# Supporting Information

## Revealing Intuitively Assessable Chemical Bonding Patterns in Organic Aromatic Molecules via Adaptive Natural Density Partitioning

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**Table S1.** Cartesian coordinates and total energies (B3LYP/3-21G level of theory) of $C_3H_3^+$ (cyclopropenyl cation), $C_5H_5^-$ (cyclopentadienyl anion), $C_6H_6$ (benzene), $C_{10}H_8$ (naphthalene), $C_{14}H_{10}$ (anthracene), $C_{14}H_{10}$ (phenanthrene), $C_{18}H_{12}$ (triphenelene), and $C_{24}H_{12}$ (coronene). All the structures are local minima with NIMAG = 0.

| $C_3H_3^+$ (cyclopropenyl cation) $E_{tot}$=-115.070896 a.u. | | | |
|---|---|---|---|
| 6 | 0.000000 | 0.794383 | 0.000000 |
| 6 | 0.687956 | -0.397191 | 0.000000 |
| 6 | -0.687956 | -0.397191 | 0.000000 |
| 1 | -1.620095 | -0.935363 | 0.000000 |
| 1 | 0.000000 | 1.870725 | 0.000000 |
| 1 | 1.620095 | -0.935363 | 0.000000 |
| $C_5H_5^-$ (cyclopentadienyl anion) $E_{tot}$=-192.435695 a.u. | | | |
| 6 | 0.000000 | 1.207909 | 0.000000 |
| 6 | 1.148790 | 0.373264 | 0.000000 |
| 6 | 0.709991 | -0.977219 | 0.000000 |
| 6 | -0.709991 | -0.977219 | 0.000000 |
| 6 | -1.148790 | 0.373264 | 0.000000 |
| 1 | -2.181823 | 0.708917 | 0.000000 |
| 1 | -1.348441 | -1.855969 | 0.000000 |
| 1 | 1.348441 | -1.855969 | 0.000000 |
| 1 | 2.181823 | 0.708917 | 0.000000 |

| | | | |
|---|---|---|---|
| 1 | 0.000000 | 2.294104 | 0.000000 |
| $C_6H_6$ (benzene) $E_{tot}$=-230.975773 a.u. | | | |
| 6 | 0.000000 | 1.397283 | 0.000000 |
| 6 | 1.210083 | 0.698642 | 0.000000 |
| 6 | 1.210083 | -0.698642 | 0.000000 |
| 6 | 0.000000 | -1.397283 | 0.000000 |
| 6 | -1.210083 | -0.698642 | 0.000000 |
| 6 | -1.210083 | 0.698642 | 0.000000 |
| 1 | 2.148940 | 1.240691 | 0.000000 |
| 1 | 2.148940 | -1.240691 | 0.000000 |
| 1 | 0.000000 | -2.481382 | 0.000000 |
| 1 | -2.148940 | -1.240691 | 0.000000 |
| 1 | -2.148940 | 1.240691 | 0.000000 |
| 1 | 0.000000 | 2.481382 | 0.000000 |
| $C_{10}H_8$ (naphthalene) $E_{tot}$=-383.771162 a.u. | | | |
| 6 | 0.000000 | 0.000000 | 0.717995 |
| 6 | 0.000000 | 0.000000 | -0.717995 |
| 6 | 0.000000 | 1.246187 | -1.404625 |
| 6 | 0.000000 | -1.246187 | -1.404625 |
| 6 | 0.000000 | 1.246187 | 1.404625 |
| 6 | 0.000000 | -1.246187 | 1.404625 |
| 6 | 0.000000 | 2.434356 | -0.709276 |
| 6 | 0.000000 | -2.434356 | -0.709276 |
| 6 | 0.000000 | 2.434356 | 0.709276 |
| 6 | 0.000000 | -2.434356 | 0.709276 |
| 1 | 0.000000 | -1.242972 | -2.489704 |
| 1 | 0.000000 | 1.242972 | -2.489704 |
| 1 | 0.000000 | 1.242972 | 2.489704 |
| 1 | 0.000000 | -1.242972 | 2.489704 |
| 1 | 0.000000 | 3.377505 | -1.243323 |
| 1 | 0.000000 | 3.377505 | 1.243323 |
| 1 | 0.000000 | -3.377505 | -1.243323 |
| 1 | 0.000000 | -3.377505 | 1.243323 |
| $C_{14}H_{10}$ (anthracene) $E_{tot}$=-536.560244 a.u. | | | |
| 6 | 0.000000 | 1.223167 | 0.723884 |
| 6 | 0.000000 | 0.000000 | 1.406526 |
| 6 | 0.000000 | -1.223167 | 0.723884 |
| 6 | 0.000000 | -1.223167 | -0.723884 |
| 6 | 0.000000 | 0.000000 | -1.406526 |
| 6 | 0.000000 | 1.223167 | -0.723884 |
| 6 | 0.000000 | 2.481022 | -1.408700 |
| 6 | 0.000000 | 2.481022 | 1.408700 |
| 6 | 0.000000 | 3.661002 | 0.714010 |

| | | | |
|---|---|---|---|
| 6 | 0.000000 | 3.661002 | -0.714010 |
| 6 | 0.000000 | -2.481022 | -1.408700 |
| 6 | 0.000000 | -2.481022 | 1.408700 |
| 6 | 0.000000 | -3.661002 | -0.714010 |
| 6 | 0.000000 | -3.661002 | 0.714010 |
| 1 | 0.000000 | -2.477270 | -2.493623 |
| 1 | 0.000000 | -2.477270 | 2.493623 |
| 1 | 0.000000 | 2.477270 | -2.493623 |
| 1 | 0.000000 | 2.477270 | 2.493623 |
| 1 | 0.000000 | 4.606641 | -1.243457 |
| 1 | 0.000000 | 4.606641 | 1.243457 |
| 1 | 0.000000 | -4.606641 | 1.243457 |
| 1 | 0.000000 | -4.606641 | -1.243457 |
| 1 | 0.000000 | 0.000000 | 2.492357 |
| 1 | 0.000000 | 0.000000 | -2.492357 |
| $C_{14}H_{10}$ (phenanthrene) $E_{tot}$=-536.569057 a.u. | | | |
| 6 | 0.000000 | 0.729861 | -0.380919 |
| 6 | 0.000000 | -0.729861 | -0.380919 |
| 6 | 0.000000 | -1.423799 | 0.867944 |
| 6 | 0.000000 | -0.679429 | 2.097052 |
| 6 | 0.000000 | 0.679429 | 2.097052 |
| 6 | 0.000000 | 1.423799 | 0.867944 |
| 6 | 0.000000 | 2.839401 | 0.879947 |
| 6 | 0.000000 | 1.499501 | -1.569418 |
| 6 | 0.000000 | -2.839401 | 0.879947 |
| 6 | 0.000000 | -1.499501 | -1.569418 |
| 6 | 0.000000 | -3.560983 | -0.297227 |
| 6 | 0.000000 | -2.882019 | -1.531511 |
| 6 | 0.000000 | 3.560983 | -0.297227 |
| 6 | 0.000000 | 2.882019 | -1.531511 |
| 1 | 0.000000 | -3.349606 | 1.837481 |
| 1 | 0.000000 | 3.349606 | 1.837481 |
| 1 | 0.000000 | -1.002584 | -2.530810 |
| 1 | 0.000000 | 1.002584 | -2.530810 |
| 1 | 0.000000 | -4.644349 | -0.275243 |
| 1 | 0.000000 | -3.446451 | -2.456726 |
| 1 | 0.000000 | 3.446451 | -2.456726 |
| 1 | 0.000000 | 4.644349 | -0.275243 |
| 1 | 0.000000 | -1.232826 | 3.030086 |
| 1 | 0.000000 | 1.232826 | 3.030086 |
| $C_{18}H_{12}$ (triphenelene) $E_{tot}$=-689.364103 a.u. | | | |
| 6 | 0.711278 | 1.259281 | 0.000000 |
| 6 | 1.446208 | -0.013656 | 0.000000 |

| | | | |
|---|---|---|---|
| 6 | 0.734930 | -1.245625 | 0.000000 |
| 6 | -0.734930 | -1.245625 | 0.000000 |
| 6 | -1.446208 | -0.013656 | 0.000000 |
| 6 | -0.711278 | 1.259281 | 0.000000 |
| 6 | 2.859032 | -0.049832 | 0.000000 |
| 6 | 1.472672 | -2.451078 | 0.000000 |
| 6 | -1.472672 | -2.451078 | 0.000000 |
| 6 | -2.859032 | -0.049832 | 0.000000 |
| 6 | -1.386360 | 2.500910 | 0.000000 |
| 6 | 1.386360 | 2.500910 | 0.000000 |
| 6 | -0.701010 | 3.703317 | 0.000000 |
| 6 | 0.701010 | 3.703317 | 0.000000 |
| 6 | -3.557672 | -1.244566 | 0.000000 |
| 6 | -2.856662 | -2.458751 | 0.000000 |
| 6 | 2.856662 | -2.458751 | 0.000000 |
| 6 | 3.557672 | -1.244566 | 0.000000 |
| 1 | -3.420619 | 0.873860 | 0.000000 |
| 1 | -0.953525 | -3.399273 | 0.000000 |
| 1 | -4.641214 | -1.238938 | 0.000000 |
| 1 | -3.393559 | -3.399940 | 0.000000 |
| 1 | 2.467094 | 2.525413 | 0.000000 |
| 1 | -2.467094 | 2.525413 | 0.000000 |
| 1 | 1.247655 | 4.638878 | 0.000000 |
| 1 | -1.247655 | 4.638878 | 0.000000 |
| 1 | 3.420619 | 0.873860 | 0.000000 |
| 1 | 0.953525 | -3.399273 | 0.000000 |
| 1 | 3.393559 | -3.399940 | 0.000000 |
| 1 | 4.641214 | -1.238938 | 0.000000 |
| $C_{24}H_{12}$ (coronene) $E_{tot}$=-916.806819 a.u. | | | |
| 6 | 0.000000 | 1.429047 | 0.000000 |
| 6 | 1.237591 | 0.714523 | 0.000000 |
| 6 | 1.237591 | -0.714524 | 0.000000 |
| 6 | 0.000000 | -1.429047 | 0.000000 |
| 6 | -1.237591 | -0.714523 | 0.000000 |
| 6 | -1.237591 | 0.714524 | 0.000000 |
| 6 | 2.468798 | 1.425361 | 0.000000 |
| 6 | 2.468798 | -1.425361 | 0.000000 |
| 6 | 0.000000 | -2.850722 | 0.000000 |
| 6 | -2.468798 | -1.425361 | 0.000000 |
| 6 | -2.468798 | 1.425361 | 0.000000 |
| 6 | 0.000000 | 2.850722 | 0.000000 |
| 6 | -2.438081 | -2.851087 | 0.000000 |
| 6 | -1.250073 | -3.536984 | 0.000000 |

| | | | |
|---|---|---|---|
| 6 | -3.688154 | -0.685897 | 0.000000 |
| 6 | -3.688154 | 0.685897 | 0.000000 |
| 6 | -2.438081 | 2.851087 | 0.000000 |
| 6 | -1.250073 | 3.536984 | 0.000000 |
| 6 | 1.250073 | 3.536984 | 0.000000 |
| 6 | 2.438081 | 2.851087 | 0.000000 |
| 6 | 3.688154 | 0.685897 | 0.000000 |
| 6 | 3.688154 | -0.685897 | 0.000000 |
| 6 | 2.438081 | -2.851087 | 0.000000 |
| 6 | 1.250073 | -3.536984 | 0.000000 |
| 1 | -1.244165 | -4.621614 | 0.000000 |
| 1 | -3.380353 | -3.388285 | 0.000000 |
| 1 | -4.624518 | -1.233329 | 0.000000 |
| 1 | -4.624518 | 1.233329 | 0.000000 |
| 1 | -3.380353 | 3.388285 | 0.000000 |
| 1 | -1.244165 | 4.621614 | 0.000000 |
| 1 | 1.244165 | 4.621614 | 0.000000 |
| 1 | 3.380353 | 3.388285 | 0.000000 |
| 1 | 4.624518 | 1.233329 | 0.000000 |
| 1 | 4.624518 | -1.233329 | 0.000000 |
| 1 | 3.380353 | -3.388285 | 0.000000 |
| 1 | 1.244165 | -4.621614 | 0.000000 |

**Table S2.** Example of the AdNDP input and output files ($C_6H_6$ benzene). In addition to the AdNDP output file, the information necessary for plotting the obtained bonding pattern is written to the standard Gaussian 03 output file. The given examples correspond to the calculations at the B3LYP/3-21G level of theory.

***Input***:

**NBO filename**
benz_d6h-NBO.log
**Number of atoms**
12
**Amount of valence electronic pairs**
15
**Total amount of electronic pairs**
21
**Total amount of basis functions**
66
**Amount of basis functions on each atom**
9
9
9
9
9
9
2
2
2
2
2
2
**Occupation number thresholds**
0.1
0.1
0.
0.
0.
0.
0.
0.
0.
0.
0.
0.1
**CMO filename**
benz_d6h-MO.log

***Output***:

NBOAmnt= 21

| # | Centers | ON, \|e\| |
|---|---|---|
| 1 | 1 0 0 0 0 0 0 0 0 0 0 0 Occ | 1.99872338 |
| 2 | 2 0 0 0 0 0 0 0 0 0 0 0 Occ | 1.99872311 |
| 3 | 3 0 0 0 0 0 0 0 0 0 0 0 Occ | 1.99872311 |
| 4 | 4 0 0 0 0 0 0 0 0 0 0 0 Occ | 1.99872338 |
| 5 | 5 0 0 0 0 0 0 0 0 0 0 0 Occ | 1.99872311 |
| 6 | 6 0 0 0 0 0 0 0 0 0 0 0 Occ | 1.99872311 |
| 7 | 1 2 0 0 0 0 0 0 0 0 0 0 Occ | 1.98789777 |
| 8 | 1 6 0 0 0 0 0 0 0 0 0 0 Occ | 1.98789777 |
| 9 | 2 3 0 0 0 0 0 0 0 0 0 0 Occ | 1.98791416 |
| 10 | 3 4 0 0 0 0 0 0 0 0 0 0 Occ | 1.98789777 |
| 11 | 4 5 0 0 0 0 0 0 0 0 0 0 Occ | 1.98789777 |
| 12 | 5 6 0 0 0 0 0 0 0 0 0 0 Occ | 1.98791416 |
| 13 | 1 12 0 0 0 0 0 0 0 0 0 0 Occ | 1.98135357 |
| 14 | 2 7 0 0 0 0 0 0 0 0 0 0 Occ | 1.98135887 |
| 15 | 3 8 0 0 0 0 0 0 0 0 0 0 Occ | 1.98135887 |
| 16 | 4 9 0 0 0 0 0 0 0 0 0 0 Occ | 1.98135357 |
| 17 | 5 10 0 0 0 0 0 0 0 0 0 0 Occ | 1.98135887 |
| 18 | 6 11 0 0 0 0 0 0 0 0 0 0 Occ | 1.98135887 |
| 19 | 1 2 3 4 5 6 7 8 9 10 11 12 Occ | 2.0001004 |
| 20 | 1 2 3 4 5 6 7 8 9 10 11 12 Occ | 2.00004866 |
| 21 | 1 2 3 4 5 6 7 8 9 10 11 12 Occ | 2.00004866 |

Residual Density 0.1921

**Figure S1.** Results of the non-directed AdNDP search for the anthracene molecule. Three completely delocalized 14c-2e bonds are concentrated primarily over the central six-atomic ring, determining the choice of the fragment for the directed AdNDP search.

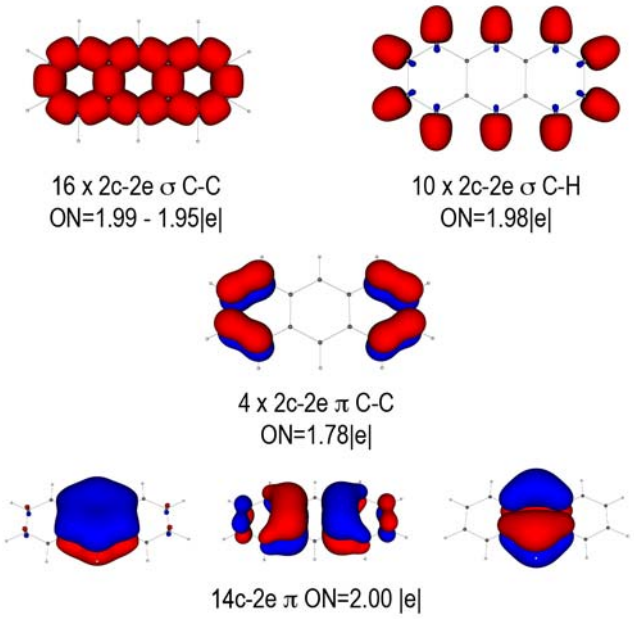


**Figure S2.** Results of the non-directed AdNDP search for the phenanthrene molecule. Six completely delocalized 14c-2e bonds are concentrated primarily over the two outer six-atomic rings, determining the choice of the fragments for the directed AdNDP search.

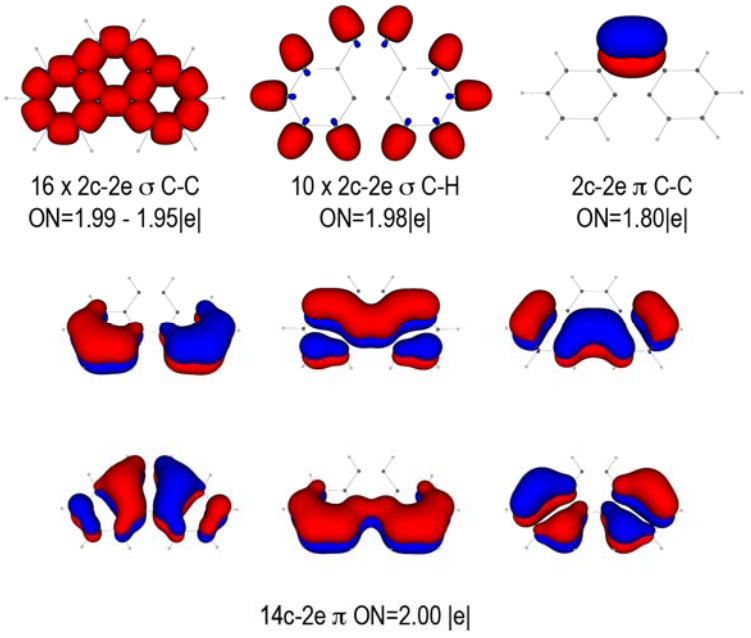

**Figure S3.** Results of the AdNDP partitioning for a) an antiaromatic cyclobutadien molecule and b) non-aromatic cyclo-pentadien molecule.