Electronic Supplementary Information for

Three Wrongs Can Make a Right: A Computational Investigation of [4*n*]–[4*n*]–[4*n*] Fused π-Systems

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1. Computational Details

All geometries were optimized at the (U)M11/6-311+G(d,p) level and vibrational frequency analyses were performed to verify the nature of the minima. **3-***Syn* and **3**-*terminal* were found to exhibit modest diradicaloid character, based on wavefunction stability tests and y_0 values computed at the UHF/6-31G(d) level (y_0 = 0.40 for **3-***syn* and y_0 = 0.54 for **3**-*terminal*). Therefore, geometries and energies for **3-***syn* and **3**-*terminal* were computed with a broken symmetry approach with the guess = mix keyword. Likewise, NICS-XY scans, SYSMOIC plots, and E(2) analyses for **3-***syn* and **3**-*terminal* were computed using UKS. All other structures investigated have stable closed-shell wavefunction.

Details for NICS-XY scans. NICS-XY-scans[1] were computed employing the Aroma package.[2] $NICS(1)_{zz}$ values were calculated using the (GIAO)[3] method at the (U)B97-2/6-311+G(d,p) level. **3-***syn* and **3**-*terminal* were found to exhibit modest diradicaloid character, and thus their NICS-XY-scans were computed with geometries obtained at the UKS level. NICS-XY-scans for all systems were computed following the same protocol: bq atoms were placed at 0.04 Å intervals along a line through the molecular framework, following a symmetry axis, and oriented parallel to the XY plane of the molecule at a constant height above it. The path of probes was defined to pass through the centers of the rings and extended across the molecular framework. Probes were located 1.0 Å above the molecular plane, and the (*zz*) component of the magnetic shielding tensor was extracted to generate the $NICS(1)_{zz}$ XY-scan profiles.

Details for SYSMOIC plots. Current density plots were computed employing SYSMOIC[4,5] package. Wavefunction files (wfx) were computed using the (CGST)[6-8] method at the (U)B97-2/6-311+G(d,p) level of theory. Current density maps were calculated in Z orientation of the magnetic field and mapped 1.0 Å (1.89 Bohr) over molecule plane. Because most of the molecules are planar, MO-decomposition was conducted to investigate only π-orbitals responsible for delocalized induced currents. Plots with current density were generated using python code plot.py presented by Paenurk and Gershoni-Poranne[9].

Details for E(2) analyses. Second-order perturbation theory analyses were computed at the (U)M11/6-311+G(d,p) level employing the Natural Bond Orbital (NBO) 7.0[10] program. For each system, E(2) energies corresponding to all π to π* donor-acceptor interactions were summed up to provide an estimate for π-electron delocalization energy. See results in Table S1.

2. NICS-XY scan paths

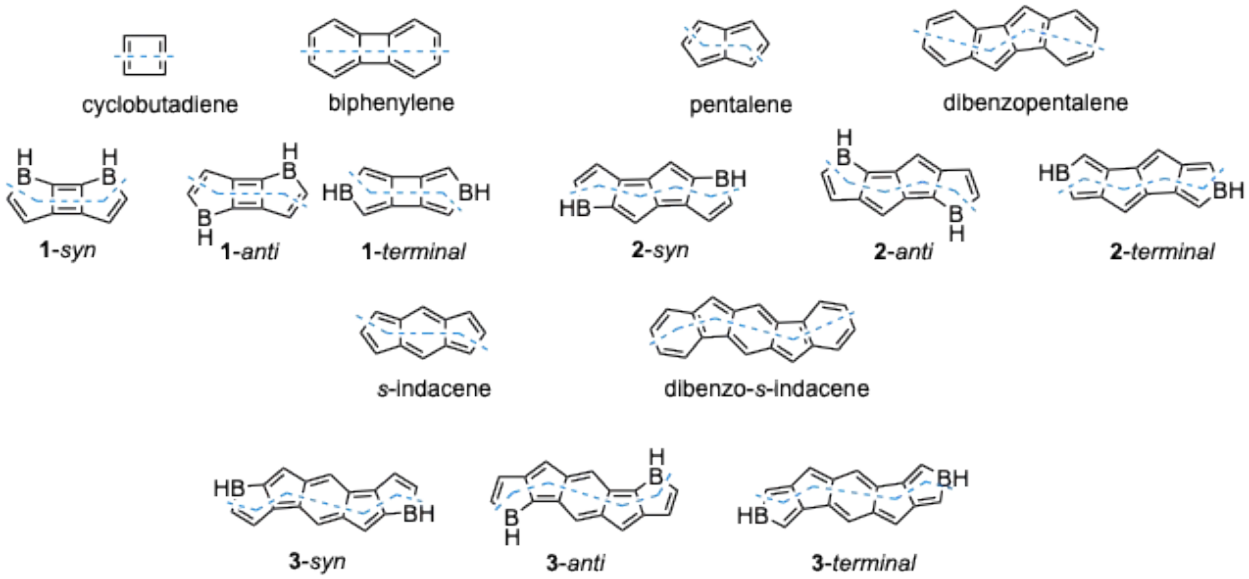

Figure S1. NICS–XY scan paths for all compounds investigated in this study.

3. Computed NICS data for compounds listed in Figure 1

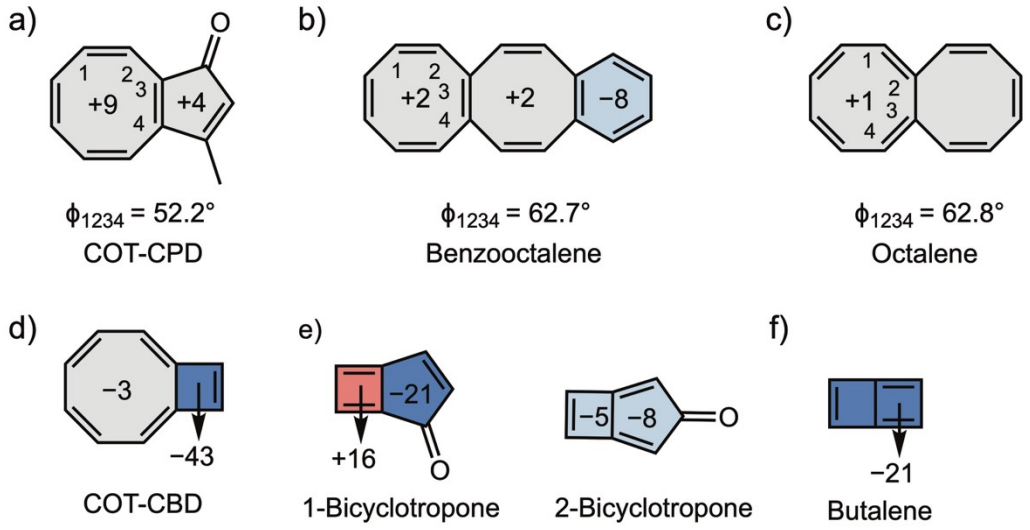

Figure S2. a)–c) Computed NICS(0) values and dihedral angles (φ_{1234}) for non-planar COT-containing systems. d)–f) Computed NICS(1)$_{zz}$ values planar [4*n*]–[4*n*] systems. All NICS values were computed at the B97-2/6-311+G(d,p)//M11/6-311+G(d,p) level.

4. Plots of HOMO orbitals for all compounds studied

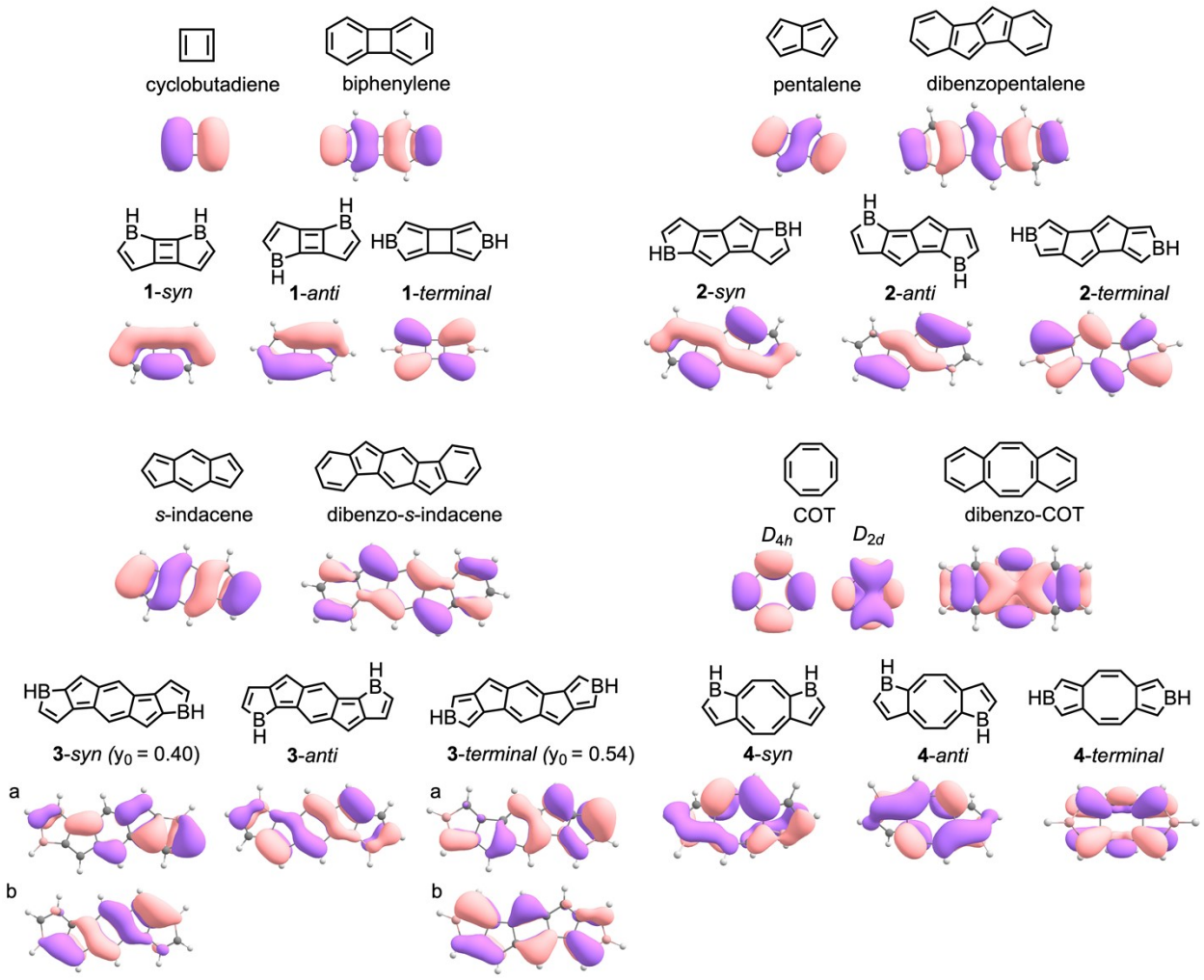

Figure S3. Plots of HOMOs for compounds with stable closed-shell wavefunctions as well as [a]SHOMO and [b]SHOMO–1 orbitals for **3**-*syn* and **3**-*terminal*.

5. Second-Order Perturbation Analysis

Table S1. Sums of second-order perturbation theory (E2) energies (kcal/mol) corresponding to all π to π* donor-acceptor interactions for the listed compounds.

Compound	E(2) (kcal/mol)	Compound	E(2) (kcal/mol)
1-*syn*	225.14	**3**-*syn*	504.09 (305.69) [a]
1-*anti*	224.26	**3**-*anti*	491.62
1-*terminal*	211.88	**3**-*terminal*	494.06 (416.06) [a]
2-*syn*	371.38	**4**-*syn*	359.13
2-*anti*	369.39	**4**-*anti*	313.80
2-*terminal*	346.21	**4**-*terminal*	219.30

[a] Both **3**-*syn* and **3**-*terminal* have modest diradicaloid character and therefore values in parentheses were evaluated with UKS.

6. Perimeter Bond Length Alternation

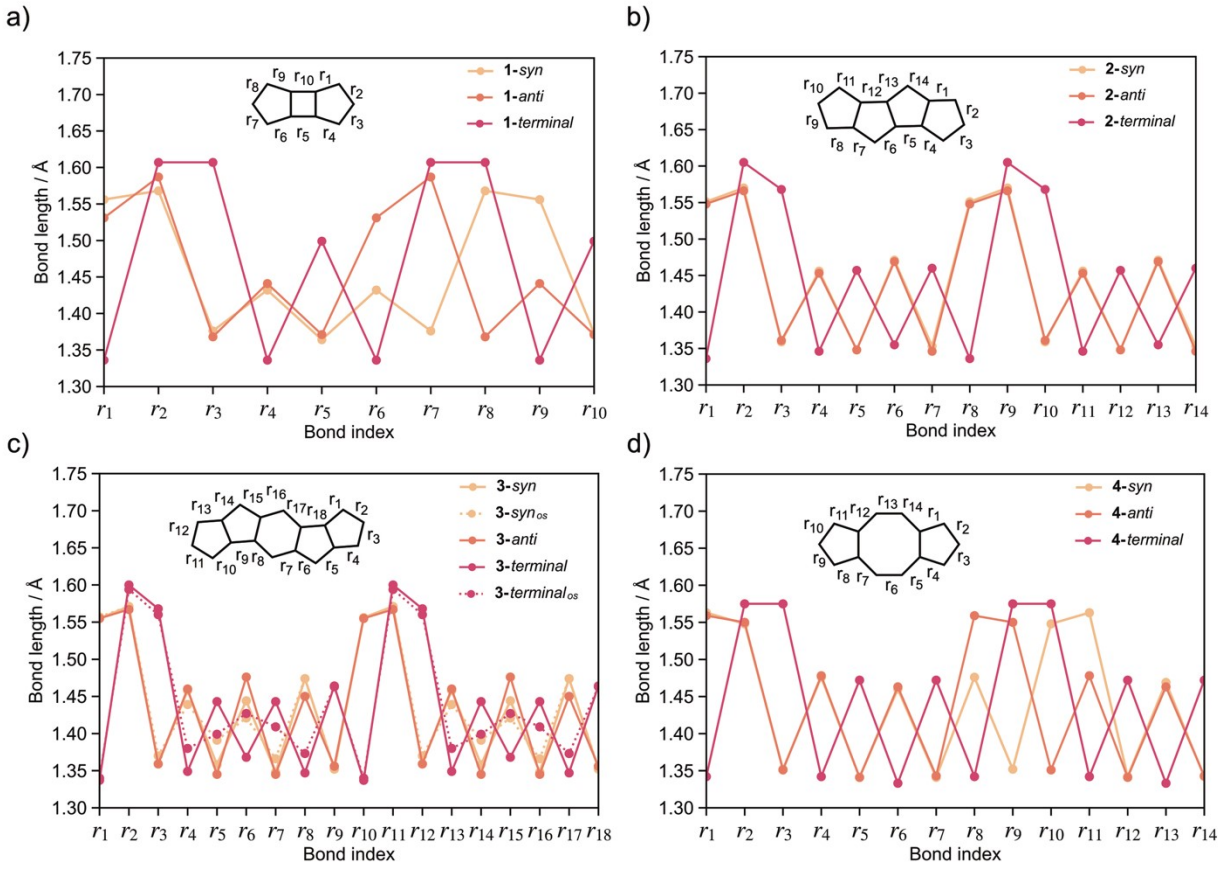

Figure S4. Comparisons of perimeter bond lengths for all borole-fused *syn*-, *anti*-, and *terminal*-isomers. Note larger bond alternations for the *terminal*-isomers.

7. Bond current strength.

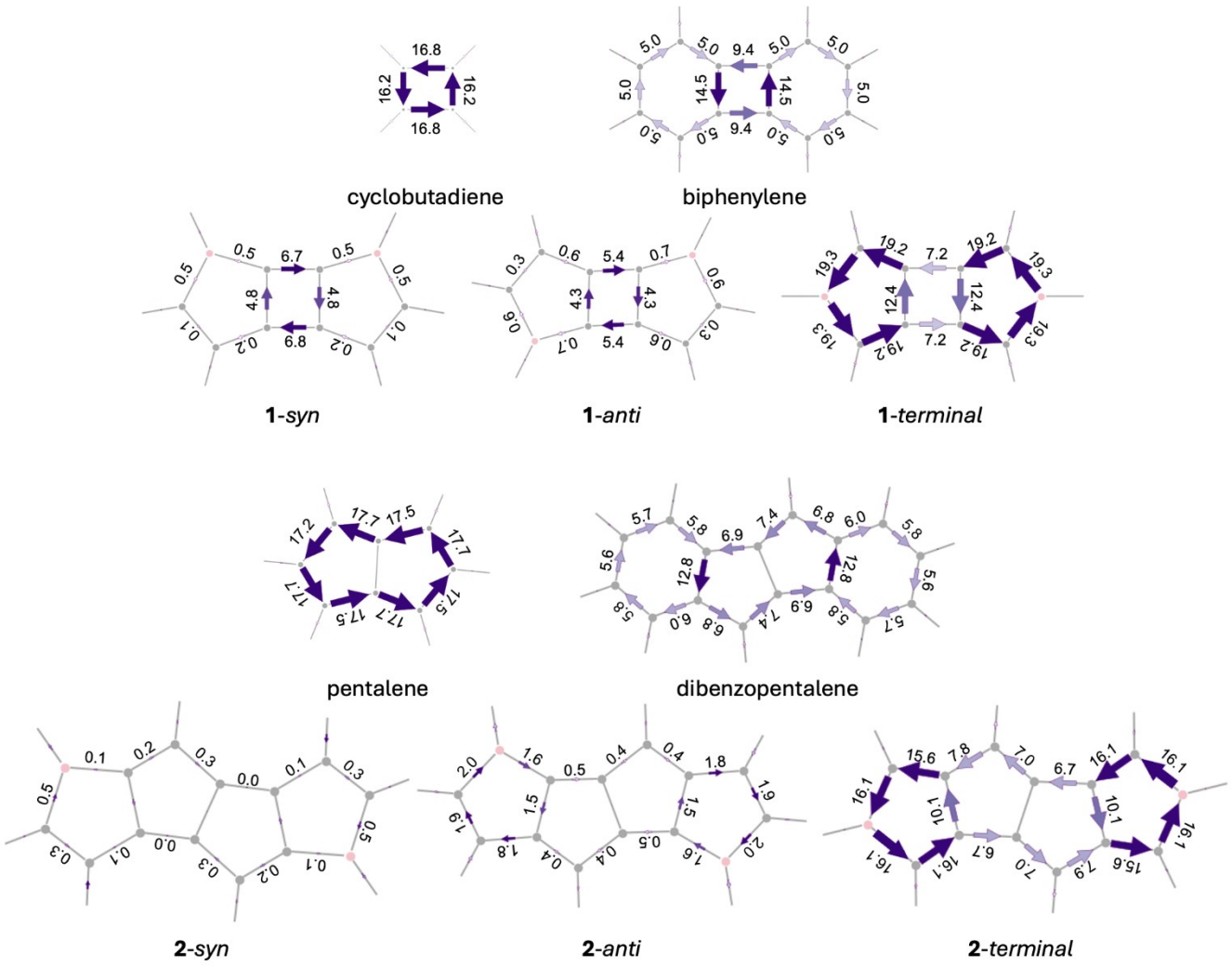

Figure S5. *Net* bond current strength in nA/T of π-electron contributions only for cyclobutadiene and pentalene derivatives.

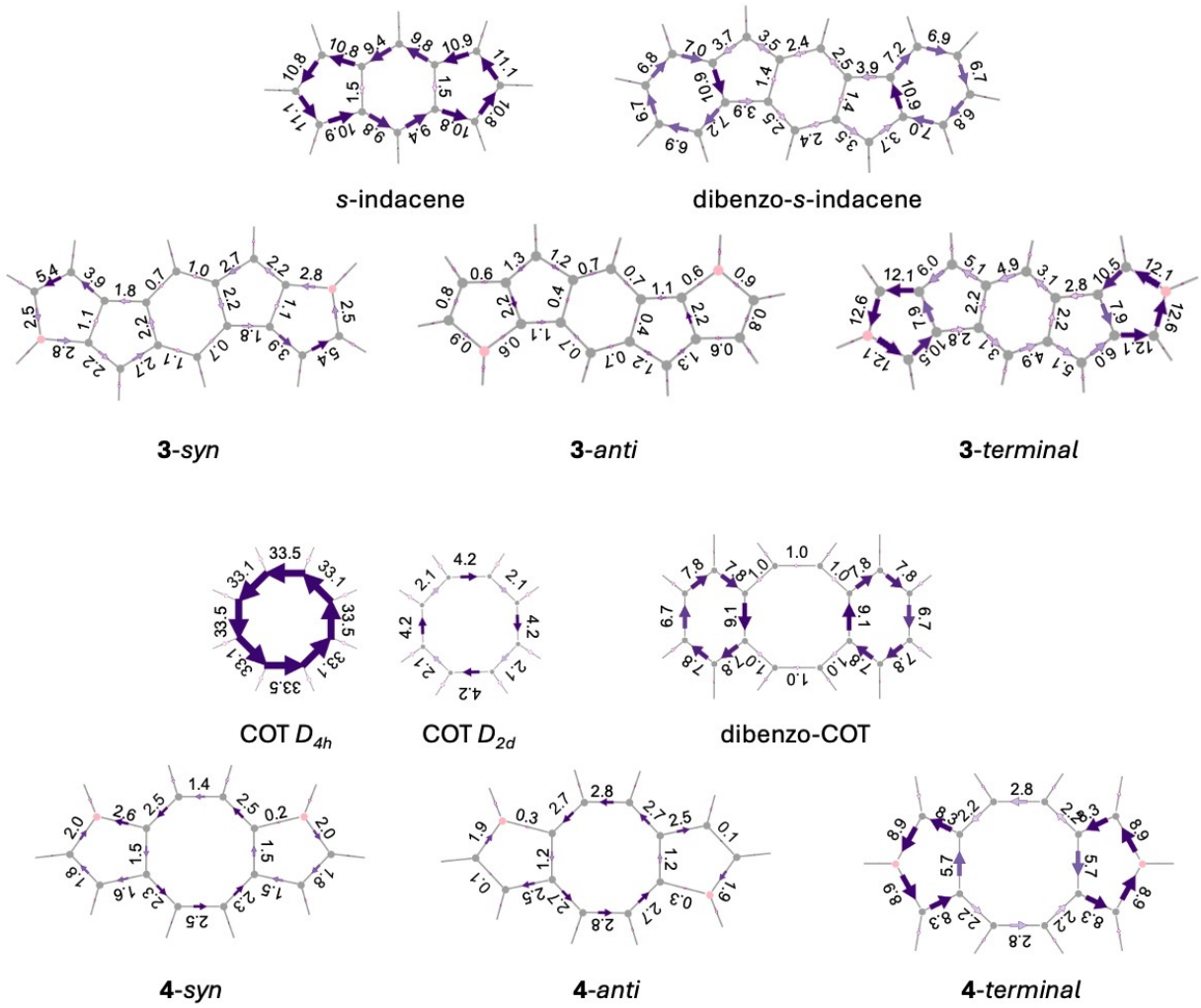

Figure S6. Net bond current strength in nA/T of π-electron contributions only for *s*-indacene and COT- derivatives. The apparent discontinuities in current in the COT-derivatives are a result of the non-planarity of the structures.

8. References

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10. E. D. Glendening, J. K. Badenhoop, A. E. Reed, J. E. Carpenter, J. A. Bohmann, C. M. Morales, P. Karafiloglou, C. R. Landis and F. Weinhold, *NBO 7.0*, Theoretical Chemistry Institute, University of Wisconsin–Madison, Madison, WI, 2018.

9. Optimized Cartesian Coordinates at (U)M11/6-311+G(d,p)

cyclobutadiene

	X	Y	Z
6	-0.785582000	0.664243000	0.000079000
6	0.786095000	0.663816000	0.000033000
6	0.785583000	-0.664243000	-0.000080000
6	-0.786096000	-0.663816000	-0.000033000
1	-1.554130000	-1.431216000	-0.000075000
1	1.553058000	-1.432224000	-0.000168000
1	-1.553056000	1.432225000	0.000169000
1	1.554128000	1.431217000	0.000076000

Total Electronic Energy = −154.550626 a.u.
Number of imaginary frequencies: 0

biphenylene

	X	Y	Z
6	0.756534000	0.707549000	0.000377000
6	1.909187000	1.439547000	-0.000208000
6	3.110881000	0.691157000	-0.000067000
6	3.110894000	-0.691134000	-0.000035000
6	1.909225000	-1.439550000	-0.000172000
6	0.756555000	-0.707576000	0.000361000
6	-0.756553000	-0.707572000	0.000013000
6	-0.756535000	0.707551000	0.000012000
6	-1.909189000	1.439546000	0.000218000
6	-3.110882000	0.691156000	-0.000231000
6	-3.110896000	-0.691136000	-0.000224000
6	-1.909220000	-1.439550000	0.000184000
1	1.926865000	2.527205000	-0.000917000
1	4.062850000	1.219247000	0.000065000
1	4.062876000	-1.219203000	0.000123000
1	1.926917000	-2.527206000	-0.000969000
1	-1.926869000	2.527202000	0.000789000
1	-4.062852000	1.219245000	-0.000616000
1	-4.062877000	-1.219207000	-0.000615000
1	-1.926918000	-2.527209000	0.000765000

Total Electronic Energy = −461.675892 a.u.
Number of imaginary frequencies: 0

1-*syn*

	X	Y	Z
6	0.686334000	0.861659000	-0.000128000
6	0.681867000	-0.652970000	-0.000164000
6	-2.901181000	-0.102556000	0.000162000
1	-2.694273000	2.372126000	0.000076000
1	-3.975771000	-0.288245000	0.000368000
6	-0.681895000	-0.652997000	-0.000162000
6	-0.686329000	0.861666000	-0.000199000
1	-2.305180000	-2.211249000	0.000161000
6	2.020628000	-1.159970000	0.000003000
6	2.901178000	-0.102585000	0.000147000
1	2.305096000	-2.211263000	0.000025000
1	3.975753000	-0.288345000	0.000304000
1	2.694379000	2.372083000	0.000213000
6	-2.020670000	-1.159974000	0.000042000
5	-2.181734000	1.290147000	0.000035000
5	2.181815000	1.290105000	0.000095000

Total Electronic Energy = −357.697875 a.u.
Number of imaginary frequencies: 0

1-*anti*

	X	Y	Z
6	0.647575000	0.830720000	-0.000114000
6	0.715514000	-0.679763000	-0.000145000
6	-2.084414000	1.130134000	-0.000020000
6	-2.900363000	0.031564000	0.000195000
1	-2.412753000	2.167800000	-0.000032000
1	-3.984751000	0.153347000	0.000418000
6	-0.647586000	-0.830713000	-0.000281000
6	-0.715555000	0.679872000	-0.000214000
5	-2.093641000	-1.334833000	0.000116000
1	-2.561366000	-2.437447000	0.000369000
6	2.084397000	-1.130169000	0.000022000
6	2.900452000	-0.031672000	0.000171000
1	2.412586000	-2.167877000	-0.000095000
1	3.984834000	-0.153483000	0.000306000
5	2.093642000	1.334892000	0.000114000
1	2.561318000	2.437525000	0.000202000

Total Electronic Energy = −357.703909 a.u.

Number of imaginary frequencies: 0

1-*terminal*

	X	Y	Z
6	0.749456000	0.758840000	-0.000010000
6	0.749456000	-0.758846000	0.000002000
6	-1.972991000	1.294652000	0.000005000
1	-2.218238000	2.352901000	-0.000006000
1	-4.127351000	-0.000014000	0.000023000
6	-0.749457000	-0.758836000	0.000020000
6	-0.749457000	0.758844000	0.000009000
1	-2.218210000	-2.352909000	0.000032000
6	1.972991000	-1.294653000	-0.000011000
1	2.218239000	-2.352901000	-0.000004000
1	4.127351000	0.000016000	-0.000037000
1	2.218219000	2.352908000	-0.000042000
6	1.972985000	1.294656000	-0.000031000
6	-1.972986000	-1.294656000	0.000028000
5	2.924956000	0.000000000	-0.000030000
5	-2.924956000	-0.000001000	0.000021000

Total Electronic Energy = −357.699174 a.u.
Number of imaginary frequencies: 0

pentalene

	X	Y	Z
6	-1.207435000	1.227473000	-0.000088000
6	-2.163417000	0.067735000	-0.000088000
6	-1.475750000	-1.087943000	-0.000030000
6	-0.039873000	-0.731380000	0.000009000
6	0.039905000	0.731354000	-0.000036000
6	1.207457000	-1.227447000	0.000098000
6	2.163390000	-0.067730000	0.000102000
6	1.475734000	1.087938000	0.000023000
1	-3.244579000	0.171097000	-0.000126000
1	-1.890929000	-2.090033000	-0.000017000
1	3.244555000	-0.171084000	0.000156000
1	1.890903000	2.090032000	0.000002000
1	1.511768000	-2.271092000	0.000161000
1	-1.511784000	2.271083000	-0.000121000

Total Electronic Energy = −308.127939 a.u.
Number of imaginary frequencies: 0

dibenzopentalene

	X	Y	Z
6	2.000038000	0.862494000	-0.000069000
6	1.747778000	-0.530810000	-0.000069000
6	2.789158000	-1.435135000	-0.000089000
6	4.100776000	-0.947192000	-0.000014000
6	4.349581000	0.417875000	0.000128000
6	3.296334000	1.338993000	0.000095000
6	0.284608000	-0.680958000	-0.000065000
6	-0.702991000	-1.590989000	0.000083000
6	-2.000037000	-0.862493000	0.000069000
6	-1.747777000	0.530812000	-0.000014000
6	-2.789159000	1.435134000	-0.000003000
6	-4.100777000	0.947194000	0.000029000
6	-4.349581000	-0.417878000	0.000010000
6	-3.296333000	-1.338995000	0.000026000
6	-0.284610000	0.680959000	-0.000070000
6	0.702993000	1.590990000	-0.000102000
1	2.598931000	-2.507156000	-0.000195000
1	4.934673000	-1.646638000	-0.000065000
1	5.377082000	0.777223000	0.000245000
1	3.499141000	2.408969000	0.000260000
1	-0.611648000	-2.674088000	0.000263000
1	-2.598931000	2.507155000	0.000016000
1	-4.934674000	1.646638000	0.000072000
1	-5.377081000	-0.777226000	-0.000029000
1	-3.499138000	-2.408972000	-0.000045000
1	0.611650000	2.674090000	-0.000187000

Total Electronic Energy = −615.238817 a.u.
Number of imaginary frequencies: 0

2-syn

	X	Y	Z
6	1.644583000	-0.506794000	0.000048000
6	1.950827000	0.967191000	0.000023000
6	0.787203000	1.657518000	0.000014000
6	-0.307605000	0.675802000	-0.000005000
6	0.307659000	-0.675708000	0.000005000
6	-0.787136000	-1.657455000	-0.000003000
1	0.668675000	2.737410000	-0.000013000
1	-0.668540000	-2.737341000	0.000018000

6	-1.950818000	-0.967251000	-0.000023000
6	-1.644746000	0.506749000	-0.000025000
6	-2.898415000	1.246728000	-0.000006000
6	-3.970342000	0.411300000	0.000011000
6	2.898583000	-1.246824000	0.000010000
6	3.970316000	-0.411433000	-0.000034000
1	4.987215000	-0.801885000	-0.000084000
1	4.183129000	2.068967000	-0.000011000
5	3.496862000	1.085799000	-0.000010000
5	-3.497064000	-1.085679000	-0.000006000
1	-4.183203000	-2.068615000	0.000000000
1	-2.949570000	2.335128000	-0.000001000
1	2.949807000	-2.335211000	0.000051000
1	-4.987152000	0.802020000	0.000034000

Total Electronic Energy = −511.287187 a.u.
Number of imaginary frequencies: 0

2-anti

	X	Y	Z
6	1.610037000	-0.665954000	-0.000048000
6	1.981395000	0.803068000	-0.000041000
6	0.896844000	1.604322000	0.000011000
6	-0.264427000	0.704853000	-0.000036000
6	0.264559000	-0.704633000	-0.000089000
6	-0.896749000	-1.604126000	-0.000106000
1	0.864631000	2.688519000	0.000071000
1	-0.864517000	-2.688327000	-0.000166000
6	-1.981341000	-0.802925000	-0.000020000
6	-1.610155000	0.666178000	0.000051000
6	-4.024826000	0.310199000	0.000029000
6	4.024632000	-0.310728000	0.000038000
1	5.109775000	-0.407392000	0.000023000
1	3.955792000	1.868148000	-0.000219000
1	-3.954889000	-1.868113000	-0.000057000
1	-3.133910000	2.630534000	0.000174000
1	3.133419000	-2.630504000	0.000558000
1	-5.110040000	0.406213000	0.000012000
5	2.946650000	-1.446935000	0.000190000
5	-2.947055000	1.446980000	0.000115000
6	-3.430019000	-0.913544000	-0.000018000
6	3.430344000	0.913405000	-0.000090000

Total Electronic Energy = −511.288402 a.u.

Number of imaginary frequencies: 0

2-terminal

	X	Y	Z
6	1.690452000	-0.640813000	0.000013000
6	2.041645000	0.847778000	-0.000003000
6	0.790384000	1.594507000	-0.000021000
6	-0.232035000	0.705420000	-0.000012000
6	0.232030000	-0.705413000	0.000007000
6	-0.790382000	-1.594498000	0.000016000
1	0.703434000	2.676467000	-0.000038000
1	-0.703430000	-2.676458000	0.000033000
6	-2.041651000	-0.847778000	0.000003000
6	-1.690456000	0.640820000	-0.000019000
1	5.177973000	-0.663494000	0.000008000
1	3.840362000	2.034299000	0.000000000
1	-3.840330000	-2.034310000	0.000018000
1	-2.771404000	2.498299000	-0.000052000
1	2.771378000	-2.498296000	0.000020000
1	-5.177977000	0.663459000	-0.000012000
6	-3.372128000	-1.053990000	0.000010000
6	3.372154000	1.053982000	0.000004000
6	-2.782227000	1.410944000	-0.000026000
6	2.782212000	-1.410940000	0.000021000
5	4.010902000	-0.377621000	0.000016000
5	-4.010901000	0.377605000	-0.000003000

Total Electronic Energy = −511.272207 a.u.
Number of imaginary frequencies: 0

***s*-Indacene**

	X	Y	Z
6	-0.604041000	1.278074000	0.000000000
6	0.851030000	1.104666000	0.000000000
6	1.437088000	-0.216938000	0.000000000
6	0.604041000	-1.278074000	0.000000000
6	-0.851030000	-1.104666000	0.000000000
6	-1.437088000	0.216938000	0.000000000
6	1.415068000	2.343882000	0.000000000
1	2.521225000	-0.334399000	0.000000000
1	-2.521225000	0.334399000	0.000000000
1	2.479803000	2.563870000	0.000000000
6	-1.415068000	-2.343882000	0.000000000

6	-0.349350000	-3.349009000	0.000000000
6	0.851030000	-2.722529000	0.000000000
1	-2.479803000	-2.563870000	0.000000000
6	-0.851030000	2.722529000	0.000000000
6	0.349350000	3.349009000	0.000000000
1	0.513343000	4.422126000	0.000000000
1	-1.830928000	3.189684000	0.000000000
1	1.830928000	-3.189684000	0.000000000
1	-0.513343000	-4.422126000	0.000000000

Total Electronic Energy = −461.665475 a.u.
Number of imaginary frequencies: 0

dibenzo-*s*-indacene

	X	Y	Z
6	-0.962564000	1.020207000	-0.000026000
6	-1.351218000	-0.403541000	0.000006000
6	-0.439150000	-1.389592000	0.000023000
6	0.962545000	-1.020129000	-0.000037000
6	1.351205000	0.403593000	-0.000079000
6	0.439147000	1.389658000	-0.000050000
6	-2.824280000	-0.427074000	0.000075000
1	-0.725002000	-2.441475000	0.000087000
1	0.725011000	2.441538000	-0.000044000
6	2.824304000	0.427099000	-0.000081000
6	3.262077000	-0.913488000	-0.000018000
6	2.080385000	-1.786251000	0.000054000
6	-2.080348000	1.786349000	-0.000027000
6	-3.262182000	0.913492000	0.000017000
6	-3.733548000	-1.468741000	-0.000036000
6	-5.095432000	-1.165271000	-0.000064000
6	-5.530115000	0.157345000	0.000047000
6	-4.616713000	1.210466000	0.000093000
1	-3.399307000	-2.505585000	-0.000090000
1	-5.826818000	-1.971345000	-0.000134000
1	-6.597497000	0.370916000	0.000045000
1	-4.962852000	2.242977000	0.000144000
6	5.095418000	1.165205000	0.000103000
6	5.530146000	-0.157418000	0.000070000
6	4.616757000	-1.210541000	-0.000053000
6	3.733550000	1.468652000	-0.000064000
1	5.826798000	1.971284000	0.000181000
1	6.597534000	-0.370969000	0.000170000
1	4.962843000	-2.243064000	-0.000054000

1	3.399330000	2.505507000	-0.000114000
1	-2.112222000	2.873058000	-0.000084000
1	2.112272000	-2.872963000	0.000184000

Total Electronic Energy = −768.766473 a.u.
Number of imaginary frequencies: 0

3-*syn*

	X	Y	Z
6	-1.346342000	-0.390180000	-0.000064000
6	-0.955610000	1.036683000	-0.000116000
6	0.336331000	1.422289000	-0.000136000
6	1.346298000	0.390211000	0.000080000
6	0.955556000	-1.036659000	0.000121000
6	-0.336378000	-1.422269000	0.000137000
6	-2.202511000	1.823368000	0.000126000
1	0.621883000	2.473957000	-0.000344000
1	-0.621934000	-2.473936000	0.000330000
1	-2.238078000	2.909989000	0.000201000
6	2.202453000	-1.823368000	-0.000177000
6	3.245408000	-0.963560000	-0.000315000
6	2.703534000	0.417464000	-0.000099000
6	5.009384000	0.735780000	0.000040000
6	3.807459000	1.369431000	0.000044000
1	2.238013000	-2.909988000	-0.000286000
6	-2.703576000	-0.417469000	0.000095000
6	-3.807412000	-1.369536000	0.000001000
6	-3.245500000	0.963556000	0.000259000
6	-5.009338000	-0.735921000	0.000004000
1	-5.943655000	-1.295265000	0.000014000
1	-3.667942000	-2.450708000	-0.000026000
1	3.668073000	2.450617000	0.000093000
1	5.943662000	1.295194000	0.000046000
5	4.794613000	-0.820352000	-0.000115000
1	5.635656000	-1.674782000	-0.000017000
5	-4.794372000	0.820559000	0.000106000
1	-5.635430000	1.674977000	0.000016000

Total Electronic Energy = −664.816424 a.u.
Number of imaginary frequencies: 0

3-*syn*$_{os}$ at UM11/6-311+G(d,p)

	X	Y	Z

6	1.338243000	0.389426000	0.000016000
6	0.961963000	-1.017361000	0.000034000
6	-0.347273000	-1.407810000	0.000023000
6	-1.338244000	-0.389427000	-0.000021000
6	-0.961963000	1.017360000	-0.000036000
6	0.347272000	1.407809000	-0.000026000
6	2.204828000	-1.809474000	0.000013000
1	-0.628476000	-2.460380000	0.000065000
1	0.628475000	2.460378000	-0.000065000
1	2.233549000	-2.896509000	0.000023000
6	-2.204829000	1.809473000	-0.000005000
6	-3.257151000	0.958687000	0.000062000
6	-2.729304000	-0.419930000	0.000047000
6	-5.028981000	-0.728802000	-0.000094000
6	-3.815520000	-1.364422000	-0.000009000
1	-2.233549000	2.896508000	-0.000011000
6	2.729302000	0.419928000	-0.000039000
6	3.815520000	1.364420000	0.000006000
6	3.257149000	-0.958687000	-0.000045000
6	5.028980000	0.728800000	0.000081000
1	5.962093000	1.289335000	0.000117000
1	3.676038000	2.445488000	-0.000023000
1	-3.676036000	-2.445490000	0.000021000
1	-5.962097000	-1.289332000	-0.000139000
5	-4.807997000	0.826225000	-0.000076000
1	-5.644610000	1.684776000	-0.000187000
5	4.808006000	-0.826213000	0.000071000
1	5.644615000	-1.684767000	0.000167000

Total Electronic Energy = −665.820717 a.u.
Number of imaginary frequencies: 0

3-*anti*

	X	Y	Z
6	0.007512000	1.401857000	0.000000000
6	1.273971000	0.621137000	0.000000000
6	1.273971000	-0.723448000	0.000000000
6	-0.007512000	-1.401857000	0.000000000
6	-1.273971000	-0.621137000	0.000000000
6	-1.273971000	0.723448000	0.000000000
6	2.379008000	1.599893000	0.000000000
1	2.192272000	-1.309158000	0.000000000
1	-2.192272000	1.309158000	0.000000000
1	3.433962000	1.343362000	0.000000000

6	-2.379008000	-1.599893000	0.000000000
6	-1.812485000	-2.820280000	0.000000000
6	-0.326640000	-2.719500000	0.000000000
6	-1.096191000	-5.039585000	0.000000000
6	0.326640000	2.719500000	0.000000000
6	1.812485000	2.820280000	0.000000000
6	1.096191000	5.039585000	0.000000000
6	-2.188284000	-4.231573000	0.000000000
6	2.188284000	4.231573000	0.000000000
1	3.223310000	4.573107000	0.000000000
1	1.196650000	6.123941000	0.000000000
1	-3.433962000	-1.343362000	0.000000000
1	-1.196650000	-6.123941000	0.000000000
1	-3.223310000	-4.573107000	0.000000000
5	-0.212395000	4.178000000	0.000000000
1	-1.347638000	4.564945000	0.000000000
5	0.212395000	-4.178000000	0.000000000
1	1.347638000	-4.564945000	0.000000000

Total Electronic Energy = −664.816084 a.u.
Number of imaginary frequencies: 0

3-*terminal*

	X	Y	Z
6	0.017839000	1.399476000	0.000000000
6	1.273974000	0.614908000	0.000000000
6	1.201417000	-0.826119000	0.000000000
6	-0.017839000	-1.399476000	0.000000000
6	-1.273974000	-0.614908000	0.000000000
6	-1.201417000	0.826119000	0.000000000
6	2.373127000	1.428885000	0.000000000
1	2.111751000	-1.423008000	0.000000000
1	-2.111751000	1.423008000	0.000000000
1	3.402316000	1.080662000	0.000000000
6	-2.373127000	-1.428885000	0.000000000
6	-1.952651000	-2.808949000	0.000000000
6	-0.432838000	-2.803080000	0.000000000
6	0.432838000	2.803080000	0.000000000
6	1.952651000	2.808949000	0.000000000
6	-2.454603000	-4.060580000	0.000000000
6	2.454603000	4.060580000	0.000000000
1	3.515354000	4.295871000	0.000000000
1	1.186335000	6.206222000	0.000000000

1	-3.402316000	-1.080662000	0.000000000
1	-1.186335000	-6.206222000	0.000000000
1	-3.515354000	-4.295871000	0.000000000
1	-1.138010000	4.272188000	0.000000000
1	1.138010000	-4.272188000	0.000000000
6	-0.075640000	4.039501000	0.000000000
6	0.075640000	-4.039501000	0.000000000
5	1.201417000	5.003676000	0.000000000
5	-1.201417000	-5.003676000	0.000000000

Total Electronic Energy = −664.797397 a.u.
Number of imaginary frequencies: 0

3-*terminal*$_{os}$ at UM11/6-311+G(d,p)

	X	Y	Z
6	0.017839000	1.399476000	0.000000000
6	1.273974000	0.614908000	0.000000000
6	1.201417000	-0.826119000	0.000000000
6	-0.017839000	-1.399476000	0.000000000
6	-1.273974000	-0.614908000	0.000000000
6	-1.201417000	0.826119000	0.000000000
6	2.373127000	1.428885000	0.000000000
1	2.111751000	-1.423008000	0.000000000
1	-2.111751000	1.423008000	0.000000000
1	3.402316000	1.080662000	0.000000000
6	-2.373127000	-1.428885000	0.000000000
6	-1.952651000	-2.808949000	0.000000000
6	-0.432838000	-2.803080000	0.000000000
6	0.432838000	2.803080000	0.000000000
6	1.952651000	2.808949000	0.000000000
6	-2.454603000	-4.060580000	0.000000000
6	2.454603000	4.060580000	0.000000000
1	3.515354000	4.295871000	0.000000000
1	1.186335000	6.206222000	0.000000000
1	-3.402316000	-1.080662000	0.000000000
1	-1.186335000	-6.206222000	0.000000000
1	-3.515354000	-4.295871000	0.000000000
1	-1.138010000	4.272188000	0.000000000
1	1.138010000	-4.272188000	0.000000000
6	-0.075640000	4.039501000	0.000000000
6	0.075640000	-4.039501000	0.000000000
5	1.201417000	5.003676000	0.000000000
5	-1.201417000	-5.003676000	0.000000000

Total Electronic Energy = −664.803283 a.u.
Number of imaginary frequencies: 0

cyclooctatetraene (D_{2d})

	X	Y	Z
6	1.252243000	-1.110191000	0.409096000
6	1.666366000	0.155963000	0.408992000
6	-1.666398000	-0.156009000	0.408943000
6	1.110262000	1.252126000	-0.409060000
6	-1.252373000	1.110140000	0.409014000
6	-0.155902000	1.666274000	-0.408919000
6	0.156040000	-1.666113000	-0.409032000
6	-1.110223000	-1.252216000	-0.409007000
1	1.805482000	-1.832901000	1.013304000
1	0.412357000	-2.539376000	-1.013323000
1	-1.805790000	1.832881000	1.013025000
1	-0.412129000	2.539701000	-1.013007000
1	1.832949000	1.805530000	-1.013144000
1	-2.539850000	-0.412277000	1.012979000
1	-1.832808000	-1.805637000	-1.013193000
1	2.539696000	0.412234000	1.013200000

Total Electronic Energy = −309.318161 a.u.
Number of imaginary frequencies: 0

cyclooctatetraene (D_{4h})

	X	Y	Z
6	0.667192000	1.712244000	0.000000000
6	-0.667192000	1.712244000	0.000000000
6	0.667192000	-1.712244000	0.000000000
6	-1.712244000	0.667192000	0.000000000
6	-0.667192000	-1.712244000	0.000000000
6	-1.712244000	-0.667192000	0.000000000
6	1.712244000	0.667192000	0.000000000
6	1.712244000	-0.667192000	0.000000000
1	1.105826000	2.711263000	0.000000000
1	2.711263000	1.105826000	0.000000000
1	-1.105826000	-2.711263000	0.000000000
1	-2.711263000	-1.105826000	0.000000000
1	2.711263000	-1.105826000	0.000000000
1	1.105826000	-2.711263000	0.000000000
1	-1.105826000	2.711263000	0.000000000

1	-2.711263000	1.105826000	0.000000000

Total Electronic Energy = −309.292392 a.u.
Number of imaginary frequencies: 1

dibenzo-COT

	X	Y	Z
6	0.664854000	-1.505134000	1.304254000
6	1.537634000	-0.699637000	0.412591000
6	-1.537640000	0.699524000	0.412725000
6	1.537647000	0.699599000	0.412656000
6	-0.664862000	1.504996000	1.304367000
6	0.664882000	1.505049000	1.304327000
6	-0.664816000	-1.505314000	1.304165000
6	-1.537634000	-0.699763000	0.412556000
1	1.181430000	-2.204485000	1.965190000
1	-1.181297000	-2.204835000	1.964994000
1	-1.181441000	2.204445000	1.965206000
1	1.181420000	2.204572000	1.965114000
6	2.437030000	1.379875000	-0.413926000
6	3.304923000	0.695687000	-1.248661000
6	3.305003000	-0.695488000	-1.248698000
6	2.437167000	-1.379819000	-0.414023000
1	2.442454000	2.469506000	-0.397358000
1	3.988094000	1.245689000	-1.893333000
1	3.988258000	-1.245375000	-1.893380000
1	2.442727000	-2.469448000	-0.397488000
6	-2.437080000	1.379881000	-0.413777000
6	-2.437173000	-1.379828000	-0.414074000
6	-3.304995000	-0.695439000	-1.248749000
6	-3.304961000	0.695719000	-1.248621000
1	-2.442517000	2.469510000	-0.397112000
1	-2.442726000	-2.469458000	-0.397675000
1	-3.988179000	-1.245308000	-1.893521000
1	-3.988106000	1.245750000	-1.893294000

Total Electronic Energy = −616.414374 a.u.
Number of imaginary frequencies: 0

4-syn

	X	Y	Z
6	1.621015000	-0.660138000	-0.206527000
6	0.689222000	-1.624464000	-0.239991000
6	-0.667132000	1.668749000	-0.306603000

6	-0.689475000	-1.624419000	0.240167000
6	-1.612387000	0.717990000	-0.359170000
6	-1.621047000	-0.659949000	0.206862000
6	1.612571000	0.717863000	0.359335000
6	0.667320000	1.668663000	0.307117000
6	3.030462000	-0.968193000	-0.518384000
6	3.912401000	-0.044034000	-0.074583000
1	3.290467000	-1.902277000	-1.021170000
1	4.986032000	-0.166244000	-0.202046000
5	3.110000000	1.082946000	0.618869000
1	3.502911000	2.067336000	1.183723000
6	-3.912441000	-0.043945000	0.073994000
1	-3.502539000	2.067043000	-1.184752000
1	-4.986117000	-0.166156000	0.201091000
1	-3.290829000	-1.901880000	1.021463000
1	-0.956027000	2.646051000	-0.704412000
1	0.956292000	2.645898000	0.705033000
1	-1.030722000	-2.600071000	0.596050000
1	1.030340000	-2.600122000	-0.595988000
6	-3.030655000	-0.967914000	0.518447000
5	-3.109787000	1.082885000	-0.619465000

Total Electronic Energy = −512.480277 a.u.
Number of imaginary frequencies: 0

4-anti

	X	Y	Z
6	1.623104000	-0.660700000	0.202453000
6	0.703651000	-1.636772000	0.214007000
6	-0.703720000	1.636743000	0.213733000
6	-0.654947000	-1.657472000	-0.328801000
6	-1.623075000	0.660602000	0.202717000
6	-1.615892000	-0.719402000	-0.358597000
6	1.615874000	0.719251000	-0.358845000
6	0.654975000	1.657393000	-0.328746000
6	3.026308000	-0.953333000	0.562287000
6	3.909138000	-0.018314000	0.147740000
1	3.279864000	-1.884971000	1.072532000
1	4.979683000	-0.126123000	0.310207000
5	3.112267000	1.106826000	-0.561092000
1	3.512492000	2.104673000	-1.096703000
6	-3.026255000	0.953349000	0.562411000
6	-3.909104000	0.018448000	0.147707000
1	-3.279703000	1.885052000	1.072597000

1	-4.979665000	0.126415000	0.309994000
5	-3.112325000	-1.106739000	-0.561177000
1	-3.512707000	-2.104385000	-1.097056000
1	-1.043228000	2.606425000	0.586900000
1	0.951111000	2.642484000	-0.701203000
1	-0.950916000	-2.642409000	-0.701808000
1	1.043028000	-2.606368000	0.587489000

Total Electronic Energy = −512.480765 a.u.
Number of imaginary frequencies: 0

4-terminal

	X	Y	Z
6	-0.666762000	1.606947000	-1.008282000
6	-1.549452000	0.771114000	-0.177601000
6	1.549391000	-0.771075000	-0.177598000
6	-1.549345000	-0.771148000	-0.177553000
6	0.666713000	-1.606823000	-1.008315000
6	-0.666691000	-1.606886000	-1.008295000
6	0.666676000	1.607012000	-1.008191000
6	1.549337000	0.771183000	-0.177478000
6	-2.521986000	-1.243646000	0.617281000
1	-2.707332000	-2.308636000	0.737767000
1	-4.069999000	-0.000145000	2.133026000
1	-2.707641000	2.308509000	0.737589000
6	2.522048000	1.243578000	0.617344000
1	2.707419000	2.308556000	0.737884000
1	4.070003000	-0.000087000	2.133020000
1	2.707657000	-2.308614000	0.737359000
6	2.522153000	-1.243580000	0.617085000
6	-2.522134000	1.243517000	0.617226000
5	-3.219087000	-0.000089000	1.285746000
5	3.219136000	-0.000041000	1.285696000
1	1.176229000	-2.363897000	-1.606880000
1	-1.176178000	-2.364031000	-1.606794000
1	1.176211000	2.363979000	-1.606875000
1	-1.176296000	2.363858000	-1.607041000

Total Electronic Energy = −512.442175 a.u.
Number of imaginary frequencies: 0