A theoretical study on application of BN/CC isosterism to modify topology of coronene aromaticity and HOMO-LUMO energy gaps

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S1. Comparison of the performance of different density functionals

A comparison of calculated and experimental[1] bond lengths of **Cor** is given in Table S1. It can be seen that all three functionals yielded structures in close agreement with the experimental one. Since the latter was obtained by the X-ray analysis, some deviations between the calculated (isolated molecule in gas phase) and experimental data are expected. The largest deviation, 0.013 Å, was found for the rim double bond calculated with the B3LYP-D3(BJ).

The calculated HOMA, FLU, PDI and $EDDB_P$ using all three functionals are collected in Tables S2-S5 and correlation diagrams are presented in Figure S1. It can be seen that for all aromaticity indices the best correlations were obtained between ωB97XD and M06-2X: HOMA, $R^2 = 0.9994$, $y = 0.9857x + 0.0203$; FLU, $R^2 = 0.9996$, $y = 0.9956x - 0.0000$; PDI, $R^2 = 0.9997$, $y = 1.0181x - 0.0006$ and $EDDB_P$, $R^2 = 0.9998$, $y = 0.9945x - 0.0050$. Only slightly worse were the correlations with the B3LYP functional: R^2 varied from 0.9818 to 0.9987, the slope of the regression line from 0.9638 to 1.1390 and the intercept from 0.0008 to 0.0797. The FLU and PDI showed the least variation when calculated with different functionals and HOMA the largest, although all variations were very small, as shown by the line equation and correlation coefficients.

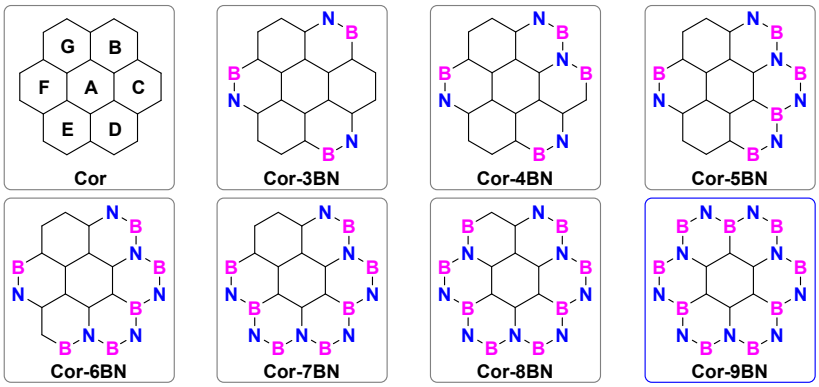
$NICS_{\pi zz}$-xy scans obtained with all three functionals are shown in Figure S2. They are also very similar and the main difference is the total shielding of the central ring in the studied systems. B3LYP indicates the largest difference between shielding of this ring in **Cor** and **Cor-9BN**, where it is more shielded in the former compound, although the difference is small ≈ 2 ppm. This difference disappears when calculated with the M06-2X and reverses with ωB97XD when the central ring of **Cor-9BN** is more shielded by only 0.7 ppm.

Based on the above discussion, we conclude that all three functionals correctly describe the studied systems and can be considered reliable.

Table S1. Calculated and experimental (X-ray)[1] bond lengths (Å) of coronene, averaged to D_{6h} symmetry.

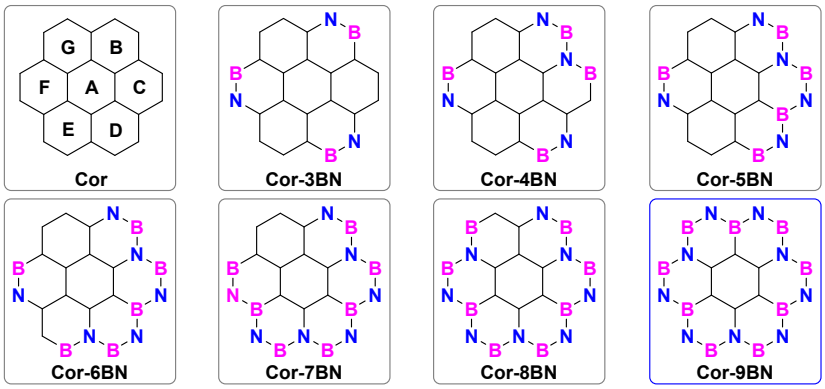
Bond type	**B3LYP-D3(BJ)**	**M06-2X**	**ωB97XD**	**exp.**
Inner benzene	1.425	1.425	1.424	1.423
Spoke bond	1.418	1.410	1.408	1.416
Rim single bond	1.422	1.423	1.422	1.421
Rim double bond	1.370	1.365	1.363	1.357

Table S2. Calculated HOMA values for individual rings **A-G**, molecular primeter (**peri**) and perimeter of carbocyclic subunits (**carbo-peri**) of coronene and its BN analogues using different functionals and 6-311+G(d,p) basis set.



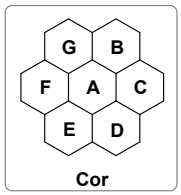
	A	B	C	D	E	F	G	peri	carbo-peri
Cor									
B3LYP-D3(BJ) D_{6h}	0.649	0.750	0.750	0.750	0.750	0.750	0.750	0.774	/
M06-2X D_{6h}	0.651	0.774	0.774	0.774	0.774	0.774	0.774	0.747	/
ωB97XD C_{2h}	0.657	0.782	0.782	0.782	0.782	0.782	0.782	0.746	/
Cor C_3									
B3LYP	0.651	0.750	0.750	0.750	0.750	0.750	0.750	0.774	/
M06-2X	0.648	0.772	0.772	0.772	0.772	0.772	0.772	0.743	/
ωB97XD	0.657	0.782	0.781	0.782	0.781	0.782	0.781	0.745	/
Cor-3BN C_{3h}									
B3LYP-D3(BJ)	0.448	0.604	0.846	0.604	0.846	0.604	0.846	0.785	0.764
M06-2X	0.423	0.593	0.890	0.593	0.890	0.593	0.890	0.770	0.776
ωB97XD	0.437	0.607	0.896	0.607	0.896	0.607	0.896	0.777	0.782
Cor-4BN C_s									
B3LYP-D3(BJ)	0.519	0.725	0.694	0.458	0.844	0.616	0.854	0.813	0.752
M06-2X	0.504	0.718	0.697	0.430	0.889	0.611	0.899	0.801	0.758
ωB97XD	0.518	0.729	0.710	0.449	0.898	0.624	0.908	0.809	0.765
Cor-5BN C_s									
B3LYP-D3(BJ)	0.572	0.689	0.671	0.426	0.839	0.603	0.851	0.816	0.771
M06-2X	0.555	0.686	0.666	0.391	0.884	0.598	0.895	0.806	0.775
ωB97XD	0.568	0.698	0.672	0.403	0.893	0.610	0.904	0.813	0.782
Cor-6BN C_s									
B3LYP-D3(BJ)	0.680	0.725	0.695	0.650	0.656	0.479	0.821	0.848	0.772
M06-2X	0.697	0.731	0.689	0.633	0.647	0.457	0.857	0.839	0.784
ωB97XD	0.712	0.744	0.696	0.643	0.662	0.476	0.865	0.847	0.793
Cor-7BN C_s									
B3LYP-D3(BJ)	0.745	0.723	0.698	0.633	0.670	0.453	0.800	0.858	0.799
M06-2X	0.764	0.731	0.695	0.622	0.666	0.428	0.831	0.851	0.807
ωB97XD	0.781	0.745	0.703	0.634	0.674	0.439	0.840	0.858	0.818
Cor-8BN C_s									
B3LYP-D3(BJ)	0.821	0.634	0.684	0.665	0.680	0.691	0.617	0.884	/
M06-2X	0.859	0.630	0.680	0.660	0.677	0.686	0.599	0.880	/
ωB97XD	0.875	0.647	0.690	0.671	0.687	0.695	0.614	0.887	/
Cor-9BN									
B3LYP-D3(BJ) D_{3h}	0.872	0.677	0.677	0.677	0.677	0.677	0.677	0.914	/
M06-2X C_{3h}	0.906	0.673	0.673	0.673	0.673	0.673	0.673	0.916	/
ωB97XD C_{3h}	0.919	0.682	0.683	0.682	0.683	0.682	0.683	0.922	/

Table S3. Calculated FLU values for individual rings **A-G**, molecular primeter (**peri**) and perimeter of carbocyclic subunits (**carbo-peri**) of coronene and its BN analogues using different functionals and 6-311+G(d,p) basis set.

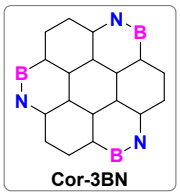


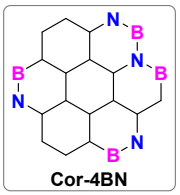
	A	B	C	D	E	F	G	peri	carbo-peri
Cor									
B3LYP-D3(BJ) D_{6h}	0.0265	0.0181	0.0181	0.0181	0.0181	0.0181	0.0181	0.0137	/
M06-2X D_{6h}	0.0290	0.0184	0.0184	0.0184	0.0184	0.0184	0.0184	0.0159	/
ωB97XD C_{2h}	0.0295	0.0183	0.0183	0.0183	0.0183	0.0183	0.0183	0.0163	/
Cor C_3									
B3LYP-D3(BJ)	0.0265	0.0181	0.0181	0.0181	0.0181	0.0181	0.0181	0.0137	/
M06-2X	0.0291	0.0184	0.0184	0.0184	0.0184	0.0184	0.0184	0.0160	/
ωB97XD	0.0295	0.0183	0.0183	0.0183	0.0183	0.0183	0.0183	0.0163	/
Cor-3BN C_{3h}									
B3LYP-D3(BJ)	0.0294	0.0326	0.0116	0.0326	0.0116	0.0326	0.0116	0.0230	0.0145
M06-2X	0.0318	0.0347	0.0108	0.0347	0.0108	0.0347	0.0108	0.0248	0.0148
ωB97XD	0.0319	0.0343	0.0106	0.0343	0.0106	0.0343	0.0106	0.0246	0.0148
Cor-4BN C_s									
B3LYP-D3(BJ)	0.0265	0.0271	0.0221	0.0378	0.0115	0.0333	0.0116	0.0208	0.0152
M06-2X	0.0282	0.0285	0.0224	0.0408	0.0106	0.0355	0.0107	0.0223	0.0156
ωB97XD	0.0282	0.0286	0.0220	0.0404	0.0104	0.0352	0.0105	0.0219	0.0156
Cor-5BN C_s									
B3LYP-D3(BJ)	0.0246	0.0297	0.0311	0.0416	0.0115	0.0337	0.0114	0.0177	0.0144
M06-2X	0.0263	0.0310	0.0314	0.0440	0.0107	0.0360	0.0106	0.0185	0.0149
ωB97XD	0.0263	0.0311	0.0312	0.0435	0.0105	0.0357	0.0104	0.0185	0.0149
Cor-6BN C_s									
B3LYP-D3(BJ)	0.0207	0.0292	0.0311	0.0321	0.0238	0.0381	0.0124	0.0154	0.0153
M06-2X	0.0212	0.0304	0.0314	0.0335	0.0247	0.0409	0.0120	0.0162	0.0158
ωB97XD	0.0211	0.0305	0.0312	0.0334	0.0243	0.0406	0.0118	0.0159	0.0157
Cor-7BN C_s									
B3LYP-D3(BJ)	0.0184	0.0293	0.0309	0.0335	0.0312	0.0409	0.0130	0.0119	0.0141
M06-2X	0.0186	0.0304	0.0313	0.0347	0.0317	0.0431	0.0128	0.0122	0.0146
ωB97XD	0.0184	0.0305	0.0312	0.0346	0.0315	0.0426	0.0127	0.0120	0.0145
Cor-8BN C_s									
B3LYP-D3(BJ)	0.0154	0.0315	0.0319	0.0325	0.0318	0.0307	0.0266	0.0097	/
M06-2X	0.0149	0.0328	0.0325	0.0333	0.0324	0.0317	0.0281	0.0099	/
ωB97XD	0.0147	0.0327	0.0324	0.0332	0.0322	0.0315	0.0279	0.0097	/
Cor-9BN									
B3LYP-D3(BJ) D_{3h}	0.0135	0.0319	0.0319	0.0319	0.0319	0.0319	0.0319	0.0055	/
M06-2X C_{3h}	0.0129	0.0327	0.0327	0.0327	0.0327	0.0327	0.0327	0.0052	/
ωB97XD C_{3h}	0.0127	0.0326	0.0326	0.0326	0.0326	0.0326	0.0326	0.0051	/

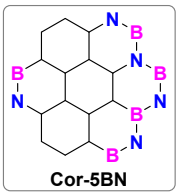
Table S4. Calculated PDI (e) values for individual rings **A-G** of coronene and its BN analogues using different functionals and 6-311+G(d,p) basis set.

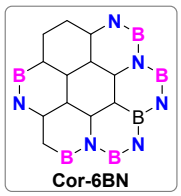


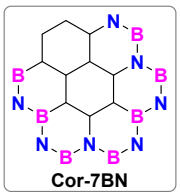
Cor

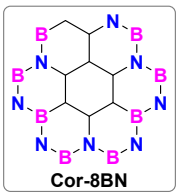

Cor-3BN

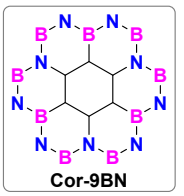

Cor-4BN


Cor-5BN


Cor-6BN

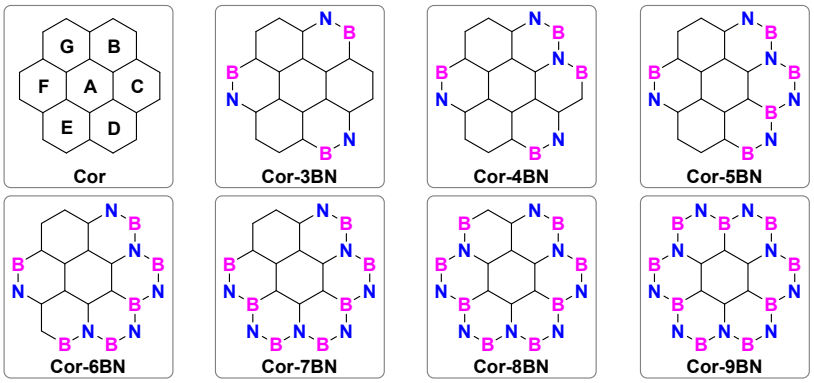

Cor-7BN


Cor-8BN


Cor-9BN

	A	B	C	D	E	F	G
Cor							
B3LYP-D3(BJ) D_{6h}	0.0330	0.0540	0.0540	0.0540	0.0540	0.0540	0.0540
M06-2X D_{6h}	0.0304	0.0561	0.0561	0.0561	0.0561	0.0561	0.0561
ωB97XD C_{2h}	0.0294	0.0570	0.0570	0.0570	0.0570	0.0570	0.0570
Cor C_3							
B3LYP-D3(BJ)	0.0328	0.0539	0.0539	0.0539	0.0539	0.0539	0.0539
M06-2X	0.0303	0.0560	0.0565	0.0560	0.0565	0.0560	0.0565
ωB97XD	0.0293	0.0570	0.0570	0.0570	0.0570	0.0570	0.0570
Cor-3BN C_{3h}							
B3LYP-D3(BJ)	0.0302	0.0339	0.0657	0.0339	0.0657	0.0339	0.0657
M06-2X	0.0287	0.0328	0.0693	0.0328	0.0693	0.0328	0.0693
ωB97XD	0.0282	0.0329	0.0699	0.0329	0.0699	0.0329	0.0699
Cor-4BN C_s							
B3LYP-D3(BJ)	0.0358	0.0280	0.0493	0.0275	0.0653	0.0333	0.0653
M06-2X	0.0352	0.0267	0.0500	0.0257	0.0687	0.0318	0.0688
ωB97XD	0.0350	0.0265	0.0506	0.0257	0.0695	0.0318	0.0695
Cor-5BN C_s							
B3LYP-D3(BJ)	0.0400	0.0256	0.0313	0.0246	0.0651	0.0327	0.0655
M06-2X	0.0396	0.0245	0.0307	0.0229	0.0683	0.0312	0.0688
ωB97XD	0.0395	0.0242	0.0309	0.0230	0.0690	0.0310	0.0694
Cor-6BN C_s							
B3LYP-D3(BJ)	0.0473	0.0261	0.0295	0.0248	0.0453	0.0273	0.0633
M06-2X	0.0484	0.0250	0.0288	0.0231	0.0453	0.0253	0.0658
ωB97XD	0.0487	0.0247	0.0289	0.0231	0.0457	0.0252	0.0663
Cor-7BN C_s							
B3LYP-D3(BJ)	0.0522	0.0263	0.0290	0.0237	0.0286	0.0253	0.0625
M06-2X	0.0536	0.0251	0.0281	0.0223	0.0277	0.0235	0.0646
ωB97XD	0.0540	0.0249	0.0281	0.0223	0.0278	0.0236	0.0649
Cor-8BN C_s							
B3LYP-D3(BJ)	0.0575	0.0240	0.0269	0.0253	0.0268	0.0270	0.0405
M06-2X	0.0597	0.0230	0.0258	0.0241	0.0256	0.0256	0.0395
ωB97XD	0.0603	0.0229	0.0258	0.0241	0.0257	0.0256	0.0397
Cor-9BN							
B3LYP-D3(BJ) D_{3h}	0.0612	0.0260	0.0260	0.0260	0.0260	0.0260	0.0260
M06-2X C_{3h}	0.0633	0.0204	0.0249	0.0204	0.0249	0.0244	0.0249
ωB97XD C_{3h}	0.0638	0.0249	0.0249	0.0249	0.0249	0.0249	0.0249

Table S5. Calculated $EDDB_P$ (e) values for individual rings **A-G**, molecular primeter (**peri**) and perimeter of carbocyclic subunits (**carbo-peri**) of coronene and its BN analogues using different functionals and 6-311+G(d,p) basis set.



	A	B	C	D	E	F	G	peri	carbo-peri
Cor									
B3LYP D_{6h}	2.5736	2.6959	2.6959	2.6959	2.6959	2.6959	2.6959	8.3128	/
M06-2X D_{6h}	2.4243	2.5328	2.5328	2.5328	2.5328	2.5328	2.5328	7.5158	/
ωB97XD C_{2h}	2.3764	2.4948	2.4948	2.4948	2.4948	2.4948	2.4948	7.3593	/
Cor C_3									
B3LYP	2.5744	2.6971	2.6962	2.6971	2.6962	2.6971	2.6962	8.3170	/
M06-2X	2.4175	2.5608	2.5288	2.5608	2.5288	2.5608	2.5288	7.5085	/
ωB97XD	2.3745	2.4903	2.4948	2.4903	2.4948	2.4903	2.4948	7.3513	/
Cor-3BN C_{3h}									
B3LYP	2.0596	1.8013	3.7144	1.8013	3.7144	1.8013	3.7144	7.7155	10.6958
M06-2X	1.7198	1.5012	3.8379	1.5012	3.8379	1.5012	3.8379	7.2061	10.4514
ωB97XD	1.6609	1.4809	3.8357	1.4809	3.8357	1.4809	3.8357	7.1944	10.3483
Cor-4BN C_s									
B3LYP	2.1762	2.1556	2.2320	1.7561	3.7593	1.8603	3.7324	7.4600	8.0344
M06-2X	1.8545	1.9825	2.0857	1.5363	3.8940	1.6053	3.8679	6.9998	7.8119
ωB97XD	1.7831	1.9512	2.0933	1.5294	3.9013	1.5837	3.8746	7.0066	7.7252
Cor-5BN C_s									
B3LYP	2.1881	2.0258	1.8791	1.7254	3.7500	1.8673	3.7832	8.2172	8.1441
M06-2X	1.8941	1.8975	1.8151	1.5627	3.8790	1.6349	3.9111	7.9326	7.9639
ωB97XD	1.8307	1.8644	1.8080	1.5727	3.8857	1.6191	3.9127	7.9104	7.8968
Cor-6BN C_s									
B3LYP	2.6866	2.0376	1.9476	2.1974	2.1293	1.7990	3.7171	7.9959	5.6509
M06-2X	2.4886	1.9451	1.8673	2.0912	1.9403	1.6194	3.7061	7.6249	5.4130
ωB97XD	2.4379	1.9149	1.8587	2.0974	1.9385	1.6236	3.7024	7.6362	5.3560
Cor-7BN C_s									
B3LYP	2.9830	2.0632	1.9533	2.0871	1.9361	1.7779	3.5402	8.8023	5.8141
M06-2X	2.8162	1.9755	1.8665	1.9922	1.8500	1.6418	3.4694	8.5448	5.5676
ωB97XD	2.7955	1.9456	1.8595	1.9848	1.8434	1.6557	3.4524	8.5222	5.5307
Cor-8BN C_s									
B3LYP	3.5656	1.9204	1.9678	2.0228	1.9876	2.1433	1.9864	8.6439	/
M06-2X	3.6405	1.8182	1.8771	1.9273	1.8962	2.0341	1.7919	8.4322	/
ωB97XD	3.6334	1.8017	1.8683	1.9199	1.8870	2.0349	1.7859	8.4265	/
Cor-9BN									
B3LYP D_{3h}	2.8491	2.0033	2.0033	2.0033	2.0033	2.0033	2.0033	9.7073	/
M06-2X C_{3h}	3.9477	1.9069	1.9100	1.9069	1.9100	1.9069	1.9100	9.5941	/
ωB97XD C_{3h}	3.9429	1.8990	1.9029	1.8990	1.9029	1.8990	1.9029	9.5668	/

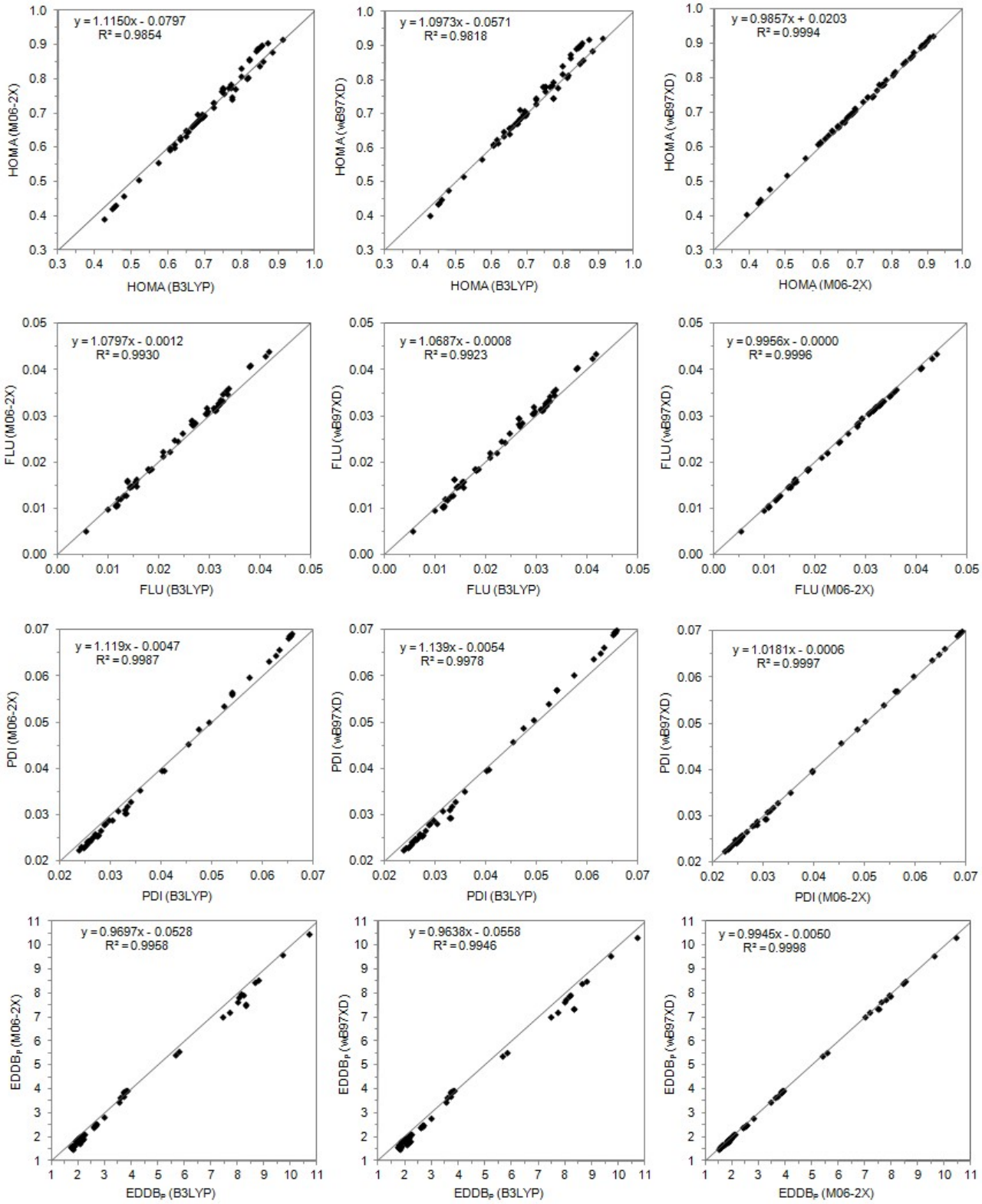


Figure S1. Correlations of HOMA, FLU, PDI and $EDDB_P$ calculated using different functionals.

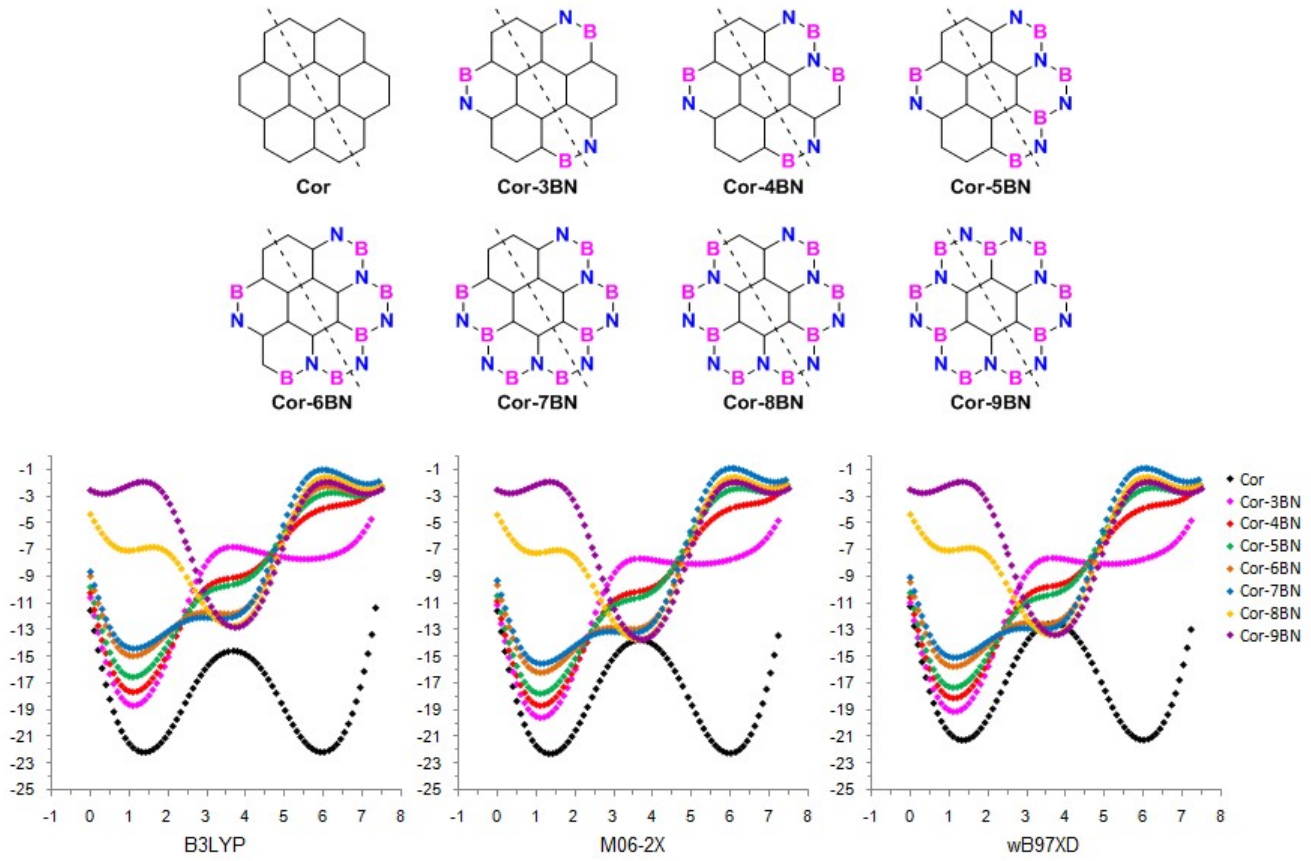


Figure S2. $NICS_{\pi zz}$-xy scans of coronene and its BN analogues calculated using different functionals and 6-311+G(d,p) basis set. The scan direction was along the dashed line starting from the upper-left ring. Distance from the ring plane was 1.7 Å. The x-axis shows the distance (Å) from the first Bq atom and the y-axis represents the NICS values (ppm). In the structures, the hydrogen atoms and double bonds are omitted.

S2. Comparison of the performance of different aromaticity indices

Figure S3 presents the correlation between the different electronic indices used in this work (FLU, PDI and $EDDB_P$), as well as between the electronic and structural HOMA indices, obtained at the ωB97XD/6-311+G(d,p) level of theory. Correlations were made separately for the central benzene ring, outer benzene, molecular perimeter and BN rings. The corresponding values can be found Table S6 and the correlation coefficients are also collected in Table S7. The data reveal that aromaticity of the outer benzene of the studied compounds is best described by the indices used, followed by the central ring. For the latter, the outlier point in the correlation graphs in Figure S3 belongs to coronene for all but PDI/FLU and EDDB/HOMA correlations. The two groups disagree on the degree of its aromaticity: either PDI and FLU underestimate it, or EDDB and HOMA overestimate it. We conclude that the central benzene of coronene is more influenced by the surrounding six rings than the more aromatic outer ring and is therefore more difficult to describe it with aromaticity indices. Nevertheless, a careful analysis of the numerical data shows that all indices show the same numerical trend for both type of benzene rings and can be considered safe for monitoring changes in the aromaticity of these rings. When the central ring of coronene is excluded from the correlation, the R^2 values become 0.9989 (PDI/FLU), 0.9364 (EDDB/FLU), 0.9230 (EDDB/PDI), 0.9981 (PDI/HOMA), 0.9991 (FLU/HOMA) and 0.9367 (EDDB/HOMA). Therefore, replacing the peripheral CC bonds with BN bonds reduces the effects of the outer rings on the central ring, so that its aromaticity becomes easier to describe.

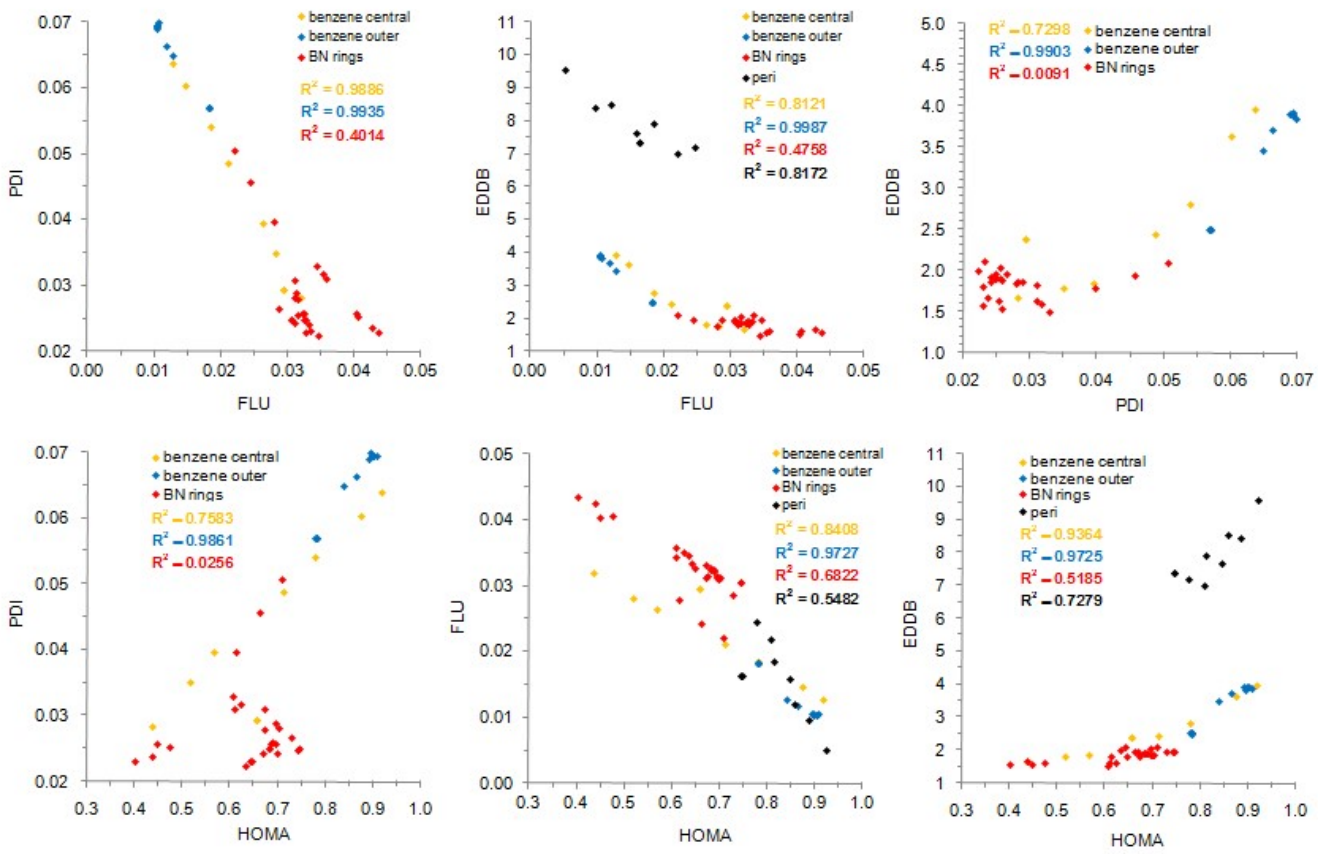
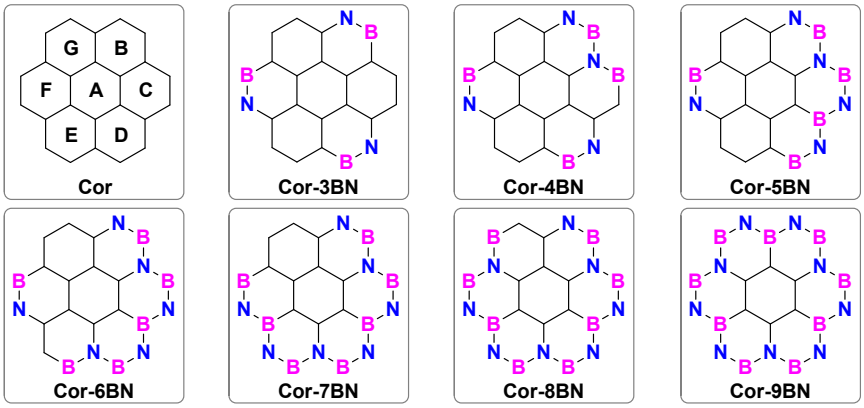


Figure S3. Correlations between different aromaticity indices calculated at the ωB97XD/6-311+G(d,p) level of theory.

Table S6. Calculated HOMA, FLU, PDI (e), $EDDB_P$ (e) and $NICS(1.7)_{\pi zz}$ (ppm) values for individual rings **A-G**, molecular perimeter (**peri**) and perimeter of carbocyclic subunits (**carbo-peri**) of coronene and its BN analogues at the wB97XD/6-311+G(d,p) level of theory.[a]



HOMA	A	B	C	D	E	F	G	peri	carbo-peri
Cor	0.657	0.782	0.782	0.782	0.782	0.782	0.782	0.746	/
Cor-3BN	0.437	0.607	0.896	0.607	0.896	0.607	0.896	0.777	0.782
Cor-4BN	0.518	0.729	0.710	0.449	0.898	0.624	0.908	0.809	0.765
Cor-5BN	0.568	0.698	0.672	0.403	0.893	0.610	0.904	0.813	0.782
Cor-6BN	0.712	0.744	0.696	0.643	0.662	0.476	0.865	0.847	0.793
Cor-7BN	0.781	0.745	0.703	0.634	0.674	0.439	0.840	0.858	0.818
Cor-8BN	0.875	0.647	0.690	0.671	0.687	0.695	0.614	0.887	/
Cor-9BN	0.919	0.682	0.683	0.682	0.683	0.682	0.683	0.922	/
FLU	**A**	**B**	**C**	**D**	**E**	**F**	**G**	**peri**	**carbo-peri**
Cor	0.0295	0.0183	0.0183	0.0183	0.0183	0.0183	0.0183	0.0163	/
Cor-3BN	0.0319	0.0343	0.0106	0.0343	0.0106	0.0343	0.0106	0.0246	0.0148
Cor-4BN	0.0282	0.0286	0.0220	0.0404	0.0104	0.0352	0.0105	0.0219	0.0156
Cor-5BN	0.0263	0.0311	0.0312	0.0435	0.0105	0.0357	0.0104	0.0185	0.0149
Cor-6BN	0.0211	0.0305	0.0312	0.0334	0.0243	0.0406	0.0118	0.0159	0.0157
Cor-7BN	0.0184	0.0305	0.0312	0.0346	0.0315	0.0426	0.0127	0.0120	0.0145
Cor-8BN	0.0147	0.0327	0.0324	0.0332	0.0322	0.0315	0.0279	0.0097	/
Cor-9BN	0.0127	0.0326	0.0326	0.0326	0.0326	0.0326	0.0326	0.0051	/
PDI	**A**	**B**	**C**	**D**	**E**	**F**	**G**		
Cor	0.0294	0.0570	0.0570	0.0570	0.0570	0.0570	0.0570		
Cor-3BN	0.0282	0.0329	0.0699	0.0329	0.0699	0.0329	0.0699		
Cor-4BN	0.0350	0.0265	0.0506	0.0257	0.0695	0.0318	0.0695		
Cor-5BN	0.0395	0.0242	0.0309	0.0230	0.0690	0.0310	0.0694		
Cor-6BN	0.0487	0.0247	0.0289	0.0231	0.0457	0.0252	0.0663		
Cor-7BN	0.0540	0.0249	0.0281	0.0223	0.0278	0.0236	0.0649		
Cor-8BN	0.0603	0.0229	0.0258	0.0241	0.0257	0.0256	0.0397		
Cor-9BN	0.0638	0.0249	0.0249	0.0249	0.0249	0.0249	0.0249		
$EDDB_P$	**A**	**B**	**C**	**D**	**E**	**F**	**G**	**peri**	**carbo-peri**
Cor	2.3764	2.4948	2.4948	2.4948	2.4948	2.4948	2.4948	7.3593	/
Cor-3BN	1.6609	1.4809	3.8357	1.4809	3.8357	1.4809	3.8357	7.1944	10.3483 (57%)
Cor-4BN	1.7831	1.9512	2.0933	1.5294	3.9013	1.5837	3.8746	7.0066	7.7252 (55%)
Cor-5BN	1.8307	1.8644	1.8080	1.5727	3.8857	1.6191	3.9127	7.9104	7.8968 (56%)
Cor-6BN	2.4379	1.9149	1.8587	2.0974	1.9385	1.6236	3.7024	7.6362	5.3560 (54%)
Cor-7BN	2.7955	1.9456	1.8595	1.9848	1.8434	1.6557	3.4524	8.5222	5.5307 (55%)
Cor-8BN	3.6334	1.8017	1.8683	1.9199	1.8870	2.0349	1.7859	8.4265	/
Cor-9BN	3.9429	1.8990	1.9029	1.8990	1.9029	1.8990	1.9029	9.5668	/
$NICS(1.7)_{\pi zz}$	**A**	**B**	**C**	**D**	**E**	**F**	**G**		

Cor	-12.46	-21.17	-21.17	-21.17	-21.17	-21.17	-21.17		
Cor-3BN	-7.58	-7.46	-19.08	-7.46	-19.08	-7.46	-19.08		
Cor-4BN	-9.70	-2.15	-11.17	-3.76	-18.49	-6.84	-18.07		
Cor-5BN	-10.32	0.54	-3.66	-2.40	-17.94	-6.53	-17.24		
Cor-6BN	-12.49	0.31	-2.96	-1.88	-9.33	-3.29	-15.72		
Cor-7BN	-12.89	-0.09	-2.38	-0.93	-3.17	-2.86	-15.06		
Cor-8BN	-13.32	0.12	-1.94	-1.60	-2.22	-2.62	-6.95		
Cor-9BN	-13.36	-1.88	-1.89	-1.88	-1.89	-1.88	-1.89		
[a] Percent values correspond to the number of delocalized electrons with respect to the total number of π-electrons.									

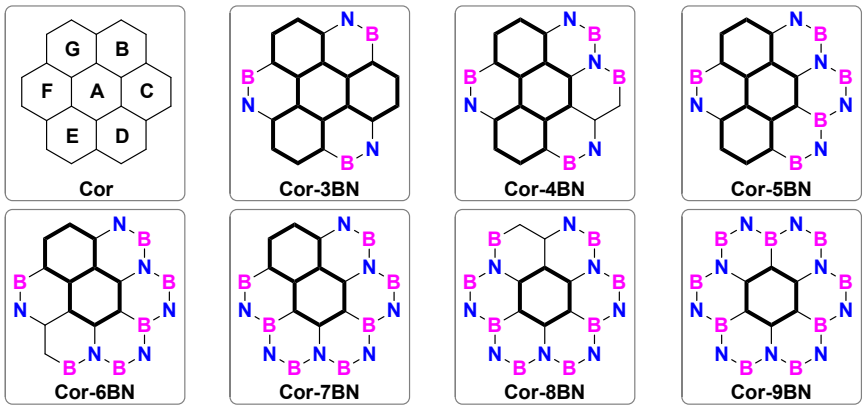
Table S7. Correlation coefficients between various aromaticity indices, calculated at the ωB97XD/6-311+G(d,p) level of theory.

	PDI/FLU	EDDB/FLU	EDDB/PDI	PDI/HOMA	FLU/HOMA	EDDB/HOMA
Central benzene ring	0.9886	0.8121	0.7298	0.7583	0.8408	0.9364
Outer benzene ring	0.9935	0.9987	0.9903	0.9861	0.9727	0.9725
BN rings	0.4014	0.4758	0.0091	0.0256	0.6822	0.5185
Molecular perimeter	/	0.8172	/	/	0.5482	0.7279

Table S7 and Figure S3 show that the agreement between the indices used to quantify aromaticity of molecular perimeter is worse. In particular, the effect of introduction of the first three BN units on peripheral aromaticity is described in the same way by FLU and EDDB, but differently by HOMA. Then, in BN coronenes, HOMA and FLU show the same trend with $R^2 = 0.9749$, while EDDB slightly disagrees showing some fluctuations in aromaticity (Table S6).

It is generally accepted that aromaticity of benzene consistently decreases with increasing number of BN units replacing its CC bonds. This change is attributed to electronegativity differences between boron, nitrogen and carbon atoms.[2] The agreement between the indices used to quantify the aromaticity of the BN rings of the studied compounds vary from poor (EDDB/PDI, HOMA/PDI and FLU/PDI) to moderate (EDDB/FLU, EDDB/HOMA and FLU/HOMA). Thus, the reduced aromaticity of the peripheral coronene rings after BN substitution, with subtle differences between them, appears to be better described by HOMA, FLU and EDDB, although there are linear PDI/FLU and PDI/HOMA correlations for a certain number of compounds (Figure S3).

Table S8. Calculated HOMA, FLU, PDI (e), $EDDB_P$ (e) and $NICS(1.7)_{\pi zz}$ (ppm) values for isolated reference carbocyclic compounds at the ωB97XD/6-311+G(d,p) level of theory. Carbocyclic subunits are marked with thick bonds in each BN-coronene.[a]



HOMA	**A**	**B**	**C**	**D**	**E**	**F**	**G**	**carbo-peri**
Triphenylene	0.128	/	0.936	/	0.936	/	0.936	0.682
Phenanthrene	0.482	/	/	/	0.905	/	0.905	0.745
Naphthalene	0.811	/	/	/	/	/	0.811	0.830
Benzene	0.998	/	/	/	/	/	/	0.998
FLU	**A**	**B**	**C**	**D**	**E**	**F**	**G**	**carbo-peri**
Triphenylene	0.0335	/	0.0051	/	0.0051	/	0.0051	0.0126
Phenanthrene	0.0263	/	/	/	0.0071	/	0.0071	0.0131
Naphthalene	0.0118	/	/	/	/	/	0.0118	0.0100
Benzene	0.0000	/	/	/	/	/	/	0.0000
PDI	**A**	**B**	**C**	**D**	**E**	**F**	**G**	
Triphenylene	0.0293	/	0.0882	/	0.0882	/	0.0882	/
Phenanthrene	0.0483	/	/	/	0.0842	/	0.0842	/
Naphthalene	0.0772	/	/	/	/	/	0.0772	/
Benzene	0.1045	/	/	/	/	/	/	/
$EDDB_P$	**A**	**B**	**C**	**D**	**E**	**F**	**G**	**carbo-peri**
Triphenylene	0.7747	/	4.3838	/	4.3838	/	4.3838	10.2968 (57%)
Phenanthrene	1.3965	/	/	/	3.9659	/	3.9659	7.3359 (52%)
Naphthalene	3.0415	/	/	/	/	/	3.0415	5.3350 (53%)
Benzene	5.4812	/	/	/	/	/	/	5.4812 (91%)
$NICS(1.7)_{\pi zz}$	**A**	**B**	**C**	**D**	**E**	**F**	**G**	
Triphenylene	-9.36	/	-16.38	/	-16.38	/	-16.38	
Phenanthrene	-14.20	/	/	/	-18.01	/	-18.01	
Naphthalene	-18.13	/	/	/	/	/	-18.13	
Benzene	-17.77	/	/	/	/	/	/	

[a] Percent values correspond to the number of delocalized electrons with respect to the total number of π-electrons.

Table S9. Energies (eV) of HOMO and LUMO orbitals and their difference (HOMO-LUMO energy gap) calculated with different functionals and 6-311+G(d,p) basis set.

	B3LYP-D3(BJ)			M06-2X			ωB97XD		
	HOMO	LUMO	energy gap	HOMO	LUMO	energy gap	HOMO	LUMO	energy gap
Cor	-5.78	-1.77	**4.01**	-6.88	-1.03	**5.84**	-7.45	-0.14	**7.31**
Cor-3BN	-5.87	-1.60	**4.27**	-6.99	-0.78	**6.21**	-7.60	0.11	**7.71**
Cor-4BN	-5.56	-1.90	**3.66**	-6.63	-1.08	**5.54**	-7.26	-0.21	**7.05**
Cor-5BN	-5.49	-1.76	**3.73**	-6.56	-0.93	**5.63**	-7.18	-0.05	**7.13**
Cor-6BN	-5.41	-1.87	**3.54**	-6.47	-1.04	**5.43**	-7.11	-0.16	**6.95**
Cor-7BN	-5.49	-1.61	**3.88**	-6.56	-0.74	**5.82**	-7.21	0.15	**7.35**
Cor-8BN	-5.79	-1.38	**4.41**	-6.94	-0.48	**6.46**	-7.60	0.41	**8.01**
Cor-9BN	-6.15	-0.89	**5.26**	-7.34	-0.12	**7.22**	-7.99	0.95	**8.94**
benzene	-7.08	-0.47	**6.61**	-8.42	0.45	**8.88**	-9.08	1.46	**10.54**
naphthalene	-6.15	-1.39	**4.75**	-7.38	-0.49	**6.89**	-8.02	0.44	**8.46**
phenanthrene	-6.09	-1.40	**4.69**	-7.30	-0.52	**6.78**	-7.93	0.40	**8.33**
triphenylene	-6.20	-1.36	**4.84**	-7.41	-0.51	**6.90**	-8.03	0.42	**8.46**

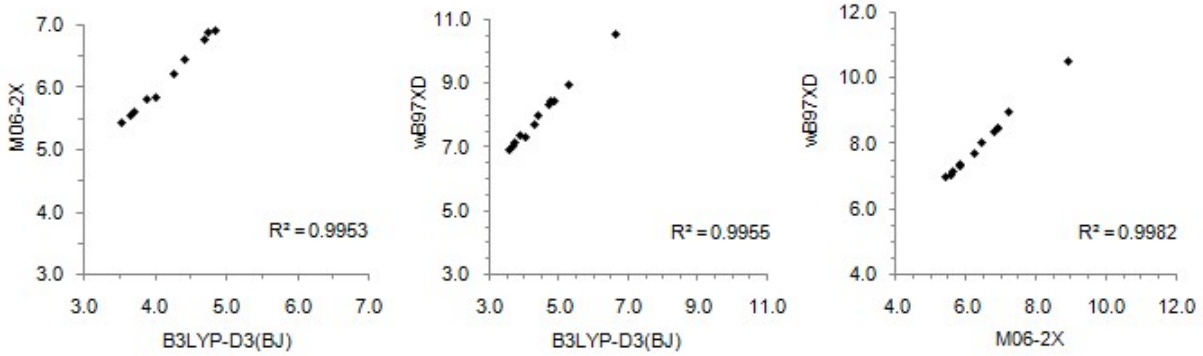


Figure S4. Correlations between HOMO-LUMO gaps calculated with different functionals and 6-311+G(d,p) basis set.

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2. a) M. Baranac-Stojanović, Aromaticity and Stability of Azaborines. *Chem. Eur. J.* **2014**, *20*, 16558-16565; b) R. Carion, V. Liégeois, B. Champagne, D. Bonifazi, S. Pelloni, P. Lazzeretti, On the Aromatic Character of 1,2-Dihydro-1,2-azaborine According to Magnetic Criteria. *J. Phys. Chem. Lett.* **2010**, *1*, 1563-1568; c) R. A. Iwaki, T. Udagawa, Effect of heteroatoms on aromaticity analyzed by geometric, magnetic, and electronic criteria. *Chem. Phys. Lett.* **2020**, *745*, 137271; d) M. d. R. Merino-García, L. A. Soriano-Agueda, J. d. D. Guzmán-Hernández, D. Martínez-Otero, B. L. Rivera, F. Cortés-Guzmán, J. E. Barquera-Lozada, V. Jancik, Benzene and Borazine, so Different, yet so Similar: Insight from Experimental Charge Density Analysis. *Inorg. Chem.* **2022**, *61*, 6785-6797.

Absolute energies (a.u.) and x, y, z coordinates of structures optimized using the ωB97XD functional and 6-311+G(d,p) basis set

Coronene (C_{2h})
E = -921.76968 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.244956	3.519733	0.000000
2	6	0	0.000000	2.832539	0.000000
3	6	0	0.000000	1.424527	0.000000
4	6	0	1.233586	0.712309	0.000000
5	6	0	2.452856	1.416347	0.000000
6	6	0	2.425403	2.838322	0.000000
7	6	0	-1.233586	0.712309	0.000000
8	6	0	1.233586	-0.712309	0.000000
9	6	0	0.000000	-1.424527	0.000000
10	6	0	-1.233586	-0.712309	0.000000
11	6	0	0.000000	-2.832539	0.000000
12	6	0	1.244956	-3.519733	0.000000
13	6	0	2.425403	-2.838322	0.000000
14	6	0	2.452856	-1.416347	0.000000
15	6	0	3.670414	-0.681546	0.000000
16	6	0	3.670414	0.681546	0.000000
17	1	0	4.608511	1.227054	0.000000
18	1	0	4.608511	-1.227055	0.000000
19	1	0	1.241017	4.604949	0.000000
20	1	0	3.367243	3.377333	0.000000
21	1	0	1.241017	-4.604949	0.000000
22	1	0	3.367243	-3.377333	0.000000
23	6	0	-1.244956	3.519733	0.000000
24	6	0	-2.425403	2.838322	0.000000
25	6	0	-2.452856	1.416347	0.000000
26	1	0	-1.241017	4.604949	0.000000
27	1	0	-3.367243	3.377333	0.000000
28	6	0	-3.670414	0.681546	0.000000
29	6	0	-3.670414	-0.681546	0.000000
30	6	0	-2.452856	-1.416347	0.000000
31	1	0	-4.608511	1.227055	0.000000
32	1	0	-4.608511	-1.227054	0.000000
33	6	0	-1.244956	-3.519733	0.000000
34	1	0	-1.241017	-4.604949	0.000000
35	6	0	-2.425403	-2.838322	0.000000
36	1	0	-3.367243	-3.377333	0.000000

Coronene (C_3)
E = -921.7696793 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.838257	-2.425456	0.000122
2	6	0	-1.416275	-2.452753	0.000043
3	6	0	-0.712277	-1.233543	-0.002241
4	6	0	-1.424558	-0.000028	0.002069

5	6	0	-2.832507	0.000000	0.000024
6	6	0	-3.519934	-1.245066	0.000286
7	6	0	0.712304	-1.233690	0.002069
8	6	0	-0.712141	1.233622	-0.002241
9	6	0	0.712255	1.233718	0.002069
10	6	0	1.424418	-0.000079	-0.002241
11	6	0	1.416254	2.453023	0.000024
12	6	0	0.681709	3.670885	0.000286
13	6	0	-0.681378	3.670731	0.000122
14	6	0	-1.416009	2.452907	0.000043
15	6	0	-2.838189	2.425417	-0.000382
16	6	0	-3.519900	1.245069	0.000006
17	1	0	-4.605003	1.240964	-0.000141
18	1	0	-3.377312	3.367163	-0.000074
19	1	0	-3.377343	-3.367262	0.000485
20	1	0	-4.605036	-1.241111	0.000167
21	1	0	1.227684	4.608634	0.000167
22	1	0	-1.227462	4.608496	0.000485
23	6	0	-0.681378	-3.670652	-0.000382
24	6	0	0.681688	-3.670858	0.000006
25	6	0	1.416253	-2.453023	0.000024
26	1	0	-1.227393	-4.608419	-0.000074
27	1	0	1.227796	-4.608532	-0.000141
28	6	0	2.838225	-2.425819	0.000286
29	6	0	3.519635	-1.245274	0.000122
30	6	0	2.832284	-0.000154	0.000043
31	1	0	3.377352	-3.367523	0.000167
32	1	0	4.604806	-1.241234	0.000485
33	6	0	2.838212	2.425788	0.000006
34	1	0	3.377208	3.367568	-0.000141
35	6	0	3.519567	1.245235	-0.000382
36	1	0	4.604705	1.241256	-0.000074

Cor-3BN

E = -932.1098344 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.425140	2.841061	0.000000
2	6	0	2.459738	1.438859	0.000000
3	6	0	1.236702	0.734051	0.000000
4	6	0	0.000000	1.426429	0.000000
5	6	0	0.018489	2.835483	0.000000
6	6	0	1.235553	3.530668	0.000000
7	6	0	1.235324	-0.713215	0.000000
8	6	0	-1.254058	0.703990	0.000000
9	6	0	-1.235324	-0.713215	0.000000
10	6	0	0.017356	-1.438041	0.000000
11	6	0	-2.464845	-1.401730	0.000000
12	6	0	-3.675424	-0.695314	0.000000
13	6	0	-3.673001	0.679702	0.000000
14	6	0	-2.475958	1.410766	0.000000
15	1	0	-1.072525	4.543224	0.000000
16	1	0	-3.422860	3.634387	0.000000
17	1	0	3.361711	3.389931	0.000000
18	1	0	1.223727	4.616488	0.000000
19	1	0	-4.609859	-1.248465	0.000000

20	1	0	-4.616622	1.216362	0.000000
21	6	0	2.446356	-1.433754	0.000000
22	1	0	4.858902	1.147090	0.000000
23	1	0	4.470810	-1.342778	0.000000
24	6	0	2.439872	-2.835354	0.000000
25	6	0	1.247861	-3.520763	0.000000
26	6	0	0.016220	-2.849625	0.000000
27	1	0	3.386132	-3.368023	0.000000
28	1	0	1.254911	-4.606293	0.000000
29	1	0	-3.398285	-3.200446	0.000000
30	1	0	-1.436041	-4.781477	0.000000
31	7	0	-1.173557	3.539559	0.000000
32	7	0	-2.478570	-2.786109	0.000000
33	7	0	3.652126	-0.753450	0.000000
34	5	0	-2.451967	2.938546	0.000000
35	5	0	-1.318872	-3.592739	0.000000
36	5	0	3.770839	0.654193	0.000000

Cor-4BN

E = -935.561233 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.666941	-0.675068	0.000000
2	6	0	2.476323	-1.404930	0.000000
3	6	0	1.247177	-0.702168	0.000000
4	6	0	1.226990	0.712601	0.000000
5	6	0	2.458609	1.398601	0.000000
6	6	0	3.667812	0.705220	0.000000
7	6	0	0.000000	-1.418484	0.000000
8	6	0	-0.027662	1.431260	0.000000
9	6	0	-1.233975	0.732917	0.000000
10	6	0	-1.229687	-0.716815	0.000000
11	6	0	-2.481108	1.468262	0.000000
12	6	0	-2.511053	2.841650	0.000000
13	1	0	3.343481	3.236070	0.000000
14	1	0	1.291350	4.717555	0.000000
15	1	0	4.612036	-1.208647	0.000000
16	1	0	4.599908	1.260884	0.000000
17	1	0	-3.484255	3.325724	0.000000
18	1	0	-1.123986	4.785681	0.000000
19	6	0	-0.016539	-2.833529	0.000000
20	1	0	3.427318	-3.626842	0.000000
21	1	0	1.079055	-4.537963	0.000000
22	6	0	-1.226142	-3.527761	0.000000
23	6	0	-2.415671	-2.828845	0.000000
24	6	0	-2.449079	-1.432683	0.000000
25	1	0	-1.219172	-4.613145	0.000000
26	1	0	-3.354257	-3.374048	0.000000
27	1	0	-4.492444	1.323928	0.000000
28	1	0	-4.848789	-1.166774	0.000000
29	7	0	2.443930	2.782506	0.000000
30	7	0	-3.666187	0.745316	0.000000
31	7	0	1.179282	-3.534264	0.000000
32	5	0	1.255237	3.532322	0.000000
33	5	0	-3.767434	-0.659699	0.000000
34	5	0	2.455444	-2.933285	0.000000

35	5	0	-1.230860	3.598339	0.000000
36	7	0	-0.001282	2.818986	0.000000

Cor-5BN

E = -939.0839759 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.666194	-0.738680	0.000000
2	6	0	-2.469923	-1.455929	0.000000
3	6	0	-1.247766	-0.736642	0.000000
4	6	0	-1.251001	0.679508	0.000000
5	6	0	-2.488852	1.353804	0.000000
6	6	0	-3.687038	0.645121	0.000000
7	6	0	0.006982	-1.438407	0.000000
8	6	0	0.000000	1.401078	0.000000
9	6	0	1.200909	0.726359	0.000000
10	6	0	1.222001	-0.714953	0.000000
11	1	0	-3.384787	3.187955	0.000000
12	1	0	-1.347891	4.689458	0.000000
13	1	0	-4.605830	-1.282369	0.000000
14	1	0	-4.627915	1.185932	0.000000
15	1	0	3.264464	3.511211	0.000000
16	1	0	1.093384	4.784315	0.000000
17	6	0	0.047714	-2.853633	0.000000
18	1	0	-3.386590	-3.693457	0.000000
19	1	0	-1.027441	-4.573250	0.000000
20	6	0	1.271475	-3.518300	0.000000
21	6	0	2.451323	-2.792245	0.000000
22	6	0	2.466024	-1.397079	0.000000
23	1	0	1.290710	-4.603724	0.000000
24	1	0	3.397230	-3.325675	0.000000
25	1	0	4.640482	1.304225	0.000000
26	1	0	4.856547	-1.192508	0.000000
27	7	0	-2.482309	2.740955	0.000000
28	7	0	3.767895	0.797280	0.000000
29	7	0	-1.140300	-3.570900	0.000000
30	5	0	-1.297068	3.502954	0.000000
31	5	0	3.802036	-0.621858	0.000000
32	5	0	-2.424493	-2.985447	0.000000
33	5	0	1.181243	3.596415	0.000000
34	7	0	-0.036858	2.808581	0.000000
35	7	0	2.430977	2.943100	0.000000
36	5	0	2.523858	1.510888	0.000000

Cor-6BN

E = -942.5428374 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.651592	-0.725227	0.000000
2	6	0	-2.463674	-1.442289	0.000000

3	6	0	-1.226904	-0.735892	0.000000
4	6	0	-1.237987	0.682051	0.000000
5	6	0	-2.481610	1.363612	0.000000
6	6	0	-3.676586	0.664416	0.000000
7	6	0	0.018275	-1.446529	0.000000
8	6	0	0.000000	1.395250	0.000000
9	6	0	1.204589	0.710552	0.000000
10	6	0	1.218298	-0.720237	0.000000
11	1	0	-3.364654	3.201851	0.000000
12	1	0	-1.319489	4.692464	0.000000
13	1	0	-4.591117	-1.269224	0.000000
14	1	0	-4.617759	1.204040	0.000000
15	1	0	3.283402	3.488550	0.000000
16	1	0	1.116235	4.774339	0.000000
17	6	0	0.045776	-2.896761	0.000000
18	1	0	-3.416117	-3.660821	0.000000
19	1	0	-1.070666	-4.577609	0.000000
20	6	0	1.227736	-3.587945	0.000000
21	1	0	1.182299	-4.674016	0.000000
22	1	0	3.594792	-3.332856	0.000000
23	1	0	4.636137	1.215067	0.000000
24	1	0	4.725445	-1.282443	0.000000
25	7	0	-2.464384	2.750146	0.000000
26	7	0	3.739211	0.754823	0.000000
27	7	0	-1.168470	-3.573617	0.000000
28	5	0	-1.277230	3.505887	0.000000
29	5	0	3.713062	-0.658489	0.000000
30	5	0	-2.440830	-2.970874	0.000000
31	5	0	1.198183	3.586622	0.000000
32	7	0	-0.021049	2.802921	0.000000
33	7	0	2.445304	2.927829	0.000000
34	5	0	2.520974	1.498228	0.000000
35	5	0	2.513586	-2.829968	0.000000
36	7	0	2.447223	-1.376727	0.000000

Cor-7BN

E = -946.0678844 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.457664	-2.791150	0.000000
2	6	0	-2.482422	-1.405053	0.000000
3	6	0	-1.235177	-0.705622	0.000000
4	6	0	-0.018451	-1.433053	0.000000
5	6	0	-0.058880	-2.852098	0.000000
6	6	0	-1.268284	-3.521587	0.000000
7	6	0	-1.219853	0.719031	0.000000
8	6	0	1.216576	-0.719860	0.000000
9	6	0	1.233859	0.670112	0.000000
10	6	0	0.000000	1.384181	0.000000
11	1	0	1.091613	-4.537963	0.000000
12	1	0	3.406411	-3.514333	0.000000
13	1	0	-3.400443	-3.330588	0.000000
14	1	0	-1.284758	-4.606581	0.000000
15	1	0	4.676343	1.076843	0.000000
16	1	0	4.700747	-1.439883	0.000000
17	1	0	-4.873445	-1.208453	0.000000

18	1	0	-4.659392	1.291272	0.000000
19	1	0	-3.271551	3.506716	0.000000
20	1	0	-1.108991	4.765200	0.000000
21	1	0	3.371385	3.397227	0.000000
22	1	0	1.250730	4.721300	0.000000
23	7	0	1.150939	-3.532412	0.000000
24	7	0	2.526526	2.847431	0.000000
25	7	0	-3.786755	0.784270	0.000000
26	5	0	2.400419	-2.882770	0.000000
27	5	0	1.285309	3.530839	0.000000
28	5	0	-3.820683	-0.634230	0.000000
29	5	0	3.712304	-0.775408	0.000000
30	7	0	2.425356	-1.442471	0.000000
31	7	0	3.769477	0.635821	0.000000
32	5	0	2.570006	1.418985	0.000000
33	5	0	-1.186316	3.576374	0.000000
34	7	0	0.036720	2.796103	0.000000
35	7	0	-2.443773	2.930773	0.000000
36	5	0	-2.542298	1.500857	0.000000

Cor-8BN

E = -949.5332997 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.236036	-0.710793	0.000000
2	6	0	0.025350	-1.443648	0.000000
3	6	0	0.052641	-2.893729	0.000000
4	6	0	1.222488	-3.594571	0.000000
5	6	0	1.225695	0.701684	0.000000
6	6	0	-1.196011	-0.726030	0.000000
7	6	0	-1.220953	0.674159	0.000000
8	6	0	0.000000	1.377978	0.000000
9	1	0	-1.136789	-4.536894	0.000000
10	1	0	-3.433391	-3.482408	0.000000
11	1	0	3.590839	-3.347938	0.000000
12	1	0	1.169332	-4.680016	0.000000
13	1	0	-4.664211	1.101836	0.000000
14	1	0	-4.692285	-1.414282	0.000000
15	1	0	4.738280	-1.302462	0.000000
16	1	0	4.655739	1.198835	0.000000
17	1	0	3.293018	3.482834	0.000000
18	1	0	1.134007	4.754709	0.000000
19	1	0	-3.347468	3.409728	0.000000
20	1	0	-1.218837	4.725412	0.000000
21	7	0	-1.180121	-3.530124	0.000000
22	7	0	-2.503971	2.857723	0.000000
23	7	0	3.758082	0.739812	0.000000
24	5	0	-2.418507	-2.865367	0.000000
25	5	0	-1.261939	3.535571	0.000000
26	5	0	3.728896	-0.673017	0.000000
27	5	0	-3.701775	-0.753206	0.000000
28	7	0	-2.419532	-1.427163	0.000000
29	7	0	-3.759077	0.657860	0.000000
30	5	0	-2.554894	1.429727	0.000000
31	5	0	1.205714	3.566182	0.000000
32	7	0	-0.019094	2.790436	0.000000

33	7	0	2.460180	2.914805	0.000000
34	5	0	2.541053	1.487261	0.000000
35	5	0	2.513811	-2.837064	0.000000
36	7	0	2.460461	-1.384791	0.000000

Cor-9BN

E = -953.0614075 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.697635	1.208258	0.000000
2	6	0	-1.416119	0.000000	0.000000
3	6	0	0.708060	1.226395	0.000000
4	6	0	-0.697565	-1.208299	0.000000
5	6	0	0.708060	-1.226395	0.000000
6	6	0	1.395200	0.000041	0.000000
7	1	0	-4.609861	-1.337986	0.000000
8	1	0	-3.401157	-3.528430	0.000000
9	1	0	-3.401157	3.528430	0.000000
10	1	0	-4.609861	1.337986	0.000000
11	1	0	1.146201	-4.661250	0.000000
12	1	0	-1.355132	-4.709703	0.000000
13	1	0	-1.355131	4.709703	0.000000
14	1	0	1.146201	4.661250	0.000000
15	1	0	3.463660	3.323264	0.000000
16	1	0	4.756289	1.181273	0.000000
17	1	0	3.463660	-3.323264	0.000000
18	1	0	4.756289	-1.181273	0.000000
19	5	0	-2.946180	0.000000	0.000000
20	5	0	-2.853674	-2.470509	0.000000
21	5	0	-0.712725	-3.706367	0.000000
22	5	0	-2.853445	2.470421	0.000000
23	5	0	-0.712687	3.706609	0.000000
24	5	0	1.473090	2.551467	0.000000
25	5	0	3.566170	1.235946	0.000000
26	5	0	3.566361	-1.236100	0.000000
27	5	0	1.473090	-2.551467	0.000000
28	7	0	-1.404647	-2.432743	0.000000
29	7	0	-3.604041	-1.270045	0.000000
30	7	0	-3.604041	1.270045	0.000000
31	7	0	-1.404494	2.432832	0.000000
32	7	0	0.702129	3.756214	0.000000
33	7	0	2.901912	2.486169	0.000000
34	7	0	2.809141	-0.000089	0.000000
35	7	0	2.901912	-2.486169	0.000000
36	7	0	0.702129	-3.756214	0.000000

Benzene

E = -232.2209145 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.390845	0.000000
2	6	0	1.204507	0.695423	0.000000

3	6	0	1.204507	-0.695423	0.000000
4	6	0	0.000000	-1.390845	0.000000
5	6	0	-1.204507	-0.695423	0.000000
6	6	0	-1.204507	0.695423	0.000000
7	1	0	0.000000	2.475315	0.000000
8	1	0	2.143686	1.237658	0.000000
9	1	0	2.143686	-1.237658	0.000000
10	1	0	0.000000	-2.475315	0.000000
11	1	0	-2.143686	-1.237658	0.000000
12	1	0	-2.143686	1.237658	0.000000

Naphthalene

E = -385.8430462 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-2.423063	-0.706912
2	6	0	0.000000	-1.241437	-1.396633
3	6	0	0.000000	0.000000	-0.710665
4	6	0	0.000000	0.000000	0.710665
5	6	0	0.000000	-1.241437	1.396633
6	6	0	0.000000	-2.423063	0.706912
7	1	0	0.000000	1.239064	-2.482169
8	1	0	0.000000	-3.365755	-1.242693
9	1	0	0.000000	-1.239064	-2.482169
10	6	0	0.000000	1.241437	-1.396633
11	6	0	0.000000	1.241437	1.396633
12	1	0	0.000000	-1.239064	2.482169
13	1	0	0.000000	-3.365755	1.242693
14	6	0	0.000000	2.423063	0.706912
15	6	0	0.000000	2.423063	-0.706912
16	1	0	0.000000	1.239064	2.482169
17	1	0	0.000000	3.365755	1.242693
18	1	0	0.000000	3.365755	-1.242693

Phenanthrene

E= -539.4689893 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-3.545961	-0.295539
2	6	0	0.000000	-2.826019	0.874098
3	6	0	0.000000	-1.416170	0.859089
4	6	0	0.000000	-0.728336	-0.376070
5	6	0	0.000000	-1.493770	-1.560578
6	6	0	0.000000	-2.869044	-1.524086
7	6	0	0.000000	-0.674779	2.088468
8	6	0	0.000000	0.728336	-0.376070
9	6	0	0.000000	1.416170	0.859089
10	6	0	0.000000	0.674779	2.088468
11	6	0	0.000000	2.826019	0.874098
12	1	0	0.000000	3.335900	1.832231
13	6	0	0.000000	3.545961	-0.295539
14	6	0	0.000000	2.869044	-1.524086

15	6	0	0.000000	1.493770	-1.560578
16	1	0	0.000000	-1.226363	3.023041
17	1	0	0.000000	-4.629771	-0.271635
18	1	0	0.000000	-3.335900	1.832231
19	1	0	0.000000	-1.001292	-2.524694
20	1	0	0.000000	-3.431115	-2.451235
21	1	0	0.000000	1.226363	3.023041
22	1	0	0.000000	4.629771	-0.271635
23	1	0	0.000000	3.431115	-2.451235
24	1	0	0.000000	1.001292	-2.524694

Triphenylene

E = -693.0932701 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.697695	3.687138	0.000000
2	6	0	-1.377692	2.489934	0.000000
3	6	0	-0.704391	1.254001	0.000000
4	6	0	0.704391	1.254001	0.000000
5	6	0	1.377692	2.489934	0.000000
6	6	0	0.697695	3.687138	0.000000
7	6	0	-1.438192	-0.016980	0.000000
8	6	0	1.438192	-0.016980	0.000000
9	6	0	0.733801	-1.237021	0.000000
10	6	0	-0.733801	-1.237021	0.000000
11	6	0	1.467500	-2.438083	0.000000
12	6	0	2.844308	-2.447791	0.000000
13	6	0	3.542003	-1.239348	0.000000
14	6	0	2.845192	-0.051851	0.000000
15	1	0	-1.247156	4.621556	0.000000
16	1	0	1.247156	4.621556	0.000000
17	1	0	3.378807	-3.390846	0.000000
18	1	0	4.625963	-1.230709	0.000000
19	6	0	-2.845192	-0.051851	0.000000
20	6	0	-3.542003	-1.239348	0.000000
21	6	0	-2.844308	-2.447791	0.000000
22	6	0	-1.467500	-2.438083	0.000000
23	1	0	-4.625963	-1.230709	0.000000
24	1	0	-3.378807	-3.390846	0.000000
25	1	0	-0.951759	-3.388551	0.000000
26	1	0	0.951759	-3.388551	0.000000
27	1	0	3.410451	0.870028	0.000000
28	1	0	2.458692	2.518523	0.000000
29	1	0	-2.458692	2.518523	0.000000
30	1	0	-3.410451	0.870028	0.000000

Absolute energies (a.u.) and x, y, z coordinates of structures optimized using the B3LYP-D3(BJ) functional and 6-311+G(d,p) basis set

Coronene (C_3)

E = -922.20533 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.346493	3.490807	0.000140
2	6	0	-1.848165	2.160409	-0.000050
3	6	0	-0.926250	1.082676	0.001911
4	6	0	0.474542	1.343441	-0.002045
5	6	0	0.946836	2.680777	-0.000054
6	6	0	0.000000	3.741480	-0.000017
7	6	0	-1.400725	-0.260755	-0.002045
8	6	0	1.400750	0.260817	0.001911
9	6	0	0.926183	-1.082686	-0.002045
10	6	0	-0.474500	-1.343494	0.001911
11	6	0	1.848203	-2.160373	-0.000054
12	6	0	3.240217	-1.870740	-0.000017
13	6	0	3.696374	-0.579307	0.000140
14	6	0	2.795052	0.520353	-0.000050
15	6	0	3.240174	1.870864	0.000071
16	6	0	2.349834	2.911597	-0.000020
17	1	0	2.707759	3.935416	0.000270
18	1	0	4.306999	2.066229	-0.000190
19	1	0	-2.054014	4.312832	-0.000031
20	1	0	0.364424	4.762990	0.000337
21	1	0	3.942658	-2.697095	0.000337
22	1	0	4.762029	-0.377588	-0.000031
23	6	0	-3.240303	1.870641	0.000071
24	6	0	-3.696434	0.579217	-0.000020
25	6	0	-2.795039	-0.520405	-0.000054
26	1	0	-3.942906	2.696856	-0.000190
27	1	0	-4.762050	0.377280	0.000270
28	6	0	-3.240217	-1.870740	-0.000017
29	6	0	-2.349881	-2.911500	0.000140
30	6	0	-0.946887	-2.680762	-0.000050
31	1	0	-4.307082	-2.065895	0.000337
32	1	0	-2.708015	-3.935244	-0.000031
33	6	0	1.346600	-3.490814	-0.000020
34	1	0	2.054291	-4.312697	0.000270
35	6	0	0.000129	-3.741505	0.000071
36	1	0	-0.364093	-4.763085	-0.000190

Cor-3BN

E = -932.5406516 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.435310	2.843340	0.000000
2	6	0	2.470037	1.437963	0.000000
3	6	0	1.240094	0.730063	0.000000
4	6	0	0.000000	1.427046	0.000000

5	6	0	0.021621	2.842963	0.000000
6	6	0	1.242304	3.536125	0.000000
7	6	0	1.235858	-0.713523	0.000000
8	6	0	-1.252300	0.708921	0.000000
9	6	0	-1.235858	-0.713523	0.000000
10	6	0	0.012206	-1.438985	0.000000
11	6	0	-2.472889	-1.402757	0.000000
12	6	0	-3.683526	-0.692196	0.000000
13	6	0	-3.680060	0.687371	0.000000
14	6	0	-2.480331	1.420133	0.000000
15	1	0	-1.069777	4.551029	0.000000
16	1	0	-3.419398	3.640781	0.000000
17	1	0	3.371537	3.390871	0.000000
18	1	0	1.231753	4.621409	0.000000
19	1	0	-4.618134	-1.243975	0.000000
20	1	0	-4.622349	1.224401	0.000000
21	6	0	2.451267	-1.440206	0.000000
22	1	0	4.862708	1.140896	0.000000
23	1	0	4.476195	-1.349060	0.000000
24	6	0	2.441222	-2.843929	0.000000
25	6	0	1.244749	-3.530711	0.000000
26	6	0	0.010294	-2.858096	0.000000
27	1	0	3.386381	-3.377434	0.000000
28	1	0	1.250812	-4.615272	0.000000
29	1	0	-3.406418	-3.201968	0.000000
30	1	0	-1.443309	-4.781676	0.000000
31	7	0	-1.172563	3.545885	0.000000
32	7	0	-2.484545	-2.788412	0.000000
33	7	0	3.657108	-0.757473	0.000000
34	5	0	-2.454383	2.943856	0.000000
35	5	0	-1.322263	-3.597486	0.000000
36	5	0	3.776646	0.653630	0.000000

Cor-4BN

E = -935.9920366 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.675017	0.681123	0.000000
2	6	0	-2.480781	1.413625	0.000000
3	6	0	-1.246104	0.707166	0.000000
4	6	0	-1.227899	-0.714754	0.000000
5	6	0	-2.466180	-1.400875	0.000000
6	6	0	-3.676531	-0.702497	0.000000
7	6	0	0.000000	1.419817	0.000000
8	6	0	0.021236	-1.434278	0.000000
9	6	0	1.237159	-0.732879	0.000000
10	6	0	1.235180	0.713940	0.000000
11	6	0	2.483426	-1.470075	0.000000
12	6	0	2.508759	-2.849319	0.000000
13	1	0	-3.351826	-3.239144	0.000000
14	1	0	-1.297743	-4.721160	0.000000
15	1	0	-4.618735	1.215548	0.000000
16	1	0	-4.608052	-1.258590	0.000000
17	1	0	3.481997	-3.332944	0.000000
18	1	0	1.125657	-4.789923	0.000000
19	6	0	0.019252	2.840269	0.000000

20	1	0	-3.425430	3.631295	0.000000
21	1	0	-1.076288	4.545047	0.000000
22	6	0	1.233910	3.533620	0.000000
23	6	0	2.426097	2.833087	0.000000
24	6	0	2.460566	1.432397	0.000000
25	1	0	1.226068	4.618618	0.000000
26	1	0	3.364169	3.377591	0.000000
27	1	0	4.495910	-1.330785	0.000000
28	1	0	4.853906	1.162318	0.000000
29	7	0	-2.449918	-2.786386	0.000000
30	7	0	3.670431	-0.748029	0.000000
31	7	0	-1.178156	3.539735	0.000000
32	5	0	-1.260161	-3.540025	0.000000
33	5	0	3.774492	0.660099	0.000000
34	5	0	-2.458362	2.937861	0.000000
35	5	0	1.231441	-3.606907	0.000000
36	7	0	-0.003088	-2.827492	0.000000

Cor-5BN

E = -939.5122935 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.676740	-0.731135	0.000000
2	6	0	-2.479087	-1.455323	0.000000
3	6	0	-1.249335	-0.736877	0.000000
4	6	0	-1.249193	0.686383	0.000000
5	6	0	-2.490266	1.365009	0.000000
6	6	0	-3.692719	0.655738	0.000000
7	6	0	0.002242	-1.439386	0.000000
8	6	0	0.000000	1.404142	0.000000
9	6	0	1.207929	0.722893	0.000000
10	6	0	1.225983	-0.715784	0.000000
11	1	0	-3.381210	3.203185	0.000000
12	1	0	-1.336381	4.697529	0.000000
13	1	0	-4.616976	-1.272108	0.000000
14	1	0	-4.631208	1.200146	0.000000
15	1	0	3.277196	3.503815	0.000000
16	1	0	1.111261	4.783667	0.000000
17	6	0	0.039750	-2.859426	0.000000
18	1	0	-3.398608	-3.684113	0.000000
19	1	0	-1.041167	-4.575888	0.000000
20	6	0	1.266383	-3.528319	0.000000
21	6	0	2.451185	-2.805568	0.000000
22	6	0	2.472272	-1.405555	0.000000
23	1	0	1.280263	-4.613446	0.000000
24	1	0	3.394639	-3.341548	0.000000
25	1	0	4.646409	1.293421	0.000000
26	1	0	4.856804	-1.204614	0.000000
27	7	0	-2.477971	2.753951	0.000000
28	7	0	3.772003	0.785821	0.000000
29	7	0	-1.152043	-3.571562	0.000000
30	5	0	-1.289463	3.515059	0.000000
31	5	0	3.805921	-0.635745	0.000000
32	5	0	-2.438005	-2.980732	0.000000
33	5	0	1.193294	3.599665	0.000000
34	7	0	-0.030264	2.816245	0.000000

35	7	0	2.439655	2.938314	0.000000
36	5	0	2.530029	1.503718	0.000000

Cor-6BN

E = -942.9705586 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.662739	-0.720077	0.000000
2	6	0	-2.471803	-1.444213	0.000000
3	6	0	-1.230060	-0.738218	0.000000
4	6	0	-1.237953	0.687182	0.000000
5	6	0	-2.483223	1.371929	0.000000
6	6	0	-3.683198	0.671067	0.000000
7	6	0	0.014714	-1.450037	0.000000
8	6	0	0.000000	1.398791	0.000000
9	6	0	1.210775	0.708683	0.000000
10	6	0	1.223523	-0.721340	0.000000
11	1	0	-3.363590	3.213652	0.000000
12	1	0	-1.312616	4.699210	0.000000
13	1	0	-4.602322	-1.262258	0.000000
14	1	0	-4.621654	1.214785	0.000000
15	1	0	3.293863	3.482457	0.000000
16	1	0	1.128695	4.774505	0.000000
17	6	0	0.039631	-2.899033	0.000000
18	1	0	-3.423662	-3.656339	0.000000
19	1	0	-1.078733	-4.580056	0.000000
20	6	0	1.227116	-3.593868	0.000000
21	1	0	1.177641	-4.679517	0.000000
22	1	0	3.591572	-3.344149	0.000000
23	1	0	4.641285	1.210250	0.000000
24	1	0	4.727858	-1.291417	0.000000
25	7	0	-2.462058	2.760616	0.000000
26	7	0	3.743840	0.746945	0.000000
27	7	0	-1.177095	-3.574319	0.000000
28	5	0	-1.272610	3.516916	0.000000
29	5	0	3.720584	-0.667593	0.000000
30	5	0	-2.451641	-2.968979	0.000000
31	5	0	1.207532	3.591053	0.000000
32	7	0	-0.016685	2.810138	0.000000
33	7	0	2.451456	2.924766	0.000000
34	5	0	2.525267	1.492794	0.000000
35	5	0	2.513986	-2.842885	0.000000
36	7	0	2.452741	-1.384269	0.000000

Cor-7BN

E = -946.492969 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.459048	-2.803067	0.000000
2	6	0	-2.488223	-1.410677	0.000000
3	6	0	-1.239963	-0.706684	0.000000
4	6	0	-0.014912	-1.435168	0.000000

5	6	0	-0.052691	-2.856268	0.000000
6	6	0	-1.266448	-3.529928	0.000000
7	6	0	-1.225397	0.718664	0.000000
8	6	0	1.219802	-0.720996	0.000000
9	6	0	1.235678	0.676086	0.000000
10	6	0	0.000000	1.389309	0.000000
11	1	0	1.100805	-4.542255	0.000000
12	1	0	3.414476	-3.512796	0.000000
13	1	0	-3.399774	-3.344169	0.000000
14	1	0	-1.278538	-4.614653	0.000000
15	1	0	4.676788	1.087708	0.000000
16	1	0	4.707542	-1.428932	0.000000
17	1	0	-4.873044	-1.215327	0.000000
18	1	0	-4.663246	1.285099	0.000000
19	1	0	-3.281052	3.503504	0.000000
20	1	0	-1.120289	4.766750	0.000000
21	1	0	3.369184	3.404984	0.000000
22	1	0	1.245954	4.727299	0.000000
23	7	0	1.160337	-3.535020	0.000000
24	7	0	2.522128	2.855106	0.000000
25	7	0	-3.788972	0.777125	0.000000
26	5	0	2.411486	-2.884426	0.000000
27	5	0	1.281429	3.541261	0.000000
28	5	0	-3.823600	-0.643578	0.000000
29	5	0	3.720537	-0.770185	0.000000
30	7	0	2.433984	-1.442580	0.000000
31	7	0	3.770039	0.642199	0.000000
32	5	0	2.567771	1.425040	0.000000
33	5	0	-1.194701	3.582171	0.000000
34	7	0	0.032412	2.804081	0.000000
35	7	0	-2.449360	2.929894	0.000000
36	5	0	-2.546035	1.497619	0.000000

Cor-8BN

E = -949.956896 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.240826	-0.712163	0.000000
2	6	0	0.024078	-1.447343	0.000000
3	6	0	0.049969	-2.895000	0.000000
4	6	0	1.225908	-3.597906	0.000000
5	6	0	1.229981	0.703328	0.000000
6	6	0	-1.200631	-0.727420	0.000000
7	6	0	-1.224312	0.677696	0.000000
8	6	0	0.000000	1.383074	0.000000
9	1	0	-1.139035	-4.541867	0.000000
10	1	0	-3.437380	-3.485013	0.000000
11	1	0	3.590096	-3.355180	0.000000
12	1	0	1.171365	-4.683048	0.000000
13	1	0	-4.666382	1.107101	0.000000
14	1	0	-4.698041	-1.409758	0.000000
15	1	0	4.741611	-1.304439	0.000000
16	1	0	4.659136	1.198790	0.000000
17	1	0	3.298613	3.482942	0.000000
18	1	0	1.140236	4.757432	0.000000
19	1	0	-3.349376	3.413339	0.000000

20	1	0	-1.219678	4.729607	0.000000
21	7	0	-1.185169	-3.533606	0.000000
22	7	0	-2.503153	2.862045	0.000000
23	7	0	3.760798	0.736917	0.000000
24	5	0	-2.425849	-2.870452	0.000000
25	5	0	-1.262378	3.544106	0.000000
26	5	0	3.735909	-0.677196	0.000000
27	5	0	-3.709967	-0.752891	0.000000
28	7	0	-2.427318	-1.430080	0.000000
29	7	0	-3.760975	0.659440	0.000000
30	5	0	-2.554931	1.432152	0.000000
31	5	0	1.210025	3.573144	0.000000
32	7	0	-0.017725	2.798415	0.000000
33	7	0	2.462591	2.916215	0.000000
34	5	0	2.543023	1.486588	0.000000
35	5	0	2.516964	-2.846107	0.000000
36	7	0	2.466656	-1.389664	0.000000

Cor-9BN

E = -953.4826925 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.399872	0.000000
2	6	0	1.230098	0.710198	0.000000
3	6	0	-1.230098	0.710198	0.000000
4	6	0	1.212325	-0.699936	0.000000
5	6	0	0.000000	-1.420395	0.000000
6	6	0	-1.212325	-0.699936	0.000000
7	1	0	4.663870	1.149165	0.000000
8	1	0	4.713391	-1.354752	0.000000
9	1	0	1.183446	4.759292	0.000000
10	1	0	3.327141	3.464447	0.000000
11	1	0	1.336729	-4.613612	0.000000
12	1	0	3.529945	-3.404540	0.000000
13	1	0	-1.183446	4.759292	0.000000
14	1	0	-3.327141	3.464447	0.000000
15	1	0	-4.663870	1.149165	0.000000
16	1	0	-4.713391	-1.354752	0.000000
17	1	0	-1.336729	-4.613612	0.000000
18	1	0	-3.529945	-3.404540	0.000000
19	5	0	2.551961	1.473376	0.000000
20	5	0	3.714298	-0.714385	0.000000
21	5	0	2.475825	-2.859484	0.000000
22	5	0	1.238473	3.573869	0.000000
23	5	0	-1.238473	3.573869	0.000000
24	5	0	-2.551961	1.473376	0.000000
25	5	0	-3.714298	-0.714385	0.000000
26	5	0	-2.475825	-2.859484	0.000000
27	5	0	0.000000	-2.946751	0.000000
28	7	0	2.439214	-1.408281	0.000000
29	7	0	3.758466	0.701483	0.000000
30	7	0	2.486735	2.904185	0.000000
31	7	0	0.000000	2.816561	0.000000
32	7	0	-2.486735	2.904185	0.000000
33	7	0	-3.758466	0.701483	0.000000
34	7	0	-2.439214	-1.408281	0.000000

35	7	0	-1.271731	-3.605668	0.000000
36	7	0	1.271731	-3.605668	0.000000

Benzene

E = -232.3301645 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.393673	0.000000
2	6	0	1.206956	0.696836	0.000000
3	6	0	1.206956	-0.696836	0.000000
4	6	0	0.000000	-1.393673	0.000000
5	6	0	-1.206956	-0.696836	0.000000
6	6	0	-1.206956	0.696836	0.000000
7	1	0	0.000000	2.477417	0.000000
8	1	0	2.145506	1.238709	0.000000
9	1	0	2.145506	-1.238709	0.000000
10	1	0	0.000000	-2.477417	0.000000
11	1	0	-2.145506	-1.238709	0.000000
12	1	0	-2.145506	1.238709	0.000000

Naphthalene

E = -386.0253963 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-2.428658	-0.707261
2	6	0	0.000000	-1.242423	-1.400144
3	6	0	0.000000	0.000000	-0.715450
4	6	0	0.000000	0.000000	0.715450
5	6	0	0.000000	-1.242423	1.400144
6	6	0	0.000000	-2.428658	0.707261
7	1	0	0.000000	1.240326	-2.484981
8	1	0	0.000000	-3.370768	-1.243320
9	1	0	0.000000	-1.240326	-2.484981
10	6	0	0.000000	1.242423	-1.400144
11	6	0	0.000000	1.242423	1.400144
12	1	0	0.000000	-1.240326	2.484981
13	1	0	0.000000	-3.370768	1.243320
14	6	0	0.000000	2.428658	0.707261
15	6	0	0.000000	2.428658	-0.707261
16	1	0	0.000000	1.240326	2.484981
17	1	0	0.000000	3.370768	1.243320
18	1	0	0.000000	3.370768	-1.243320

Phenanthrene

E = -539.7235154 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-3.552548	-0.297476

2	6	0	0.000000	-2.831890	0.876750
3	6	0	0.000000	-1.419745	0.865172
4	6	0	0.000000	-0.726911	-0.378053
5	6	0	0.000000	-1.493800	-1.563560
6	6	0	0.000000	-2.873389	-1.528001
7	6	0	0.000000	-0.678322	2.091247
8	6	0	0.000000	0.726911	-0.378053
9	6	0	0.000000	1.419745	0.865172
10	6	0	0.000000	0.678322	2.091247
11	6	0	0.000000	2.831890	0.876750
12	1	0	0.000000	3.342553	1.833801
13	6	0	0.000000	3.552548	-0.297476
14	6	0	0.000000	2.873389	-1.528001
15	6	0	0.000000	1.493800	-1.563560
16	1	0	0.000000	-1.229673	3.025285
17	1	0	0.000000	-4.635971	-0.275156
18	1	0	0.000000	-3.342553	1.833801
19	1	0	0.000000	-0.999165	-2.525644
20	1	0	0.000000	-3.435334	-2.454759
21	1	0	0.000000	1.229673	3.025285
22	1	0	0.000000	4.635971	-0.275156
23	1	0	0.000000	3.435334	-2.454759
24	1	0	0.000000	0.999165	-2.525644

Triphenylene

E = -693.4194058 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.699588	3.693421	0.000000
2	6	0	-1.381871	2.493438	0.000000
3	6	0	-0.708599	1.254066	0.000000
4	6	0	0.708599	1.254066	0.000000
5	6	0	1.381871	2.493438	0.000000
6	6	0	0.699588	3.693421	0.000000
7	6	0	-1.440352	-0.013369	0.000000
8	6	0	1.440352	-0.013369	0.000000
9	6	0	0.731754	-1.240697	0.000000
10	6	0	-0.731754	-1.240697	0.000000
11	6	0	1.468445	-2.443454	0.000000
12	6	0	2.848802	-2.452572	0.000000
13	6	0	3.548391	-1.240849	0.000000
14	6	0	2.850316	-0.049983	0.000000
15	1	0	-1.248101	4.627949	0.000000
16	1	0	1.248101	4.627949	0.000000
17	1	0	3.383871	-3.394862	0.000000
18	1	0	4.631972	-1.233087	0.000000
19	6	0	-2.850316	-0.049983	0.000000
20	6	0	-3.548391	-1.240849	0.000000
21	6	0	-2.848802	-2.452572	0.000000
22	6	0	-1.468445	-2.443454	0.000000
23	1	0	-4.631972	-1.233087	0.000000
24	1	0	-3.383871	-3.394862	0.000000
25	1	0	-0.951347	-3.392280	0.000000
26	1	0	0.951347	-3.392280	0.000000
27	1	0	3.413474	0.872249	0.000000
28	1	0	2.462127	2.520030	0.000000

29	1	0	-2.462127	2.520030	0.000000
30	1	0	-3.413474	0.872249	0.000000

Absolute energies (a.u.) and x, y, z coordinates of structures optimized using the M06-2X functional and 6-311+G(d,p) basis set

Coronene (C_3)

E = -921.737221 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.342125	3.487042	0.000254
2	6	0	1.842104	2.154624	0.000608
3	6	0	0.925933	1.082970	-0.004039
4	6	0	-0.475021	1.343496	0.003688
5	6	0	-0.945095	2.672517	-0.000572
6	6	0	0.000000	3.736529	0.000026
7	6	0	1.401012	-0.260367	0.003688
8	6	0	-1.400846	0.260397	-0.004039
9	6	0	-0.925991	-1.083128	0.003688
10	6	0	0.474912	-1.343367	-0.004039
11	6	0	-1.841920	-2.154734	-0.000572
12	6	0	-3.235929	-1.868264	0.000026
13	6	0	-3.690929	-0.581207	0.000254
14	6	0	-2.787011	0.517997	0.000608
15	6	0	-3.235865	1.868506	0.000077
16	6	0	-2.348963	2.906072	-0.000103
17	1	0	-2.704640	3.930836	-0.000951
18	1	0	-4.303472	2.060446	0.000905
19	1	0	2.051827	4.307478	0.001187
20	1	0	-0.367256	4.757216	-0.000779
21	1	0	-3.936242	-2.696661	-0.000779
22	1	0	-4.756299	-0.376805	0.001187
23	6	0	3.236106	1.868088	0.000077
24	6	0	3.691214	0.581226	-0.000103
25	6	0	2.787015	-0.517783	-0.000572
26	1	0	3.936135	2.696693	0.000905
27	1	0	4.756524	0.376869	-0.000951
28	6	0	3.235929	-1.868264	0.000026
29	6	0	2.348804	-2.905835	0.000254
30	6	0	0.944907	-2.672621	0.000608
31	1	0	4.303498	-2.060555	-0.000779
32	1	0	2.704472	-3.930673	0.001187
33	6	0	-1.342251	-3.487298	-0.000103
34	1	0	-2.051884	-4.307705	-0.000951
35	6	0	-0.000241	-3.736594	0.000077
36	1	0	0.367338	-4.757139	0.000905

Cor-3BN

E = -932.078611 a.u.

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	2.427251	2.842220	0.000000
2	6	0	2.461360	1.439664	0.000000
3	6	0	1.237734	0.734469	0.000000
4	6	0	0.000000	1.426626	0.000000
5	6	0	0.018236	2.837255	0.000000
6	6	0	1.235664	3.533236	0.000000
7	6	0	1.235494	-0.713313	0.000000
8	6	0	-1.254936	0.704675	0.000000
9	6	0	-1.235494	-0.713313	0.000000
10	6	0	0.017201	-1.439144	0.000000
11	6	0	-2.466253	-1.402834	0.000000
12	6	0	-3.677704	-0.696502	0.000000
13	6	0	-3.675060	0.680950	0.000000
14	6	0	-2.477466	1.411769	0.000000
15	1	0	-1.070972	4.546126	0.000000
16	1	0	-3.422265	3.633000	0.000000
17	1	0	3.363622	3.390195	0.000000
18	1	0	1.222240	4.618231	0.000000
19	1	0	-4.610625	-1.250624	0.000000
20	1	0	-4.617806	1.217884	0.000000
21	6	0	2.448017	-1.434421	0.000000
22	1	0	4.857403	1.147268	0.000000
23	1	0	4.472547	-1.345574	0.000000
24	6	0	2.442041	-2.836734	0.000000
25	6	0	1.247810	-3.523171	0.000000
26	6	0	0.016106	-2.851433	0.000000
27	1	0	3.388385	-3.367606	0.000000
28	1	0	1.254184	-4.608079	0.000000
29	1	0	-3.401575	-3.200552	0.000000
30	1	0	-1.435138	-4.780268	0.000000
31	7	0	-1.175085	3.541338	0.000000
32	7	0	-2.479346	-2.788323	0.000000
33	7	0	3.654431	-0.753016	0.000000
34	5	0	-2.454848	2.941084	0.000000
35	5	0	-1.319630	-3.596503	0.000000
36	5	0	3.774478	0.655419	0.000000

Cor-4BN

E = -935.5332581 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.669382	-0.676707	0.000000
2	6	0	2.477580	-1.406354	0.000000
3	6	0	1.247861	-0.703395	0.000000
4	6	0	1.227222	0.712970	0.000000
5	6	0	2.460249	1.399768	0.000000
6	6	0	3.670536	0.705619	0.000000
7	6	0	0.000000	-1.419214	0.000000
8	6	0	-0.027194	1.432880	0.000000
9	6	0	-1.234888	0.732642	0.000000
10	6	0	-1.231296	-0.717422	0.000000
11	6	0	-2.482330	1.469907	0.000000
12	6	0	-2.512752	2.844026	0.000000
13	1	0	3.348431	3.235946	0.000000

14	1	0	1.288037	4.717840	0.000000
15	1	0	4.613323	-1.211657	0.000000
16	1	0	4.600236	1.264262	0.000000
17	1	0	-3.487039	3.323970	0.000000
18	1	0	-1.124603	4.784778	0.000000
19	6	0	-0.016240	-2.835722	0.000000
20	1	0	3.428838	-3.622946	0.000000
21	1	0	1.077122	-4.541512	0.000000
22	6	0	-1.226840	-3.530571	0.000000
23	6	0	-2.418319	-2.830611	0.000000
24	6	0	-2.451472	-1.433879	0.000000
25	1	0	-1.217051	-4.615228	0.000000
26	1	0	-3.356571	-3.375662	0.000000
27	1	0	-4.494108	1.327220	0.000000
28	1	0	-4.847591	-1.168001	0.000000
29	7	0	2.445968	2.784854	0.000000
30	7	0	-3.668020	0.745485	0.000000
31	7	0	1.180632	-3.536584	0.000000
32	5	0	1.256618	3.536682	0.000000
33	5	0	-3.771340	-0.660422	0.000000
34	5	0	2.458425	-2.936020	0.000000
35	5	0	-1.231626	3.602170	0.000000
36	7	0	-0.001208	2.821292	0.000000

Cor-5BN

E = -939.0595283 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.668545	-0.740901	0.000000
2	6	0	-2.470780	-1.457663	0.000000
3	6	0	-1.248448	-0.737898	0.000000
4	6	0	-1.251223	0.679730	0.000000
5	6	0	-2.490319	1.354631	0.000000
6	6	0	-3.689684	0.644678	0.000000
7	6	0	0.007157	-1.439087	0.000000
8	6	0	0.000000	1.402632	0.000000
9	6	0	1.202578	0.726375	0.000000
10	6	0	1.223829	-0.715094	0.000000
11	1	0	-3.390378	3.187043	0.000000
12	1	0	-1.344991	4.689274	0.000000
13	1	0	-4.606850	-1.286130	0.000000
14	1	0	-4.628287	1.188289	0.000000
15	1	0	3.267182	3.513020	0.000000
16	1	0	1.092768	4.783759	0.000000
17	6	0	0.047450	-2.855605	0.000000
18	1	0	-3.388354	-3.688821	0.000000
19	1	0	-1.025147	-4.576913	0.000000
20	6	0	1.272545	-3.520754	0.000000
21	6	0	2.453991	-2.793554	0.000000
22	6	0	2.468419	-1.397559	0.000000
23	1	0	1.288490	-4.605482	0.000000
24	1	0	3.399638	-3.326625	0.000000
25	1	0	4.642752	1.306950	0.000000
26	1	0	4.853945	-1.193744	0.000000
27	7	0	-2.484952	2.742797	0.000000
28	7	0	3.769897	0.797774	0.000000

29	7	0	-1.141241	-3.573390	0.000000
30	5	0	-1.298994	3.506872	0.000000
31	5	0	3.805786	-0.622356	0.000000
32	5	0	-2.427048	-2.988338	0.000000
33	5	0	1.181513	3.600597	0.000000
34	7	0	-0.037702	2.811059	0.000000
35	7	0	2.431667	2.945204	0.000000
36	5	0	2.525489	1.512358	0.000000

Cor-6BN

E = -942.5215989 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.654176	-0.726344	0.000000
2	6	0	-2.464941	-1.443321	0.000000
3	6	0	-1.227717	-0.737029	0.000000
4	6	0	-1.238557	0.682530	0.000000
5	6	0	-2.483056	1.364874	0.000000
6	6	0	-3.679525	0.665045	0.000000
7	6	0	0.017996	-1.447723	0.000000
8	6	0	0.000000	1.397119	0.000000
9	6	0	1.205836	0.710721	0.000000
10	6	0	1.219759	-0.720734	0.000000
11	1	0	-3.369594	3.201806	0.000000
12	1	0	-1.316481	4.692869	0.000000
13	1	0	-4.592370	-1.271971	0.000000
14	1	0	-4.618072	1.207978	0.000000
15	1	0	3.287044	3.489018	0.000000
16	1	0	1.115692	4.773785	0.000000
17	6	0	0.046532	-2.899313	0.000000
18	1	0	-3.417179	-3.656895	0.000000
19	1	0	-1.069489	-4.580847	0.000000
20	6	0	1.228995	-3.591727	0.000000
21	1	0	1.179883	-4.676697	0.000000
22	1	0	3.595171	-3.329665	0.000000
23	1	0	4.638954	1.217421	0.000000
24	1	0	4.722417	-1.285937	0.000000
25	7	0	-2.466372	2.752711	0.000000
26	7	0	3.741700	0.754854	0.000000
27	7	0	-1.169920	-3.575569	0.000000
28	5	0	-1.278589	3.510435	0.000000
29	5	0	3.717123	-0.659797	0.000000
30	5	0	-2.443689	-2.973354	0.000000
31	5	0	1.199230	3.590874	0.000000
32	7	0	-0.021452	2.805525	0.000000
33	7	0	2.446364	2.929397	0.000000
34	5	0	2.522603	1.499029	0.000000
35	5	0	2.516220	-2.832809	0.000000
36	7	0	2.448630	-1.377966	0.000000

Cor-7BN

E = -946.0500351 a.u.

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-2.460621	-2.792075	0.000000
2	6	0	-2.484731	-1.404933	0.000000
3	6	0	-1.237096	-0.705433	0.000000
4	6	0	-0.018978	-1.433790	0.000000
5	6	0	-0.059290	-2.853717	0.000000
6	6	0	-1.270182	-3.523951	0.000000
7	6	0	-1.221236	0.719717	0.000000
8	6	0	1.218096	-0.720884	0.000000
9	6	0	1.234923	0.670520	0.000000
10	6	0	0.000000	1.385723	0.000000
11	1	0	1.087676	-4.542080	0.000000
12	1	0	3.405945	-3.514652	0.000000
13	1	0	-3.403368	-3.330889	0.000000
14	1	0	-1.283371	-4.608194	0.000000
15	1	0	4.679095	1.078254	0.000000
16	1	0	4.698181	-1.443100	0.000000
17	1	0	-4.870679	-1.209370	0.000000
18	1	0	-4.661397	1.294636	0.000000
19	1	0	-3.274680	3.508236	0.000000
20	1	0	-1.106962	4.764784	0.000000
21	1	0	3.375967	3.397158	0.000000
22	1	0	1.249891	4.720178	0.000000
23	7	0	1.151151	-3.535238	0.000000
24	7	0	2.528552	2.848624	0.000000
25	7	0	-3.788585	0.785246	0.000000
26	5	0	2.402843	-2.886817	0.000000
27	5	0	1.287158	3.534586	0.000000
28	5	0	-3.824494	-0.634226	0.000000
29	5	0	3.716290	-0.777757	0.000000
30	7	0	2.427036	-1.444611	0.000000
31	7	0	3.771889	0.634866	0.000000
32	5	0	2.571863	1.419452	0.000000
33	5	0	-1.186642	3.580961	0.000000
34	7	0	0.037428	2.798369	0.000000
35	7	0	-2.444367	2.933263	0.000000
36	5	0	-2.543685	1.502672	0.000000

Cor-8BN

E = -949.5186283 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.237380	-0.711188	0.000000
2	6	0	0.025064	-1.444801	0.000000
3	6	0	0.053164	-2.896105	0.000000
4	6	0	1.223634	-3.598227	0.000000
5	6	0	1.226906	0.702080	0.000000
6	6	0	-1.197809	-0.726648	0.000000
7	6	0	-1.221972	0.675110	0.000000
8	6	0	0.000000	1.379506	0.000000
9	1	0	-1.135299	-4.540374	0.000000
10	1	0	-3.434147	-3.480833	0.000000
11	1	0	3.590376	-3.345868	0.000000
12	1	0	1.167243	-4.682581	0.000000
13	1	0	-4.666985	1.105202	0.000000

14	1	0	-4.690751	-1.414773	0.000000
15	1	0	4.735167	-1.306125	0.000000
16	1	0	4.658832	1.200104	0.000000
17	1	0	3.297353	3.483467	0.000000
18	1	0	1.134409	4.753849	0.000000
19	1	0	-3.350557	3.411559	0.000000
20	1	0	-1.216744	4.725095	0.000000
21	7	0	-1.181354	-3.532252	0.000000
22	7	0	-2.504861	2.860245	0.000000
23	7	0	3.760604	0.739270	0.000000
24	5	0	-2.421554	-2.868149	0.000000
25	5	0	-1.262373	3.539996	0.000000
26	5	0	3.732571	-0.674853	0.000000
27	5	0	-3.706010	-0.753786	0.000000
28	7	0	-2.422140	-1.427900	0.000000
29	7	0	-3.761537	0.658881	0.000000
30	5	0	-2.556389	1.431388	0.000000
31	5	0	1.207360	3.570083	0.000000
32	7	0	-0.018669	2.793028	0.000000
33	7	0	2.462095	2.916320	0.000000
34	5	0	2.542888	1.488006	0.000000
35	5	0	2.515920	-2.839849	0.000000
36	7	0	2.461697	-1.386342	0.000000

Cor-9BN

E = -953.0504806 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.396550	0.000000
2	6	0	-1.227496	0.708655	0.000000
3	6	0	1.227461	0.708715	0.000000
4	6	0	-1.209448	-0.698275	0.000000
5	6	0	0.000035	-1.417370	0.000000
6	6	0	1.209448	-0.698275	0.000000
7	1	0	-4.664170	1.148489	0.000000
8	1	0	-4.707052	-1.357182	0.000000
9	1	0	-1.179154	4.755365	0.000000
10	1	0	-3.326797	3.464990	0.000000
11	1	0	-1.337371	-4.613586	0.000000
12	1	0	-3.528690	-3.398860	0.000000
13	1	0	1.178172	4.755018	0.000000
14	1	0	3.326706	3.465045	0.000000
15	1	0	4.664168	1.148596	0.000000
16	1	0	4.707844	-1.356505	0.000000
17	1	0	1.337464	-4.613534	0.000000
18	1	0	3.528880	-3.397836	0.000000
19	5	0	-2.553016	1.474192	0.000000
20	5	0	-3.710351	-0.713848	0.000000
21	5	0	-2.473491	-2.856473	0.000000
22	5	0	-1.237033	3.570343	0.000000
23	5	0	1.236965	3.570182	0.000000
24	5	0	2.553196	1.473881	0.000000
25	5	0	3.710524	-0.713870	0.000000
26	5	0	2.473386	-2.856334	0.000000
27	5	0	-0.000180	-2.948073	0.000000
28	7	0	-2.434789	-1.405701	0.000000

29	7	0	-3.758641	0.702410	0.000000
30	7	0	-2.487464	2.903936	0.000000
31	7	0	0.000022	2.811440	0.000000
32	7	0	2.487625	2.903874	0.000000
33	7	0	3.758614	0.702239	0.000000
34	7	0	2.434767	-1.405739	0.000000
35	7	0	1.271016	-3.606284	0.000000
36	7	0	-1.271150	-3.606175	0.000000

Benzene

E = -232.1983428 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.391689	0.000000
2	6	0	1.205238	0.695845	0.000000
3	6	0	1.205238	-0.695845	0.000000
4	6	0	0.000000	-1.391689	0.000000
5	6	0	-1.205238	-0.695845	0.000000
6	6	0	-1.205238	0.695845	0.000000
7	1	0	0.000000	2.475425	0.000000
8	1	0	2.143781	1.237713	0.000000
9	1	0	2.143781	-1.237713	0.000000
10	1	0	0.000000	-2.475425	0.000000
11	1	0	-2.143781	-1.237713	0.000000
12	1	0	-2.143781	1.237713	0.000000

Naphthalene

E = -385.81533 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-2.424140	-0.707750
2	6	0	0.000000	-1.241445	-1.397951
3	6	0	0.000000	0.000000	-0.710916
4	6	0	0.000000	0.000000	0.710916
5	6	0	0.000000	-1.241445	1.397951
6	6	0	0.000000	-2.424140	0.707750
7	1	0	0.000000	1.236690	-2.482850
8	1	0	0.000000	-3.365870	-1.243747
9	1	0	0.000000	-1.236690	-2.482850
10	6	0	0.000000	1.241445	-1.397951
11	6	0	0.000000	1.241445	1.397951
12	1	0	0.000000	-1.236690	2.482850
13	1	0	0.000000	-3.365870	1.243747
14	6	0	0.000000	2.424140	0.707750
15	6	0	0.000000	2.424140	-0.707750
16	1	0	0.000000	1.236690	2.482850
17	1	0	0.000000	3.365870	1.243747
18	1	0	0.000000	3.365870	-1.243747

Phenanthrene

E = -539.4359032 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-3.547617	-0.294831
2	6	0	0.000000	-2.826625	0.875508
3	6	0	0.000000	-1.416227	0.859111
4	6	0	0.000000	-0.728426	-0.377107
5	6	0	0.000000	-1.493870	-1.562634
6	6	0	0.000000	-2.870391	-1.525011
7	6	0	0.000000	-0.675539	2.090171
8	6	0	0.000000	0.728426	-0.377107
9	6	0	0.000000	1.416227	0.859111
10	6	0	0.000000	0.675539	2.090171
11	6	0	0.000000	2.826625	0.875508
12	1	0	0.000000	3.334246	1.834315
13	6	0	0.000000	3.547617	-0.294831
14	6	0	0.000000	2.870391	-1.525011
15	6	0	0.000000	1.493870	-1.562634
16	1	0	0.000000	-1.230216	3.022328
17	1	0	0.000000	-4.630626	-0.271254
18	1	0	0.000000	-3.334246	1.834315
19	1	0	0.000000	-1.001414	-2.525958
20	1	0	0.000000	-3.433571	-2.450668
21	1	0	0.000000	1.230216	3.022328
22	1	0	0.000000	4.630626	-0.271254
23	1	0	0.000000	3.433571	-2.450668
24	1	0	0.000000	1.001414	-2.525958

Triphenylene

E = -693.0544321 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.698428	3.689217	0.000000
2	6	0	-1.379554	2.491082	0.000000
3	6	0	-0.705094	1.254850	0.000000
4	6	0	0.705094	1.254850	0.000000
5	6	0	1.379554	2.491082	0.000000
6	6	0	0.698428	3.689217	0.000000
7	6	0	-1.439279	-0.016796	0.000000
8	6	0	1.439279	-0.016796	0.000000
9	6	0	0.734185	-1.238054	0.000000
10	6	0	-0.734185	-1.238054	0.000000
11	6	0	1.467563	-2.440269	0.000000
12	6	0	2.845741	-2.449465	0.000000
13	6	0	3.544169	-1.239752	0.000000
14	6	0	2.847117	-0.050812	0.000000
15	1	0	-1.246875	4.623380	0.000000
16	1	0	1.246875	4.623380	0.000000
17	1	0	3.380527	-3.391515	0.000000
18	1	0	4.627402	-1.231865	0.000000
19	6	0	-2.847117	-0.050812	0.000000
20	6	0	-3.544169	-1.239752	0.000000
21	6	0	-2.845741	-2.449465	0.000000

22	6	0	-1.467563	-2.440269	0.000000
23	1	0	-4.627402	-1.231865	0.000000
24	1	0	-3.380527	-3.391515	0.000000
25	1	0	-0.953527	-3.390663	0.000000
26	1	0	0.953527	-3.390663	0.000000
27	1	0	3.413164	0.869553	0.000000
28	1	0	2.459637	2.521110	0.000000
29	1	0	-2.459637	2.521110	0.000000
30	1	0	-3.413164	0.869553	0.000000