Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Excited-state singlet-triplet inversion in hexagonal aromatic and heteroaromatic compounds

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Electronic supplementary information

Section S1. Comparison of cc-pVDZ and cc-pVTZ excitation energies for borazine

Table S1. Vertical excitation energies ΔE (in eV) of the singlet and triplet valence excited states of borazine computed with the ADC(2), CC2 and EOM-CCSD methods and the cc-pVDZ and cc-pVTZ basis sets. Δ_{ST} is the energy gap between the lowest singlet and triplet states.

cc-pVDZ				cc-pVTZ			
State	ADC(2)	CC2	EOM-CCSD	State	ADC(2)	CC2	EOM-CCSD
$^1A_2'$	6.703	6.771	6.833	$^1A_2'$	6.755	6.792	6.886
$^3A_1'$	6.831	6.774	6.720	$^3A_1'$	6.952	6.882	6.867
$^3E'$	6.904	6.948	6.884	$^3E'$	6.950	6.967	6.932
$^3A_2'$	7.025	7.147	7.090	$^3A_2'$	7.012	7.095	7.055
$^1A_1'$	7.819	7.886	7.996	$^1A_1'$	7.811	7.837	8.005
$^1E'$	7.923	8.064	8.220	$^1E'$	7.893	7.986	8.172
Δ_{ST}	-0.127	-0.003	0.113	Δ_{ST}	-0.195	-0.090	0.019

Section S2. Electron densities of HOMO and LUMO

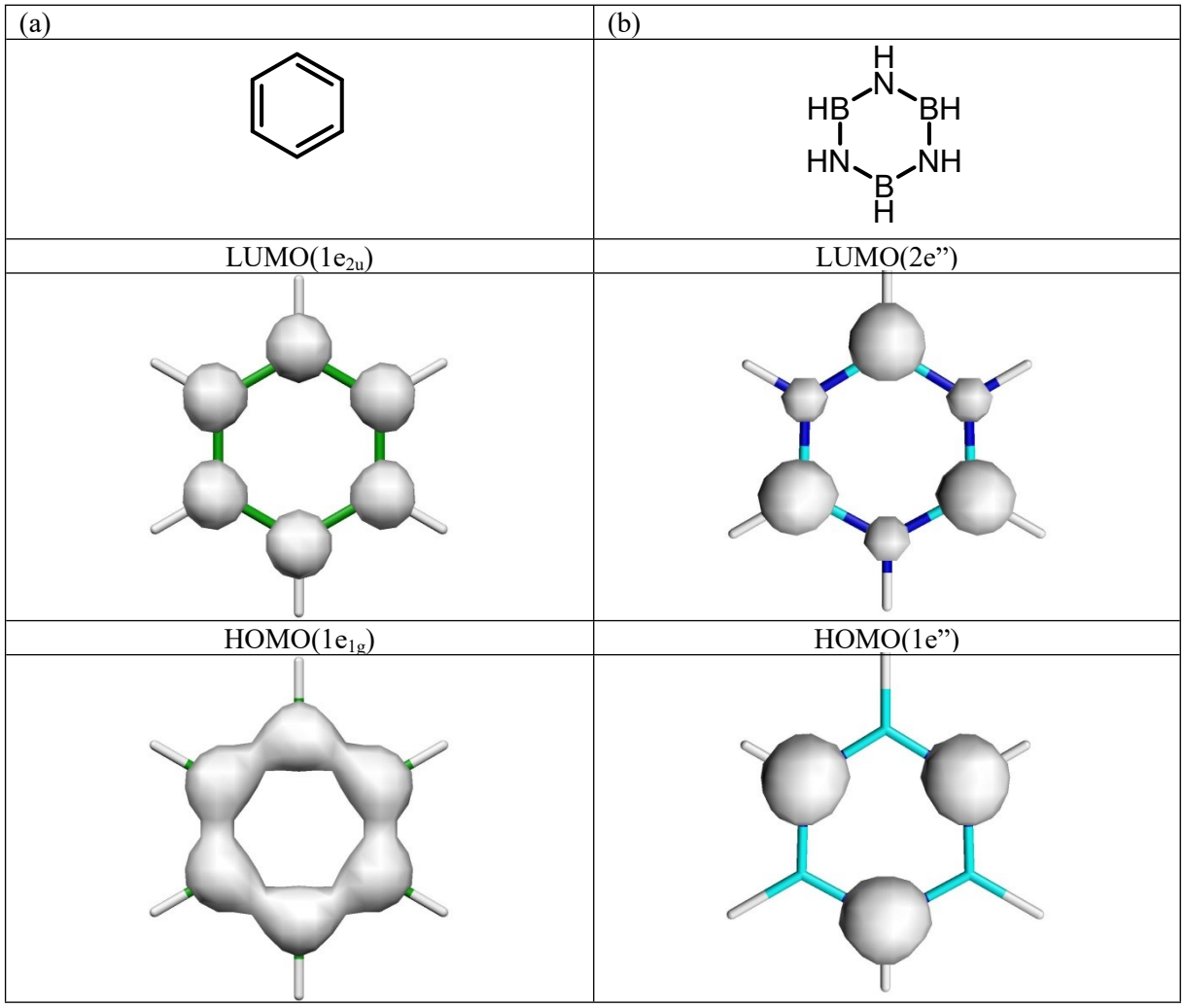

Fig. S1: Electron densities of HOMO and LUMO of (a) benzene and (b) borazine.

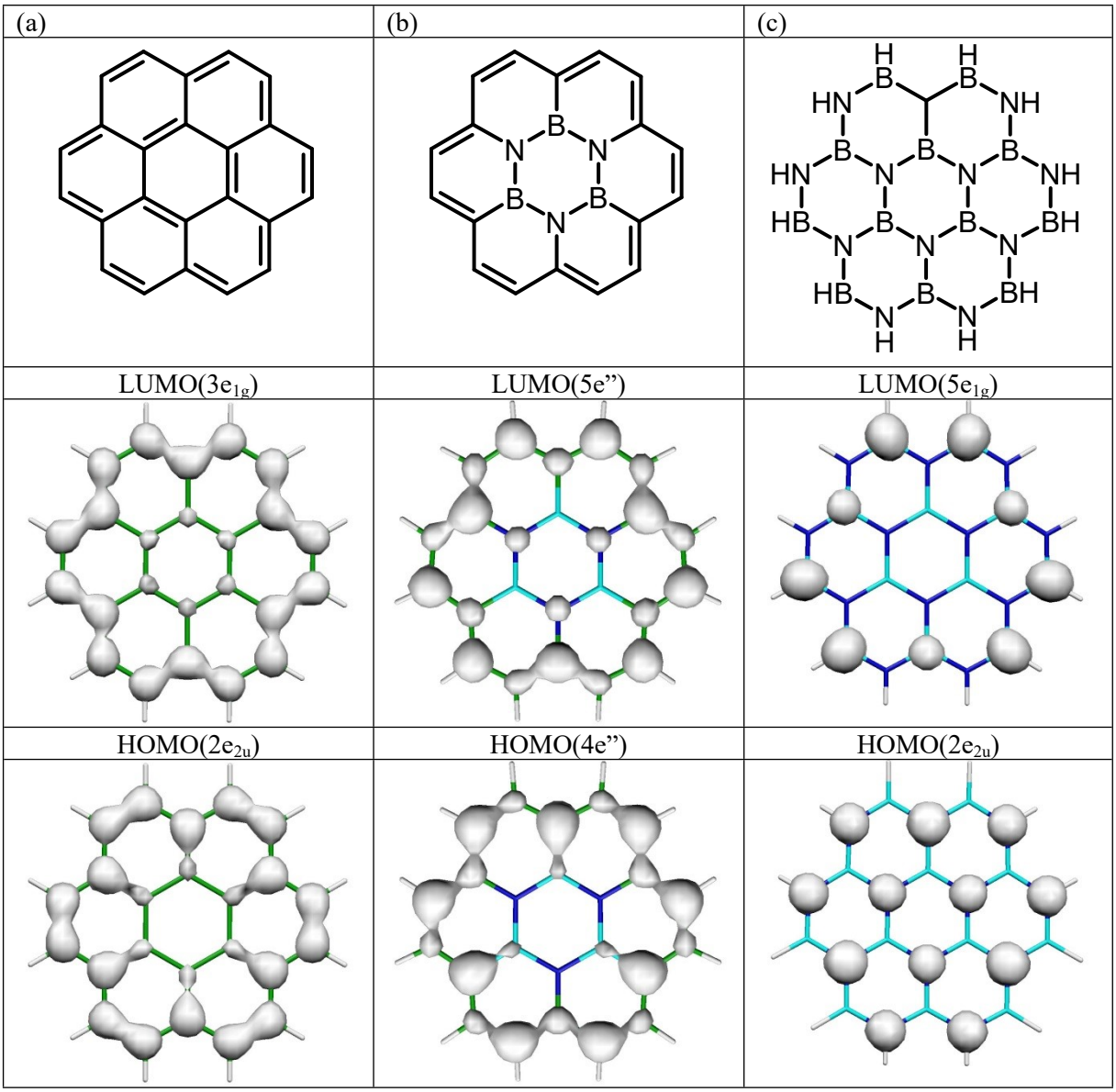

Fig. S2: Electron densities of HOMO and LUMO of (a) coronene (**1.1**), (b) partially BN-substituted coronene (**1.2**) and (c) fully BN-substituted coronene (**1.3**).

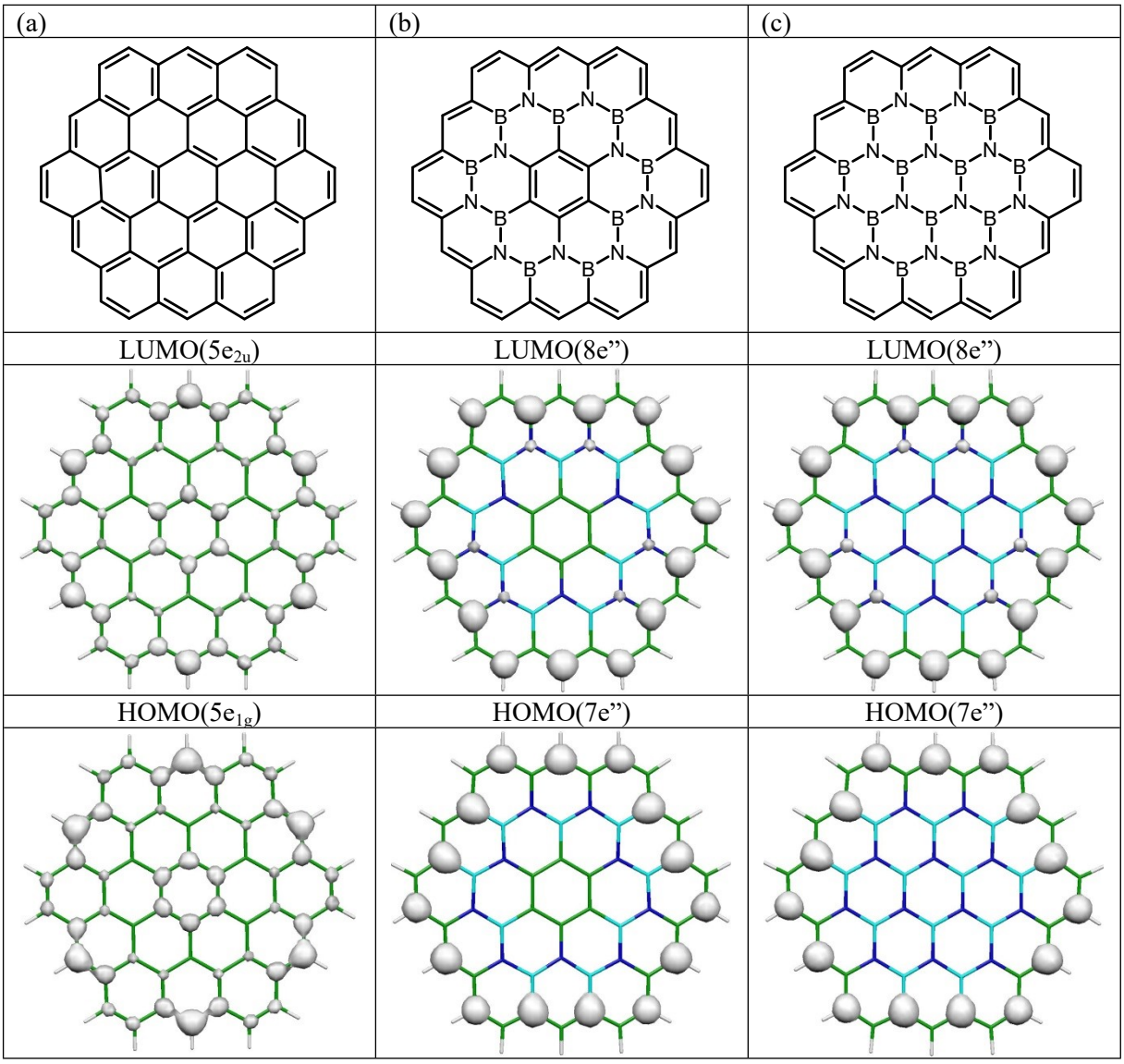

Fig. S3: Electron densities of HOMO and LUMO of (a) circumcoronene (**3.1**) and (b, c) two partially BN-substituted derivatives of circumcoronene (**3.2** and **3.3**).

Section S3: Effect of weak out-of-plane distortions at the MP2 level on vertical excitation energies for the example of coronene

Table S2. Comparison of vertical ADC(2) excitation energies ΔE (in eV) of the singlet and triplet valence excited states of coronene (**1.1**) at the planar (left) and one of the non-planar (right) MP2-optimized geometries. Δ_{ST} is the energy gap between the lowest singlet and triplet states. The D_{3d} structure is 0.045 eV lower in energy than the D_{6h} structure.

Coronene(D_{6h}) (E = 0)		Coronene(D_{3d}) (E = -0.045 eV)	
State	ΔE	State	ΔE
$^3B_{1u}$	2.810	$^3B_{1u}$	2.806
$^1B_{2u}$	3.221	$^1B_{2u}$	3.216
$^3E_{1u}$	2.242	$^3E_{1u}$	2.236
$^3B_{2u}$	3.646	$^3B_{2u}$	3.638
$^1B_{1u}$	3.781	$^1B_{1u}$	3.774
$^1E_{1u}$	4.314	$^1E_{1u}$	4.302
Δ_{ST}	0.411	Δ_{ST}	0.410

Section S4. Hexabenzocoronene and BN-substituted derivatives

Adding symmetrically six more benzene rings to coronene, one obtains hexabenzocoronene (HBC). The structures of HBC (**2.1**) and two partially BN-substituted derivatives of HBC (**2.2**, **2.3**) are shown in Chart S1. In contrast to coronene and circumcoronene, the equilibrium geometry of HBC is slightly non-planar at the DFT and MP2 levels due to steric repulsion of hydrogen atoms of neighbouring rings. However, the effect of non-planarity on the vertical excitation energies is minor as is shown in Table S3, which lists the vertical ADC(2) excitation energies of the planar and non-planar conformers of **2.1** – **2.3**.

Partial BN-substitution decreases the excitation energies. In all three systems, the energies of singlet and triplet states of B_{2u}/A_2' symmetry are inverted, albeit the energy gap is very small in HBC. While the energy gap between the lowest singlet and triplet states, Δ_{ST}, of planar HBC is positive (0.378 eV) and only marginally smaller than Δ_{ST} of coronene (0.411 eV), BN-substitution of planar HBC along a single circle (**2.2**) results in a slightly negative Δ_{ST} (-0.073 eV) and substitution with two BN circles (**2.3**) results in a robustly negative Δ_{ST} (-0.245 eV). An overview of the energy level schemes of **2.1 – 2.3** is given in Fig. S4. The electron densities of HOMO and LUMO of the three

compounds are displayed in Fig. S5. While the densities of HOMO and LUMO of HBC exhibit overlap on all atoms (Fig. S5(a)), only tiny populations along the outer rim exhibit overlap in **2.2** (Fig. S5(b)). In **2.3**, the HOMO and LUMO densities are completely non-overlapping (Fig. S5(c)).

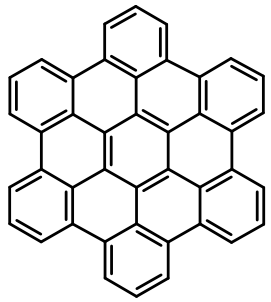	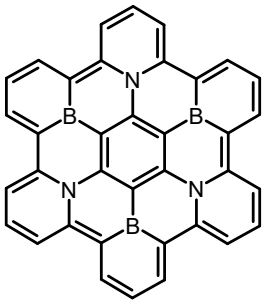	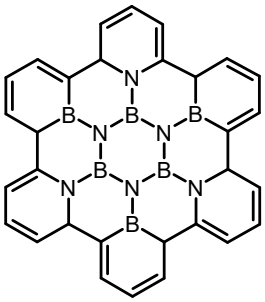
2.1	**2.2**	**2.3**

Chart S1: HBC (**2.1**), and its BN-substituted derivatives (**2.2** and **2.3**).

Table S3. Vertical excitation energies ΔE (in eV) of the singlet and triplet excited states of HBC (**2.1**) and two partially BN-substituted derivatives **2.2** and **2.3** (see Chart S1), ordered with increasing energy. The upper part gives the excitation energies of the planar structures, the lower part the excitation energies of the structures which are slightly non-planar due to steric repulsion. Δ_{ST} is the energy gap between the lowest singlet and triplet states. Oscillator strengths are given in parentheses.

2.1		**2.2**		**2.3**	
D_{6h}		D_{3h}		D_{3h}	
State	ΔE	State	ΔE	State	ΔE
$^3B_{1u}$'	2.568	$^1A_2$'	2.060(0.0)	$^1A_2$'	1.792(0.0)
$^1B_{2u}$'	2.946(0.0)	$^3A_1$'	2.133	$^3A_2$'	2.037
$^3B_{2u}$'	2.966	^3E	2.274	^3E'	2.094
$^3E_{1u}$	3.006	$^3A_2$'	2.349	$^3A_1$'	2.320
$^1B_{1u}$'	3.372(0.0)	$^1A_1$'	2.492(0.0)	^1E'	2.410(1.641)
$^1E_{1u}$	3.512(0.0)	^1E'	2.727(2.036)	$^1A_1$'	2.548(0.0)
Δ_{ST}	0.378	Δ_{ST}	-0.073	Δ_{ST}	-0.245
D_{3d} (E = -0.142eV)		C_{3v} (E = -0.011eV)		C_{3v} (E = -0.003eV)	
State	ΔE	State	ΔE	State	ΔE
$^3A_{2u}$	2.564	$^1A_2$	2.049(0.0)	$^1A_2$	1.788(0.0)
$^1A_{1u}$	2.932(0.0)	$^3A_1$	2.130	$^3A_2$	2.032
^3E_g	2.961	^3E	2.264	^3E	2.091
$^3A_{1u}$	2.991	$^3A_2$	2.337	$^3A_1$	2.474
$^1A_{2u}$	3.355(0.0)	$^1A_1$	2.478(0.0)	^1E	2.404(1.626)
^1E_g	3.484(0.0)	^1E	2.713(2.008)	$^1A_1$	2.542(0.0)
Δ_{ST}	0.368	Δ_{ST}	-0.081	Δ_{ST}	-0.244

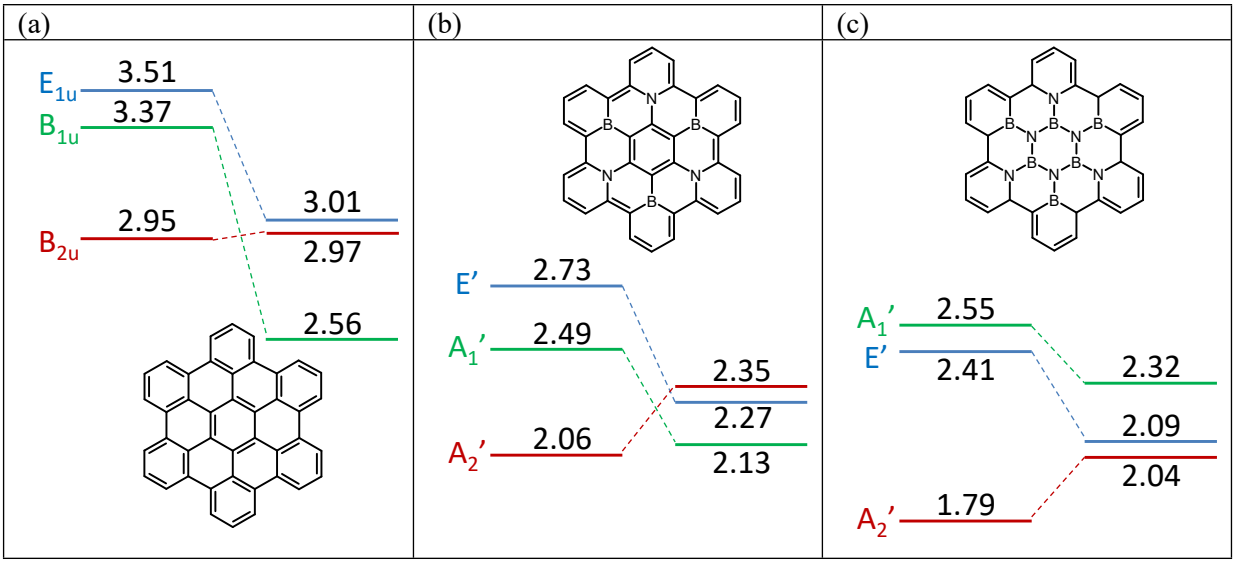

Fig. S4: ADC(2) energy level schemes of (a) HBC (**2.1**) and (b, c) two partially BN-substituted derivatives (**2.2**, **2.3**). Singlets left, triplets right.

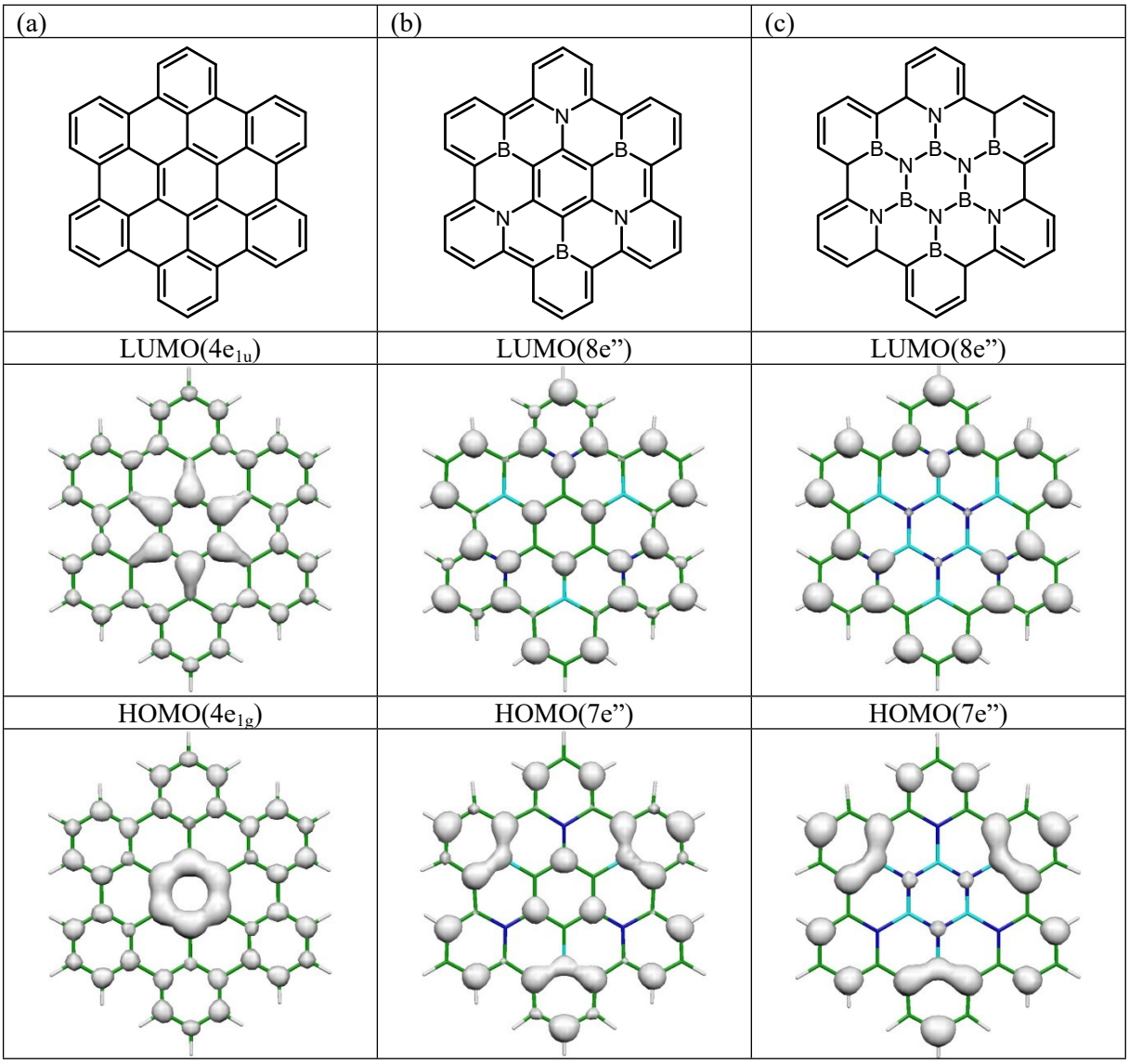

Fig. S5: Electron densities of HOMO and LUMO of (a) HBC (**2.1**) and (b, c) two partially BN-substituted derivatives of HBC (**2.2** and **2.3**).

Section S5. Cartesian coordinates of ground-state MP2/cc-pVDZ equilibrium geometries for compounds 1.2, 1.3, 2.1, 2.2, 2.3, 3.1, 3.2, 3.3

1.2 (D_{3h})

36
FINAL HEAT OF FORMATION = -929.412414
C -2.840340 -2.436392 0.000000
C -3.612178 -1.271257 0.000000
C -2.977036 0.000000 0.000000
B -1.455002 0.000000 0.000000

N	-0.720640	-1.248185	0.000000
C	-1.420699	-2.460724	0.000000
N	-0.720640	1.248185	0.000000
C	-1.420699	2.460724	0.000000
C	-2.840340	2.436392	0.000000
C	-3.612178	1.271257	0.000000
B	0.727501	1.260069	0.000000
C	1.488518	2.578188	0.000000
C	0.705148	3.763867	0.000000
C	-0.689808	3.678003	0.000000
N	1.441280	0.000000	0.000000
C	2.841399	0.000000	0.000000
C	3.530148	1.241610	0.000000
C	2.907030	2.492609	0.000000
B	0.727501	-1.260069	0.000000
C	1.488518	-2.578188	0.000000
C	2.907030	-2.492609	0.000000
C	3.530148	-1.241610	0.000000
C	-0.689808	-3.678003	0.000000
C	0.705148	-3.763867	0.000000
H	-4.707852	-1.355231	0.000000
H	-4.707852	1.355231	0.000000
H	4.625533	-1.190703	0.000000
H	4.625533	1.190703	0.000000
H	3.527590	-3.399503	0.000000
H	1.180261	-4.754735	0.000000
H	-1.281587	-4.601180	0.000000
H	-3.343945	-3.410477	0.000000
H	3.527590	3.399503	0.000000
H	1.180261	4.754735	0.000000
H	-1.281587	4.601180	0.000000
H	-3.343945	3.410477	0.000000

1.3 (D_{3h})

36

FINAL HEAT OF FORMATION = -960.830159

N	-3.595776	1.268778	0.000000
B	-2.908141	0.000000	0.000000
N	-3.595776	-1.268778	0.000000
B	-2.911635	-2.523289	0.000000
N	-1.458403	-2.526028	0.000000
B	-0.729415	-3.783194	0.000000
N	0.699094	-3.748422	0.000000
B	1.454070	-2.518524	0.000000
N	2.896682	-2.479644	0.000000
B	3.641050	-1.259905	0.000000
N	2.916806	0.000000	0.000000
B	3.641050	1.259905	0.000000
N	2.896682	2.479644	0.000000
B	1.454070	2.518524	0.000000
N	0.699094	3.748422	0.000000

B	-0.729415	3.783194	0.000000
N	-1.458403	2.526028	0.000000
B	-0.727823	1.260626	0.000000
N	0.726258	1.257917	0.000000
B	1.455646	0.000000	0.000000
N	0.726258	-1.257917	0.000000
B	-0.727823	-1.260626	0.000000
N	-1.452517	0.000000	0.000000
B	-2.911635	2.523289	0.000000
H	-3.529394	3.558514	0.000000
H	-1.317067	4.835802	0.000000
H	1.194177	-4.634706	0.000000
H	3.416685	-3.351541	0.000000
H	-1.317067	-4.835802	0.000000
H	-3.529394	-3.558514	0.000000
H	-4.610862	-1.283165	0.000000
H	-4.610862	1.283165	0.000000
H	4.846461	-1.277288	0.000000
H	4.846461	1.277288	0.000000
H	3.416685	3.351541	0.000000
H	1.194177	4.634706	0.000000

2.1 (D_{3d})

60

FINAL HEAT OF FORMATION = -1606.675440

C	1.211732	5.008087	-0.165698
C	1.237409	3.600326	-0.059009
C	0.000000	2.879305	-0.006030
C	-1.237409	3.600326	-0.059009
C	-1.211732	5.008087	-0.165698
C	0.000000	5.702409	-0.243268
C	0.000000	1.432314	-0.014183
C	1.240421	0.716157	0.014183
C	2.493551	1.439652	0.006030
C	2.499270	2.871790	0.059009
C	1.240421	-0.716157	-0.014183
C	0.000000	-1.432314	0.014183
C	-1.240421	-0.716157	-0.014183
C	-1.240421	0.716157	0.014183
C	2.493551	-1.439652	-0.006030
C	2.499270	-2.871790	-0.059009
C	1.237409	-3.600326	0.059009
C	0.000000	-2.879305	0.006030
C	-1.237409	-3.600326	0.059009
C	-1.211732	-5.008087	0.165698
C	0.000000	-5.702409	0.243268
C	1.211732	-5.008087	0.165698
C	-2.493551	-1.439652	-0.006030
C	-2.499270	-2.871790	-0.059009
C	-2.493551	1.439652	0.006030
C	-3.736678	0.728536	0.059009

C	-3.736678	-0.728536	-0.059009
C	-4.942996	-1.454653	-0.165698
C	-4.938431	-2.851205	-0.243268
C	-3.731264	-3.553434	-0.165698
C	-2.499270	2.871790	0.059009
C	-3.731264	3.553434	0.165698
C	-4.938431	2.851205	0.243268
C	-4.942996	1.454653	0.165698
C	3.736678	-0.728536	-0.059009
C	4.942996	-1.454653	-0.165698
C	4.938431	-2.851205	-0.243268
C	3.731264	-3.553434	-0.165698
C	3.736678	0.728536	0.059009
C	3.731264	3.553434	0.165698
C	4.938431	2.851205	0.243268
C	4.942996	1.454653	0.165698
H	2.144705	-5.571093	0.240033
H	-2.144705	-5.571093	0.240033
H	-5.897061	-0.928178	-0.240033
H	-3.752356	-4.642916	-0.240033
H	-3.752356	4.642916	0.240033
H	-5.897061	0.928178	0.240033
H	5.897061	-0.928178	-0.240033
H	3.752356	-4.642916	-0.240033
H	3.752356	4.642916	0.240033
H	5.897061	0.928178	0.240033
H	-2.144705	5.571093	-0.240033
H	2.144705	5.571093	-0.240033
H	-5.881979	-3.395962	-0.352487
H	5.881979	-3.395962	-0.352487
H	0.000000	6.791924	-0.352487
H	-5.881979	3.395962	0.352487
H	5.881979	3.395962	0.352487
H	0.000000	-6.791924	0.352487

2.2 (C_{3v})

60

FINAL HEAT OF FORMATION = -1616.715540

C	5.011206	-1.179599	0.190856
C	3.612444	-1.217750	0.047228
N	2.866773	0.000000	0.040541
C	3.612444	1.217750	0.047228
C	5.011206	1.179599	0.190856
C	5.739429	0.000000	0.282214
C	2.959028	2.501647	-0.060572
B	1.461130	2.530752	-0.014799
C	0.716400	1.240841	0.039507
C	1.426548	0.000000	0.022463
C	0.686975	3.813417	-0.060572
C	1.441581	5.002086	-0.198400
C	2.849314	4.935157	-0.267894

C	3.611143	3.749489	-0.198400
C	-0.713274	1.235427	0.022463
N	-1.433387	2.482699	0.040541
C	-0.751619	3.737344	0.047228
C	-1.432800	0.000000	0.039507
C	-0.713274	-1.235427	0.022463
C	0.716400	-1.240841	0.039507
B	1.461130	-2.530752	-0.014799
C	2.959028	-2.501647	-0.060572
C	0.686975	-3.813417	-0.060572
C	-0.751619	-3.737344	0.047228
N	-1.433387	-2.482699	0.040541
C	-2.860825	-2.519593	0.047228
C	-3.646004	-1.311770	-0.060572
B	-2.922260	0.000000	-0.014799
C	-3.646004	1.311770	-0.060572
C	-2.860825	2.519593	0.047228
C	3.611143	-3.749489	-0.198400
C	2.849314	-4.935157	-0.267894
C	1.441581	-5.002086	-0.198400
C	-3.527166	-3.750032	0.190856
C	-2.869715	-4.970491	0.282214
C	-1.484040	-4.929631	0.190856
C	-5.052724	1.252597	-0.198400
C	-5.698628	0.000000	-0.267894
C	-5.052724	-1.252597	-0.198400
C	-1.484040	4.929631	0.190856
C	-2.869715	4.970491	0.282214
C	-3.527166	3.750032	0.190856
H	-0.901294	-5.850722	0.245566
H	-4.616227	-3.705904	0.245566
H	-5.685344	2.146167	-0.285973
H	-5.685344	-2.146167	-0.285973
H	-0.901294	5.850722	0.245566
H	-4.616227	3.705904	0.245566
H	4.701307	-3.850569	-0.285973
H	0.984037	-5.996735	-0.285973
H	5.517521	2.144818	0.245566
H	5.517521	-2.144818	0.245566
H	0.984037	5.996735	-0.285973
H	4.701307	3.850569	-0.285973
H	-6.788382	0.000000	-0.395693
H	3.394191	-5.878911	-0.395693
H	3.394191	5.878911	-0.395693
H	-3.412470	5.910571	0.416252
H	6.824940	0.000000	0.416252
H	-3.412470	-5.910571	0.416252

2.3 (C_{3v})

60

FINAL HEAT OF FORMATION = -1627.265830

C	5.033553	-1.240551	0.145692
C	3.624164	-1.313758	0.045195
B	2.882716	0.000000	0.021680
C	3.624164	1.313758	0.045195
C	5.033553	1.240551	0.145692
C	5.696556	0.000000	0.198530
C	2.893943	2.565991	-0.032787
N	1.482125	2.567116	-0.014648
B	0.719202	1.245694	-0.015479
N	1.429541	0.000000	-0.021364
C	0.775242	3.789223	-0.032787
C	1.499633	4.990853	-0.144883
C	2.890413	5.006342	-0.207017
C	3.572389	3.794147	-0.144883
N	-0.714771	1.238019	-0.021364
B	-1.441358	2.496505	0.021680
C	-0.674334	3.795497	0.045195
B	-1.438404	0.000000	-0.015479
N	-0.714771	-1.238019	-0.021364
B	0.719202	-1.245694	-0.015479
N	1.482125	-2.567116	-0.014648
C	2.893943	-2.565991	-0.032787
C	0.775242	-3.789223	-0.032787
C	-0.674334	-3.795497	0.045195
B	-1.441358	-2.496505	0.021680
C	-2.949830	-2.481739	0.045195
C	-3.669185	-1.223233	-0.032787
N	-2.964251	0.000000	-0.014648
C	-3.669185	1.223233	-0.032787
C	-2.949830	2.481739	0.045195
C	3.572389	-3.794147	-0.144883
C	2.890413	-5.006342	-0.207017
C	1.499633	-4.990853	-0.144883
C	-3.591125	-3.738910	0.145692
C	-2.848278	-4.933362	0.198530
C	-1.442428	-4.979461	0.145692
C	-5.072022	1.196706	-0.144883
C	-5.780825	0.000000	-0.207017
C	-5.072022	-1.196706	-0.144883
C	-1.442428	4.979461	0.145692
C	-2.848278	4.933362	0.198530
C	-3.591125	3.738910	0.145692
H	-0.976543	-5.971943	0.209031
H	-4.683583	-3.831682	0.209031
H	-5.598539	2.149948	-0.196229
H	-5.598539	-2.149948	-0.196229
H	-0.976543	5.971943	0.209031
H	-4.683583	3.831682	0.209031
H	4.661179	-3.773502	-0.196229
H	0.937359	-5.923451	-0.196229
H	5.660126	2.140261	0.209031

H	5.660126	-2.140261	0.209031
H	0.937359	5.923451	-0.196229
H	4.661179	3.773502	-0.196229
H	-6.871153	0.000000	-0.307651
H	3.435577	-5.950593	-0.307651
H	3.435577	5.950593	-0.307651
H	-3.394096	5.878746	0.293914
H	6.788191	0.000000	0.293914
H	-3.394096	-5.878746	0.293914

3.1 (D_{6h})

72
FINAL HEAT OF FORMATION = -2062.782290

C	-5.703296	-2.495877	0.000000
C	-5.013993	-1.233242	0.000000
C	-5.699824	0.000000	0.000000
C	-5.013993	1.233242	0.000000
C	-5.703296	2.495877	0.000000
C	-5.013141	3.691260	0.000000
C	-3.575016	3.725624	0.000000
C	-2.849912	4.936192	0.000000
C	-1.438977	4.958867	0.000000
C	-0.690155	6.187137	0.000000
C	0.690155	6.187137	0.000000
C	1.438977	4.958867	0.000000
C	2.849912	4.936192	0.000000
C	3.575016	3.725624	0.000000
C	5.013141	3.691260	0.000000
C	5.703296	2.495877	0.000000
C	5.013993	1.233242	0.000000
C	5.699824	0.000000	0.000000
C	5.013993	-1.233242	0.000000
C	5.703296	-2.495877	0.000000
C	5.013141	-3.691260	0.000000
C	3.575016	-3.725624	0.000000
C	2.849912	-4.936192	0.000000
C	1.438977	-4.958867	0.000000
C	0.690155	-6.187137	0.000000
C	-0.690155	-6.187137	0.000000
C	-1.438977	-4.958867	0.000000
C	-2.849912	-4.936192	0.000000
C	-3.575016	-3.725624	0.000000
C	-2.860700	-2.475165	0.000000
C	-3.573906	-1.239856	0.000000
C	-2.858680	0.000000	0.000000
C	-3.573906	1.239856	0.000000
C	-2.860700	2.475165	0.000000
C	-1.429340	2.475690	0.000000
C	-0.713206	3.715022	0.000000
C	0.713206	3.715022	0.000000
C	1.429340	2.475690	0.000000

C	2.860700	2.475165	0.000000
C	3.573906	1.239856	0.000000
C	2.858680	0.000000	0.000000
C	3.573906	-1.239856	0.000000
C	2.860700	-2.475165	0.000000
C	1.429340	-2.475690	0.000000
C	0.713206	-3.715022	0.000000
C	-0.713206	-3.715022	0.000000
C	-1.429340	-2.475690	0.000000
C	-0.715179	-1.238726	0.000000
C	0.715179	-1.238726	0.000000
C	1.430358	0.000000	0.000000
C	0.715179	1.238726	0.000000
C	-0.715179	1.238726	0.000000
C	-1.430358	0.000000	0.000000
C	-5.013141	-3.691260	0.000000
H	-6.800031	-2.494654	0.000000
H	-6.800031	2.494654	0.000000
H	-6.797910	0.000000	0.000000
H	-5.560449	4.641672	0.000000
H	-3.398955	5.887163	0.000000
H	-3.398955	-5.887163	0.000000
H	-1.239581	-7.136327	0.000000
H	1.239581	-7.136327	0.000000
H	3.398955	5.887163	0.000000
H	3.398955	-5.887163	0.000000
H	1.239581	7.136327	0.000000
H	-1.239581	7.136327	0.000000
H	-5.560449	-4.641672	0.000000
H	5.560449	4.641672	0.000000
H	5.560449	-4.641672	0.000000
H	6.800031	-2.494654	0.000000
H	6.797910	0.000000	0.000000
H	6.800031	2.494654	0.000000

3.2 (D_{3h})

72

FINAL HEAT OF FORMATION = -2093.734000

C	-5.716519	-2.503823	0.000000
C	-5.038470	-1.245994	0.000000
C	-5.702862	0.000000	0.000000
C	-5.038470	1.245994	0.000000
C	-5.716519	2.503823	0.000000
C	-5.049392	3.724540	0.000000
C	-3.621249	3.818339	0.000000
C	-2.909358	5.039155	0.000000
C	-1.496154	5.045263	0.000000
C	-0.700850	6.235172	0.000000
C	0.689885	6.202562	0.000000
C	1.440172	4.986440	0.000000

C	2.851431	4.938824	0.000000
C	3.598298	3.740446	0.000000
C	5.026634	3.698739	0.000000
C	5.750242	2.510632	0.000000
C	5.117403	1.226924	0.000000
C	5.818715	0.000000	0.000000
C	5.117403	-1.226924	0.000000
C	5.750242	-2.510632	0.000000
C	5.026634	-3.698739	0.000000
C	3.598298	-3.740446	0.000000
C	2.851431	-4.938824	0.000000
C	1.440172	-4.986440	0.000000
C	0.689885	-6.202562	0.000000
C	-0.700850	-6.235172	0.000000
C	-1.496154	-5.045263	0.000000
C	-2.909358	-5.039155	0.000000
C	-3.621249	-3.818339	0.000000
B	-2.864892	-2.487547	0.000000
N	-3.642194	-1.252210	0.000000
B	-2.935727	0.000000	0.000000
N	-3.642194	1.252210	0.000000
B	-2.864892	2.487547	0.000000
N	-1.407610	2.438053	0.000000
B	-0.721833	3.724843	0.000000
N	0.736652	3.780337	0.000000
B	1.467864	2.542414	0.000000
N	2.905542	2.528127	0.000000
B	3.586725	1.237296	0.000000
N	2.815221	0.000000	0.000000
B	3.586725	-1.237296	0.000000
N	2.905542	-2.528127	0.000000
B	1.467864	-2.542414	0.000000
N	0.736652	-3.780337	0.000000
B	-0.721833	-3.724843	0.000000
N	-1.407610	-2.438053	0.000000
C	-0.702057	-1.215999	0.000000
C	0.709283	-1.228514	0.000000
C	1.404114	0.000000	0.000000
C	0.709283	1.228514	0.000000
C	-0.702057	1.215999	0.000000
C	-1.418565	0.000000	0.000000
C	-5.049392	-3.724540	0.000000
H	-6.811578	-2.482024	0.000000
H	-6.811578	2.482024	0.000000
H	-6.797232	0.000000	0.000000
H	-5.650832	4.645826	0.000000
H	-3.461475	5.995451	0.000000
H	-3.461475	-5.995451	0.000000
H	-1.197987	-7.216677	0.000000
H	1.256293	-7.140011	0.000000
H	3.398616	5.886575	0.000000
H	3.398616	-5.886575	0.000000

H 1.256293 7.140011 0.000000
H -1.197987 7.216677 0.000000
H -5.650832 -4.645826 0.000000
H 5.555284 4.657987 0.000000
H 5.555284 -4.657987 0.000000
H 6.848820 -2.570851 0.000000
H 6.922951 0.000000 0.000000
H 6.848820 2.570851 0.000000

3.3 (D_{3h})

72
FINAL HEAT OF FORMATION = -2104.295860
C 5.015195 -3.696826 0.000000
C 5.769120 -2.526609 0.000000
C 5.154423 -1.235605 0.000000
B 3.625774 -1.236513 0.000000
N 2.881084 0.000000 0.000000
B 1.442647 0.000000 0.000000
N 0.724477 -1.254830 0.000000
B -0.721323 -1.249369 0.000000
N -1.448953 0.000000 0.000000
B -0.721323 1.249369 0.000000
N 0.724477 1.254830 0.000000
B 1.446584 2.505556 0.000000
N 2.897004 2.506419 0.000000
B 3.625774 1.236513 0.000000
C 5.154423 1.235605 0.000000
C 5.848632 0.000000 0.000000
C 3.583807 -3.722965 0.000000
N 2.897004 -2.506419 0.000000
B 1.446584 -2.505556 0.000000
N 0.722121 -3.762089 0.000000
B -0.742035 -3.758269 0.000000
N -1.440542 -2.495092 0.000000
B -2.883739 -2.521756 0.000000
N -3.619125 -1.255669 0.000000
B -2.893167 0.000000 0.000000
N -3.619125 1.255669 0.000000
B -2.883739 2.521756 0.000000
N -1.440542 2.495092 0.000000
B -0.742035 3.758269 0.000000
N 0.722121 3.762089 0.000000
C 1.432278 4.965151 0.000000
C 2.841960 4.922418 0.000000
C 3.583807 3.722965 0.000000
C 5.015195 3.696826 0.000000
C 5.769120 2.526609 0.000000
C 2.841960 -4.922418 0.000000
C 1.432278 -4.965151 0.000000
C 0.693948 -6.191699 0.000000
C -0.696453 -6.259509 0.000000

C	-1.507146	-5.081663	0.000000
C	-2.924316	-5.065064	0.000000
C	-3.647276	-3.846059	0.000000
C	-5.072667	-3.732900	0.000000
C	-5.709143	-2.494873	0.000000
C	-5.016086	-1.242186	0.000000
C	-5.683919	0.000000	0.000000
C	-5.016086	1.242186	0.000000
H	5.523819	-4.666922	0.000000
H	1.279764	-7.117228	0.000000
H	3.388905	-5.869756	0.000000
H	-1.169081	-7.253225	0.000000
H	-3.476751	-6.021910	0.000000
H	6.953502	0.000000	0.000000
C	-3.647276	3.846059	0.000000
H	6.866018	2.614159	0.000000
C	-5.709143	2.494873	0.000000
H	5.523819	4.666922	0.000000
H	-6.777810	0.000000	0.000000
H	3.388905	5.869756	0.000000
H	-6.803582	-2.450306	0.000000
C	0.693948	6.191699	0.000000
H	-5.696937	-4.639066	0.000000
H	6.866018	-2.614159	0.000000
C	-1.507146	5.081663	0.000000
C	-5.072667	3.732900	0.000000
C	-0.696453	6.259509	0.000000
C	-2.924316	5.065064	0.000000
H	-6.803582	2.450306	0.000000
H	1.279764	7.117228	0.000000
H	-1.169081	7.253225	0.000000
H	-3.476751	6.021910	0.000000
H	-5.696937	4.639066	0.000000