

Physical Chemistry Chemical Physics

ELECTRONIC SUPPLEMENTARY INFORMATION

**Local aromaticity of the five-membered rings
in acenaphthylene derivatives**

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Table S1. Cartesian coordinates and energies (in Hartrees) of the molecules studied obtained at the B3LYP/6-311+G(d,p) level.

1			
<i>E</i> =-385.9889			
H	-3.37303900	-1.24340700	-0.00000100
C	-2.43044400	-0.70761400	-0.00000100
H	-1.24265300	-2.48596400	0.00000000
C	-1.24371400	-1.40076200	0.00000000
C	-1.24371400	1.40076200	0.00000000
C	0.00000000	-0.71576500	0.00000000
C	-2.43044400	0.70761400	-0.00000100
C	0.00000000	0.71576500	0.00000000
C	1.24371400	-1.40076300	0.00000000
H	-3.37303900	1.24340700	-0.00000100
H	1.24265300	2.48596500	0.00000100
H	-1.24265300	2.48596400	0.00000000
C	2.43044400	-0.70761400	0.00000100
H	1.24265200	-2.48596500	0.00000000
H	3.37303900	-1.24340600	0.00000100
C	2.43044400	0.70761400	0.00000100
H	3.37303900	1.24340600	0.00000100
C	1.24371400	1.40076300	0.00000100
1a			
<i>E</i> =-462.1985			
H	-3.39422400	-1.59268900	0.00002700
C	-2.42669400	-1.10284600	0.00001200
H	-1.35949500	-2.96031100	0.00001700
C	-1.28159500	-1.87812500	0.00000800
C	-1.16046800	0.95020000	-0.00001900
C	0.00000000	-1.25423600	-0.00001000
C	-2.38777300	0.32092300	0.00000000
C	0.00000000	0.14036300	-0.00002700
C	1.28159500	-1.87812500	0.00000100
H	-3.31841500	0.87885200	0.00001400
C	2.42669500	-1.10284600	0.00000600
H	1.35949500	-2.96031100	0.00000900
H	3.39422400	-1.59269100	0.00001800
C	2.38777400	0.32092200	0.00000000
H	3.31841400	0.87885300	0.00002000
C	1.16046700	0.95019900	-0.00001500
C	0.68117900	2.34268300	0.00001600
H	1.31546500	3.21875700	0.00003300
C	-0.68117900	2.34268400	0.00000300
H	-1.31546300	3.21875800	0.00001000

2			
<i>E</i> =-539.6602			
H	-4.60040000	1.24481600	-0.00000100
C	-3.65593200	0.71240900	0.00000000
H	-2.47661500	2.49042200	-0.00000200
C	-2.47701300	1.40532900	-0.00000100
C	-2.47701300	-1.40532900	0.00000000
C	-1.22212100	0.72156900	0.00000000
C	-3.65593200	-0.71240900	0.00000000
C	-1.22212100	-0.72156900	0.00000000
C	0.00000000	1.40196100	0.00000000
H	-4.60040000	-1.24481600	0.00000100
H	0.00000000	-2.48791100	0.00000100
H	-2.47661600	-2.49042200	0.00000100
C	1.22212100	0.72156900	0.00000000
H	0.00000000	2.48791100	-0.00000100
C	2.47701300	1.40532900	-0.00000100
C	1.22212100	-0.72156900	0.00000100
H	2.47661500	-2.49042200	0.00000100
C	0.00000000	-1.40196100	0.00000100
C	3.65593200	0.71240900	0.00000100
H	2.47661600	2.49042200	-0.00000100
H	4.60040000	1.24481600	0.00000100
C	3.65593200	-0.71240900	0.00000000
H	4.60040000	-1.24481600	0.00000100
C	2.47701300	-1.40532900	0.00000000
2a			
<i>E</i> =-615.8707			
H	-4.85920700	-1.09122500	0.00002100
C	-3.86477800	-0.65964300	0.00001800
H	-2.87719300	-2.54898000	0.00002100
C	-2.76281400	-1.46988300	0.00001900
C	-2.46940900	1.32437300	0.00000000
C	-1.43967400	-0.92831000	0.00001400
C	-3.71478600	0.75483700	0.00000700
C	-1.29250100	0.52075600	0.00001100
C	-0.31733100	-1.77845500	0.00000400
H	-4.59831000	1.38354300	0.00000200
H	-2.36404900	2.40327700	-0.00001200
C	0.98449300	-1.25259500	-0.00000800
H	-0.47494500	-2.85270000	0.00000600
C	2.22104400	-1.97587700	-0.00001800
C	1.09025400	0.14737300	-0.00000900
C	0.01460600	1.03923200	-0.00000600
C	3.41738200	-1.29430800	-0.00002200
H	2.21218200	-3.06071300	-0.00001900

H	4.34529900	-1.85546100	-0.00002000
C	3.48929800	0.13578600	-0.00001600
H	4.46236000	0.61620200	0.00000500
C	2.32262300	0.86152800	-0.00000200
C	1.96180800	2.28424000	0.00007400
H	2.66285200	3.10738600	0.00013100
C	0.60099500	2.38824200	-0.00007100
H	0.04374800	3.31489400	-0.00011400
3 <i>E</i> =-693.3292			
C	-2.44709300	-0.72496000	-0.00000300
H	-1.23436800	-2.49066400	-0.00000900
C	-1.23400900	-1.40482900	-0.00000600
C	-1.23400800	1.40482900	-0.00000200
C	0.00000200	-0.72509400	-0.00000400
C	-2.44709300	0.72496200	-0.00000200
C	0.00000200	0.72509200	-0.00000200
C	1.23400500	-1.40483000	-0.00000400
H	1.23436700	2.49066400	0.00000400
H	-1.23436400	2.49066400	-0.00000400
C	2.44709500	-0.72495800	-0.00000100
H	1.23436800	-2.49066400	-0.00000700
C	3.70723100	-1.40762600	0.00000000
C	2.44709500	0.72495800	0.00000200
H	3.70732600	2.49269200	0.00000900
C	1.23400500	1.40482900	0.00000100
C	4.88264000	-0.71478200	0.00000300
H	3.70732700	-2.49269200	-0.00000300
H	5.82797700	-1.24559500	0.00000400
C	4.88264000	0.71478300	0.00000700
H	5.82797700	1.24559600	0.00001100
C	3.70723100	1.40762700	0.00000700
C	-3.70723300	1.40762800	-0.00000100
H	-3.70732900	2.49269400	-0.00000200
C	-4.88263900	0.71478400	0.00000100
H	-5.82797800	1.24559300	-0.00000100
C	-4.88263900	-0.71478500	0.00000300
H	-5.82797900	-1.24559400	0.00000700
C	-3.70723300	-1.40762800	0.00000100
H	-3.70732400	-2.49269400	0.00000200
3a <i>E</i> =-769.5402			
C	2.61178500	0.65338900	-0.00009100
H	1.27134200	2.32175400	-0.00063200
C	1.34773300	1.23964000	-0.00048400
C	1.56751200	-1.56056900	-0.00010600

C	0.17076400	0.47406400	-0.00075700
C	2.72523200	-0.78975300	0.00004400
C	0.28036500	-0.98618900	-0.00043700
C	-1.13530400	1.02251200	-0.00104800
H	-0.74452700	-2.88680600	-0.00009400
H	1.65476900	-2.64291300	0.00003600
C	-2.22431600	0.15799400	-0.00092900
C	-3.44426800	0.90132500	-0.00020200
C	-2.15367700	-1.24959400	-0.00045800
H	-3.42786100	-3.02732900	0.00022200
C	-0.87442900	-1.80897300	-0.00026600
C	-4.62462100	0.20243100	0.00061900
H	-5.58682500	0.70427700	0.00168400
C	-4.58749700	-1.23276000	0.00068200
H	-5.52953300	-1.76980500	0.00126900
C	-3.41080000	-1.94266800	0.00016600
C	4.03303600	-1.37531100	0.00036400
H	4.11526300	-2.45726800	0.00044800
C	5.15230500	-0.59464200	0.00054000
H	6.13594800	-1.05032800	0.00077100
C	5.04035700	0.82974400	0.00042900
H	5.94158000	1.43255800	0.00061400
C	3.81446100	1.43068000	0.00011200
H	3.73142800	2.51247300	0.00003100
C	-3.05302900	2.31380800	0.00055400
H	-3.73399300	3.15341000	0.00129500
C	-1.68863100	2.38371100	0.00025600
H	-1.10945600	3.29693500	0.00042700
3b <i>E</i> =-769.5411			
C	4.88337200	-0.91349400	-0.00001500
H	3.75194400	-2.71842000	-0.00000600
C	3.72357100	-1.63368000	-0.00000800
C	3.65089200	1.17888500	-0.00001800
C	2.44367600	-0.98899200	-0.00000300
C	2.41014100	0.47234600	-0.00000600
C	1.26488600	-1.74558000	0.00000000
H	3.63159900	2.26260000	-0.00002400
C	0.00006900	-1.11760700	0.00000100
H	1.33552700	-2.82890800	0.00000000
C	-1.26499800	-1.74560700	0.00000300
C	0.00007700	0.29167100	0.00000000
C	1.15524200	1.09522600	-0.00000600
H	-1.33532600	-2.82897400	0.00000300
C	-1.15538600	1.09525200	0.00000500
C	-0.68424300	2.48215900	0.00003000

H	-1.31174300	3.36241400	0.00005200
C	0.68410300	2.48215800	-0.00003200
H	1.31162300	3.36240200	-0.00005400
C	-2.41001400	0.47231400	0.00000500
C	-2.44356600	-0.98925600	0.00000400
C	-3.72372200	-1.63372700	0.00001000
C	-4.88332100	-0.91358200	0.00001600
C	-3.65089100	1.17892100	0.00001600
H	-3.63137100	2.26263700	0.00002100
H	-3.75203900	-2.71850000	0.00001000
C	-4.84438300	0.51223500	0.00002000
C	4.84449200	0.51204600	-0.00002100
H	-5.77569200	1.06773600	0.00002700
H	-5.84154900	-1.42035200	0.00002100
H	5.77561600	1.06787200	-0.00002900
H	5.84141600	-1.42063800	-0.00001900
4			
<i>E</i> =-846.9969			
C	3.67357200	-0.72679600	-0.00000400
H	2.46544900	-2.49223200	0.00000300
C	2.46479600	-1.40643100	0.00000000
C	2.46479800	1.40643200	-0.00000800
C	1.22479400	-0.72753700	0.00000000
C	3.67357300	0.72679500	-0.00000800
C	1.22479500	0.72754000	-0.00000400
C	-0.00000400	-1.40697300	0.00000400
H	0.00000300	2.49268700	-0.00000800
H	2.46545400	2.49223300	-0.00001100
C	-1.22478700	-0.72753600	0.00000400
H	-0.00000100	-2.49268200	0.00000700
C	-2.46480200	-1.40643000	0.00000900
C	-1.22478500	0.72754400	-0.00000100
H	-2.46545400	2.49223500	-0.00000500
C	-0.00000300	1.40697800	-0.00000500
C	-3.67356900	-0.72680400	0.00000900
H	-2.46544200	-2.49223300	0.00001200
C	-3.67356600	0.72680000	0.00000300
C	-2.46480500	1.40643300	-0.00000100
C	4.93630400	1.40886500	-0.00001200
H	4.93666500	2.49392000	-0.00001600
C	6.10997500	0.71601100	-0.00001200
H	7.05576000	1.24600000	-0.00001500
C	6.10997500	-0.71601500	-0.00000800
H	7.05575900	-1.24600600	-0.00000800
C	4.93630300	-1.40886800	-0.00000400
H	4.93666200	-2.49392300	-0.00000100

C	-4.93630800	-1.40887000	0.00001500
H	-4.93665900	-2.49392600	0.00002000
C	-4.93630800	1.40886700	0.00000200
H	-4.93666400	2.49392300	-0.00000400
C	-6.10997300	0.71601600	0.00000800
H	-7.05576300	1.24599800	0.00000500
C	-6.10997400	-0.71601900	0.00001500
H	-7.05576300	-1.24600100	0.00002200
4a			
<i>E</i> =-923.2082			
C	-3.34363900	-1.23397800	-0.00009200
H	-1.96862600	-2.89648700	-0.00003200
C	-2.07891800	-1.81646200	-0.00009000
C	-2.28892900	1.02271600	-0.00016400
C	-0.90381900	-1.01453100	-0.00010500
C	-3.38887500	0.17773000	-0.00018000
C	-0.98659900	0.45294600	-0.00011100
C	0.36320700	-1.61314800	-0.00007900
H	0.13889300	2.27839100	-0.00006800
C	1.54651400	-0.86362100	-0.00004400
H	0.43012700	-2.69684100	-0.00007800
C	2.82219800	-1.47211900	-0.00000100
C	1.46038200	0.58685000	-0.00003900
H	2.59625100	2.41931700	-0.00002200
C	0.19529500	1.19515000	-0.00007000
C	3.99032900	-0.72424200	0.00002700
H	2.88419800	-2.55614300	0.00000900
C	3.90490300	0.72598800	0.00001200
C	2.65761900	1.33535800	-0.00001800
C	-4.59861100	0.94173700	-0.00001600
C	-5.78902900	0.26250500	0.000020500
H	-6.74272200	0.78049300	0.000040600
C	-5.77710500	-1.17496300	0.00018500
H	-6.72862800	-1.69491800	0.00033200
C	-4.61412000	-1.90494300	0.00004100
H	-4.64988400	-2.98915100	0.00006800
C	5.28999500	-1.33264200	0.00007100
H	5.35275700	-2.41587500	0.00008300
C	5.12540400	1.48005600	0.00004100
H	5.06287500	2.56324700	0.00003000
C	6.33760400	0.85614900	0.00007900
H	7.25084700	1.44050900	0.00009900
C	6.42169400	-0.57294100	0.00009600
H	7.39685800	-1.04659500	0.00012900
C	-4.18460200	2.34709500	0.00011700
H	-4.85126500	3.19800000	0.00003800

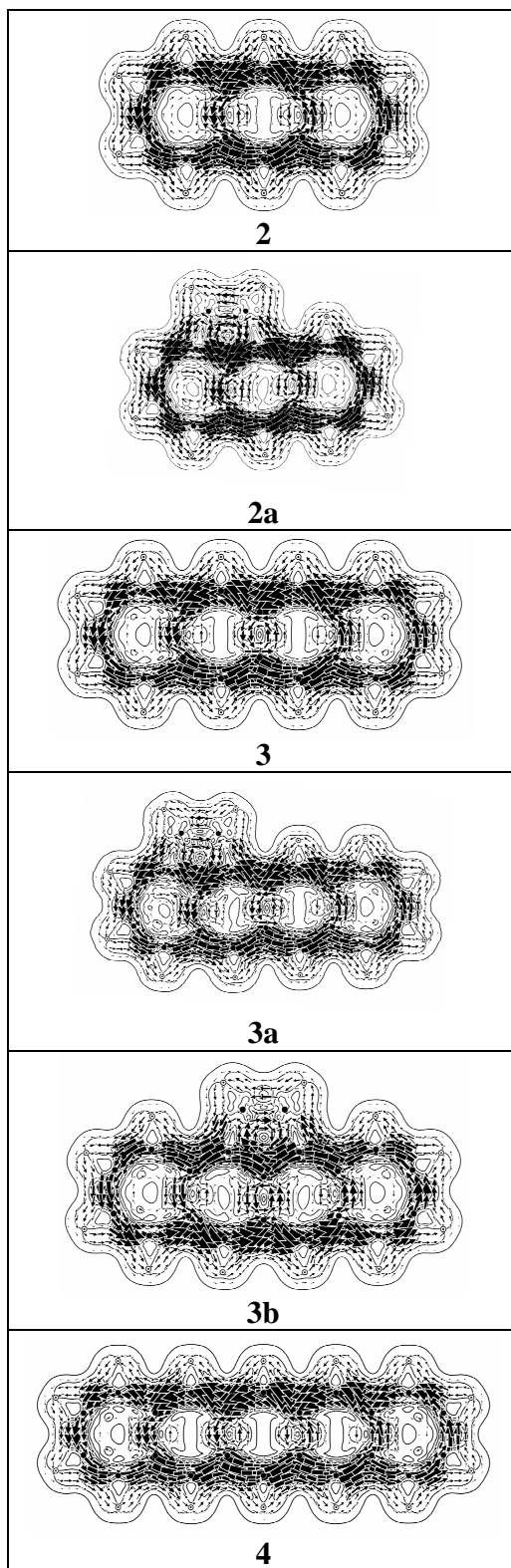
C	-2.81892700	2.39272900	-0.00001000
H	-2.22349000	3.29553600	-0.00012800
4b <i>E</i> =-923.2098			
H	6.95322300	-1.48646800	-0.00004600
C	6.00174700	-0.96719200	-0.00004100
H	4.84665700	-2.75609700	-0.00003900
C	4.83351500	-1.67107500	-0.00003800
C	4.79878900	1.14417100	-0.00002500
C	3.56066300	-1.00889600	-0.00003100
C	5.98163900	0.46066100	-0.00003300
C	3.54626700	0.45573800	-0.00002900
C	2.37527400	-1.74872300	-0.00001900
H	4.79474400	2.22797900	-0.00001600
C	1.11486700	-1.10345200	-0.00000500
H	2.43047900	-2.83291500	-0.00001800
C	-0.14866400	-1.71731700	0.00001000
C	1.13170600	0.30933800	-0.00000700
C	2.30370400	1.09728600	-0.00001300
H	-0.23129700	-2.79975700	0.00001300
C	-0.00510400	1.12722600	-0.00000300
C	0.48451000	2.50556800	-0.00005800
H	-0.13125500	3.39424800	-0.00008900
C	1.85450900	2.48877600	0.00003900
H	2.49358200	3.36047500	0.00007000
C	-1.27995100	0.52143000	0.00001400
C	-1.32921100	-0.94617000	0.00002100
C	-2.59525800	-1.57525700	0.00002900
C	-3.78121800	-0.85534200	0.00003100
C	-2.49313000	1.23421600	0.00000900
H	-2.46380000	2.31854500	-0.00000200
H	-2.63564700	-2.66039200	0.00003100
C	-3.72799500	0.59441800	0.00002000
C	-4.96454300	1.31934400	0.00001900
C	-6.16250700	0.66672000	0.00002900
H	-7.08888200	1.23015000	0.00002800
C	-6.21483600	-0.76315200	0.00004000
H	-7.17891600	-1.25883900	0.00004700
C	-5.06494900	-1.49559200	0.00004000
H	-5.10087000	-2.58008900	0.00004800
H	-4.92757900	2.40366900	0.00001100
H	6.92061200	1.00316400	-0.00003200
5 <i>E</i> =-1000.6640			
C	-2.45113800	0.72889000	-0.00018100
H	-1.23118100	2.49388200	-0.00021900

C	-1.23100500	1.40823800	-0.00017100
C	-1.23101700	-1.40819000	-0.00010400
C	0.00002300	0.72943100	-0.00013300
C	-2.45123500	-0.72884400	-0.00017100
C	-0.00003400	-0.72940900	-0.00006300
C	1.23093100	1.40821700	-0.00014700
H	1.23119100	-2.49385400	0.00012300
H	-1.23137500	-2.49383300	-0.00007900
C	2.45118600	0.72883700	-0.00004400
H	1.23128900	2.49385700	-0.00020300
C	3.69433100	1.40738200	-0.00004500
C	2.45116000	-0.72884800	0.00005600
H	3.69515500	-2.49316200	0.00017600
C	1.23093600	-1.40821600	0.00004700
C	4.90086500	0.72772200	0.00002200
H	3.69519600	2.49314200	-0.00010900
C	4.90085600	-0.72774500	0.00010300
C	3.69433700	-1.40740400	0.00012500
C	-3.69446500	-1.40739800	-0.00028900
H	-3.69537300	-2.49313300	-0.00037500
C	-4.90082900	0.72775800	-0.00013400
C	-3.69429200	1.40736900	-0.00015500
H	-3.69508400	2.49316900	-0.00010100
C	6.16504500	1.40956600	0.00001200
H	6.16526600	2.49461200	-0.00004100
C	6.16505000	-1.40959100	0.00015400
H	6.16525600	-2.49463700	0.00020300
C	7.33778100	-0.71671900	0.00014000
H	8.28390400	-1.24612500	0.00018100
C	7.33778300	0.71669700	0.00007100
H	8.28390300	1.24610800	0.00006500
C	-6.16491700	1.40961400	0.00028000
C	-7.33773400	0.71673800	0.00056200
C	-7.33772200	-0.71668300	0.00027900
C	-6.16506100	-1.40956200	-0.00003300
C	-4.90083000	-0.72784700	-0.00029900
H	-6.16512700	2.49462400	0.00020700
H	-8.28382700	1.24616200	0.00107000
H	-8.28380400	-1.24616200	0.00012300
H	-6.16541900	-2.49465500	-0.00031800
5a			
<i>E</i> =-1076.8755			
C	-2.80053200	-0.79692500	-0.00000800
H	-1.65894500	-2.61441000	-0.00002200
C	-1.61149200	-1.52977000	-0.00002900
C	-1.48300300	1.28322000	-0.00004400

C	-0.35291800	-0.90432900	-0.00005900
C	-2.73400700	0.65870600	-0.00001500
C	-0.28529400	0.55121100	-0.00006600
C	0.84549900	-1.63870200	-0.00008400
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H	-1.43544100	2.36774400	-0.00004900
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C	2.16498300	0.44738700	-0.00012600
C	0.97846900	1.17411900	-0.00010600
C	4.54340100	-1.21415600	-0.00011500
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C	3.46380900	1.03165200	-0.00017700
C	-3.94484300	1.39161300	0.00000800
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C	5.77378400	0.97766400	-0.00003000
C	6.97112200	0.31182100	0.00023800
H	7.91897300	0.84046600	0.00044000
C	6.97612800	-1.12665600	0.00025300
H	7.93383700	-1.63510400	0.00042800
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H	-8.64998400	-1.05311000	0.00009800
H	-8.53723200	1.43629800	0.00009300
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C	5.34445600	2.37778200	0.00007000
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C	-0.17300400	-0.94619300	-0.00007600
C	-2.57642100	0.59490300	-0.00000400
C	-0.12529000	0.52594000	0.00000200
C	1.01313400	-1.71731300	-0.00009800
H	5.95559600	2.22620800	0.00012000
H	-1.30230800	2.31988100	0.00009700
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C	1.15632500	1.13027500	0.00004200
C	4.71807100	-1.01035400	0.00004300
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H	-3.92309300	-2.58559400	-0.00017400
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H	8.11066100	-1.49059700	0.00012800
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C	-7.50850100	-0.69269900	-0.00008500
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H	-8.38773000	1.29999400	0.00001800
H	-6.22953100	2.47791800	0.00008600
C	3.01806700	2.48988600	-0.00003200
H	3.65720200	3.36141400	-0.00008900
C	1.64684900	2.50687200	0.00014700
H	1.03197300	3.39623500	0.00021300
5c			
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C	-3.70547700	-1.58955400	0.00002400
C	-3.64236300	1.22239900	0.00001700

C	-2.44647900	-0.94207500	0.00001900
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H	-1.32623600	-2.77988500	0.00000700
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C	-0.00004700	0.35081800	0.00000100
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C	-0.68609600	2.53607900	-0.00003000
H	-1.31345500	3.41645300	-0.00005100
C	2.41673000	0.52816600	-0.00001700
C	2.44638700	-0.94219000	-0.00002300
C	3.70555700	-1.58960200	-0.00003000
C	4.89992400	-0.88708900	-0.00003100
C	3.64239400	1.22236300	-0.00001300
H	3.62897400	2.30693300	-0.00000300
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C	4.86643400	0.56473400	-0.00002200
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C	7.30202600	0.60214500	-0.00002900
H	8.23635500	1.15229800	-0.00002800
C	7.33477500	-0.82929400	-0.00003900
H	8.29204100	-1.33795600	-0.00004500
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H	6.19584300	-2.63027600	-0.00004600
H	6.09260100	2.35650200	-0.00001400
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C	-6.11408700	1.27177300	0.00002500
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H	-6.09269900	2.35647300	0.00002100



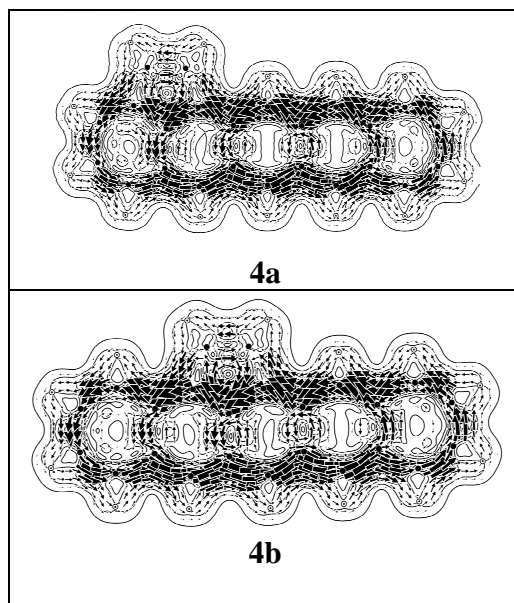
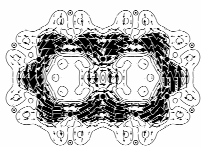
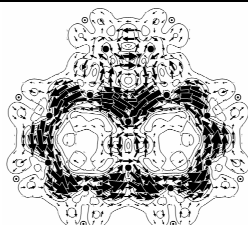


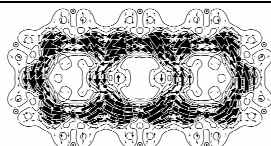
Figure S1. Ring current plots of the molecules studied obtained at the CTOCD-DZ/HF/6-31G/B3LYP/6-311+G(d,p) level.



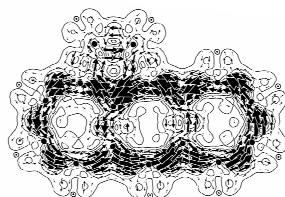
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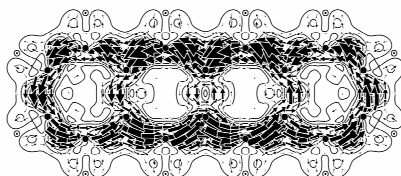
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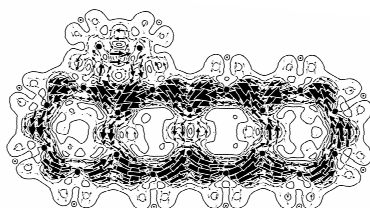
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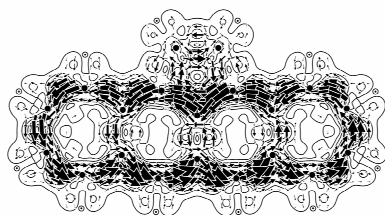
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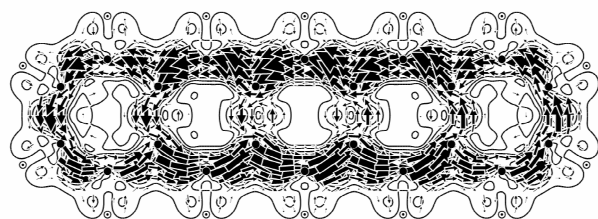
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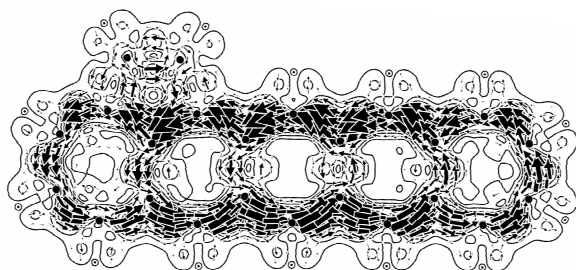
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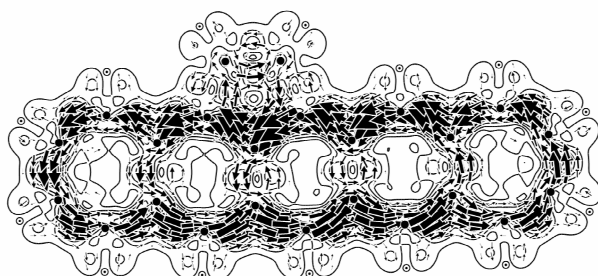
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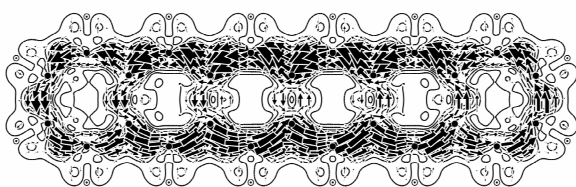
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4a



4b



5

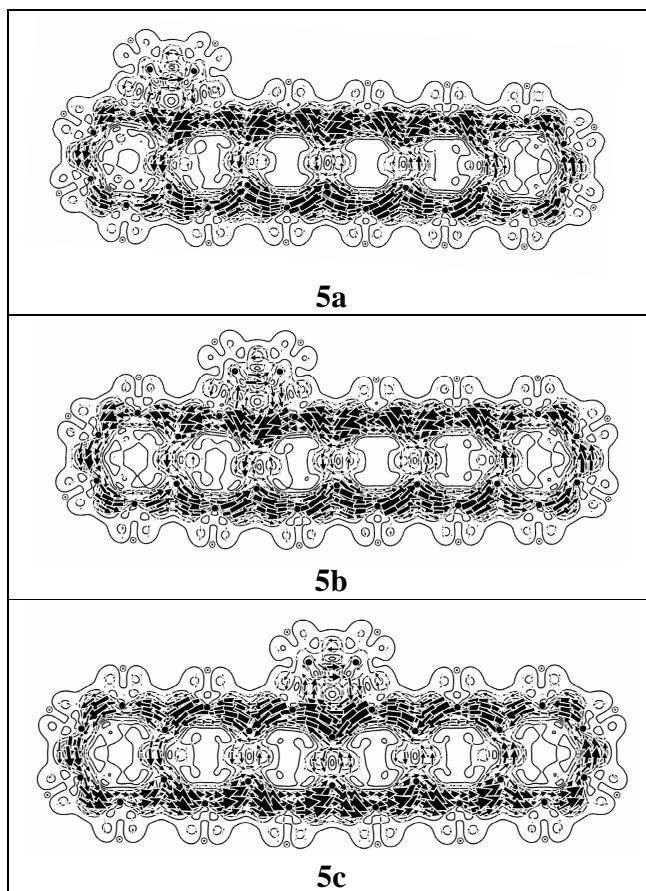
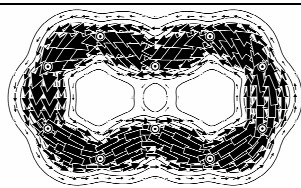
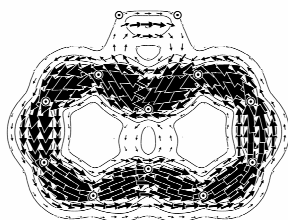


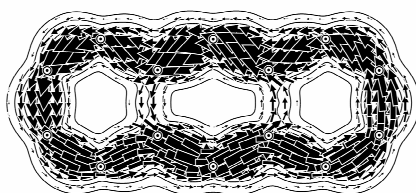
Figure S2. Ring current plots of the molecules studied obtained at the CTOCD-DZ/HF/STO-3G/B3LYP/6-311+G(d,p) level.



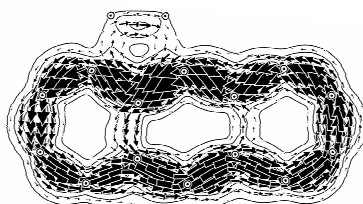
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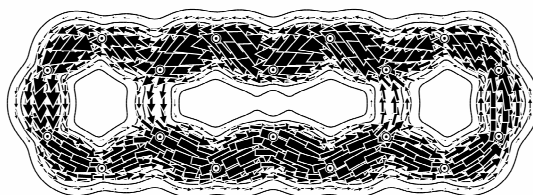
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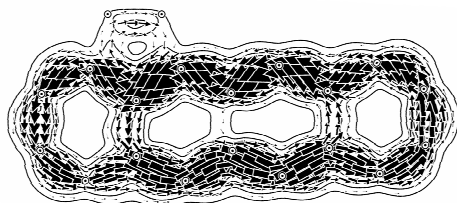
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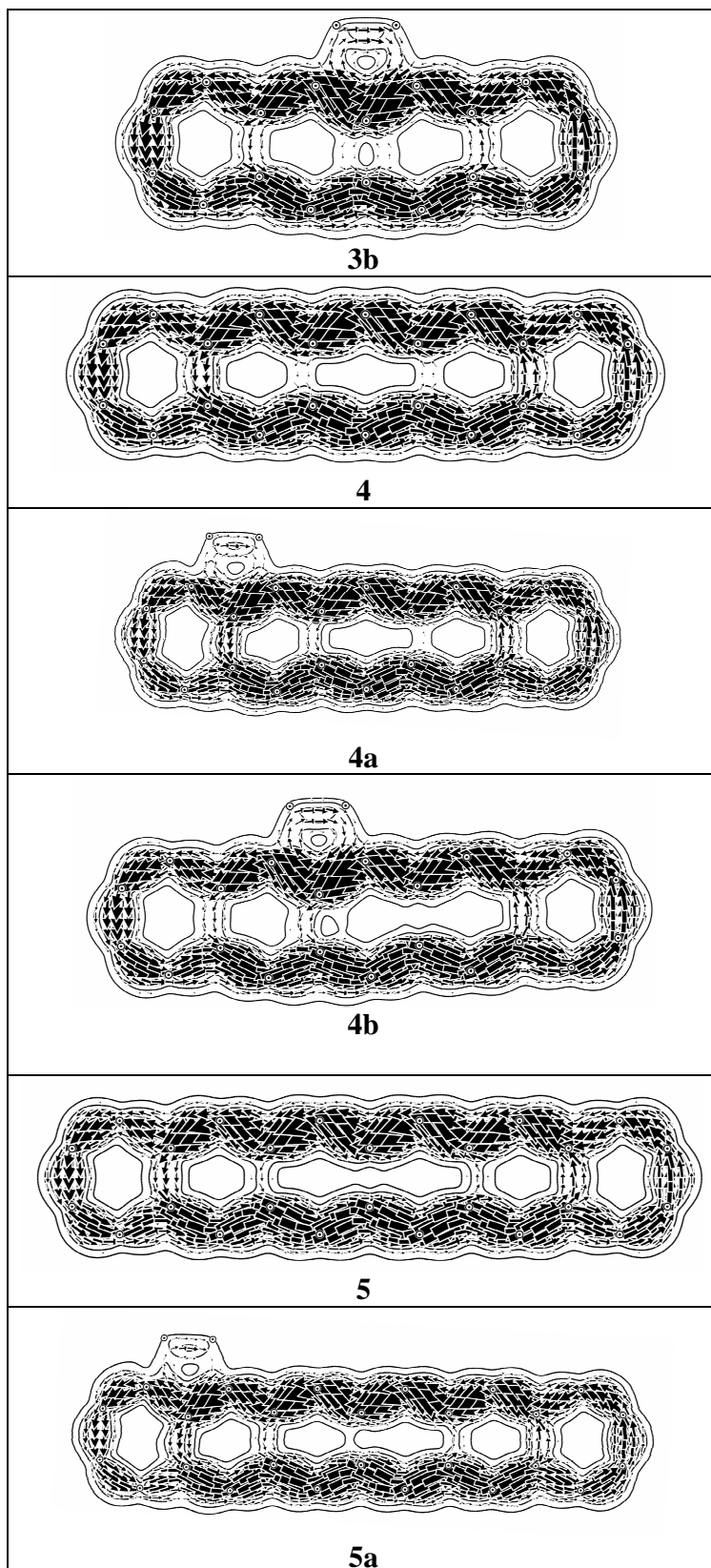
2a



3



3a



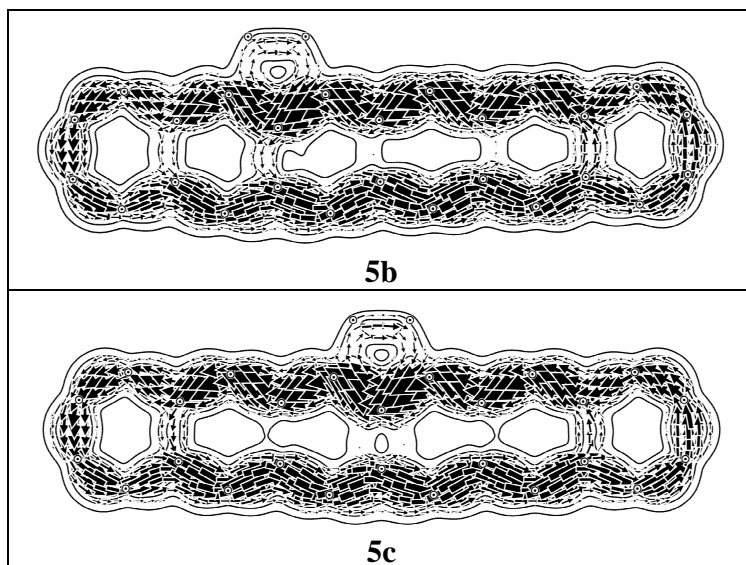


Figure S3. Ring current plots of the molecules studied obtained using the pseudo- π method.

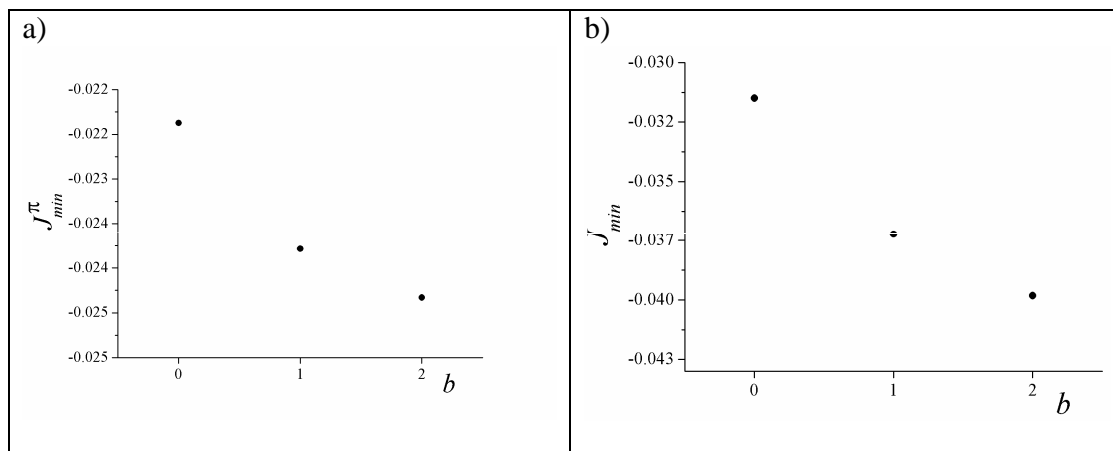


Figure S4. Dependence of the J_{min}^{π} and J_{min} of the γ -type C-C bonds obtained a) at the CT OCD-DZ/HF/STO-3G/B3LYP/6-311+G(d,p) level and b) with the pseudo- π method, respectively, on the number b of hexagons in the series of molecules **5a**, **5b**, and **5c**. For details see text.