Supplementary Information for

Deciphering Aromaticity in Porphyrinoids via Adaptive Natural Density Partitioning

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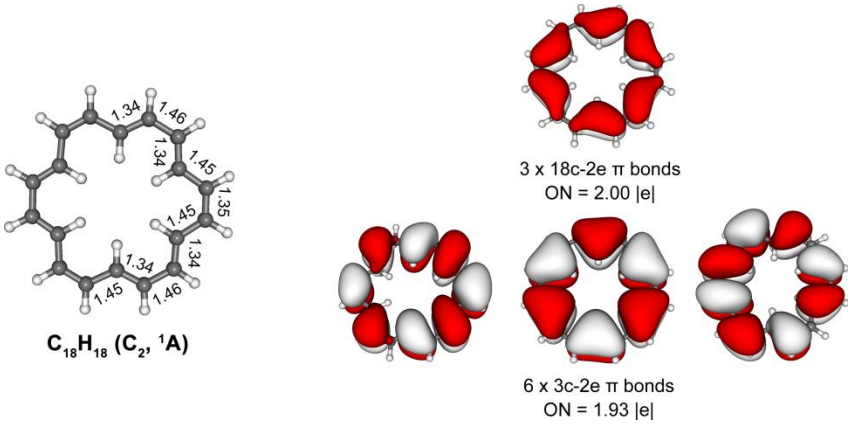

Fig. S1. AdNDP π bonding pattern for C_2 symmetric bond-alternate [18]annulene. The corresponding point group symmetry and spectroscopic state are given in parenthesis.

1) Cartesian coordinates of C_2 symmetric bond-alternate [18]annulene at the KMLYP/6-311++G** level of theory:

C	0.000000000	3.585336000	-1.291759000
C	0.000366000	2.947313000	0.007624000
C	0.000163000	1.467028000	-2.555552000
C	0.000003000	2.911470000	-2.458641000
C	-0.000366000	-2.947313000	0.007624000
C	0.000000000	-3.585336000	-1.291759000
C	-0.000003000	-2.911470000	-2.458641000
C	-0.000163000	-1.467028000	-2.555552000
C	-0.000002000	-0.730306000	-3.675647000
C	0.000002000	0.730306000	-3.675647000
H	-0.000073000	1.221100000	-4.644392000
H	0.000073000	-1.221100000	-4.644392000
H	-0.000296000	4.671213000	-1.307621000
H	-0.000286000	3.468013000	-3.391189000
H	0.000296000	-4.671213000	-1.307621000
H	0.000286000	-3.468013000	-3.391189000
C	-0.000594000	3.549113000	1.205604000
C	-0.000530000	2.818684000	2.470389000
C	-0.000233000	1.480289000	2.547909000
H	-0.001466000	4.633454000	1.264969000
H	-0.000806000	3.412066000	3.379912000
C	-0.000062000	0.673750000	3.750071000

C	0.000062000	-0.673750000	3.750071000
C	0.000233000	-1.480289000	2.547909000
H	-0.000077000	1.202911000	4.698419000
H	0.000077000	-1.202911000	4.698419000
C	0.000594000	-3.549113000	1.205604000
H	0.001466000	-4.633454000	1.264969000
C	0.000530000	-2.818684000	2.470389000
H	0.000806000	-3.412066000	3.379912000
H	-0.000091000	0.927717000	1.618760000
H	0.001460000	1.866349000	-0.006637000
H	0.000367000	0.939058000	-1.612188000
H	-0.000367000	-0.939058000	-1.612188000
H	-0.001460000	-1.866349000	-0.006637000
H	0.000091000	-0.927717000	1.618760000

2) Cartesian coordinates of all studied structures at the B3LYP/6-311++G** level of theory:

1. D_{6h} [18]annulene:

C	0.704854642	-3.731579818	0.000000000
C	1.490460251	-2.581552881	0.000000000
C	-1.490460251	-2.581552881	0.000000000
C	-0.704854642	-3.731579818	0.000000000
C	-1.490460251	2.581552881	0.000000000
C	-2.879215598	2.476211935	0.000000000
C	-3.584070240	1.255367883	0.000000000
C	-2.980920501	0.000000000	0.000000000
C	-3.584070240	-1.255367883	0.000000000
C	-2.879215598	-2.476211935	0.000000000
H	-3.464561863	-3.392226805	0.000000000
H	-4.670035520	-1.304285184	0.000000000
H	1.205473657	-4.696511989	0.000000000
H	-1.205473657	-4.696511989	0.000000000
H	-3.464561863	3.392226805	0.000000000
H	-4.670035520	1.304285184	0.000000000
C	2.879215598	-2.476211935	0.000000000
C	3.584070240	-1.255367883	0.000000000
C	2.980920501	0.000000000	0.000000000
H	3.464561863	-3.392226805	0.000000000
H	4.670035520	-1.304285184	0.000000000
C	3.584070240	1.255367883	0.000000000
C	2.879215598	2.476211935	0.000000000
C	1.490460251	2.581552881	0.000000000
H	4.670035520	1.304285184	0.000000000
H	3.464561863	3.392226805	0.000000000
C	-0.704854642	3.731579818	0.000000000
H	-1.205473657	4.696511989	0.000000000
C	0.704854642	3.731579818	0.000000000
H	1.205473657	4.696511989	0.000000000
H	1.898442175	0.000000000	0.000000000
H	0.949221088	-1.644099152	0.000000000
H	-0.949221088	-1.644099152	0.000000000
H	-1.898442175	0.000000000	0.000000000
H	-0.949221088	1.644099152	0.000000000
H	0.949221088	1.644099152	0.000000000

2. D_{2h} dideazaporphyrin:

H	0.000000000	3.247268000	3.514902000
N	0.000000000	0.000000000	2.590165000
N	0.000000000	0.000000000	-2.590165000
C	0.000000000	-2.546625000	1.467606000
C	0.000000000	-2.546625000	-1.467606000
C	0.000000000	2.546625000	1.467606000
C	0.000000000	2.546625000	-1.467606000
C	0.000000000	-1.085426000	3.389771000
C	0.000000000	1.085426000	3.389771000
C	0.000000000	-1.085426000	-3.389771000
C	0.000000000	1.085426000	-3.389771000
C	0.000000000	-3.715550000	0.703013000

C	0.000000000	-3.715550000	-0.703013000
C	0.000000000	3.715550000	0.703013000
C	0.000000000	3.715550000	-0.703013000
C	0.000000000	-0.680142000	4.797954000
C	0.000000000	0.680142000	4.797954000
C	0.000000000	-0.680142000	-4.797954000
C	0.000000000	0.680142000	-4.797954000
C	0.000000000	-2.392023000	2.845432000
C	0.000000000	-2.392023000	-2.845432000
C	0.000000000	2.392023000	-2.845432000
C	0.000000000	2.392023000	2.845432000
H	0.000000000	-4.677081000	1.210294000
H	0.000000000	-4.677081000	-1.210294000
H	0.000000000	4.677081000	1.210294000
H	0.000000000	4.677081000	-1.210294000
H	0.000000000	-1.343323000	5.651626000
H	0.000000000	1.343323000	5.651626000
H	0.000000000	-1.343323000	-5.651626000
H	0.000000000	1.343323000	-5.651626000
H	0.000000000	-3.247268000	3.514902000
H	0.000000000	-3.247268000	-3.514902000
H	0.000000000	3.247268000	-3.514902000
H	0.000000000	-1.601647000	-0.940107000
H	0.000000000	-1.601647000	0.940107000
H	0.000000000	1.601647000	-0.940107000
H	0.000000000	1.601647000	0.940107000

3. D_{2h} porphyrin:

H	0.000000000	3.214800000	3.177620000
N	0.000000000	0.000000000	-2.113143000
N	0.000000000	2.034655000	0.000000000
N	0.000000000	0.000000000	2.113143000
N	0.000000000	-2.034655000	0.000000000
C	0.000000000	1.129114000	-2.891249000
C	0.000000000	-1.129114000	-2.891249000
C	0.000000000	1.129114000	2.891249000
C	0.000000000	-1.129114000	2.891249000
C	0.000000000	2.856174000	-1.085330000
C	0.000000000	2.856174000	1.085330000
C	0.000000000	-2.856174000	-1.085330000
C	0.000000000	-2.856174000	1.085330000
C	0.000000000	0.685356000	-4.254695000
C	0.000000000	-0.685356000	-4.254695000
C	0.000000000	0.685356000	4.254695000
C	0.000000000	-0.685356000	4.254695000
C	0.000000000	4.257515000	-0.677501000
C	0.000000000	4.257515000	0.677501000
C	0.000000000	-4.257515000	-0.677501000
C	0.000000000	-4.257515000	0.677501000
C	0.000000000	2.439222000	-2.420175000
C	0.000000000	-2.439222000	-2.420175000
C	0.000000000	-2.439222000	2.420175000
C	0.000000000	2.439222000	2.420175000
H	0.000000000	1.343862000	-5.110064000
H	0.000000000	-1.343862000	-5.110064000
H	0.000000000	1.343862000	5.110064000
H	0.000000000	-1.343862000	5.110064000
H	0.000000000	5.105807000	-1.347168000
H	0.000000000	5.105807000	1.347168000
H	0.000000000	-5.105807000	-1.347168000
H	0.000000000	-5.105807000	1.347168000
H	0.000000000	3.214800000	-3.177620000
H	0.000000000	-3.214800000	-3.177620000
H	0.000000000	-3.214800000	3.177620000
H	0.000000000	0.000000000	-1.099347000
H	0.000000000	0.000000000	1.099347000

4. C_{2v} dihydrodideazaporphyrin:

H	-3.303929000	3.489192000	-0.189773000
N	0.000000000	2.684088000	-0.117805000
N	0.000000000	-2.684088000	-0.117805000
C	2.604535000	1.486910000	0.030779000

C	2.604535000	-1.486910000	0.030779000
C	-2.604535000	1.486910000	0.030779000
C	-2.604535000	-1.486910000	0.030779000
C	1.140804000	3.449603000	0.000209000
C	-1.140804000	3.449603000	0.000209000
C	1.140804000	-3.449603000	0.000209000
C	-1.140804000	-3.449603000	0.000209000
C	3.793844000	0.683830000	-0.099848000
C	3.793844000	-0.683830000	-0.099848000
C	-3.793844000	0.683830000	-0.099848000
C	-3.793844000	-0.683830000	-0.099848000
C	0.708844000	4.758431000	0.207991000
C	-0.708844000	4.758431000	0.207991000
C	0.708844000	-4.758431000	0.207991000
C	-0.708844000	-4.758431000	0.207991000
C	2.449322000	2.832110000	-0.059931000
C	2.449322000	-2.832110000	-0.059931000
C	-2.449322000	-2.832110000	-0.059931000
C	-2.449322000	2.832110000	-0.059931000
H	4.739914000	1.200674000	-0.234634000
H	4.739914000	-1.200674000	-0.234634000
H	-4.739914000	1.200674000	-0.234634000
H	-4.739914000	-1.200674000	-0.234634000
H	1.352014000	5.608596000	0.376530000
H	-1.352014000	5.608596000	0.376530000
H	1.352014000	-5.608596000	0.376530000
H	-1.352014000	-5.608596000	0.376530000
H	3.303929000	3.489192000	-0.189773000
H	3.303929000	-3.489192000	-0.189773000
H	-3.303929000	-3.489192000	-0.189773000
H	1.699352000	-0.925937000	0.229799000
H	1.699352000	0.925937000	0.229799000
H	-1.699352000	-0.925937000	0.229799000
H	-1.699352000	0.925937000	0.229799000
H	0.000000000	-1.750859000	-0.489615000
H	0.000000000	1.750859000	-0.489615000