Electronic supplementary information

Multiple-decker and ring sandwich formation of manganese-benzene organometallic cluster anions: $Mn_nBz_n^-$ (n=1–5 and 18)

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Details of the computational methods

The density functional theory (DFT) calculations were performed at the unrestricted BP86[S1,S2] level, implemented in the Gaussian 09 program package[S3] using the def2-TZVP[S4] basis sets. A convergence criterion of 10^{-8} Hartree on total energy was adopted for all the self-consistent field calculations. Vibrational frequency analyses were performed at each stationary point during the geometry optimizations, and the geometries were allowed to relax through vibrational modes with imaginary frequencies until no further imaginary frequencies were found. For each optimized anion, the first vertical detachment energy (VDE) was calculated as the energy difference between the ground state of the anion and the neutral whose geometry is the same as the anion. The vertical excitation energies of the neutral were further calculated by means of the time-dependent DFT method, and added to the first VDE to obtain the higher VDEs, where only one-electron transitions were considered. Zero-point energy corrections were neglected because they were small (only brought at most ~0.1 eV differences to the relative energies).

It is important to correctly evaluate the energy orderings of different spin states of $Mn_nBz_n^-$ clusters, as a recent study[S5] has pointed out that the current DFT methods for transition metal-based organometallic systems have a specific problem that the spin multiplicity of a global-minimum structure depends on the functional employed. In this study, $Mn_1Bz_1^{-/0}$ were optimized using various functionals to calculate the ADE/VDE values of $Mn_1Bz_1^-$, and the BP86 was adopted on the basis of the reasonable agreements with the experimental values (see Tables S1 and S2 on page 11).

One could argue that DFT-GGA method often underestimates the on-site correlation effect in the 3d transition metal atom. On the other hand, theoretical studies have mentioned the reliability of GGA with regard to the magnetic properties of similar sandwich systems by demonstrating the well agreement between GGA and GGA+U calculations.[S6,S7] Taken into account that our BP86 calculations well reproduced experimental results of $Mn_1Bz_1^{-/0}$, we decided to adopt the BP86 method for all sizes of the clusters, including $Mn_{18}Bz_{18}^{-/0}$.

References

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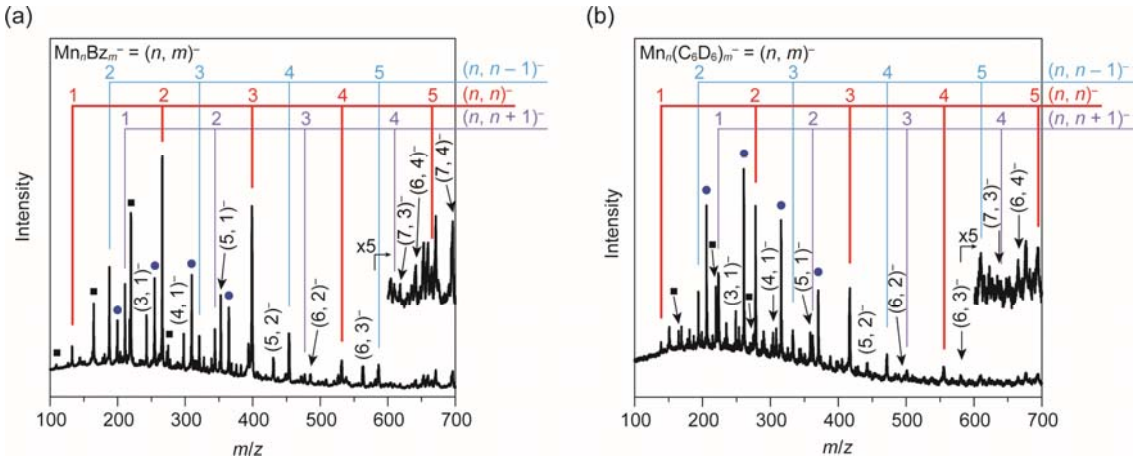

Fig. S1 Mass spectra of (a) $Mn_nBz_m^-$ and (b) $Mn_n(C_6D_6)_m^-$ clusters. The peak assignments for $(n, m)^-$ = $(n, n-1)^-$, $(n, n)^-$, and $(n, n+1)^-$ are indicated with vertical lines. Several dominant $(n, m)^-$ clusters with $m \leq n-2$ are also labeled. Coexistent naked Mn_n^- clusters and incomplete Mn-Bz cluster anions are marked by ■ and ●, respectively.

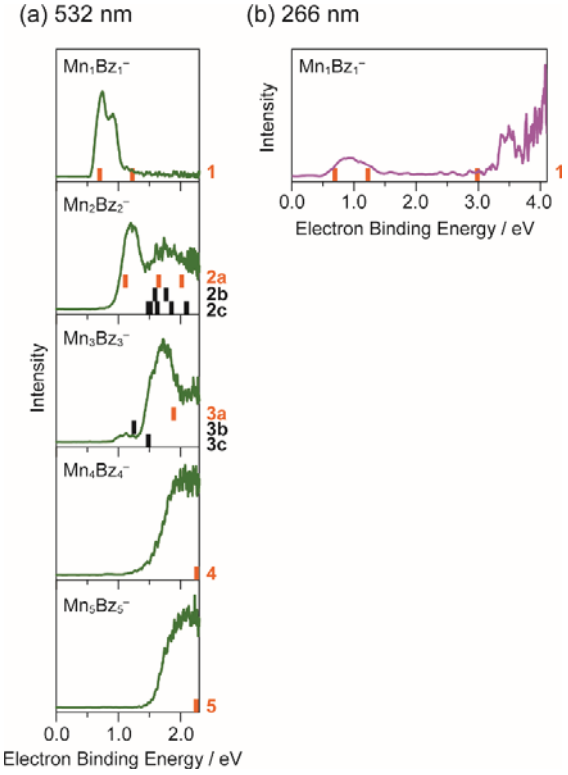

Fig. S2 Photoelectron spectra of $Mn_nBz_n^-$ (n = 1–5) taken with (a) 532 nm (2.33 eV) and (b) 266 nm (4.66 eV) radiation. The calculated VDEs of the plausible structures are indicated below the spectra with vertical bars. Bold-faced labels right to the VDE bars are denoted to identify the structures (see Fig. 3b and c). The 266 nm spectrum of $Mn_1Bz_1^-$ was measured to ascertain the peak center at ~3.5 eV, which was barely observed in the 355 nm spectrum (Fig. 3a).

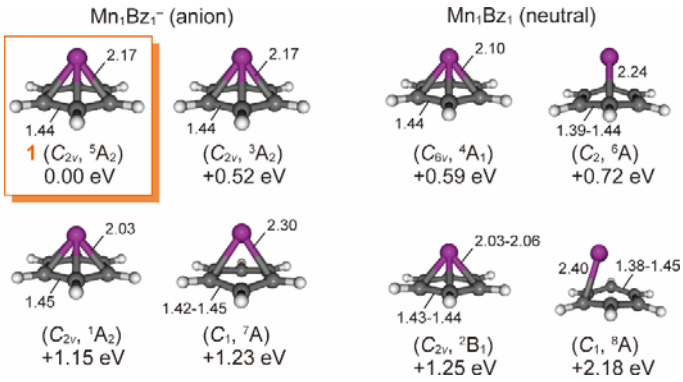

Fig. S3 Low-lying structures of $Mn_1Bz_1^{-/0}$ clusters with their symmetries, electronic states, and relative energies to **1** (enclosed in a frame). Typical bond lengths are indicated in Å. Bonds are visible for C–C, C–H, and Mn–C with distances of < 2.4 Å only to guide the eyes. They do not necessarily represent single bonds.

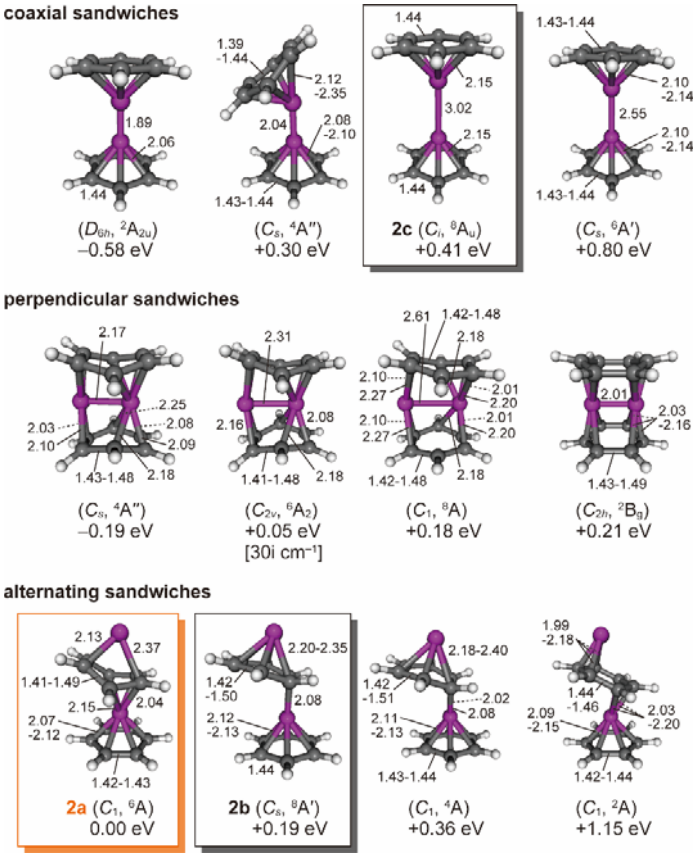

Fig. S4 Low-lying isomers of $Mn_2Bz_2^-$ clusters with their symmetries, electronic states, and relative energies to **2a**. The isomers are classified into three types of sandwich structures: namely, coaxial, perpendicular, and alternating sandwiches. Three isomers identified in the photoelectron spectra, including major and minor ones, are shown in frames. The indications are shown in the same manner as Fig. S3. Note that the $^6A_2$-state perpendicular sandwich isomer has an imaginary vibrational mode of 30i cm^{-1} (A_2 symmetry).

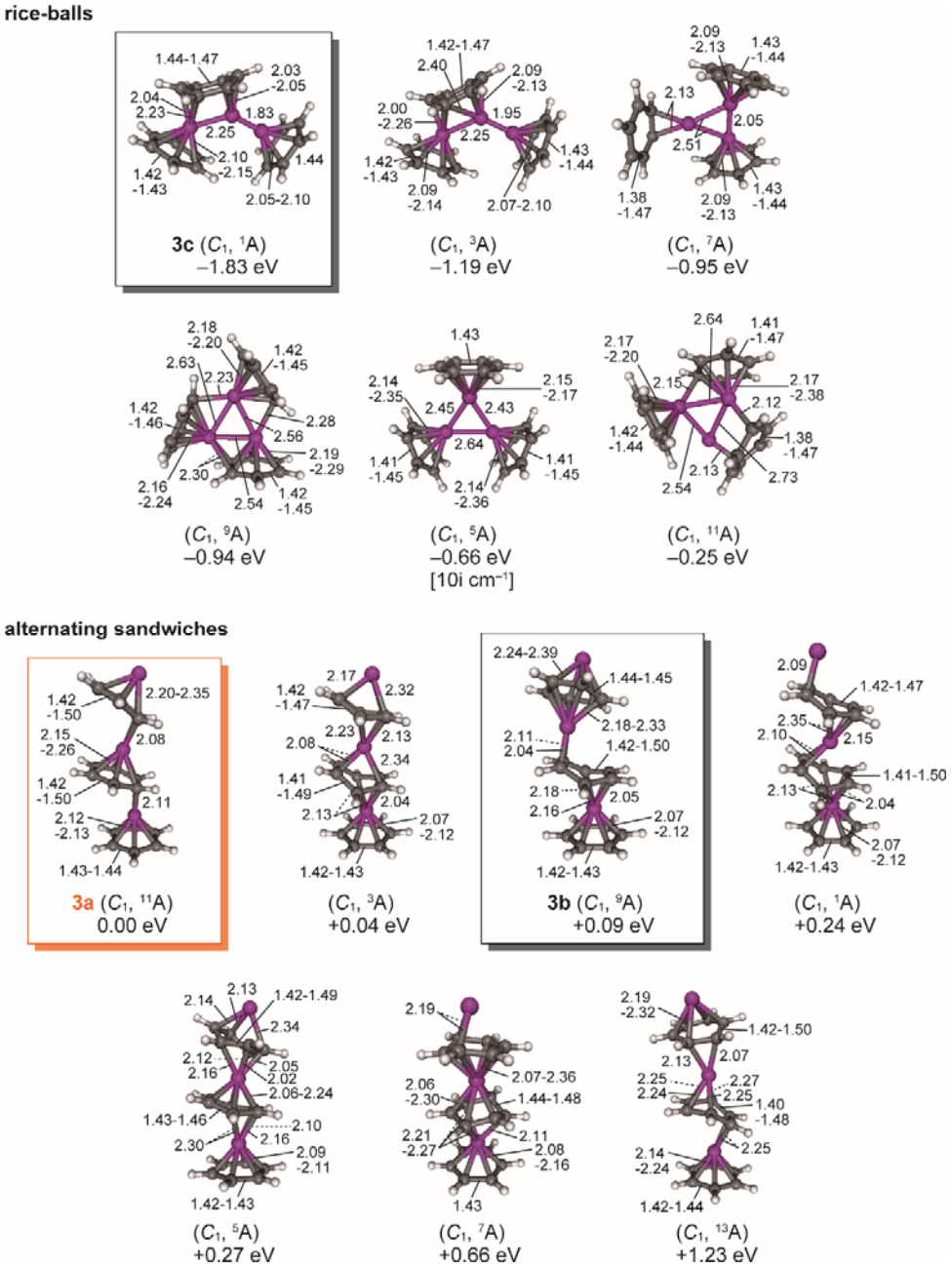

Fig. S5 Low-lying isomers of $Mn_2Bz_2^-$ clusters with their symmetries, electronic states, and relative energies to **3a**. Each isomer is classified into either rice-ball (metal core covered by ligands) or alternating sandwich structure. Three isomers identified in the photoelectron spectra, including major and minor ones, are shown in frames. The indications are shown in the same manner as Fig. S3. Note that the ^{5}A-state rice-ball isomer has an imaginary vibrational mode of 10i cm^{-1}.

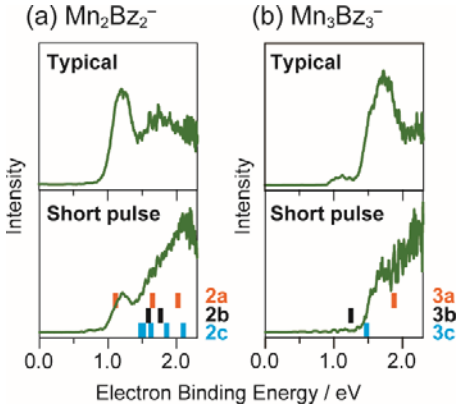

Fig. S6 Photoelectron spectra of (a) $Mn_2Bz_2^-$ and (b) $Mn_3Bz_3^-$ taken with 532 nm under the condition with using typical (≥ 280 μs, upper part) and short (250 μs, lower part) pulses for the Bz pulsed valve. Comparison with Fig. 2 shows that the thermodynamic condition diminishes the kinetically favorable isomers (**2a**, **2b**, **3a**, and **3b**), while thermodynamic species (**2c** and **3c**, colored in blue) remain in the spectra, presumably due to the difference of the reaction pathways. Note that the relaxation of higher-lying **2c** to its ground singlet state is unlikely to occur due to the significant structural difference in the Mn-Mn bond length (see Fig. S4).

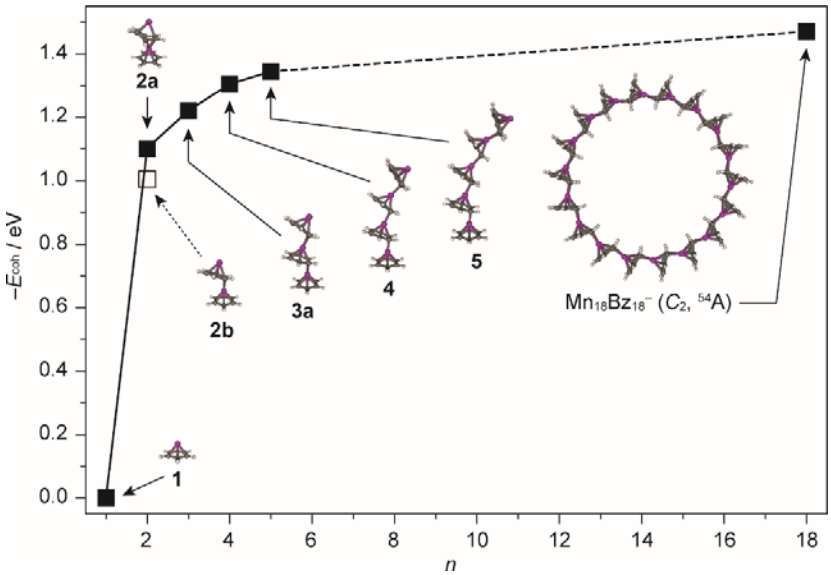

Fig. S7 Calculated cohesive energies per $Mn_1(\eta^6\text{-}Bz)_1$ unit for $Mn_nBz_n^-$ (n = 1–5 and 18) clusters (E_{coh}). E_{coh} was obtained by the formula $E_{coh} = [E(Mn_nBz_n^-) - \{(n-1)E(Mn_1Bz_1) + E(Mn_1Bz_1^-)\}] / n$, where E(cluster) represents the cluster's total energy. The cohesive energy of a minor product of the tilted sandwich $Mn_2Bz_2^-$ (**2b)** is explicitly indicated with a white square, because the structure determined for $Mn_2Bz_2^-$ (**2a**) has a different bonding scheme from the tilted sandwiches (e.g., **3a**, **4**, and **5**). Basis set superposition error (BSSE) corrections were neglected because they were considerably small (e.g., ~0.03 eV for **2b**). The lines are provided only for the eyes.

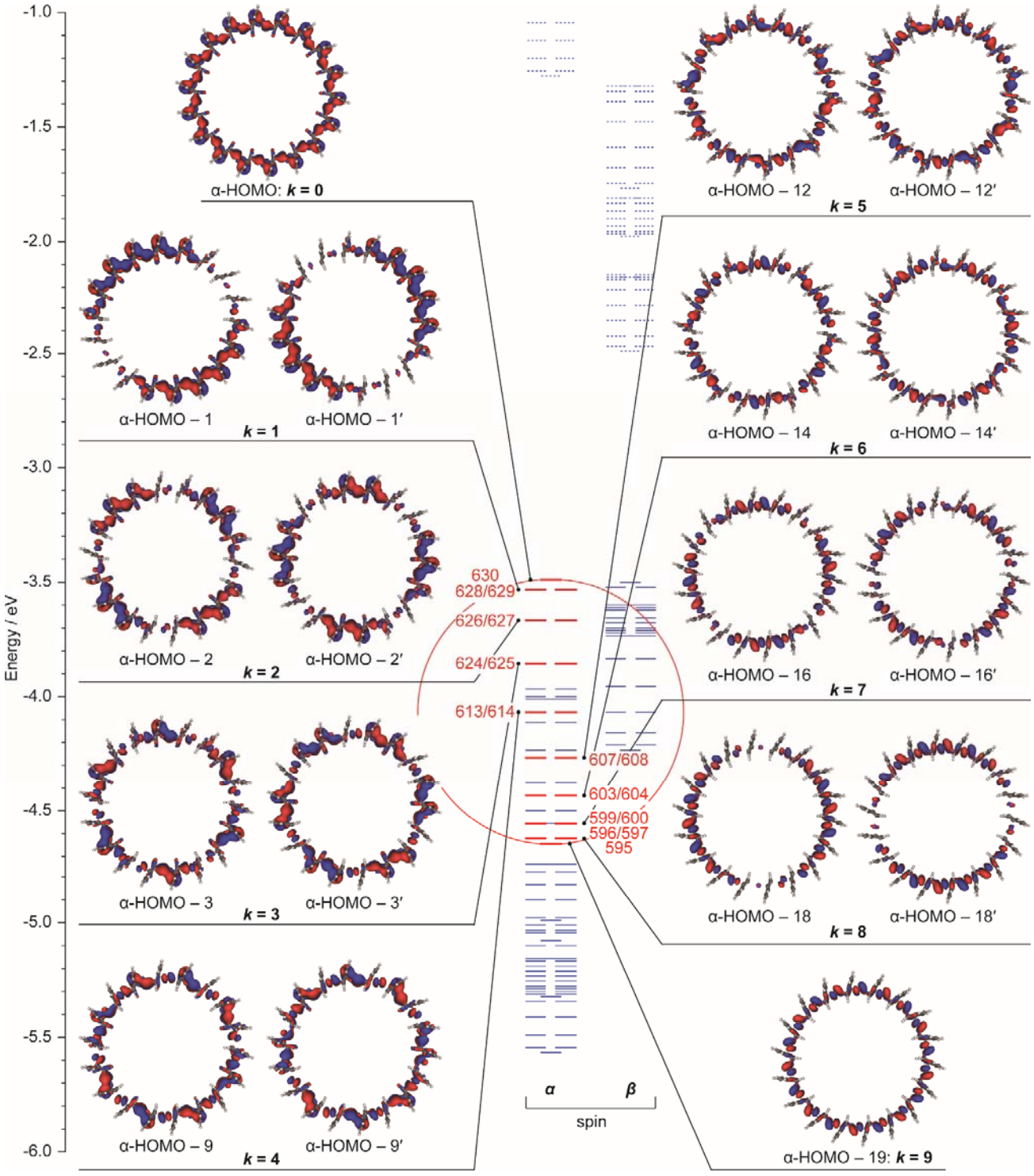

Fig. S8 Kohn–Sham orbital energy levels of the neutral (C_{18h}, $^{55}B_u$) $Mn_{18}Bz_{18}$. Occupied and unoccupied orbitals are denoted by solid and dashed lines, respectively. The simple Hückel model was employed for the orbitals colored in red, whose isosurface plots (isosurface value = 0.01) and numbers of nodes *k* are also shown (see also Fig. 6a and c).

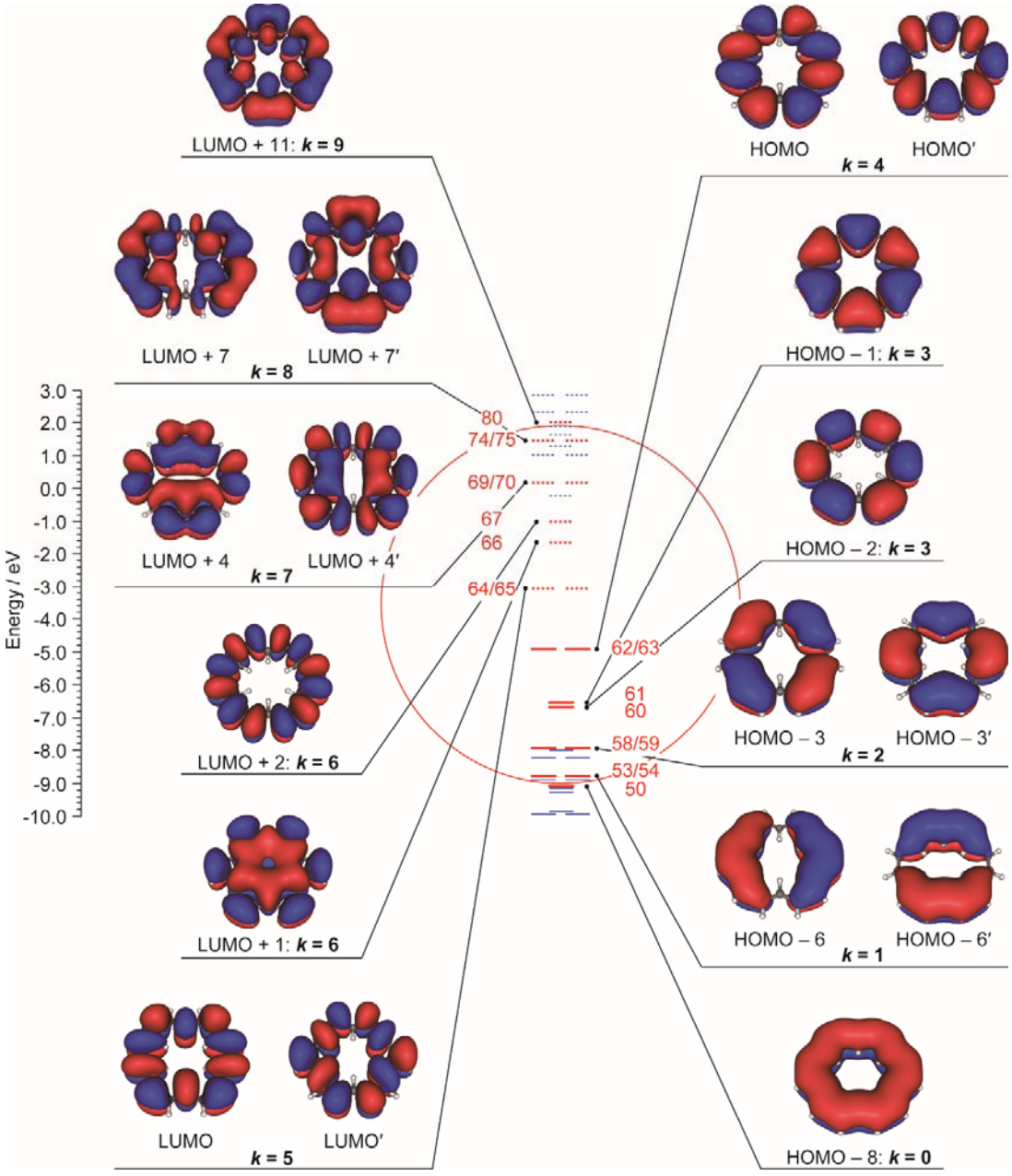

Fig. S9 Kohn–Sham orbital energy levels of the neutral (D_{3d}, $^1A_{1g}$) [18]annulene ($C_{18}H_{18}$). Occupied and unoccupied orbitals are denoted by solid and dashed lines, respectively. The simple Hückel model was employed for the orbitals colored in red, whose isosurface plots (isosurface value = 0.01) and numbers of nodes k are also shown (see also Fig. 6b and 6d). Note that the k = 3 and 6 orbitals are not degenerate under the D_{3d} symmetry in our geometry optimization.

Table S1 Total energies (in Hartree) of $Mn_1Bz_1^{-/0}$ with different DFT functionals

$2S+1$	BP86	PBE	PBE0	B3LYP	M06
			$Mn_1Bz_1^-$ (anion)		
1	−1383.44532675	−1382.73851935	−1382.71996082	−1383.24932802	−1382.98791071
3	−1383.46862514	−1382.76245684	−1382.73844967	−1383.30791859	−1383.05791695
5	**−1383.48767837**	**−1382.78122532**	**−1382.80540406**	**−1383.32291468**	**−1383.06170821**
7	−1383.44251566	−1382.73541991	−1382.77493109	−1383.32017620	−1383.02370947
			Mn_1Bz_1 (neutral)		
2	−1383.44186211	−1382.73762490	−1382.73890662	−1383.26547699	−1382.99497021
4	**−1383.46589142**	**−1382.76345844**	−1382.78286250	−1383.30170180	−1383.04912620
6	−1383.46107427	−1382.75795986	**−1382.80222934**	**−1383.31952986**	**−1383.08419939**
8	−1383.40739168	−1382.70475107	−1382.76694134	−1383.27899150[a]	−1383.00949903

[a] An imaginary vibrational mode of 30i cm^{-1} (B symmetry) is remaining only for Mn_1Bz_1 (neutral) with B3LYP at $2S + 1 = 8$.

Table S2 Calculated ADEs and VDEs (in eV) of the lowest-energy spin states of $Mn_1Bz_1^-$

	BP86	PBE	PBE0	B3LYP	M06	Expt.
ADE	0.59	0.48	0.09	0.09	–0.61	0.58 ± 0.07
VDE	0.69	0.58	0.54	0.54	0.48	0.76 ± 0.02

Table S3 Symmetries, electronic states, total energies (E), energies relative to 1 (ΔE), imaginary frequencies, $<S^2>$ values, calculated VDEs, and corresponding labels of various spin states ($2S + 1$) of $Mn_1Bz_1^{-/0}$

$2S+1$	symm./state	E / Hartree	ΔE / eV	imaginary freq.	$<S^2>$	VDE	label
			$Mn_1Bz_1^-$ (anion)				
1	$C_{2v}/^1A_2$	–1383.44532675	1.15	none	1.02	0.17	
3	$C_{2v}/^3A_2$	–1383.46862514	0.52	none	3.26	0.16	
5	$C_{2v}/^5A_2$	–1383.48767837	**0.00**	none	6.31	0.69	**1**
7	$C_2/^7A$	–1383.44251566	1.23	none	12.14	–0.22	
			Mn_1Bz_1 (neutral)				
2	$C_{2v}/^2B_1$	–1383.44186211	1.25	none	0.77		
4	$C_{6v}/^4A_1$	–1383.46589142	0.59	none	3.91		
6	$C_2/^6A$	–1383.46107427	0.72	none	8.91		
8	$C_1/^8A$	–1383.40739168	2.18	none	15.76		

Table S4 Symmetries, electronic states, total energies (E), energies relative to 2a (ΔE), imaginary frequencies, $<S^2>$ values, calculated VDEs, and corresponding labels of various spin states ($2S + 1$) of $Mn_2Bz_2^-$

$2S + 1$	symm./state	E / Hartree	ΔE / eV	imaginary freq.	$<S^2>$	VDE	label
			coaxial sandwich				
2	$D_{6h}/^2A_{2u}$	–2767.05557307	–0.58	none	0.77	0.75	
4	$C_s/^4A''$	–2767.02319165	0.30	none	3.88	0.81	
6	$C_s/^6A'$	–2767.00490239	0.80	none	9.01	1.33	
8	$C_i/^8A_u$	–2767.01915573	0.41	none	16.26	1.47	**2c**
			perpendicular sandwich				
2	$C_{2h}/^2B_g$	–2767.02665972	0.21	none	0.79	0.72	
4	$C_s/^4A''$	–2767.04116392	–0.19	none	3.93	0.86	
6	$C_{2v}/^6A_2$	–2767.03270769	0.05	30i cm^{-1} (A_2)	8.86	0.35	
8	$C_1/^8A$	–2767.02786784	0.18	none	16.01	0.80	
			alternating sandwich				
2	$C_1/^2A$	–2766.99213452	1.15	none	3.76	0.64	
4	$C_1/^4A$	–2767.02121071	0.36	none	5.93	1.48	
6	$C_1/^6A$	–2767.03436193	**0.00**	none	8.92	1.10	**2a**
8	$C_s/^8A'$	–2767.02739251	0.19	none	16.12	1.58	**2b**

Table S5 Symmetries, electronic states, total energies (E), energies relative to 3a (ΔE), imaginary frequencies, $<S^2>$ values, calculated VDEs, and corresponding labels of various spin states ($2S + 1$) of $Mn_3Bz_3^-$

$2S + 1$	symm./state	E / Hartree	ΔE / eV	imaginary freq.	$<S^2>$	VDE	label
			rice-ball				
1	$C_1/^1A$	–4150.62136589	–1.83	none	0.00	1.48	
3	$C_1/^3A$	–4150.59751017	–1.19	none	2.08	0.94	**3c**
5	$C_1/^5A$	–4150.57823391	–0.66	10i cm^{-1} (A)	8.53	1.36	
7	$C_1/^7A$	–4150.58898914	–0.95	none	12.16	1.44	
9	$C_1/^9A$	–4150.58841419	–0.94	none	20.63	1.37	
11	$C_1/^{11}A$	–4150.56326267	–0.25	none	30.40	1.01	
			alternating sandwich				
1	$C_1/^1A$	–4150.54519222	0.24	none	3.90	2.01	
3	$C_1/^3A$	–4150.55230581	0.04	none	5.13	1.44	
5	$C_1/^5A$	–4150.54409952	0.27	none	7.18	1.20	

Table S5 (continued)

7	C_1/^{7}A	–4150.52984254	0.66	none	12.23	1.13	
9	C_1/^{9}A	–4150.55069917	0.09	none	20.40	1.25	**3b**
11	C_1/^{11}A	–4150.55394089	**0.00**	none	30.57	1.88	**3a**
13	C_1/^{13}A	–4150.50883573	1.23	none	42.49	1.29	

Table S6 Symmetries, electronic states, total energies (E), imaginary frequencies, $<S^2>$ values, calculated VDEs, and corresponding labels of $Mn_4Bz_4^-$ and $Mn_5Bz_5^-$

$2S+1$	symm./state	E / Hartree	imaginary freq.	$<S^2>$	VDE	label
		$Mn_4Bz_4^-$ (alternating sandwich)				
14	C_1/^{14}A	–5534.07709982	none	49.52	2.25	**4**
		$Mn_5Bz_5^-$ (alternating sandwich)				
17	C_1/^{17}A	–6917.59827709	none	72.96	2.24	**5**

Table S7 Symmetries, electronic states, total energies (E), imaginary frequencies, and $<S^2>$ values of ring $Mn_{18}Bz_{18}^{-/0}$

$2S+1$	symm./state	E / Hartree	imaginary freq.	$<S^2>$
		$Mn_{18}Bz_{18}^-$ (ring anion)		
54	C_2/^{54}A	–24903.3803001	none	732.24
		$Mn_{18}Bz_{18}$ (ring neutral)		
55	C_{18h}/$^{55}B_u$	–24903.3149639	none	759.51

Table S8 Cartesian coordinates (in Å)

Structure **1**:

C	0.000000	1.435650	-0.614433
C	-1.243307	0.717823	-0.614294
C	-1.243307	-0.717823	-0.614294
C	0.000000	-1.435650	-0.614433
C	1.243307	-0.717823	-0.614294
C	1.243307	0.717823	-0.614294
H	0.000000	2.524897	-0.551953
H	-2.186637	1.262431	-0.551858
H	-2.186637	-1.262431	-0.551858

H	0.000000	-2.524897	-0.551953
H	2.186637	-1.262431	-0.551858
H	2.186637	1.262431	-0.551858
Mn	0.000000	0.000000	1.017103

Structure **2a**:

C	-2.471844	-0.626164	-1.236369
C	-2.320062	0.786511	-1.229242
C	-2.221741	1.510498	0.000554
C	-2.319608	0.785940	1.229964
C	-2.471245	-0.626757	1.236422
C	-2.472618	-1.346590	-0.000165
H	-2.439113	-1.169071	-2.186218
H	-2.169672	1.313091	-2.176129
H	-2.047529	2.587988	0.000757
H	-2.168486	1.311927	2.177063
H	-2.437580	-1.170266	2.185893
H	-2.509499	-2.441331	-0.000399
Mn	-0.846777	-0.067714	-0.000150
C	0.782615	-1.058119	-0.724835
C	0.814828	0.297579	-1.309925
C	1.758555	1.284280	-0.706684
C	1.758521	1.284094	0.706975
C	0.815273	0.296878	1.309909
C	0.782479	-1.058422	0.724096
H	0.697545	-1.979728	-1.306874
H	0.697292	0.339104	-2.399193
H	2.199757	2.083302	-1.306978
H	2.199709	2.082830	1.307651
H	0.697405	0.338094	2.399134
H	0.697680	-1.980283	1.305775
Mn	2.925640	-0.352047	-0.000037

Structure **2b**:

C	0.163739	-2.623996	1.434214
C	1.375196	-2.341684	0.717738

C	1.375196	-2.341684	-0.717738
C	0.163739	-2.623996	-1.434214
C	-1.052923	-2.893011	-0.718768
C	-1.052923	-2.893011	0.718768
H	0.149430	-2.556924	2.523163
H	2.279793	-2.068939	1.263223
H	2.279793	-2.068939	-1.263223
H	0.149430	-2.556924	-2.523163
H	-1.984132	-3.054269	-1.264709
H	-1.984132	-3.054269	1.264709
Mn	-0.193419	-1.092814	0.000000
C	0.283562	1.549790	1.433363
C	1.387391	2.077443	0.714339
C	1.387391	2.077443	-0.714339
C	0.283562	1.549790	-1.433363
C	-0.758365	0.766443	-0.749083
C	-0.758365	0.766443	0.749083
H	0.279827	1.590409	2.523797
H	2.187561	2.588327	1.252799
H	2.187561	2.588327	-1.252799
H	0.279827	1.590409	-2.523797
H	-1.722118	0.677826	-1.262548
H	-1.722118	0.677826	1.262548
Mn	-0.573138	2.981907	0.000000

Structure **2c**:

C	0.000000	1.436258	3.110111
C	1.243674	0.717999	3.110415
C	1.243674	-0.717999	3.110414
C	0.000000	-1.436258	3.110111
C	-1.243674	-0.717999	3.110414
C	-1.243674	0.717999	3.110415
H	0.000000	2.525551	3.054541
H	2.187075	1.262711	3.055160
H	2.187075	-1.262710	3.055160
H	0.000000	-2.525551	3.054540

H	-2.187075	-1.262710	3.055160
H	-2.187075	1.262711	3.055160
Mn	0.000000	0.000000	1.510952
Mn	0.000000	0.000000	-1.510952
C	0.000000	1.436258	-3.110111
C	1.243674	0.717999	-3.110414
C	1.243674	-0.717999	-3.110415
C	0.000000	-1.436258	-3.110111
C	-1.243674	-0.717999	-3.110415
C	-1.243674	0.717999	-3.110414
H	0.000000	2.525551	-3.054540
H	2.187075	1.262710	-3.055160
H	2.187075	-1.262711	-3.055160
H	0.000000	-2.525551	-3.054541
H	-2.187075	-1.262711	-3.055160
H	-2.187075	1.262710	-3.055160

Structure **3a**:

Mn	4.883802	-0.947609	-0.033767
C	4.313355	1.175109	-0.634070
C	3.629080	0.208381	-1.417145
C	2.669814	-0.718857	-0.791660
C	2.656154	-0.803184	0.702144
C	3.601410	0.047133	1.446217
C	4.299543	1.094961	0.790270
H	4.953150	1.910098	-1.125014
H	3.679715	0.257443	-2.505493
H	2.412560	-1.618935	-1.360733
H	2.388059	-1.760755	1.161763
H	3.630939	-0.026557	2.533952
H	4.928857	1.769556	1.372884
Mn	0.941094	0.137635	-0.011827
C	-0.200649	1.883038	-0.666481
C	-0.560697	0.736378	-1.423645
C	-1.094648	-0.464956	-0.771307
C	-1.088473	-0.514249	0.724497

C	-0.548564	0.641581	1.450256
C	-0.194711	1.835695	0.767542
H	0.161390	2.776102	-1.177689
H	-0.522647	0.771188	-2.513157
H	-1.047020	-1.407114	-1.326045
H	-1.035173	-1.490981	1.215203
H	-0.501157	0.604254	2.539290
H	0.171611	2.693330	1.333461
Mn	-3.048809	-0.268177	-0.006884
C	-4.563874	1.043209	-0.721943
C	-4.626950	-0.203584	-1.430798
C	-4.674124	-1.444015	-0.708701
C	-4.664673	-1.435707	0.727781
C	-4.609045	-0.187474	1.435933
C	-4.554737	1.051284	0.712855
H	-4.464882	1.978937	-1.273525
H	-4.569427	-0.211656	-2.520113
H	-4.674499	-2.391678	-1.249545
H	-4.656007	-2.377223	1.279176
H	-4.537230	-0.183877	2.524388
H	-4.449677	1.993192	1.252698

Structure **3b**:

Mn	0.380113	0.930641	-0.071572
C	-1.914150	1.868143	-0.542707
C	-1.742711	1.781154	0.886082
C	-0.424608	2.108857	1.452210
C	0.519695	2.876164	0.676008
C	0.361871	2.928536	-0.740827
C	-0.749594	2.250125	-1.349214
H	-2.916499	1.950559	-0.974109
H	-2.617248	1.778327	1.543753
H	-0.280551	2.005627	2.528265
H	1.429646	3.261789	1.138258
H	1.157811	3.341911	-1.363147
H	-0.833132	2.225025	-2.436228

Mn	-1.770003	-0.196163	0.022113
C	-1.683312	-2.115933	0.949899
C	-2.873340	-1.450893	1.370497
C	-3.789626	-0.924762	0.396346
C	-3.493907	-1.053034	-0.995329
C	-2.289092	-1.683112	-1.425593
C	-1.367415	-2.195754	-0.447296
H	-0.960736	-2.462800	1.688348
H	-3.070341	-1.307727	2.434567
H	-4.683424	-0.387279	0.718807
H	-4.158873	-0.595753	-1.731892
H	-2.033218	-1.716116	-2.484948
H	-0.425027	-2.634880	-0.766301
Mn	1.759828	-0.234541	0.004608
C	3.750970	0.131918	-0.377081
C	3.577233	-0.211353	1.010542
C	2.852760	-1.401168	1.371410
C	2.313585	-2.252864	0.349563
C	2.478610	-1.909063	-1.034314
C	3.194114	-0.715344	-1.401092
H	4.249696	1.062667	-0.649925
H	3.930828	0.466926	1.787938
H	2.655531	-1.619928	2.421195
H	1.712517	-3.118784	0.627625
H	2.002398	-2.514300	-1.806221
H	3.265698	-0.423384	-2.449336

Structure **3c**:

Mn	4.809851	-0.690555	0.040897
C	3.726176	1.318781	0.275418
C	3.422153	0.947218	-1.092010
C	3.044606	-0.423015	-1.368162
C	2.631223	-1.282814	-0.285964
C	2.656503	-0.796657	1.075635
C	3.384943	0.426009	1.359624
H	4.145353	2.299301	0.496582

H	3.748159	1.591188	-1.908542
H	2.902616	-0.751244	-2.396536
H	2.192699	-2.254268	-0.507320
H	2.381872	-1.462333	1.892551
H	3.496877	0.763101	2.389070
Mn	1.534999	0.719504	-0.014975
C	-1.242469	0.877056	1.129539
C	-0.362874	1.464965	0.071394
C	-0.259904	0.654750	-1.115213
C	-1.026914	-0.617381	-1.072188
C	-1.175541	-1.346636	0.162624
C	-1.275325	-0.550138	1.339958
H	-1.451187	1.510149	1.999921
H	-0.365941	2.559319	-0.025542
H	-0.145056	1.130836	-2.095546
H	-1.082127	-1.193759	-2.002630
H	-1.244953	-2.439322	0.199820
H	-1.426513	-1.000448	2.327209
Mn	-2.824968	-0.136170	0.062124
C	-4.360735	1.230817	0.482648
C	-4.176058	1.133336	-0.930489
C	-4.186214	-0.162751	-1.535322
C	-4.368986	-1.335793	-0.752005
C	-4.478570	-1.226915	0.668529
C	-4.539163	0.064833	1.278679
H	-4.274161	2.205330	0.971948
H	-3.992181	2.026555	-1.531102
H	-3.961373	-0.261171	-2.601264
H	-4.282699	-2.320612	-1.221182
H	-4.534717	-2.129401	1.286609
H	-4.580806	0.153312	2.368626

Structure **4**:

Mn	6.652536	-1.506238	-0.001801
C	6.383537	0.649610	-0.710216
C	5.553000	-0.246984	-1.432778

C	4.475883	-0.984438	-0.748701
C	4.475234	-0.987035	0.746101
C	5.552534	-0.252968	1.433627
C	6.383425	0.646555	0.715093
H	7.114993	1.255929	-1.246594
H	5.591710	-0.263837	-2.522474
H	4.074742	-1.862561	-1.266450
H	4.073609	-1.867114	1.260160
H	5.590818	-0.274349	2.523258
H	7.114823	1.250528	1.254186
Mn	2.920690	0.171465	0.000058
C	2.108748	2.073330	-0.713671
C	1.550241	0.987324	-1.438390
C	0.813644	-0.079801	-0.748765
C	0.813075	-0.082368	0.747186
C	1.549776	0.981999	1.440973
C	2.108573	2.070660	0.720488
H	2.623799	2.871021	-1.250180
H	1.589718	0.980675	-2.527964
H	0.681085	-1.029865	-1.275638
H	0.680253	-1.034339	1.270554
H	1.588902	0.971303	2.530527
H	2.623441	2.866375	1.260096
Mn	-1.061684	0.515638	-0.000588
C	-2.467254	2.016666	-0.719613
C	-2.626108	0.801050	-1.438157
C	-2.953532	-0.450218	-0.747212
C	-2.953786	-0.448532	0.748627
C	-2.625712	0.804180	1.436753
C	-2.466942	2.018208	0.715497
H	-2.256366	2.940110	-1.260235
H	-2.583840	0.805262	-2.527940
H	-2.753603	-1.389556	-1.271230
H	-2.753644	-1.386739	1.274612
H	-2.583636	0.810889	2.526531
H	-2.256102	2.942882	1.254032

Mn	-4.925792	-0.547612	0.000770
C	-6.643725	0.490096	-0.703794
C	-6.483245	-0.735684	-1.433041
C	-6.317090	-1.977520	-0.731682
C	-6.315809	-1.993350	0.704151
C	-6.480520	-0.767087	1.432702
C	-6.642346	0.474390	0.730601
H	-6.711203	1.437761	-1.239306
H	-6.421606	-0.714959	-2.521804
H	-6.148649	-2.900681	-1.288150
H	-6.147050	-2.928602	1.239951
H	-6.417055	-0.770102	2.521562
H	-6.708507	1.410136	1.286823

Structure **5**:

Mn	8.289738	-2.184674	0.070683
C	8.288417	-0.071631	-0.807357
C	7.327309	-0.903487	-1.440115
C	6.178472	-1.428693	-0.680524
C	6.218598	-1.314078	0.808445
C	7.403549	-0.682076	1.415930
C	8.326178	0.038531	0.612415
H	9.079260	0.385989	-1.403483
H	7.334266	-1.012475	-2.525077
H	5.647174	-2.280828	-1.118314
H	5.715439	-2.087131	1.399453
H	7.468740	-0.622806	2.502806
H	9.145471	0.579455	1.088220
Mn	4.821975	-0.011390	-0.003217
C	4.279376	1.935406	-0.852221
C	3.551415	0.894391	-1.485388
C	2.679692	0.003776	-0.707313
C	2.713801	0.110378	0.784043
C	3.613716	1.103719	1.385879
C	4.309678	2.039977	0.577042
H	4.894237	2.605874	-1.453605

H	3.564464	0.801126	-2.571528
H	2.396074	-0.952214	-1.158593
H	2.455444	-0.770425	1.380226
H	3.674545	1.169145	2.472431
H	4.947032	2.789235	1.047865
Mn	0.942535	0.935587	0.018210
C	-0.161807	2.655145	-0.743727
C	-0.537498	1.473870	-1.437178
C	-1.091482	0.321068	-0.717388
C	-1.091105	0.356660	0.777655
C	-0.540920	1.544584	1.440747
C	-0.163933	2.690537	0.690351
H	0.215839	3.511729	-1.302947
H	-0.495620	1.444143	-2.526169
H	-1.077402	-0.650501	-1.220454
H	-1.078535	-0.589041	1.327823
H	-0.501647	1.569054	2.530018
H	0.212626	3.573439	1.207786
Mn	-3.041134	0.638592	0.022336
C	-4.658576	1.899396	-0.699876
C	-4.620192	0.676366	-1.423089
C	-4.747184	-0.613173	-0.737928
C	-4.754688	-0.617915	0.757094
C	-4.635928	0.667278	1.451392
C	-4.666433	1.894811	0.735262
H	-4.595646	2.846644	-1.236560
H	-4.573426	0.691344	-2.512500
H	-4.404563	-1.508272	-1.264999
H	-4.418728	-1.516565	1.282421
H	-4.600844	0.675782	2.541347
H	-4.608788	2.838557	1.278676
Mn	-6.688473	-1.010998	-0.003056
C	-8.540075	-0.237051	-0.705658
C	-8.192969	-1.415958	-1.447065
C	-7.844830	-2.626563	-0.758229
C	-7.847040	-2.658667	0.677018

C	-8.196981	-1.479700	1.417713
C	-8.542004	-0.268979	0.728209
H	-8.748113	0.695543	-1.231278
H	-8.131942	-1.374076	-2.535185
H	-7.537456	-3.507316	-1.323802
H	-7.542341	-3.564121	1.203713
H	-8.139583	-1.486155	2.506831
H	-8.751307	0.639423	1.294145

Structure of the $Mn_{18}Bz_{18}^{-}$ ring (anion):

Mn	10.242738	5.170891	0.003176
C	12.261989	4.757944	0.722205
C	11.307621	3.992486	1.443377
C	10.412707	3.057048	0.750408
C	10.414624	3.056745	-0.743500
C	11.310828	3.992441	-1.434506
C	12.263542	4.757996	-0.711252
H	12.940649	5.419746	1.261194
H	11.289085	4.029680	2.532812
H	9.511644	2.726709	1.276181
H	9.514749	2.726405	-1.271303
H	11.294719	4.029588	-2.523981
H	12.943392	5.419825	-1.248717
Mn	11.394572	1.354955	0.004981
C	13.150691	0.276982	0.725071
C	11.991679	-0.116729	1.445161
C	10.831788	-0.690238	0.751010
C	10.834568	-0.690273	-0.742908
C	11.997073	-0.116904	-1.432787
C	13.153379	0.276907	-0.708379
H	14.014098	0.667167	1.264844
H	11.986035	-0.075710	2.534607
H	9.871642	-0.692952	1.275978
H	9.876403	-0.693109	-1.271472
H	11.995509	-0.076014	-2.522251

H	14.018783	0.667013	-1.244989
Mn	7.856403	8.363522	-0.000614
C	9.895747	8.666488	0.716176
C	9.261060	7.621910	1.439303
C	8.739226	6.436004	0.748380
C	8.739706	6.434462	-0.745594
C	9.261501	7.619205	-1.438610
C	9.895900	8.665181	-0.717261
H	10.307674	9.521176	1.253660
H	9.231708	7.652104	2.528714
H	8.005833	5.818298	1.275666
H	8.006469	5.815759	-1.271939
H	9.232518	7.647291	-2.528087
H	10.307987	9.518877	-1.256205
Mn	4.522543	10.548523	-0.003064
C	6.336121	11.530776	0.711512
C	6.097341	10.332705	1.435737
C	6.011563	9.039387	0.745800
C	6.011224	9.036989	-0.748103
C	6.096300	10.328148	-1.442203
C	6.335579	11.528520	-0.721956
H	6.431674	12.475179	1.248201
H	6.060511	10.351801	2.525176
H	5.533761	8.208645	1.274039
H	5.533040	8.204586	-1.273380
H	6.058655	10.343796	-2.531669
H	6.430725	12.471230	-1.261690
Mn	0.642329	11.461428	-0.005045
C	2.010843	13.005477	0.707635
C	2.196540	11.798639	1.432819
C	2.558109	10.553366	0.743851
C	2.558108	10.549722	-0.750056
C	2.195923	11.791489	-1.445053
C	2.010490	13.001912	-0.725819
H	1.777859	13.926066	1.243641
H	2.155882	11.804974	2.522269

H	2.393564	9.609750	1.272983
H	2.393383	9.603489	-1.274453
H	2.154784	11.792369	-2.534504
H	1.777218	13.919833	-1.266281
Mn	-3.315911	10.991475	-0.004429
C	-2.558108	12.910146	0.708991
C	-1.970174	11.839250	1.433115
C	-1.204535	10.793509	0.742950
C	-1.204453	10.790951	-0.751030
C	-1.970132	11.834262	-1.444819
C	-2.558082	12.907668	-0.724443
H	-3.091868	13.694987	1.245835
H	-2.009985	11.830463	2.522576
H	-1.035925	9.850195	1.271353
H	-1.035780	9.845835	-1.276177
H	-2.009932	11.821701	-2.534245
H	-3.091844	13.690639	-1.264004
Mn	-6.874033	9.194520	-0.001861
C	-6.818406	11.255858	0.713606
C	-5.898490	10.450407	1.436032
C	-4.821638	9.730862	0.744113
C	-4.822300	9.729703	-0.749823
C	-5.899436	10.448642	-1.441922
C	-6.818830	11.255007	-0.719860
H	-7.588154	11.809897	1.251735
H	-5.931824	10.427466	2.525512
H	-4.339795	8.901724	1.271222
H	-4.340759	8.899936	-1.276203
H	-5.933475	10.424375	-2.531352
H	-7.588909	11.808406	-1.258178
Mn	-9.602572	6.288691	0.002660
C	-10.254265	8.244518	0.720215
C	-9.113398	7.801726	1.440745
C	-7.856403	7.494077	0.746855
C	-7.858644	7.493983	-0.747072
C	-9.117780	7.801459	-1.437161

C	-10.256448	8.244395	-0.713231
H	-11.166282	8.501713	1.259797
H	-9.135258	7.768230	2.530243
H	-7.119125	6.879658	1.272580
H	-7.123033	6.879401	-1.274938
H	-9.142990	7.767745	-2.526579
H	-11.170111	8.501493	-1.250080
Mn	-11.172951	2.625111	0.004773
C	-12.454182	4.239346	0.723814
C	-11.230478	4.213066	1.444022
C	-9.944273	4.354468	0.749916
C	-9.946780	4.354642	-0.744060
C	-11.235270	4.213455	-1.433909
C	-12.456580	4.239539	-0.709624
H	-13.398998	4.168458	1.263593
H	-11.239286	4.173132	2.533480
H	-9.041211	4.028830	1.275187
H	-9.045477	4.029158	-1.272442
H	-11.247724	4.173801	-2.523342
H	-13.403183	4.168785	-1.246287
Mn	-11.394572	-1.354955	0.004981
C	-13.150691	-0.276982	0.725071
C	-11.991679	0.116729	1.445161
C	-10.831788	0.690238	0.751010
C	-10.834568	0.690273	-0.742908
C	-11.997073	0.116904	-1.432787
C	-13.153379	-0.276907	-0.708379
H	-14.014098	-0.667167	1.264844
H	-11.986035	0.075710	2.534607
H	-9.871642	0.692952	1.275978
H	-9.876403	0.693109	-1.271472
H	-11.995509	0.076014	-2.522251
H	-14.018783	-0.667013	-1.244989
Mn	-10.242738	-5.170891	0.003176
C	-12.261989	-4.757944	0.722205
C	-11.307621	-3.992486	1.443377

C	-10.412707	-3.057048	0.750408
C	-10.414624	-3.056745	-0.743500
C	-11.310828	-3.992441	-1.434506
C	-12.263542	-4.757996	-0.711252
H	-12.940649	-5.419746	1.261194
H	-11.289085	-4.029680	2.532812
H	-9.511644	-2.726709	1.276181
H	-9.514749	-2.726405	-1.271303
H	-11.294719	-4.029588	-2.523981
H	-12.943392	-5.419825	-1.248717
Mn	-7.856403	-8.363522	-0.000614
C	-9.895747	-8.666488	0.716176
C	-9.261060	-7.621910	1.439303
C	-8.739226	-6.436004	0.748380
C	-8.739706	-6.434462	-0.745594
C	-9.261501	-7.619205	-1.438610
C	-9.895900	-8.665181	-0.717261
H	-10.307674	-9.521176	1.253660
H	-9.231708	-7.652104	2.528714
H	-8.005833	-5.818298	1.275666
H	-8.006469	-5.815759	-1.271939
H	-9.232518	-7.647291	-2.528087
H	-10.307987	-9.518877	-1.256205
Mn	-4.522543	-10.548523	-0.003064
C	-6.336121	-11.530776	0.711512
C	-6.097341	-10.332705	1.435737
C	-6.011563	-9.039387	0.745800
C	-6.011224	-9.036989	-0.748103
C	-6.096300	-10.328148	-1.442203
C	-6.335579	-11.528520	-0.721956
H	-6.431674	-12.475179	1.248201
H	-6.060511	-10.351801	2.525176
H	-5.533761	-8.208645	1.274039
H	-5.533040	-8.204586	-1.273380
H	-6.058655	-10.343796	-2.531669
H	-6.430725	-12.471230	-1.261690

Mn	-0.642329	-11.461428	-0.005045
C	-2.010843	-13.005477	0.707635
C	-2.196540	-11.798639	1.432819
C	-2.558109	-10.553366	0.743851
C	-2.558108	-10.549722	-0.750056
C	-2.195923	-11.791489	-1.445053
C	-2.010490	-13.001912	-0.725819
H	-1.777859	-13.926066	1.243641
H	-2.155882	-11.804974	2.522269
H	-2.393564	-9.609750	1.272983
H	-2.393383	-9.603489	-1.274453
H	-2.154784	-11.792369	-2.534504
H	-1.777218	-13.919833	-1.266281
Mn	3.315911	-10.991475	-0.004429
C	2.558108	-12.910146	0.708991
C	1.970174	-11.839250	1.433115
C	1.204535	-10.793509	0.742950
C	1.204453	-10.790951	-0.751030
C	1.970132	-11.834262	-1.444819
C	2.558082	-12.907668	-0.724443
H	3.091868	-13.694987	1.245835
H	2.009985	-11.830463	2.522576
H	1.035925	-9.850195	1.271353
H	1.035780	-9.845835	-1.276177
H	2.009932	-11.821701	-2.534245
H	3.091844	-13.690639	-1.264004
Mn	6.874033	-9.194520	-0.001861
C	6.818406	-11.255858	0.713606
C	5.898490	-10.450407	1.436032
C	4.821638	-9.730862	0.744113
C	4.822300	-9.729703	-0.749823
C	5.899436	-10.448642	-1.441922
C	6.818830	-11.255007	-0.719860
H	7.588154	-11.809897	1.251735
H	5.931824	-10.427466	2.525512
H	4.339795	-8.901724	1.271222

H	4.340759	-8.899936	-1.276203
H	5.933475	-10.424375	-2.531352
H	7.588909	-11.808406	-1.258178
Mn	9.602572	-6.288691	0.002660
C	10.254265	-8.244518	0.720215
C	9.113398	-7.801726	1.440745
C	7.856403	-7.494077	0.746855
C	7.858644	-7.493983	-0.747072
C	9.117780	-7.801459	-1.437161
C	10.256448	-8.244395	-0.713231
H	11.166282	-8.501713	1.259797
H	9.135258	-7.768230	2.530243
H	7.119125	-6.879658	1.272580
H	7.123033	-6.879401	-1.274938
H	9.142990	-7.767745	-2.526579
H	11.170111	-8.501493	-1.250080
Mn	11.172951	-2.625111	0.004773
C	12.454182	-4.239346	0.723814
C	11.230478	-4.213066	1.444022
C	9.944273	-4.354468	0.749916
C	9.946780	-4.354642	-0.744060
C	11.235270	-4.213455	-1.433909
C	12.456580	-4.239539	-0.709624
H	13.398998	-4.168458	1.263593
H	11.239286	-4.173132	2.533480
H	9.041211	-4.028830	1.275187
H	9.045477	-4.029158	-1.272442
H	11.247724	-4.173801	-2.523342
H	13.403183	-4.168785	-1.246287

Structure of the $Mn_{18}Bz_{18}$ ring (neutral):

Mn	-0.178122	11.481056	0.000000
C	1.074863	13.122321	0.716652
C	1.349647	11.931854	1.439492
C	1.800105	10.717653	0.747589

C	1.800105	10.717653	-0.747589
C	1.349647	11.931854	-1.439492
C	1.074863	13.122321	-0.716652
H	0.777782	14.022646	1.254740
H	1.307672	11.932513	2.528641
H	1.704959	9.763611	1.275126
H	1.704959	9.763611	-1.275126
H	1.307672	11.932513	-2.528641
H	0.777782	14.022646	-1.254740
Mn	3.759372	10.849585	0.000000
C	5.498138	11.963323	0.716652
C	5.349188	10.750668	1.439492
C	5.357199	9.455627	0.747589
C	5.357199	9.455627	-0.747589
C	5.349188	10.750668	-1.439492
C	5.498138	11.963323	-0.716652
H	5.526903	12.910960	1.254740
H	5.309969	10.765644	2.528641
H	4.941489	8.591663	1.275126
H	4.941489	8.591663	-1.275126
H	5.309969	10.765644	-2.528641
H	5.526903	12.910960	-1.254740
Mn	-4.094133	10.727742	0.000000
C	-3.478057	12.698572	0.716652
C	-2.812681	11.673881	1.439492
C	-1.974107	10.686971	0.747589
C	-1.974107	10.686971	-0.747589
C	-2.812681	11.673881	-1.439492
C	-3.478057	12.698572	-0.716652
H	-4.065151	13.442994	1.254740
H	-2.852350	11.660144	2.528641
H	-1.737214	9.757923	1.275126
H	-1.737214	9.757923	-1.275126
H	-2.852350	11.660144	-2.528641
H	-4.065151	13.442994	-1.254740
Mn	-7.516330	8.680505	0.000000

C	-7.611472	10.743189	0.716652
C	-6.635758	10.007867	1.439492
C	-5.510213	9.367284	0.747589
C	-5.510213	9.367284	-0.747589
C	-6.635758	10.007867	-1.439492
C	-7.611472	10.743189	-0.716652
H	-8.417768	11.241918	1.254740
H	-6.668337	9.981390	2.528641
H	-4.969854	8.575286	1.275126
H	-4.969854	8.575286	-1.275126
H	-6.668337	9.981390	-2.528641
H	-8.417768	11.241918	-1.254740
Mn	-10.031947	5.586270	0.000000
C	-10.826832	7.492019	0.716652
C	-9.658465	7.134756	1.439492
C	-8.381707	6.917763	0.747589
C	-8.381707	6.917763	-0.747589
C	-9.658465	7.134756	-1.439492
C	-10.826832	7.492019	-0.716652
H	-11.755077	7.684902	1.254740
H	-9.680023	7.098733	2.528641
H	-7.603055	6.358343	1.275126
H	-7.603055	6.358343	-1.275126
H	-9.680023	7.098733	-2.528641
H	-11.755077	7.684902	-1.254740
Mn	-11.337564	1.818248	0.000000
C	-12.736315	3.337200	0.716652
C	-11.516218	3.401088	1.439492
C	-10.242242	3.633859	0.747589
C	-10.242242	3.633859	-0.747589
C	-11.516218	3.401088	-1.439492
C	-12.736315	3.337200	-0.716652
H	-13.674550	3.200972	1.254740
H	-11.524156	3.359864	2.528641
H	-9.319216	3.374490	1.275126
H	-9.319216	3.374490	-1.275126

H	-11.524156	3.359864	-2.528641
H	-13.674550	3.200972	-1.254740
Mn	-11.275703	-2.169081	0.000000
C	-13.109611	-1.220134	0.716652
C	-11.984946	-0.742802	1.439492
C	-10.867412	-0.088343	0.747589
C	-10.867412	-0.088343	-0.747589
C	-11.984946	-0.742802	-1.439492
C	-13.109611	-1.220134	-0.716652
H	-13.944671	-1.669041	1.254740
H	-11.978306	-0.784254	2.528641
H	-9.911342	-0.016377	1.275126
H	-9.911342	-0.016377	-1.275126
H	-11.978306	-0.784254	-2.528641
H	-13.944671	-1.669041	-1.254740
Mn	-9.853825	-5.894786	0.000000
C	-11.901694	-5.630302	0.716652
C	-11.008112	-4.797098	1.439492
C	-10.181812	-3.799889	0.747589
C	-10.181812	-3.799889	-0.747589
C	-11.008112	-4.797098	-1.439492
C	-11.901694	-5.630302	-0.716652
H	-12.532858	-6.337744	1.254740
H	-10.987695	-4.833780	2.528641
H	-9.308014	-3.405268	1.275126
H	-9.308014	-3.405268	-1.275126
H	-10.987695	-4.833780	-2.528641
H	-12.532858	-6.337744	-1.254740
Mn	-7.243431	-8.909494	0.000000
C	-9.258258	-9.361372	0.716652
C	-8.703537	-8.272794	1.439492
C	-8.268135	-7.053113	0.747589
C	-8.268135	-7.053113	-0.747589
C	-8.703537	-8.272794	-1.439492
C	-9.258258	-9.361372	-0.716652
H	-9.609398	-10.242021	1.254740

H	-8.671806	-8.300280	2.528641
H	-7.582002	-6.383433	1.275126
H	-7.582002	-6.383433	-1.275126
H	-8.671806	-8.300280	-2.528641
H	-9.609398	-10.242021	-1.254740
Mn	-3.759372	-10.849585	0.000000
C	-5.498138	-11.963323	0.716652
C	-5.349188	-10.750668	1.439492
C	-5.357199	-9.455627	0.747589
C	-5.357199	-9.455627	-0.747589
C	-5.349188	-10.750668	-1.439492
C	-5.498138	-11.963323	-0.716652
H	-5.526903	-12.910960	1.254740
H	-5.309969	-10.765644	2.528641
H	-4.941489	-8.591663	1.275126
H	-4.941489	-8.591663	-1.275126
H	-5.309969	-10.765644	-2.528641
H	-5.526903	-12.910960	-1.254740
Mn	0.178122	-11.481056	0.000000
C	-1.074863	-13.122321	0.716652
C	-1.349647	-11.931854	1.439492
C	-1.800105	-10.717653	0.747589
C	-1.800105	-10.717653	-0.747589
C	-1.349647	-11.931854	-1.439492
C	-1.074863	-13.122321	-0.716652
H	-0.777782	-14.022646	1.254740
H	-1.307672	-11.932513	2.528641
H	-1.704959	-9.763611	1.275126
H	-1.704959	-9.763611	-1.275126
H	-1.307672	-11.932513	-2.528641
H	-0.777782	-14.022646	-1.254740
Mn	4.094133	-10.727742	0.000000
C	3.478057	-12.698572	0.716652
C	2.812681	-11.673881	1.439492
C	1.974107	-10.686971	0.747589
C	1.974107	-10.686971	-0.747589

C	2.812681	-11.673881	-1.439492
C	3.478057	-12.698572	-0.716652
H	4.065151	-13.442994	1.254740
H	2.852350	-11.660144	2.528641
H	1.737214	-9.757923	1.275126
H	1.737214	-9.757923	-1.275126
H	2.852350	-11.660144	-2.528641
H	4.065151	-13.442994	-1.254740
Mn	7.516330	-8.680505	0.000000
C	7.611472	-10.743189	0.716652
C	6.635758	-10.007867	1.439492
C	5.510213	-9.367284	0.747589
C	5.510213	-9.367284	-0.747589
C	6.635758	-10.007867	-1.439492
C	7.611472	-10.743189	-0.716652
H	8.417768	-11.241918	1.254740
H	6.668337	-9.981390	2.528641
H	4.969854	-8.575286	1.275126
H	4.969854	-8.575286	-1.275126
H	6.668337	-9.981390	-2.528641
H	8.417768	-11.241918	-1.254740
Mn	10.031947	-5.586270	0.000000
C	10.826832	-7.492019	0.716652
C	9.658465	-7.134756	1.439492
C	8.381707	-6.917763	0.747589
C	8.381707	-6.917763	-0.747589
C	9.658465	-7.134756	-1.439492
C	10.826832	-7.492019	-0.716652
H	11.755077	-7.684902	1.254740
H	9.680023	-7.098733	2.528641
H	7.603055	-6.358343	1.275126
H	7.603055	-6.358343	-1.275126
H	9.680023	-7.098733	-2.528641
H	11.755077	-7.684902	-1.254740
Mn	11.337564	-1.818248	0.000000
C	12.736315	-3.337200	0.716652

C	11.516218	-3.401088	1.439492
C	10.242242	-3.633859	0.747589
C	10.242242	-3.633859	-0.747589
C	11.516218	-3.401088	-1.439492
C	12.736315	-3.337200	-0.716652
H	13.674550	-3.200972	1.254740
H	11.524156	-3.359864	2.528641
H	9.319216	-3.374490	1.275126
H	9.319216	-3.374490	-1.275126
H	11.524156	-3.359864	-2.528641
H	13.674550	-3.200972	-1.254740
Mn	11.275703	2.169081	0.000000
C	13.109611	1.220134	0.716652
C	11.984946	0.742802	1.439492
C	10.867412	0.088343	0.747589
C	10.867412	0.088343	-0.747589
C	11.984946	0.742802	-1.439492
C	13.109611	1.220134	-0.716652
H	13.944671	1.669041	1.254740
H	11.978306	0.784254	2.528641
H	9.911342	0.016377	1.275126
H	9.911342	0.016377	-1.275126
H	11.978306	0.784254	-2.528641
H	13.944671	1.669041	-1.254740
Mn	9.853825	5.894786	0.000000
C	11.901694	5.630302	0.716652
C	11.008112	4.797098	1.439492
C	10.181812	3.799889	0.747589
C	10.181812	3.799889	-0.747589
C	11.008112	4.797098	-1.439492
C	11.901694	5.630302	-0.716652
H	12.532858	6.337744	1.254740
H	10.987695	4.833780	2.528641
H	9.308014	3.405268	1.275126
H	9.308014	3.405268	-1.275126
H	10.987695	4.833780	-2.528641

H	12.532858	6.337744	-1.254740
Mn	7.243431	8.909494	0.000000
C	9.258258	9.361372	0.716652
C	8.703537	8.272794	1.439492
C	8.268135	7.053113	0.747589
C	8.268135	7.053113	-0.747589
C	8.703537	8.272794	-1.439492
C	9.258258	9.361372	-0.716652
H	9.609398	10.242021	1.254740
H	8.671806	8.300280	2.528641
H	7.582002	6.383433	1.275126
H	7.582002	6.383433	-1.275126
H	8.671806	8.300280	-2.528641
H	9.609398	10.242021	-1.254740

Structure of [18]annulene (E = –696.880864774 Hartree):

C	-1.258241	3.593035	0.001218
C	0.000000	2.987813	-0.009810
C	1.258241	3.593035	0.001218
C	2.482540	2.886186	-0.001218
C	2.587522	1.493907	0.009810
C	3.740780	0.706849	-0.001218
C	3.740780	-0.706849	0.001218
C	2.587522	-1.493907	-0.009810
C	2.482540	-2.886186	0.001218
C	1.258241	-3.593035	-0.001218
C	0.000000	-2.987813	0.009810
C	-1.258241	-3.593035	-0.001218
C	-2.482540	-2.886186	0.001218
C	-2.587522	-1.493907	-0.009810
C	-3.740780	-0.706849	0.001218
C	-3.740780	0.706849	-0.001218
C	-2.587522	1.493907	0.009810
C	-2.482540	2.886186	-0.001218
H	-1.306275	4.686928	0.010547

H	0.000000	1.896023	-0.034859
H	1.306275	4.686928	0.010547
H	3.405861	3.474732	-0.010547
H	1.642004	0.948011	0.034859
H	4.712137	1.212197	-0.010547
H	4.712137	-1.212197	0.010547
H	1.642004	-0.948011	-0.034859
H	3.405861	-3.474732	0.010547
H	1.306275	-4.686928	-0.010547
H	0.000000	-1.896023	0.034859
H	-1.306275	-4.686928	-0.010547
H	-3.405861	-3.474732	0.010547
H	-1.642004	-0.948011	-0.034859
H	-4.712137	-1.212197	0.010547
H	-4.712137	1.212197	-0.010547
H	-1.642004	0.948011	0.034859
H	-3.405861	3.474732	-0.010547