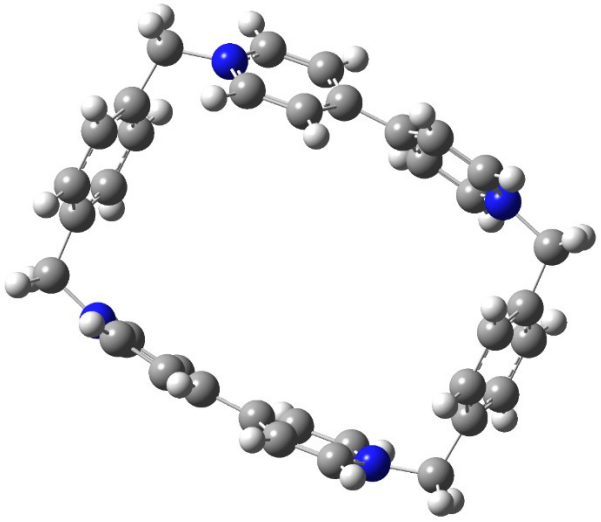
^{3}**BB**$^{2+}$ (HF = - 1608.9683613; Zero Point Energy = 0.6070129)



	X	Y	Z
C	-0.004	-0.0158	-0.1015
C	-0.072	-0.087	1.2554
C	1.1086	-0.2152	2.0538
C	2.3352	-0.1469	1.3227
C	2.3456	-0.0673	-0.0383
N	1.1905	-0.0295	-0.7638
C	1.0585	-0.4551	3.4573
C	-0.1747	-0.5434	4.1772
C	-0.2063	-0.9232	5.4832
N	0.9348	-1.2104	6.1767
C	2.1391	-1.0627	5.5526
C	2.2288	-0.6874	4.2452
C	0.1848	-7.128	-1.3179
C	0.0942	-7.502	-0.0101
C	-0.9578	-7.0204	0.8297
C	-1.9399	-6.2232	0.161
C	-1.7971	-5.8746	-1.1465
N	-0.7313	-6.2945	-1.8908
C	-0.9971	-7.2602	2.2333
C	0.0396	-7.9578	2.928
C	0.0497	-8.0401	4.2887
N	-0.9378	-7.4848	5.0488
C	-1.9889	-6.8773	4.4224
C	-2.0497	-6.7675	3.0677
C	1.3402	-4.2331	6.8345
C	0.9513	-5.5429	6.5995
C	-0.3584	-5.9515	6.8711
C	-1.2593	-5.0363	7.4091

C	-0.8682	-3.7183	7.645
C	0.427	-3.3048	7.3453
C	1.6091	-2.6907	-2.2147
C	1.2065	-3.9952	-2.4488
C	-0.027	-4.2572	-3.0553
C	-0.8327	-3.1926	-3.4475
C	-0.4269	-1.878	-3.2117
C	0.787	-1.6197	-2.5825
C	0.8343	-1.8557	7.5001
C	-0.7975	-7.3545	6.5121
C	-0.4939	-5.6883	-3.2144
C	1.1978	-0.2064	-2.2283
H	-0.8883	0.04	-0.7261
H	-1.0577	-0.0633	1.7006
H	3.2948	-0.1618	1.8224
H	3.2664	-0.0295	-0.6091
H	-1.1225	-0.3192	3.7066
H	-1.1332	-1.0239	6.0365
H	3.0157	-1.2616	6.1584
H	3.2221	-0.5888	3.8277
H	0.9826	-7.4741	-1.965
H	0.8536	-8.176	0.3639
H	-2.8155	-5.8523	0.6767
H	-2.5088	-5.2383	-1.6603
H	0.8586	-8.4285	2.4003
H	0.8382	-8.5493	4.8308
H	-2.7622	-6.4846	5.0727
H	-2.9254	-6.2879	2.6512
H	2.3623	-3.9305	6.6209
H	1.6718	-6.254	6.2033
H	-2.2715	-5.3472	7.6537
H	-1.5796	-3.0155	8.0704
H	2.568	-2.5019	-1.7385
H	1.8526	-4.8185	-2.1543
H	-1.7839	-3.3806	-3.9384
H	-1.0655	-1.0549	-3.5213
H	1.8082	-1.7586	7.985
H	0.1055	-1.2994	8.095
H	-1.7599	-7.5984	6.9692
H	-0.0708	-8.1015	6.839
H	0.2509	-6.3026	-3.7257
H	-1.423	-5.7401	-3.7875
H	0.5149	0.526	-2.6659
H	2.2066	0.0225	-2.5796

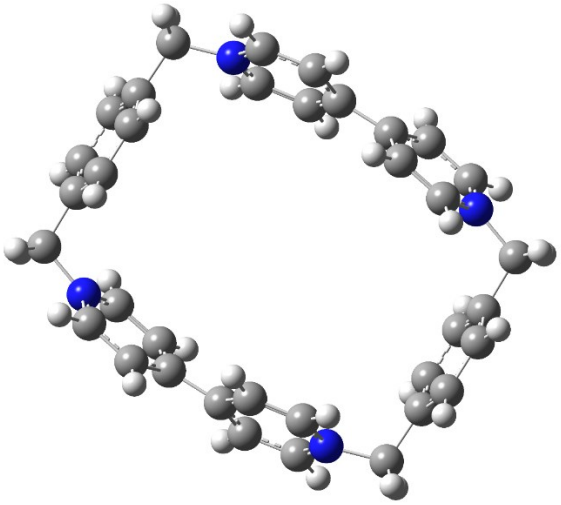
BB$^{3+\bullet}$ (HF = -1608.5887233; Zero Point Energy = 0.6087403)



	X	Y	Z
C	-0.004	-0.0158	-0.1015
C	-0.072	-0.087	1.2554
C	1.1086	-0.2152	2.0538
C	2.3352	-0.1469	1.3227
C	2.3456	-0.0673	-0.0383
N	1.1905	-0.0295	-0.7638
C	1.0585	-0.4551	3.4573
C	-0.1747	-0.5434	4.1772
C	-0.2063	-0.9232	5.4832
N	0.9348	-1.2104	6.1767
C	2.1391	-1.0627	5.5526
C	2.2288	-0.6874	4.2452
C	0.1848	-7.128	-1.3179
C	0.0942	-7.502	-0.0101
C	-0.9578	-7.0204	0.8297
C	-1.9399	-6.2232	0.161
C	-1.7971	-5.8746	-1.1465
N	-0.7313	-6.2945	-1.8908
C	-0.9971	-7.2602	2.2333
C	0.0396	-7.9578	2.928
C	0.0497	-8.0401	4.2887
N	-0.9378	-7.4848	5.0488
C	-1.9889	-6.8773	4.4224
C	-2.0497	-6.7675	3.0677
C	1.3402	-4.2331	6.8345
C	0.9513	-5.5429	6.5995
C	-0.3584	-5.9515	6.8711
C	-1.2593	-5.0363	7.4091

C	-0.8682	-3.7183	7.645
C	0.427	-3.3048	7.3453
C	1.6091	-2.6907	-2.2147
C	1.2065	-3.9952	-2.4488
C	-0.027	-4.2572	-3.0553
C	-0.8327	-3.1926	-3.4475
C	-0.4269	-1.878	-3.2117
C	0.787	-1.6197	-2.5825
C	0.8343	-1.8557	7.5001
C	-0.7975	-7.3545	6.5121
C	-0.4939	-5.6883	-3.2144
C	1.1978	-0.2064	-2.2283
H	-0.8883	0.04	-0.7261
H	-1.0577	-0.0633	1.7006
H	3.2948	-0.1618	1.8224
H	3.2664	-0.0295	-0.6091
H	-1.1225	-0.3192	3.7066
H	-1.1332	-1.0239	6.0365
H	3.0157	-1.2616	6.1584
H	3.2221	-0.5888	3.8277
H	0.9826	-7.4741	-1.965
H	0.8536	-8.176	0.3639
H	-2.8155	-5.8523	0.6767
H	-2.5088	-5.2383	-1.6603
H	0.8586	-8.4285	2.4003
H	0.8382	-8.5493	4.8308
H	-2.7622	-6.4846	5.0727
H	-2.9254	-6.2879	2.6512
H	2.3623	-3.9305	6.6209
H	1.6718	-6.254	6.2033
H	-2.2715	-5.3472	7.6537
H	-1.5796	-3.0155	8.0704
H	2.568	-2.5019	-1.7385
H	1.8526	-4.8185	-2.1543
H	-1.7839	-3.3806	-3.9384
H	-1.0655	-1.0549	-3.5213
H	1.8082	-1.7586	7.985
H	0.1055	-1.2994	8.095
H	-1.7599	-7.5984	6.9692
H	-0.0708	-8.1015	6.839
H	0.2509	-6.3026	-3.7257
H	-1.423	-5.7401	-3.7875
H	0.5149	0.526	-2.6659
H	2.2066	0.0225	-2.5796

BB^{4+} (HF = -1608.1367096; Zero Point Energy = 0.609964)

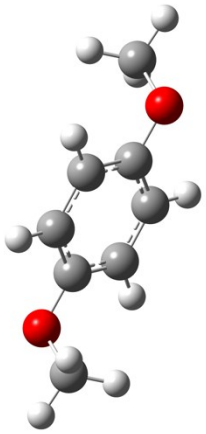


	X	Y	Z
C	-0.004	-0.0158	-0.1015
C	-0.072	-0.087	1.2554
C	1.1086	-0.2152	2.0538
C	2.3352	-0.1469	1.3227
C	2.3456	-0.0673	-0.0383
N	1.1905	-0.0295	-0.7638
C	1.0585	-0.4551	3.4573
C	-0.1747	-0.5434	4.1772
C	-0.2063	-0.9232	5.4832
N	0.9348	-1.2104	6.1767
C	2.1391	-1.0627	5.5526
C	2.2288	-0.6874	4.2452
C	0.1848	-7.128	-1.3179
C	0.0942	-7.502	-0.0101
C	-0.9578	-7.0204	0.8297
C	-1.9399	-6.2232	0.161
C	-1.7971	-5.8746	-1.1465
N	-0.7313	-6.2945	-1.8908
C	-0.9971	-7.2602	2.2333
C	0.0396	-7.9578	2.928
C	0.0497	-8.0401	4.2887
N	-0.9378	-7.4848	5.0488
C	-1.9889	-6.8773	4.4224
C	-2.0497	-6.7675	3.0677
C	1.3402	-4.2331	6.8345
C	0.9513	-5.5429	6.5995
C	-0.3584	-5.9515	6.8711
C	-1.2593	-5.0363	7.4091
C	-0.8682	-3.7183	7.645

C	0.427	-3.3048	7.3453
C	1.6091	-2.6907	-2.2147
C	1.2065	-3.9952	-2.4488
C	-0.027	-4.2572	-3.0553
C	-0.8327	-3.1926	-3.4475
C	-0.4269	-1.878	-3.2117
C	0.787	-1.6197	-2.5825
C	0.8343	-1.8557	7.5001
C	-0.7975	-7.3545	6.5121
C	-0.4939	-5.6883	-3.2144
C	1.1978	-0.2064	-2.2283
H	-0.8883	0.04	-0.7261
H	-1.0577	-0.0633	1.7006
H	3.2948	-0.1618	1.8224
H	3.2664	-0.0295	-0.6091
H	-1.1225	-0.3192	3.7066
H	-1.1332	-1.0239	6.0365
H	3.0157	-1.2616	6.1584
H	3.2221	-0.5888	3.8277
H	0.9826	-7.4741	-1.965
H	0.8536	-8.176	0.3639
H	-2.8155	-5.8523	0.6767
H	-2.5088	-5.2383	-1.6603
H	0.8586	-8.4285	2.4003
H	0.8382	-8.5493	4.8308
H	-2.7622	-6.4846	5.0727
H	-2.9254	-6.2879	2.6512
H	2.3623	-3.9305	6.6209
H	1.6718	-6.254	6.2033
H	-2.2715	-5.3472	7.6537
H	-1.5796	-3.0155	8.0704
H	2.568	-2.5019	-1.7385
H	1.8526	-4.8185	-2.1543
H	-1.7839	-3.3806	-3.9384
H	-1.0655	-1.0549	-3.5213
H	1.8082	-1.7586	7.985
H	0.1055	-1.2994	8.095
H	-1.7599	-7.5984	6.9692
H	-0.0708	-8.1015	6.839
H	0.2509	-6.3026	-3.7257
H	-1.423	-5.7401	-3.7875
H	0.5149	0.526	-2.6659
H	2.2066	0.0225	-2.5796

1,4-dimethoxybenzene

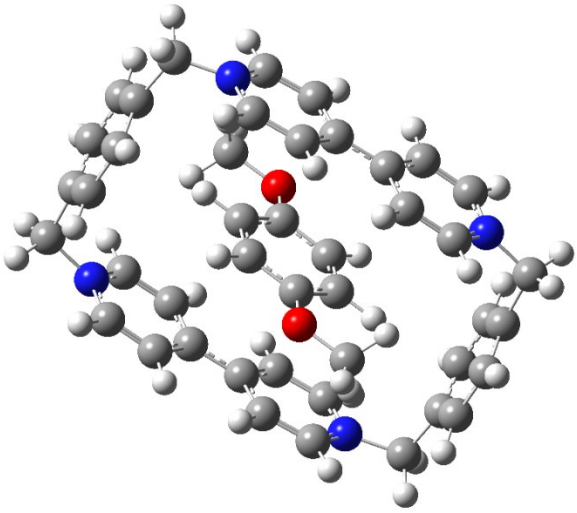
HF = -461.0935764; Zero Point Energy = 0.1664514



	X	Y	Z
C	-0.488488	-1.21964	0.032778
C	0.904581	-1.226813	0.019714
C	1.60099	-0.023607	-0.018195
C	0.90082	1.180526	-0.033545
C	-0.492245	1.1877	-0.020475
C	-1.188657	-0.015511	0.017433
H	1.424624	-2.179487	0.029621
H	2.686014	0.000266	-0.026299
H	-1.012307	2.140364	-0.030374
H	-2.273681	-0.039363	0.025529
O	-1.17718	-2.410489	0.044982
O	1.589551	2.371353	-0.045761
C	-1.446148	-2.881229	1.354469
H	-2.06326	-2.16611	1.912789
H	-1.98553	-3.823405	1.249404
H	-0.516099	-3.052566	1.910899
C	1.858185	2.842262	-1.355256
H	2.397737	3.784342	-1.250209
H	2.475021	2.127136	-1.91387
H	0.927995	3.013824	-1.91138

$^{1}BB^{2+}$ with *p*-dimethoxybenzene guest

HF = -2070.0711569; Zero Point Energy = 0.7754779



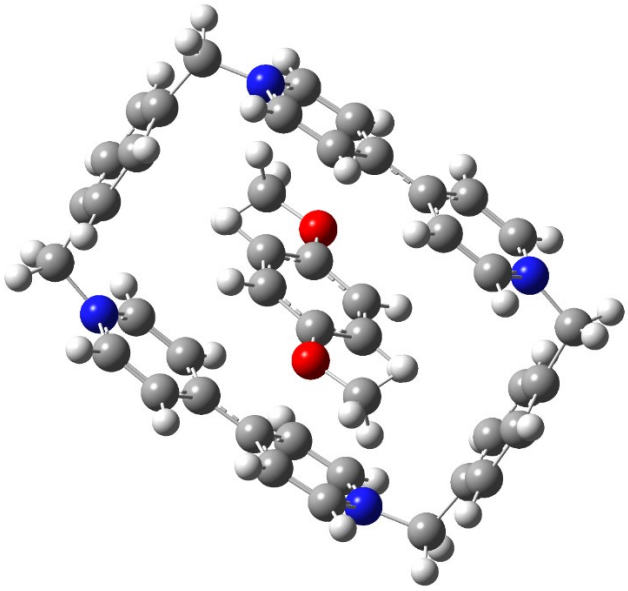
	X	Y	Z
C	0.2591	0.2902	0.1048
C	0.1699	0.0894	1.449
C	1.2777	-0.4082	2.1991
C	2.4721	-0.6207	1.4469
C	2.5067	-0.4019	0.1017
N	1.4122	0.0402	-0.5829
C	1.1932	-0.6817	3.5956
C	-0.0235	-0.548	4.3298
C	-0.0878	-0.8706	5.6526
N	1.0045	-1.3194	6.3366
C	2.1979	-1.4246	5.6812
C	2.3179	-1.1152	4.36
C	0.7847	-6.5422	-1.2028
C	0.7205	-6.865	0.1199
C	-0.496	-6.731	0.8544
C	-1.6206	-6.2968	0.0903
C	-1.5008	-5.9873	-1.2309
N	-0.3075	-6.0928	-1.8866
C	-0.5804	-7.0047	2.2508
C	0.5273	-7.5027	3.0008
C	0.4383	-7.7035	4.345
N	-0.7147	-7.4532	5.0328
C	-1.8091	-7.0109	4.3484
C	-1.7747	-6.792	3.0032
C	1.4076	-4.3375	7.241
C	1.0401	-5.6465	6.965
C	-0.3089	-6.0134	6.9463

C	-1.281	-5.0558	7.2377
C	-0.912	-3.7415	7.5147
C	0.433	-3.3708	7.5054
C	1.9783	-2.3569	-2.7876
C	1.6091	-3.6713	-3.0646
C	0.264	-4.0417	-3.0557
C	-0.7105	-3.0746	-2.792
C	-0.3427	-1.7657	-2.516
C	1.0063	-1.3992	-2.4966
C	0.836	-1.9249	7.6704
C	-0.7012	-7.4039	6.5065
C	-0.1392	-5.4875	-3.2204
C	1.3988	-0.0088	-2.0565
H	-0.5712	0.6661	-0.4814
H	-0.7736	0.3265	1.9225
H	3.3814	-0.9796	1.9117
H	3.4014	-0.5635	-0.4893
H	-0.9364	-0.2045	3.8605
H	-1.0036	-0.7858	6.2272
H	3.0401	-1.7541	6.2782
H	3.3013	-1.2081	3.9186
H	1.7003	-6.6274	-1.7776
H	1.6332	-7.2093	0.5889
H	-2.604	-6.2036	0.5319
H	-2.343	-5.6572	-1.8276
H	1.4707	-7.7399	2.5272
H	1.2685	-8.0797	4.9311
H	-2.7038	-6.8491	4.9395
H	-2.684	-6.4331	2.5384
H	2.4609	-4.0705	7.2697
H	1.809	-6.3925	6.782
H	-2.331	-5.3377	7.2661
H	-1.6768	-3.0069	7.7563
H	3.0284	-2.0753	-2.8156
H	2.3739	-4.406	-3.3057
H	-1.7638	-3.3414	-2.8211
H	-1.1116	-1.0195	-2.3334
H	1.784	-1.8244	8.2039
H	0.0791	-1.3506	8.2095
H	-1.6967	-7.6784	6.8626
H	0.0067	-8.1574	6.8596
H	0.6175	-6.0621	-3.7596
H	-1.0874	-5.5879	-3.7537
H	0.6912	0.745	-2.4095

H	2.3945	0.2655	-2.4125
C	-0.0059	-3.8974	3.5678
C	1.2936	-4.1408	3.1384
C	1.6589	-3.9525	1.8037
C	0.7023	-3.5148	0.8819
C	-0.5972	-3.2714	1.3114
C	-0.9625	-3.4596	2.6461
H	-0.2559	-4.0578	4.6141
H	2.0496	-4.4828	3.8387
H	0.9523	-3.3544	-0.1644
H	-1.3531	-2.9293	0.611
O	2.9623	-4.2175	1.5002
O	-2.2657	-3.1942	2.9497
C	-2.6564	-3.3408	4.2967
H	-3.7108	-3.0699	4.343
H	-2.5216	-4.3737	4.6434
H	-2.0732	-2.6841	4.9554
C	3.3529	-4.0719	0.1531
H	3.2184	-3.0392	-0.1942
H	4.4071	-4.3433	0.1068
H	2.7693	-4.7288	-0.5051

$^3BB^{2+}$ with *p*-dimethoxybenzene guest

HF = -2070.1096756; Zero Point Energy = 0.7763981



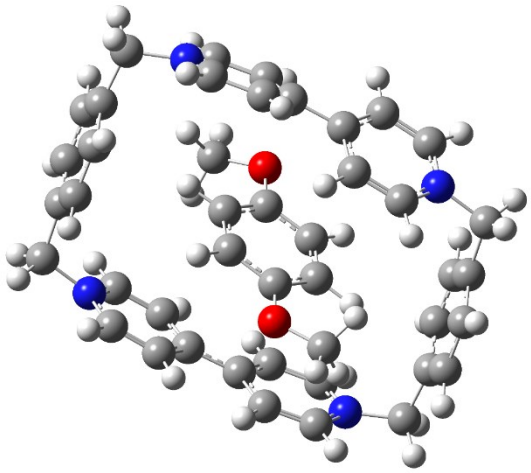
	X	Y	Z
C	0.2591	0.2902	0.1048
C	0.1699	0.0894	1.449
C	1.2777	-0.4082	2.1991
C	2.4721	-0.6207	1.4469
C	2.5067	-0.4019	0.1017
N	1.4122	0.0402	-0.5829
C	1.1932	-0.6817	3.5956
C	-0.0235	-0.548	4.3298
C	-0.0878	-0.8706	5.6526
N	1.0045	-1.3194	6.3366
C	2.1979	-1.4246	5.6812
C	2.3179	-1.1152	4.36
C	0.7847	-6.5422	-1.2028
C	0.7205	-6.865	0.1199
C	-0.496	-6.731	0.8544
C	-1.6206	-6.2968	0.0903
C	-1.5008	-5.9873	-1.2309
N	-0.3075	-6.0928	-1.8866
C	-0.5804	-7.0047	2.2508
C	0.5273	-7.5027	3.0008
C	0.4383	-7.7035	4.345
N	-0.7147	-7.4532	5.0328
C	-1.8091	-7.0109	4.3484
C	-1.7747	-6.792	3.0032
C	1.4076	-4.3375	7.241

C	1.0401	-5.6465	6.965
C	-0.3089	-6.0134	6.9463
C	-1.281	-5.0558	7.2377
C	-0.912	-3.7415	7.5147
C	0.433	-3.3708	7.5054
C	1.9783	-2.3569	-2.7876
C	1.6091	-3.6713	-3.0646
C	0.264	-4.0417	-3.0557
C	-0.7105	-3.0746	-2.792
C	-0.3427	-1.7657	-2.516
C	1.0063	-1.3992	-2.4966
C	0.836	-1.9249	7.6704
C	-0.7012	-7.4039	6.5065
C	-0.1392	-5.4875	-3.2204
C	1.3988	-0.0088	-2.0565
H	-0.5712	0.6661	-0.4814
H	-0.7736	0.3265	1.9225
H	3.3814	-0.9796	1.9117
H	3.4014	-0.5635	-0.4893
H	-0.9364	-0.2045	3.8605
H	-1.0036	-0.7858	6.2272
H	3.0401	-1.7541	6.2782
H	3.3013	-1.2081	3.9186
H	1.7003	-6.6274	-1.7776
H	1.6332	-7.2093	0.5889
H	-2.604	-6.2036	0.5319
H	-2.343	-5.6572	-1.8276
H	1.4707	-7.7399	2.5272
H	1.2685	-8.0797	4.9311
H	-2.7038	-6.8491	4.9395
H	-2.684	-6.4331	2.5384
H	2.4609	-4.0705	7.2697
H	1.809	-6.3925	6.782
H	-2.331	-5.3377	7.2661
H	-1.6768	-3.0069	7.7563
H	3.0284	-2.0753	-2.8156
H	2.3739	-4.406	-3.3057
H	-1.7638	-3.3414	-2.8211
H	-1.1116	-1.0195	-2.3334
H	1.784	-1.8244	8.2039
H	0.0791	-1.3506	8.2095
H	-1.6967	-7.6784	6.8626
H	0.0067	-8.1574	6.8596
H	0.6175	-6.0621	-3.7596

H	-1.0874	-5.5879	-3.7537
H	0.6912	0.745	-2.4095
H	2.3945	0.2655	-2.4125
C	-0.0059	-3.8974	3.5678
C	1.2936	-4.1408	3.1384
C	1.6589	-3.9525	1.8037
C	0.7023	-3.5148	0.8819
C	-0.5972	-3.2714	1.3114
C	-0.9625	-3.4596	2.6461
H	-0.2559	-4.0578	4.6141
H	2.0496	-4.4828	3.8387
H	0.9523	-3.3544	-0.1644
H	-1.3531	-2.9293	0.611
O	2.9623	-4.2175	1.5002
O	-2.2657	-3.1942	2.9497
C	-2.6564	-3.3408	4.2967
H	-3.7108	-3.0699	4.343
H	-2.5216	-4.3737	4.6434
H	-2.0732	-2.6841	4.9554
C	3.3529	-4.0719	0.1531
H	3.2184	-3.0392	-0.1942
H	4.4071	-4.3433	0.1068
H	2.7693	-4.7288	-0.5051

$BB^{3+\bullet}$ with *p*-dimethoxybenzene guest

HF = -2069.7358605; Zero Point Energy = 0.777844



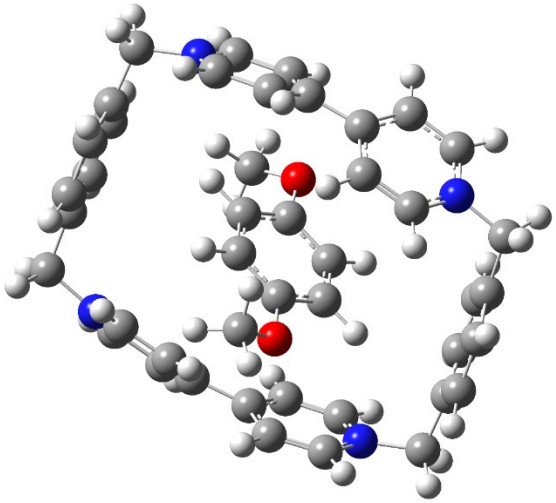
	X	Y	Z
C	0.2591	0.2902	0.1048
C	0.1699	0.0894	1.449
C	1.2777	-0.4082	2.1991
C	2.4721	-0.6207	1.4469
C	2.5067	-0.4019	0.1017
N	1.4122	0.0402	-0.5829
C	1.1932	-0.6817	3.5956
C	-0.0235	-0.548	4.3298
C	-0.0878	-0.8706	5.6526
N	1.0045	-1.3194	6.3366
C	2.1979	-1.4246	5.6812
C	2.3179	-1.1152	4.36
C	0.7847	-6.5422	-1.2028
C	0.7205	-6.865	0.1199
C	-0.496	-6.731	0.8544
C	-1.6206	-6.2968	0.0903
C	-1.5008	-5.9873	-1.2309
N	-0.3075	-6.0928	-1.8866
C	-0.5804	-7.0047	2.2508
C	0.5273	-7.5027	3.0008
C	0.4383	-7.7035	4.345
N	-0.7147	-7.4532	5.0328
C	-1.8091	-7.0109	4.3484
C	-1.7747	-6.792	3.0032
C	1.4076	-4.3375	7.241
C	1.0401	-5.6465	6.965
C	-0.3089	-6.0134	6.9463
C	-1.281	-5.0558	7.2377

C	-0.912	-3.7415	7.5147
C	0.433	-3.3708	7.5054
C	1.9783	-2.3569	-2.7876
C	1.6091	-3.6713	-3.0646
C	0.264	-4.0417	-3.0557
C	-0.7105	-3.0746	-2.792
C	-0.3427	-1.7657	-2.516
C	1.0063	-1.3992	-2.4966
C	0.836	-1.9249	7.6704
C	-0.7012	-7.4039	6.5065
C	-0.1392	-5.4875	-3.2204
C	1.3988	-0.0088	-2.0565
H	-0.5712	0.6661	-0.4814
H	-0.7736	0.3265	1.9225
H	3.3814	-0.9796	1.9117
H	3.4014	-0.5635	-0.4893
H	-0.9364	-0.2045	3.8605
H	-1.0036	-0.7858	6.2272
H	3.0401	-1.7541	6.2782
H	3.3013	-1.2081	3.9186
H	1.7003	-6.6274	-1.7776
H	1.6332	-7.2093	0.5889
H	-2.604	-6.2036	0.5319
H	-2.343	-5.6572	-1.8276
H	1.4707	-7.7399	2.5272
H	1.2685	-8.0797	4.9311
H	-2.7038	-6.8491	4.9395
H	-2.684	-6.4331	2.5384
H	2.4609	-4.0705	7.2697
H	1.809	-6.3925	6.782
H	-2.331	-5.3377	7.2661
H	-1.6768	-3.0069	7.7563
H	3.0284	-2.0753	-2.8156
H	2.3739	-4.406	-3.3057
H	-1.7638	-3.3414	-2.8211
H	-1.1116	-1.0195	-2.3334
H	1.784	-1.8244	8.2039
H	0.0791	-1.3506	8.2095
H	-1.6967	-7.6784	6.8626
H	0.0067	-8.1574	6.8596
H	0.6175	-6.0621	-3.7596
H	-1.0874	-5.5879	-3.7537
H	0.6912	0.745	-2.4095
H	2.3945	0.2655	-2.4125

C	-0.0059	-3.8974	3.5678
C	1.2936	-4.1408	3.1384
C	1.6589	-3.9525	1.8037
C	0.7023	-3.5148	0.8819
C	-0.5972	-3.2714	1.3114
C	-0.9625	-3.4596	2.6461
H	-0.2559	-4.0578	4.6141
H	2.0496	-4.4828	3.8387
H	0.9523	-3.3544	-0.1644
H	-1.3531	-2.9293	0.611
O	2.9623	-4.2175	1.5002
O	-2.2657	-3.1942	2.9497
C	-2.6564	-3.3408	4.2967
H	-3.7108	-3.0699	4.343
H	-2.5216	-4.3737	4.6434
H	-2.0732	-2.6841	4.9554
C	3.3529	-4.0719	0.1531
H	3.2184	-3.0392	-0.1942
H	4.4071	-4.3433	0.1068
H	2.7693	-4.7288	-0.5051

BB^{4+} with *p*-dimethoxybenzene guest

HF = -2069.2833078; Zero Point Energy = 0.7792035



	X	Y	Z
C	0.6084	0.6326	0.0304
C	0.5426	0.5596	1.4087
C	1.6038	-0.0097	2.1233
C	2.7657	-0.3485	1.4211
C	2.7781	-0.2497	0.0416
N	1.6907	0.1769	-0.6307
C	1.4564	-0.3639	3.5602
C	0.2118	-0.809	4.0215
C	0.0883	-1.2886	5.3079
N	1.15	-1.3229	6.1365
C	2.3482	-0.8518	5.7401
C	2.5309	-0.3673	4.4541
C	0.2766	-7.0852	-1.2356
C	0.2267	-7.6017	0.0494
C	-0.7032	-7.0966	0.9656
C	-1.6246	-6.1485	0.5051
C	-1.5327	-5.6731	-0.7861
N	-0.5683	-6.1088	-1.619
C	-0.6783	-7.4478	2.4119
C	0.5243	-7.7998	3.0347
C	0.5762	-7.9161	4.4104
N	-0.5177	-7.6891	5.1631
C	-1.7088	-7.4401	4.5861
C	-1.8204	-7.327	3.2123
C	1.6187	-4.3311	6.9888
C	1.301	-5.6707	6.8052

C	-0.0176	-6.1125	6.9636
C	-1.0025	-5.207	7.3577
C	-0.6813	-3.8615	7.5487
C	0.6233	-3.4138	7.3408
C	1.9752	-2.4943	-2.5026
C	1.4899	-3.788	-2.6789
C	0.1146	-4.0194	-2.7628
C	-0.7659	-2.9359	-2.6938
C	-0.2813	-1.6437	-2.5001
C	1.0925	-1.4162	-2.3887
C	0.971	-1.9495	7.4927
C	-0.3693	-7.5533	6.6527
C	-0.4149	-5.4269	-2.9515
C	1.6196	-0.0203	-2.1174
H	-0.2007	1.0304	-0.5727
H	-0.3446	0.9374	1.9054
H	3.6328	-0.766	1.9192
H	3.6365	-0.5384	-0.5555
H	-0.6534	-0.8509	3.37
H	-0.843	-1.6839	5.6982
H	3.1503	-0.8753	6.4704
H	3.5109	0.0076	4.1788
H	0.9912	-7.4341	-1.9736
H	0.9183	-8.3967	0.3075
H	-2.377	-5.7288	1.1639
H	-2.2021	-4.9154	-1.1775
H	1.4435	-7.9398	2.4775
H	1.4894	-8.1655	4.9389
H	-2.5563	-7.3123	5.251
H	-2.8006	-7.1279	2.795
H	2.6519	-4.0075	6.8865
H	2.0954	-6.3759	6.5737
H	-2.0194	-5.5426	7.5433
H	-1.452	-3.1737	7.8878
H	3.05	-2.3272	-2.4958
H	2.1945	-4.6078	-2.7946
H	-1.833	-3.0832	-2.8426
H	-0.9803	-0.8114	-2.4864
H	1.9062	-1.8029	8.0359
H	0.1847	-1.3895	8.004
H	-1.3124	-7.863	7.106
H	0.4094	-8.2521	6.9654
H	0.2589	-6.0425	-3.5496
H	-1.3977	-5.4352	-3.4287

H	0.9679	0.7573	-2.5201
H	2.6238	0.1319	-2.5175
C	-0.2572	-4.2541	3.6763
C	1.0873	-4.0602	3.3972
C	1.4817	-3.4503	2.2029
C	0.5136	-3.034	1.2886
C	-0.8433	-3.2152	1.5711
C	-1.2348	-3.8462	2.7569
H	-0.5748	-4.7126	4.6107
H	1.8544	-4.3699	4.1008
H	0.8058	-2.5633	0.3504
H	-1.5833	-2.8737	0.8538
O	2.8204	-3.233	2.0306
O	-2.5209	-4.1533	3.0718
C	-3.5641	-3.4444	2.4039
H	-4.4886	-3.7002	2.918
H	-3.3978	-2.3639	2.4596
H	-3.6447	-3.7436	1.3515
C	3.375	-3.6558	0.7901
H	3.0005	-3.055	-0.0476
H	4.4553	-3.5367	0.8743
H	3.1392	-4.7086	0.601

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