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Aromaticity induced by electric field - the case of polycalicenes

by

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The molecular structures were optimized at B3LYP/6-311++G(d,p) level of theory using Gaussian09 package (G09, Rev. D01). Vibrational analysis was performed. No imaginary frequencies were found for all but one system, that is, **VII**, for which one imaginary frequency, of 36*i* cm^{-1} corresponds to out-of-plane vibration. However, it should be noted that frequencies of such small magnitude should be neglected, being attributed to numerical noise. Geometries are given in angstroms, total energies (E) and external electric field values (F) in au.

Table S1. Geometries and total energies of the systems **I-VIII** and H_2 molecule.

I

C	-0.044645000	-0.000030000	-0.000050000
C	-0.911047000	1.170571000	-0.000023000
C	-2.202666000	0.726814000	0.000143000
C	-2.202701000	-0.726770000	0.000062000
C	-0.911104000	-1.170589000	-0.000152000
C	1.306970000	-0.000046000	-0.000014000
C	2.569786000	0.661855000	-0.000006000
C	2.569845000	-0.661826000	0.000036000
H	-0.570587000	2.196538000	0.000021000
H	-3.089040000	1.347039000	0.000306000
H	-3.089106000	-1.346950000	0.000093000
H	-0.570690000	-2.196571000	-0.000333000
H	3.136336000	1.578554000	0.000062000
H	3.136464000	-1.578483000	-0.000115000

E= -308.3958392

II

C	-2.555342000	0.403492000	-0.000075000
C	-1.101379000	0.590893000	-0.000039000
C	-0.873781000	1.958946000	-0.000066000
C	-2.127907000	2.647774000	-0.000111000
C	-3.143637000	1.720906000	-0.000197000
C	-3.234441000	-0.769892000	0.000080000
C	-3.304067000	-2.187860000	0.000359000
C	-4.444613000	-1.512683000	0.000268000
H	0.102098000	2.423167000	-0.000027000
H	-2.247541000	3.721957000	-0.000125000
H	-4.205595000	1.923907000	-0.000285000
H	-5.522192000	-1.528055000	0.000266000
C	2.605406000	-0.358163000	-0.000038000
C	3.746833000	-1.256262000	-0.000309000
C	4.881253000	-0.489118000	0.000031000
C	4.500129000	0.909582000	0.000460000
C	3.133383000	0.994908000	0.000170000
C	1.294728000	-0.727164000	-0.000154000
C	0.284472000	-1.699785000	-0.000383000
C	-0.105143000	-0.409403000	-0.000045000
H	3.688223000	-2.336102000	-0.000589000
H	5.899255000	-0.856075000	0.000064000
H	5.190826000	1.742509000	0.000815000
H	0.022993000	-2.744831000	-0.000615000
H	-2.802384000	-3.141253000	0.000511000
H	2.538937000	1.897751000	0.000286000

E= -615.6158812

III

C	0.066423000	1.349812000	0.000159000
C	1.512473000	1.135015000	0.000192000
C	2.109842000	2.394054000	0.000420000
C	1.095613000	3.391822000	0.000600000
C	-0.138818000	2.769261000	0.000389000
C	-0.906226000	0.386711000	-0.000072000
C	-1.320417000	-0.942535000	-0.000192000
C	-2.285251000	0.006150000	-0.000161000
H	3.175785000	2.572396000	0.000500000
H	1.268330000	4.458857000	0.000826000
H	-1.103007000	3.257719000	0.000428000
C	4.812308000	-0.806667000	0.000003000
C	5.657137000	-1.986393000	-0.000123000
C	6.962248000	-1.566336000	-0.000126000
C	6.986189000	-0.118387000	0.000109000
C	5.695618000	0.344201000	0.000261000
C	3.448162000	-0.795932000	-0.000039000
C	2.210660000	-1.448731000	-0.000198000
C	2.193472000	-0.098046000	0.000020000
H	5.299823000	-3.007323000	-0.000266000
H	7.837120000	-2.203502000	-0.000258000
H	7.881245000	0.489864000	0.000182000
H	1.668551000	-2.379398000	-0.000332000
H	-1.046203000	-1.983632000	-0.000565000
H	5.375198000	1.376648000	0.000459000
C	-4.821033000	-0.453415000	-0.000174000
C	-3.634563000	0.406510000	-0.000074000
C	-4.091218000	1.719488000	0.000099000
C	-5.517753000	1.724041000	0.000107000
C	-5.964544000	0.421212000	-0.000026000
C	-4.863925000	-1.810776000	-0.000328000
C	-4.262423000	-3.094884000	-0.000460000
C	-5.586950000	-3.030601000	-0.000444000
H	-3.458867000	2.595818000	0.000192000
H	-6.138037000	2.608835000	0.000226000
H	-3.374494000	-3.705217000	-0.000519000
H	-6.994302000	0.091830000	-0.000031000
H	-6.533276000	-3.546340000	-0.000493000

E= -922.8401915

IV

C	-2.633228000	-1.871362000	-0.000075000
C	-3.909405000	-1.160758000	0.000085000
C	-4.914734000	-2.129954000	0.000638000
C	-4.317612000	-3.417900000	0.000904000
C	-2.939935000	-3.268652000	0.000381000
C	-1.380639000	-1.309406000	-0.000641000
C	-0.533072000	-0.211253000	-0.000642000
C	0.044223000	-1.439967000	-0.000718000
H	-5.975196000	-1.921067000	0.000913000
H	-4.853823000	-4.356537000	0.001390000
H	-2.208892000	-4.064935000	0.000344000
C	-6.297894000	1.835379000	-0.000109000
C	-6.661823000	3.239256000	-0.000380000
C	-8.031575000	3.317040000	0.000112000
C	-8.574025000	1.975224000	0.000377000
C	-7.535048000	1.079444000	0.000019000
C	-5.027241000	1.334650000	-0.000210000
C	-3.639921000	1.501088000	-0.000471000
C	-4.107548000	0.232071000	-0.000193000
H	-5.961374000	4.063661000	-0.000690000
H	-8.618694000	4.226381000	0.000213000
H	-9.627891000	1.729066000	0.000699000
H	-2.799517000	2.174520000	-0.000536000
H	-0.427791000	0.859921000	-0.001435000
H	-7.606684000	0.000758000	0.000048000
C	6.298018000	1.764617000	0.000133000
C	5.562842000	0.497225000	0.000024000
C	6.515374000	-0.518057000	-0.000056000
C	7.818503000	0.056356000	0.000019000
C	7.696204000	1.429639000	0.000083000
C	5.789950000	3.025498000	0.000296000
C	4.726081000	3.961211000	0.000431000
C	5.966361000	4.431353000	0.000457000
H	6.294372000	-1.575820000	-0.000149000
H	8.745109000	-0.499277000	-0.000009000
H	8.503662000	2.148579000	0.000141000
H	6.627755000	5.282325000	0.000541000
C	2.573249000	-1.874564000	-0.000115000
C	1.168705000	-2.278094000	-0.000171000
C	1.147750000	-3.676276000	-0.000168000
C	2.479207000	-4.160713000	-0.000045000
C	3.344788000	-3.077605000	0.000027000
C	3.065005000	-0.592936000	-0.000147000
C	2.899144000	0.785552000	-0.000147000
C	4.170054000	0.313241000	-0.000045000
H	0.253338000	-4.282838000	-0.000088000
H	2.766622000	-5.202447000	0.000095000
H	2.225289000	1.625168000	-0.000155000
H	3.668551000	4.167824000	0.000492000
H	4.424609000	-3.123376000	0.000269000

E= -1230.0671837

V

C	3.206382000	-7.371004000	0.000000000
C	1.759094000	-7.282895000	0.000000000
C	1.254704000	-8.641563000	0.000000000
C	2.333121000	-9.490203000	0.000000000
C	3.545720000	-8.700947000	0.000000000
H	0.209578000	-8.917962000	0.000000000
H	2.293360000	-10.571717000	0.000000000
H	4.550758000	-9.103043000	0.000000000
C	-1.641218000	-5.511554000	0.000000000
C	-2.577622000	-4.391290000	0.000000000
C	-3.891248000	-4.952256000	0.000000000
C	-3.780980000	-6.335620000	0.000000000
C	-2.406180000	-6.681900000	0.000000000
C	-0.237320000	-5.442770000	0.000000000
C	0.919069000	-4.739266000	0.000000000
C	1.022829000	-6.131435000	0.000000000
H	-4.809801000	-4.382266000	0.000000000
H	-4.603731000	-7.036850000	0.000000000
H	1.417083000	-3.784485000	0.000000000
H	-2.002410000	-7.684554000	0.000000000
C	-2.255670000	-3.054274000	0.000000000
C	-2.644160000	-1.677090000	0.000000000
C	-1.329548000	-2.025346000	0.000000000
C	-3.663475000	-0.717750000	0.000000000
H	-0.295323000	-1.728047000	0.000000000
C	-3.504666000	0.733646000	0.000000000
C	-5.041243000	-0.976915000	0.000000000
C	-4.816570000	1.289455000	0.000000000
C	-2.318661000	1.434262000	0.000000000
C	-5.741108000	0.250684000	0.000000000
H	-5.486372000	-1.961787000	0.000000000
H	-5.043259000	2.346283000	0.000000000
C	-1.608806000	2.674959000	0.000000000
C	-0.937112000	1.491342000	0.000000000
H	-6.816290000	0.360046000	0.000000000
C	-1.643988000	4.073528000	0.000000000
H	0.000000000	0.962025000	0.000000000
C	-0.504030000	4.987616000	0.000000000
C	-2.800032000	4.865265000	0.000000000
C	0.829272000	4.651160000	0.000000000
C	-1.040717000	6.309328000	0.000000000
C	-2.427230000	6.228843000	0.000000000
H	-3.811744000	4.485300000	0.000000000
C	2.204595000	5.037219000	0.000000000
C	1.860230000	3.724213000	0.000000000
H	-0.455645000	7.217994000	0.000000000
H	-3.110479000	7.065948000	0.000000000
C	3.154673000	6.070138000	0.000000000
H	2.161862000	2.690769000	0.000000000
C	4.614414000	5.944818000	0.000000000
C	2.869869000	7.434060000	0.000000000
C	5.141599000	7.281455000	0.000000000
C	5.358815000	4.806227000	0.000000000
C	4.086931000	8.170783000	0.000000000
H	1.876703000	7.859798000	0.000000000
H	6.193750000	7.530113000	0.000000000
C	6.614160000	4.150514000	0.000000000
C	5.520653000	3.399335000	0.000000000
H	4.164228000	9.248381000	0.000000000
H	5.088720000	2.412138000	0.000000000

H	3.881325000	-6.525468000	0.000000000
H	7.690392000	4.208757000	0.000000000

E= -1537.2959573

VI

C	5.994045000	-4.376496000	0.000000000
C	6.553526000	-3.039426000	0.000000000
C	7.994125000	-3.185853000	0.000000000
C	8.280522000	-4.528639000	0.000000000
C	7.038223000	-5.268558000	0.000000000
H	8.703092000	-2.369728000	0.000000000
H	9.268880000	-4.969361000	0.000000000
H	6.956048000	-6.348039000	0.000000000
C	6.415714000	0.804374000	0.000000000
C	5.786716000	2.122096000	0.000000000
C	6.840302000	3.082567000	0.000000000
C	8.054712000	2.406483000	0.000000000
C	7.799831000	1.013660000	0.000000000
C	5.761498000	-0.437955000	0.000000000
C	4.628877000	-1.181702000	0.000000000
C	5.839734000	-1.872594000	0.000000000
H	6.702971000	4.154964000	0.000000000
H	9.034024000	2.864266000	0.000000000
H	3.552868000	-1.219096000	0.000000000
H	8.544501000	0.230073000	0.000000000
C	-1.735745000	-6.997387000	0.000000000
C	-1.599777000	-5.677513000	0.000000000
C	-2.911410000	-6.209319000	0.000000000
H	-0.937517000	-4.827518000	0.000000000
C	4.432862000	2.373934000	0.000000000
C	3.319994000	3.274995000	0.000000000
C	3.125804000	1.927198000	0.000000000
C	2.816501000	4.578627000	0.000000000
H	2.446720000	1.093115000	0.000000000
C	1.407429000	4.961027000	0.000000000
C	3.562503000	5.768163000	0.000000000
C	1.367127000	6.381512000	0.000000000
C	0.330653000	4.097177000	0.000000000
C	2.674622000	6.864591000	0.000000000
H	4.642085000	5.823984000	0.000000000
H	0.465293000	6.977684000	0.000000000
C	-1.077897000	3.847592000	0.000000000
C	-0.183864000	2.818040000	0.000000000
H	2.963500000	7.906064000	0.000000000
C	-2.390847000	4.319865000	0.000000000
H	0.000000000	1.758232000	0.000000000
C	-3.604863000	3.508199000	0.000000000
C	-2.798229000	5.664535000	0.000000000
C	-3.671079000	2.129305000	0.000000000
C	-4.701077000	4.412355000	0.000000000
C	-4.206829000	5.715843000	0.000000000
H	-2.131535000	6.515470000	0.000000000
C	-4.429910000	0.917849000	0.000000000
C	-3.067407000	0.888440000	0.000000000
H	-5.743303000	4.125695000	0.000000000
H	-4.802443000	6.617527000	0.000000000
C	-5.670310000	0.276454000	0.000000000
H	-2.158947000	0.311769000	0.000000000
C	-5.917091000	-1.163832000	0.000000000
C	-6.924953000	0.904722000	0.000000000
C	-7.331128000	-1.334507000	0.000000000
C	-4.975411000	-2.168727000	0.000000000
C	-7.934669000	-0.081389000	0.000000000
H	-7.083254000	1.973885000	0.000000000
H	-7.842076000	-2.286757000	0.000000000

C	-4.646828000	-3.558869000	0.000000000
C	-3.665896000	-2.618719000	0.000000000
H	-8.998258000	0.108941000	0.000000000
C	-5.086680000	-4.889953000	0.000000000
H	-2.615589000	-2.382707000	0.000000000
C	-4.269207000	-6.105791000	0.000000000
C	-6.418877000	-5.303483000	0.000000000
C	-5.181827000	-7.213769000	0.000000000
C	-6.472534000	-6.723307000	0.000000000
H	-7.273451000	-4.642019000	0.000000000
H	-4.889117000	-8.254550000	0.000000000
H	-7.376772000	-7.314459000	0.000000000
H	4.937045000	-4.608615000	0.000000000
H	-1.270595000	-7.969737000	0.000000000

E= -1844.5265485

VII

C	-0.461309000	-6.454476000	0.000000000
C	-1.890264000	-6.233435000	0.000000000
C	-2.516387000	-7.535200000	0.000000000
C	-1.521630000	-8.484349000	0.000000000
C	-0.243937000	-7.813773000	0.000000000
H	-3.582554000	-7.713120000	0.000000000
H	-1.662860000	-9.556835000	0.000000000
H	0.715359000	-8.318108000	0.000000000
C	-5.074016000	-4.062561000	0.000000000
C	-5.841423000	-2.820477000	0.000000000
C	-7.215610000	-3.185323000	0.000000000
C	-7.306654000	-4.575618000	0.000000000
C	-6.001786000	-5.115383000	0.000000000
C	-3.678984000	-4.180073000	0.000000000
C	-2.441558000	-3.619104000	0.000000000
C	-2.505606000	-5.007096000	0.000000000
H	-8.042905000	-2.489281000	0.000000000
H	-8.222961000	-5.149026000	0.000000000
H	-1.839272000	-2.726858000	0.000000000
H	-5.747089000	-6.166018000	0.000000000
C	6.143488000	-3.127101000	0.000000000
C	5.530524000	-4.456936000	0.000000000
C	6.603562000	-5.403704000	0.000000000
C	7.803898000	-4.714066000	0.000000000
C	7.527895000	-3.324155000	0.000000000
C	5.495023000	-1.887200000	0.000000000
C	4.370716000	-1.118906000	0.000000000
C	5.585457000	-0.461572000	0.000000000
H	6.479319000	-6.477701000	0.000000000
H	8.789515000	-5.156386000	0.000000000
H	8.266726000	-2.535458000	0.000000000
C	3.148919000	-5.711702000	0.000000000
C	2.832830000	-4.422411000	0.000000000
C	4.200607000	-4.767056000	0.000000000
H	2.056327000	-3.676186000	0.000000000
H	3.295932000	-1.059691000	0.000000000
C	-5.317432000	-1.543309000	0.000000000
C	-5.469657000	-0.119379000	0.000000000
C	-4.232242000	-0.694430000	0.000000000
C	-6.277756000	1.017038000	0.000000000
H	-3.163183000	-0.578182000	0.000000000
C	-5.815254000	2.402101000	0.000000000
C	-7.684230000	1.055808000	0.000000000
C	-6.972515000	3.221224000	0.000000000
C	-4.496088000	2.819435000	0.000000000
C	-8.102450000	2.399937000	0.000000000
H	-8.329629000	0.188546000	0.000000000
H	-6.968644000	4.302308000	0.000000000
C	-3.505946000	3.852553000	0.000000000
C	-3.150780000	2.533232000	0.000000000
H	-9.128773000	2.738647000	0.000000000
C	-3.157546000	5.200601000	0.000000000
H	-2.372512000	1.791078000	0.000000000
C	-1.801284000	5.741969000	0.000000000
C	-4.037206000	6.300412000	0.000000000
C	-0.625382000	5.011301000	0.000000000
C	-1.924856000	7.153737000	0.000000000
C	-3.282252000	7.486655000	0.000000000
H	-5.116144000	6.232922000	0.000000000
C	0.803317000	4.946336000	0.000000000

C	0.044337000	3.809765000	0.000000000
H	-1.097981000	7.850012000	0.000000000
H	-3.686001000	8.489062000	0.000000000
C	2.040036000	5.585466000	0.000000000
H	0.000000000	2.734902000	0.000000000
C	3.353584000	4.946944000	0.000000000
C	2.261662000	6.976186000	0.000000000
C	4.313787000	5.990654000	0.000000000
C	3.617211000	3.588690000	0.000000000
C	3.646800000	7.217784000	0.000000000
H	1.485171000	7.728169000	0.000000000
H	5.385265000	5.848953000	0.000000000
C	4.552348000	2.507586000	0.000000000
C	3.206735000	2.274169000	0.000000000
H	4.115621000	8.191350000	0.000000000
C	5.875435000	2.068618000	0.000000000
H	2.396119000	1.566359000	0.000000000
C	6.350957000	0.686865000	0.000000000
C	7.016088000	2.891241000	0.000000000
C	7.770971000	0.745400000	0.000000000
C	8.167866000	2.081258000	0.000000000
H	7.001140000	3.971897000	0.000000000
H	8.427588000	-0.112920000	0.000000000
H	9.187687000	2.438170000	0.000000000
H	2.806826000	-6.734254000	0.000000000
H	0.279830000	-5.667372000	0.000000000

E= -2151.7627885

VIII

C	-4.735835000	4.876508000	0.000000000
C	-3.585435000	5.774942000	0.000000000
C	-4.096946000	7.092743000	0.000000000
C	-5.496916000	7.036765000	0.000000000
C	-5.890272000	5.691748000	0.000000000
C	-4.714294000	3.488228000	0.000000000
C	-4.046934000	2.290069000	0.000000000
C	-5.417799000	2.244126000	0.000000000
H	-3.496148000	7.991148000	0.000000000
H	-6.162301000	7.888226000	0.000000000
H	-6.907397000	5.326436000	0.000000000
C	0.099471000	6.796953000	0.000000000
C	1.548215000	6.618786000	0.000000000
C	2.118348000	7.912305000	0.000000000
C	1.088838000	8.862651000	0.000000000
C	-0.140377000	8.189725000	0.000000000
C	-0.866960000	5.800059000	0.000000000
C	-1.242291000	4.480938000	0.000000000
C	-2.244126000	5.417799000	0.000000000
H	3.178445000	8.122745000	0.000000000
H	1.220413000	9.935223000	0.000000000
H	-0.954606000	3.444110000	0.000000000
H	-3.110362000	1.760345000	0.000000000
H	-1.117908000	8.650626000	0.000000000
C	-4.876508000	-4.735835000	0.000000000
C	-5.774942000	-3.585435000	0.000000000
C	-7.092743000	-4.096946000	0.000000000
C	-7.036765000	-5.496916000	0.000000000
C	-5.691748000	-5.890272000	0.000000000
C	-3.488228000	-4.714294000	0.000000000
C	-2.290069000	-4.046934000	0.000000000
C	-2.244126000	-5.417799000	0.000000000
H	-7.991148000	-3.496148000	0.000000000
H	-7.888226000	-6.162301000	0.000000000
H	-5.326436000	-6.907397000	0.000000000
C	-6.796953000	0.099471000	0.000000000
C	-6.618786000	1.548215000	0.000000000
C	-7.912305000	2.118348000	0.000000000
C	-8.862651000	1.088838000	0.000000000
C	-8.189725000	-0.140377000	0.000000000
C	-5.800059000	-0.866960000	0.000000000
C	-4.480938000	-1.242291000	0.000000000
C	-5.417799000	-2.244126000	0.000000000
H	-8.122745000	3.178445000	0.000000000
H	-9.935223000	1.220413000	0.000000000
H	-3.444110000	-0.954606000	0.000000000
H	-1.760345000	-3.110362000	0.000000000
H	-8.650626000	-1.117908000	0.000000000
C	2.244126000	5.417799000	0.000000000
C	3.488228000	4.714294000	0.000000000
C	2.290069000	4.046934000	0.000000000
C	4.876508000	4.735835000	0.000000000
H	1.760345000	3.110362000	0.000000000
C	5.774942000	3.585435000	0.000000000
C	5.691748000	5.890272000	0.000000000
C	7.092743000	4.096946000	0.000000000
C	5.417799000	2.244126000	0.000000000
C	7.036765000	5.496916000	0.000000000
H	5.326436000	6.907397000	0.000000000
H	7.991148000	3.496148000	0.000000000

C	5.800059000	0.866960000	0.000000000
C	4.480938000	1.242291000	0.000000000
H	7.888226000	6.162301000	0.000000000
C	6.796953000	-0.099471000	0.000000000
H	3.444110000	0.954606000	0.000000000
C	6.618786000	-1.548215000	0.000000000
C	8.189725000	0.140377000	0.000000000
C	5.417799000	-2.244126000	0.000000000
C	7.912305000	-2.118348000	0.000000000
C	8.862651000	-1.088838000	0.000000000
H	8.650626000	1.117908000	0.000000000
C	4.714294000	-3.488228000	0.000000000
C	4.046934000	-2.290069000	0.000000000
H	8.122745000	-3.178445000	0.000000000
H	9.935223000	-1.220413000	0.000000000
C	4.735835000	-4.876508000	0.000000000
H	3.110362000	-1.760345000	0.000000000
C	3.585435000	-5.774942000	0.000000000
C	5.890272000	-5.691748000	0.000000000
C	4.096946000	-7.092743000	0.000000000
C	2.244126000	-5.417799000	0.000000000
C	5.496916000	-7.036765000	0.000000000
H	6.907397000	-5.326436000	0.000000000
H	3.496148000	-7.991148000	0.000000000
C	0.866960000	-5.800059000	0.000000000
C	1.242291000	-4.480938000	0.000000000
H	6.162301000	-7.888226000	0.000000000
C	-0.099471000	-6.796953000	0.000000000
H	0.954606000	-3.444110000	0.000000000
C	-1.548215000	-6.618786000	0.000000000
C	0.140377000	-8.189725000	0.000000000
C	-2.118348000	-7.912305000	0.000000000
C	-1.088838000	-8.862651000	0.000000000
H	1.117908000	-8.650626000	0.000000000
H	-3.178445000	-8.122745000	0.000000000
H	-1.220413000	-9.935223000	0.000000000

E= -2457.8434778

H_2

H	0.000000000	0.000000000	0.372075000
H	0.000000000	0.000000000	-0.372075000

E= -1.1795716

Table S2. Geometries and total energies of systems **I** in the presence of external electric field (F).

```
F= -0.0250
C       -0.062961000      0.000003000     -0.000034000
C       -0.912442000      1.155829000      0.000065000
C       -2.233656000      0.720629000      0.000105000
C       -2.233664000     -0.720600000      0.000013000
C       -0.912454000     -1.155814000     -0.000079000
C        1.345420000      0.000001000     -0.000050000
C        2.571243000      0.669946000     -0.000016000
C        2.571244000     -0.669944000     -0.000078000
H       -0.560593000      2.178448000      0.000117000
H       -3.113801000      1.364431000      0.000202000
H       -3.113815000     -1.364392000      0.000025000
H       -0.560616000     -2.178436000     -0.000159000
H        3.171953000      1.570994000      0.000040000
H        3.171957000     -1.570989000     -0.000121000

E= -308.4948439

F= -0.0225
C       -0.060554000      0.000001000     -0.000039000
C       -0.911230000      1.157208000      0.000072000
C       -2.229035000      0.720835000      0.000101000
C       -2.229045000     -0.720805000      0.000008000
C       -0.911245000     -1.157195000     -0.000074000
C        1.340361000     -0.000002000     -0.000052000
C        2.569282000      0.668871000     -0.000019000
C        2.569287000     -0.668867000     -0.000078000
H       -0.560553000      2.180172000      0.000132000
H       -3.109206000      1.362300000      0.000198000
H       -3.109224000     -1.362258000      0.000016000
H       -0.560583000     -2.180165000     -0.000150000
H        3.164774000      1.572205000      0.000031000
H        3.164787000     -1.572195000     -0.000116000

E= -308.4800065

F= -0.0200
C       -0.058250000     -0.000023000      0.000038000
C       -0.910298000      1.158616000      0.000112000
C       -2.224741000      0.721171000      0.000070000
C       -2.224768000     -0.721131000     -0.000001000
C       -0.910342000     -1.158629000     -0.000008000
C        1.335570000     -0.000021000     -0.000013000
C        2.567774000      0.667854000     -0.000009000
C        2.567809000     -0.667834000     -0.000129000
H       -0.560785000      2.181925000      0.000170000
H       -3.105099000      1.360274000      0.000084000
H       -3.105154000     -1.360198000     -0.000040000
H       -0.560876000     -2.181954000     -0.000041000
H        3.158442000      1.573310000      0.000051000
H        3.158534000     -1.573253000     -0.000254000

E= -308.4663023
```

```
F= -0.0175
C       -0.056053000      0.000008000      0.000007000
C       -0.909671000      1.160087000      0.000093000
C       -2.220805000      0.721609000      0.000092000
C       -2.220809000     -0.721582000      0.000003000
C       -0.909677000     -1.160066000     -0.000046000
C        1.331051000      0.000004000     -0.000027000
C        2.566745000      0.666875000     -0.000020000
C        2.566741000     -0.666876000     -0.000099000
H       -0.561351000      2.183752000      0.000152000
H       -3.101529000      1.358296000      0.000148000
H       -3.101536000     -1.358264000     -0.000020000
H       -0.561363000     -2.183733000     -0.000110000
H        3.153041000      1.574256000      0.000021000
H        3.153031000     -1.574260000     -0.000164000

E= -308.4537163

F= -0.0150
C       -0.053970000      0.000007000     -0.000007000
C       -0.909279000      1.161564000      0.000084000
C       -2.217199000      0.722155000      0.000091000
C       -2.217204000     -0.722127000      0.000008000
C       -0.909286000     -1.161544000     -0.000050000
C        1.326820000      0.000003000     -0.000037000
C        2.566133000      0.665967000     -0.000017000
C        2.566130000     -0.665966000     -0.000094000
H       -0.562161000      2.185589000      0.000140000
H       -3.098418000      1.356425000      0.000155000
H       -3.098426000     -1.356392000     -0.000003000
H       -0.562174000     -2.185571000     -0.000115000
H        3.148427000      1.575131000      0.000049000
H        3.148420000     -1.575134000     -0.000175000

E= -308.4422347

F= -0.0125
C       -0.052026000      0.000008000     -0.000014000
C       -0.909141000      1.163051000      0.000075000
C       -2.213957000      0.722801000      0.000099000
C       -2.213961000     -0.722774000      0.000013000
C       -0.909148000     -1.163031000     -0.000066000
C        1.322848000      0.000004000     -0.000035000
C        2.565913000      0.665119000     -0.000016000
C        2.565909000     -0.665119000     -0.000089000
H       -0.563163000      2.187417000      0.000125000
H       -3.095793000      1.354665000      0.000172000
H       -3.095800000     -1.354632000      0.000012000
H       -0.563176000     -2.187398000     -0.000139000
H        3.144660000      1.575873000      0.000046000
H        3.144650000     -1.575877000     -0.000152000

E= -308.4318447
```

```
F= -0.0100
C       -0.050205000      0.000021000     -0.000022000
C       -0.909210000      1.164565000      0.000083000
C       -2.211025000      0.723518000      0.000097000
C       -2.211019000     -0.723496000      0.000008000
C       -0.909200000     -1.164531000     -0.000061000
C        1.319160000      0.000017000     -0.000042000
C        2.566110000      0.664325000     -0.000019000
C        2.566088000     -0.664335000     -0.000088000
H       -0.564432000      2.189292000      0.000140000
H       -3.093605000      1.352963000      0.000170000
H       -3.093592000     -1.352949000      0.000003000
H       -0.564411000     -2.189254000     -0.000132000
H        3.141607000      1.576586000      0.000035000
H        3.141551000     -1.576616000     -0.000142000

E= -308.4225058

F= -0.0075
C       -0.048519000      0.000031000      0.000018000
C       -0.909483000      1.166068000      0.000091000
C       -2.208461000      0.724310000      0.000093000
C       -2.208447000     -0.724292000      0.000006000
C       -0.909461000     -1.166023000     -0.000049000
C        1.315756000      0.000026000     -0.000012000
C        2.566647000      0.663609000     -0.000015000
C        2.566610000     -0.663625000     -0.000093000
H       -0.565885000      2.191152000      0.000138000
H       -3.091888000      1.351358000      0.000145000
H       -3.091861000     -1.351359000     -0.000015000
H       -0.565837000     -2.191098000     -0.000122000
H        3.139368000      1.577169000      0.000023000
H        3.139277000     -1.577219000     -0.000179000

E= -308.4142639

F= -0.0050
C       -0.046979000      0.000073000      0.000092000
C       -0.909960000      1.167578000      0.000126000
C       -2.206249000      0.725160000      0.000080000
C       -2.206203000     -0.725158000     -0.000009000
C       -0.909887000     -1.167487000     -0.000016000
C        1.312615000      0.000060000      0.000038000
C        2.567531000      0.662950000     -0.000026000
C        2.567442000     -0.662995000     -0.000099000
H       -0.567538000      2.193019000      0.000178000
H       -3.090629000      1.349828000      0.000088000
H       -3.090540000     -1.349887000     -0.000073000
H       -0.567383000     -2.192901000     -0.000085000
H        3.137911000      1.577638000     -0.000033000
H        3.137682000     -1.577770000     -0.000229000

E= -308.4070801
```

```
F= -0.0025
C       -0.045577000      0.000072000      0.000069000
C       -0.910567000      1.169054000      0.000126000
C       -2.204343000      0.726068000      0.000083000
C       -2.204299000     -0.726066000     -0.000010000
C       -0.910495000     -1.168964000     -0.000022000
C        1.309748000      0.000059000      0.000023000
C        2.568706000      0.662377000     -0.000032000
C        2.568619000     -0.662422000     -0.000090000
H       -0.569286000      2.194845000      0.000190000
H       -3.089770000      1.348382000      0.000105000
H       -3.089683000     -1.348440000     -0.000072000
H       -0.569134000     -2.194729000     -0.000100000
H        3.137059000      1.578100000     -0.000048000
H        3.136836000     -1.578229000     -0.000193000

E= -308.4009448

F= 0.0025
C       -0.043230000      0.000089000      0.000042000
C       -0.912216000      1.171948000      0.000136000
C       -2.201505000      0.728013000      0.000100000
C       -2.201447000     -0.728017000     -0.000017000
C       -0.912123000     -1.171841000     -0.000049000
C        1.304764000      0.000074000      0.000020000
C        2.571898000      0.661435000     -0.000067000
C        2.571789000     -0.661491000     -0.000035000
H       -0.573131000      2.198419000      0.000235000
H       -3.089287000      1.345719000      0.000161000
H       -3.089176000     -1.345801000     -0.000091000
H       -0.572936000     -2.198278000     -0.000182000
H        3.137348000      1.578824000     -0.000163000
H        3.137067000     -1.578986000     -0.000060000

E= -308.3917879

F= 0.0050
C       -0.042296000      0.000066000     -0.000018000
C       -0.913209000      1.173327000      0.000071000
C       -2.200547000      0.729048000      0.000108000
C       -2.200507000     -0.729045000      0.000009000
C       -0.913144000     -1.173246000     -0.000054000
C        1.302621000      0.000057000     -0.000022000
C        2.573840000      0.661079000     -0.000005000
C        2.573759000     -0.661119000     -0.000077000
H       -0.575112000      2.200104000      0.000102000
H       -3.089604000      1.344550000      0.000190000
H       -3.089527000     -1.344598000     -0.000006000
H       -0.574976000     -2.200000000     -0.000144000
H        3.138363000      1.579131000      0.000021000
H        3.138156000     -1.579248000     -0.000146000

E= -308.3887544
```

```
F= 0.0075
C       -0.041520000      0.000033000     -0.000023000
C       -0.914299000      1.174661000      0.000070000
C       -2.199889000      0.730116000      0.000105000
C       -2.199873000     -0.730100000      0.000008000
C       -0.914273000     -1.174614000     -0.000057000
C        1.300706000      0.000029000     -0.000020000
C        2.575997000      0.660796000      0.000005000
C        2.575958000     -0.660813000     -0.000083000
H       -0.577134000      2.201729000      0.000094000
H       -3.090287000      1.343470000      0.000182000
H       -3.090258000     -1.343473000      0.000004000
H       -0.577082000     -2.201674000     -0.000129000
H        3.139933000      1.579407000      0.000045000
H        3.139835000     -1.579461000     -0.000173000

E= -308.3867467

F= 0.0100
C       -0.040905000      0.000046000     -0.000010000
C       -0.915503000      1.175976000      0.000082000
C       -2.199541000      0.731202000      0.000108000
C       -2.199516000     -0.731190000     -0.000002000
C       -0.915463000     -1.175916000     -0.000057000
C        1.299018000      0.000039000     -0.000005000
C        2.578390000      0.660567000     -0.000012000
C        2.578336000     -0.660594000     -0.000069000
H       -0.579243000      2.203329000      0.000133000
H       -3.091370000      1.342438000      0.000192000
H       -3.091323000     -1.342458000     -0.000030000
H       -0.579159000     -2.203255000     -0.000148000
H        3.142116000      1.579614000     -0.000013000
H        3.141978000     -1.579691000     -0.000138000

E= -308.3857653

F= 0.0125
C       -0.040449000      0.000064000      0.000015000
C       -0.916784000      1.177244000      0.000096000
C       -2.199483000      0.732311000      0.000095000
C       -2.199443000     -0.732307000      0.000005000
C       -0.916721000     -1.177165000     -0.000055000
C        1.297557000      0.000056000      0.000013000
C        2.580978000      0.660409000     -0.000013000
C        2.580900000     -0.660448000     -0.000070000
H       -0.581371000      2.204866000      0.000156000
H       -3.092812000      1.341483000      0.000153000
H       -3.092738000     -1.341530000     -0.000022000
H       -0.581239000     -2.204765000     -0.000156000
H        3.144811000      1.579804000     -0.000033000
H        3.144609000     -1.579918000     -0.000155000
E= -308.3858151
```

```
F= 0.0150
C       -0.040156000      0.000022000      0.000015000
C       -0.918086000      1.178422000      0.000096000
C       -2.199686000      0.733456000      0.000087000
C       -2.199679000     -0.733435000     -0.000003000
C       -0.918076000     -1.178388000     -0.000045000
C        1.296321000      0.000018000      0.000009000
C        2.583693000      0.660347000     -0.000010000
C        2.583670000     -0.660356000     -0.000073000
H       -0.583402000      2.206275000      0.000161000
H       -3.094557000      1.340666000      0.000140000
H       -3.094545000     -1.340653000     -0.000030000
H       -0.583379000     -2.206237000     -0.000109000
H        3.147878000      1.580048000     -0.000006000
H        3.147818000     -1.580079000     -0.000200000

E= -308.3869062

F= 0.0175
C       -0.040012000      0.000012000      0.000001000
C       -0.919436000      1.179555000      0.000090000
C       -2.200172000      0.734614000      0.000095000
C       -2.200172000     -0.734588000      0.000001000
C       -0.919437000     -1.179530000     -0.000053000
C        1.295340000      0.000009000     -0.000008000
C        2.586586000      0.660356000     -0.000014000
C        2.586575000     -0.660359000     -0.000073000
H       -0.585442000      2.207627000      0.000148000
H       -3.096663000      1.339914000      0.000154000
H       -3.096665000     -1.339888000     -0.000019000
H       -0.585443000     -2.207603000     -0.000121000
H        3.151392000      1.580308000      0.000008000
H        3.151365000     -1.580320000     -0.000180000

E= -308.3890568

F= 0.0200
C       -0.040004000      0.000010000     -0.000010000
C       -0.920782000      1.180615000      0.000087000
C       -2.200926000      0.735782000      0.000099000
C       -2.200928000     -0.735756000      0.000006000
C       -0.920787000     -1.180593000     -0.000060000
C        1.294648000      0.000006000     -0.000022000
C        2.589613000      0.660460000     -0.000016000
C        2.589606000     -0.660461000     -0.000072000
H       -0.587416000      2.208884000      0.000141000
H       -3.099103000      1.339254000      0.000165000
H       -3.099108000     -1.339224000     -0.000006000
H       -0.587424000     -2.208863000     -0.000138000
H        3.155222000      1.580656000      0.000015000
H        3.155205000     -1.580664000     -0.000159000

E= -308.3922961
```

Table S3. Geometry and total energy of system **I** at CAM-B3LYP/6-311++G(d,p) level of theory.

C	0.000000000	0.000000000	-0.042633000
C	0.000000000	1.166275000	-0.908861000
C	0.000000000	0.725506000	-2.192948000
C	0.000000000	-0.725506000	-2.192948000
C	0.000000000	-1.166275000	-0.908861000
C	0.000000000	0.000000000	1.302134000
C	0.000000000	0.658810000	2.559885000
C	0.000000000	-0.658810000	2.559885000
H	0.000000000	2.192325000	-0.569995000
H	0.000000000	1.345594000	-3.078702000
H	0.000000000	-1.345594000	-3.078702000
H	0.000000000	-2.192325000	-0.569995000
H	0.000000000	1.575289000	3.124816000
H	0.000000000	-1.575289000	3.124816000

E= -308.2088192

Table S4. Geometry and total energy of $(calicene)_3$ system at CAM-B3LYP/6-311++G(d,p) level of theory.

C	0.000000000	0.000000000	-8.588097000
C	0.000000000	1.165889000	-7.723922000
C	0.000000000	0.725080000	-6.439344000
C	0.000000000	-0.725080000	-6.439344000
C	0.000000000	-1.165889000	-7.723922000
C	0.000000000	0.000000000	-9.934737000
C	0.000000000	0.659180000	-11.189873000
C	0.000000000	-0.659180000	-11.189873000
H	0.000000000	2.191924000	-8.062665000
H	0.000000000	1.349382000	-5.556698000
H	0.000000000	-2.191924000	-8.062665000
H	0.000000000	1.576733000	-11.753164000
H	0.000000000	-1.576733000	-11.753164000
H	0.000000000	-1.349382000	-5.556698000
C	0.000000000	0.000000000	0.053963000
C	0.000000000	-1.165483000	0.917748000
C	0.000000000	-0.724805000	2.202902000
C	0.000000000	0.724805000	2.202902000
C	0.000000000	1.165483000	0.917748000
C	0.000000000	0.000000000	-1.293587000
C	0.000000000	-0.659016000	-2.548009000
C	0.000000000	0.659016000	-2.548009000
H	0.000000000	-2.191444000	0.578631000
H	0.000000000	-1.348144000	3.086210000
H	0.000000000	2.191444000	0.578631000
H	0.000000000	-1.572811000	-3.116907000
H	0.000000000	1.348144000	3.086210000
H	0.000000000	1.572811000	-3.116907000
C	0.000000000	0.000000000	8.698260000
C	0.000000000	1.165757000	9.564051000
C	0.000000000	0.725358000	10.848858000
C	0.000000000	-0.725358000	10.848858000
C	0.000000000	-1.165757000	9.564051000
C	0.000000000	0.658741000	6.095715000
C	0.000000000	0.000000000	7.352188000
C	0.000000000	-0.658741000	6.095715000
H	0.000000000	1.572001000	5.525962000
H	0.000000000	-1.572001000	5.525962000
H	0.000000000	2.191791000	9.224720000
H	0.000000000	1.345751000	11.734450000
H	0.000000000	-1.345751000	11.734450000
H	0.000000000	-2.191791000	9.224720000

E=-924.6281207

Table S5. Values of aromaticity descriptors used in the study for three-membered rings (QTAIM parameters values given in au).

system	ring no.	HOMA	EL	FLU	NICS	NICS(1)	NICS(1)$_{zz}$	ρ_{RCP}	H_{RCP}	EN	GEO
I	1	0.400	-0.246	0.0414	-20.9	-7.3	-11.2	0.235	-0.160	0.004	0.597
II	1	0.490	-0.298	0.0360	-22.0	-8.3	-13.8	0.237	-0.163	0.000	0.510
	2	0.651	-0.198	0.0231	-22.9	-7.5	-11.2	0.233	-0.157	0.014	0.336
III	1	0.516	-0.286	0.0338	-22.0	-8.6	-13.9	0.238	-0.164	0.000	0.484
	2	0.738	-0.203	0.0180	-23.7	-8.3	-12.9	0.235	-0.160	0.004	0.258
	3	0.675	-0.232	0.0212	-23.3	-7.4	-11.1	0.233	-0.157	0.013	0.312
IV	1	0.531	-0.281	0.0326	-22.1	-8.7	-14.1	0.238	-0.165	0.000	0.469
	2	0.766	-0.194	0.0162	-24.1	-8.3	-12.8	0.236	-0.161	0.003	0.231
	3	0.763	-0.229	0.0161	-24.0	-8.2	-12.7	0.235	-0.160	0.004	0.233
	4	0.688	-0.244	0.0202	-23.3	-7.4	-11.1	0.233	-0.157	0.013	0.299
V	1	0.540	-0.277	0.0319	-21.9	-8.7	-14.1	0.239	-0.165	0.001	0.459
	2	0.779	-0.192	0.0153	-23.8	-8.3	-12.8	0.236	-0.161	0.002	0.219
	3	0.787	-0.223	0.0145	-24.0	-8.2	-12.7	0.236	-0.161	0.002	0.210
	4	0.773	-0.246	0.0152	-24.0	-8.2	-12.5	0.235	-0.160	0.004	0.223
	5	0.694	-0.255	0.0196	-23.4	-7.4	-11.1	0.233	-0.157	0.013	0.292
VI	1	0.550	-0.276	0.0308	-22.2	-8.8	-14.2	0.239	-0.166	0.001	0.448
	2	0.785	-0.199	0.0147	-23.9	-8.4	-13.0	0.236	-0.161	0.002	0.213
	3	0.792	-0.242	0.0138	-24.0	-8.2	-12.6	0.236	-0.161	0.002	0.206
	4	0.786	-0.275	0.0139	-24.1	-8.3	-12.6	0.236	-0.161	0.002	0.212
	5	0.771	-0.293	0.0147	-24.2	-8.2	-12.4	0.235	-0.160	0.003	0.226
	6	0.699	-0.284	0.0190	-23.6	-7.3	-10.7	0.233	-0.157	0.014	0.287
VII	1	0.585	-0.274	0.0268	-22.2	-9.1	-13.9	0.240	-0.168	0.004	0.410
	2	0.796	-0.210	0.0138	-23.9	-8.3	-12.6	0.236	-0.161	0.002	0.202
	3	0.800	-0.237	0.0133	-24.1	-8.3	-12.5	0.236	-0.161	0.002	0.198
	4	0.795	-0.267	0.0133	-24.1	-8.2	-12.2	0.236	-0.161	0.002	0.203
	5	0.787	-0.296	0.0134	-24.3	-8.3	-12.5	0.236	-0.161	0.002	0.211
	6	0.777	-0.310	0.0140	-24.1	-8.2	-12.4	0.235	-0.160	0.003	0.220
	7	0.732	-0.289	0.0170	-23.8	-7.4	-10.7	0.233	-0.158	0.011	0.257
VIII		0.808	-0.235	0.0130	-24.0	-8.2	-12.6	0.236	-0.161	0.002	0.190

Table S6. Values of aromaticity descriptors used in the study for five-membered rings (QTAIM parameters values given in au).

system	ring no.	HOMA	EL	FLU	NICS	NICS(1)	$NICS(1)_{zz}$	ρ_{RCP}	H_{RCP}	EN	GEO
I	1	0.246	0.285	0.0281	-4.3	-5.3	-14.0	0.0480	0.00464	0.256	0.498
II	1	0.428	0.511	0.0193	-4.1	-5.8	-14.0	0.0479	0.00467	0.269	0.303
	2	0.341	0.366	0.0237	-5.3	-6.1	-16.3	0.0481	0.00456	0.243	0.417
III	1	0.472	0.562	0.0178	-4.2	-6.0	-14.4	0.0479	0.00466	0.260	0.268
	2	0.543	0.644	0.0147	-5.4	-6.6	-16.5	0.0480	0.00461	0.248	0.209
	3	0.376	0.397	0.0222	-5.6	-6.0	-16.8	0.0482	0.00455	0.238	0.386
IV	1	0.493	0.591	0.0170	-4.3	-6.1	-14.4	0.0480	0.00465	0.257	0.250
	2	0.587	0.719	0.0131	-5.6	-6.8	-17.0	0.0481	0.00460	0.239	0.174
	3	0.579	0.698	0.0132	-5.7	-6.8	-17.3	0.0481	0.00460	0.241	0.180
	4	0.395	0.415	0.0223	-5.8	-6.1	-17.2	0.0482	0.00455	0.236	0.369
V	1	0.504	0.609	0.0166	-4.4	-6.2	-14.7	0.0480	0.00465	0.256	0.241
	2	0.605	0.760	0.0125	-5.6	-6.9	-17.2	0.0482	0.00459	0.236	0.159
	3	0.620	0.783	0.0119	-5.9	-7.0	-17.7	0.0482	0.00458	0.233	0.147
	4	0.597	0.729	0.0125	-6.1	-7.1	-18.1	0.0481	0.00460	0.239	0.164
	5	0.405	0.426	0.0208	-6.1	-6.4	-18.0	0.0482	0.00455	0.235	0.360
VI	1	0.517	0.631	0.0160	-4.3	-6.2	-14.7	0.0480	0.00464	0.254	0.229
	2	0.615	0.792	0.0121	-5.5	-6.8	-16.9	0.0482	0.00459	0.235	0.150
	3	0.633	0.828	0.0114	-5.9	-7.0	-17.8	0.0482	0.00458	0.232	0.135
	4	0.634	0.820	0.0113	-6.1	-7.2	-18.2	0.0482	0.00458	0.232	0.134
	5	0.611	0.760	0.0120	-6.2	-7.2	-18.3	0.0481	0.00459	0.237	0.152
	6	0.424	0.440	0.0201	-6.1	-6.4	-18.0	0.0482	0.00454	0.231	0.345
VII	1	0.555	0.691	0.0146	-4.9	-6.5	-15.5	0.0481	0.00463	0.248	0.197
	2	0.627	0.833	0.0115	-5.9	-7.1	-17.7	0.0482	0.00459	0.233	0.140
	3	0.640	0.836	0.0110	-6.0	-7.1	-17.8	0.0482	0.00458	0.231	0.129
	4	0.644	0.832	0.0109	-6.2	-7.3	-18.4	0.0482	0.00458	0.231	0.126
	5	0.643	0.827	0.0109	-6.3	-7.3	-18.6	0.0482	0.00458	0.231	0.127
	6	0.630	0.812	0.0112	-6.2	-7.1	-18.3	0.0482	0.00458	0.233	0.136
	7	0.491	0.494	0.0178	-6.4	-6.6	-18.2	0.0483	0.00451	0.217	0.292
VIII		0.651	0.833	0.0107	-6.1	-7.2	-18.2	0.0482	0.00457	0.229	0.121

Table S7. Mean values of HOMA, EL and FLU for systems **I-VIII**.

system	$HOMA_{mean}$	EL_{mean}	FLU_{mean}
I	0.325	0.019	0.0347
II	0.477	0.095	0.0255
III	0.552	0.147	0.0213
IV	0.600	0.184	0.0188
V	0.632	0.211	0.0171
VI	0.654	0.225	0.0158
VII	0.679	0.246	0.0140
VIII	0.729	0.299	0.0118

Table S8. Values of energetic parameters (kcal/mol) for reaction of polycalicene formation from calicene units (ΔE – total energy, ΔE_{ZPCE} – zero-point corrected energy, ΔH_r – enthalpy, ΔG_r – Gibbs free energy of the reaction).

system	ΔE	ΔE_{ZPCE}	ΔH_r	ΔG_r
II	-2.37	-7.55	-5.96	-2.16
III	-7.42	-17.93	-14.67	-7.29
IV	-14.15	-29.90	-24.98	-13.72
V	-21.99	-43.01	-36.43	-21.31
VI	-30.98	-57.26	-49.02	-29.99
VII	-43.51	-75.00	-65.74	-38.52
VIII	-71.12	-113.18	-101.04	-73.61

Table S9. Composition (factor loadings) of first principal components needed for 99% data variance recovery for all three-membered rings.

Variable	Comp 1	Comp 2	Comp 3
HOMA	-0.16	0.53	0.06
EL	-0.12	0.17	-0.97
FLU	0.17	-0.51	-0.11
NICS	0.18	-0.50	-0.16
NICS(1)	-0.38	-0.22	0.05
$NICS(1)_{zz}$	-0.39	-0.08	0.13
ρ_{RCP}	0.41	0.04	-0.01
H_{RCP}	-0.41	0.02	0.00
G_{RCP}	0.34	0.32	0.03
V_{RCP}	-0.39	-0.15	-0.02

Table S10. Composition (factor loadings) of first principal components needed for 99% data variance recovery for all five-membered rings.

Variables	Comp 1	Comp 2	Comp 3
HOMA	0.33	0.30	0.15
EL	0.31	0.35	0.08
FLU	-0.32	-0.32	-0.20
NICS	-0.31	0.34	-0.33
NICS(1)	-0.36	-0.08	-0.28
$NICS(1)_{zz}$	-0.32	0.29	-0.34
ρ_{RCP}	0.28	-0.39	-0.36
H_{RCP}	-0.20	0.54	0.05
G_{RCP}	0.34	0.18	-0.51
V_{RCP}	-0.35	-0.04	0.48

Table S11. Composition (factor loadings) of first principal components needed for 99% data variance recovery for "head" three-membered rings.

Variables	Comp 1	Comp 2
HOMA	0.33	-0.09
EL	-0.20	-0.77
FLU	-0.33	0.23
NICS	-0.32	-0.28
NICS(1)	-0.34	0.01
$NICS(1)_{zz}$	-0.31	-0.35
ρ_{RCP}	0.33	-0.17
H_{RCP}	-0.33	0.19
G_{RCP}	0.33	-0.18
V_{RCP}	-0.33	0.19

Table S12. Composition (factor loadings) of first principal components needed for 99% data variance recovery for "tail" five-membered rings.

Variables	Comp 1	Comp 2
HOMA	0.32	-0.02
EL	0.32	0.02
FLU	-0.32	-0.07
NICS	-0.32	-0.26
NICS(1)	-0.31	-0.29
$NICS(1)_{zz}$	-0.31	-0.42
ρ_{RCP}	0.32	-0.27
H_{RCP}	-0.32	-0.21
G_{RCP}	0.29	-0.65
V_{RCP}	-0.32	0.36

Table S13. Values of aromaticity descriptors for three-membered ring of calicene molecule in the presence of electric field $\vec{F}$ (QTAIM parameters values given in au).

$\vec{F}$ [au]	HOMA	EL	FLU	NICS	NICS(1)	$NICS(1)_{zz}$	ρ_{RCP}	H_{RCP}	EN	GEO
-0.0250	0.787	0.052	0.0081	-23.99	-11.85	-20.82	0.2453	-0.1741	0.026	0.186
-0.0225	0.762	-0.020	0.0105	-23.79	-11.50	-20.14	0.2446	-0.1732	0.022	0.216
-0.0200	0.733	-0.093	0.0131	-23.65	-11.13	-19.40	0.2438	-0.1721	0.018	0.249
-0.0175	0.702	-0.168	0.0160	-23.48	-10.74	-18.59	0.2429	-0.1709	0.014	0.284
-0.0150	0.669	-0.211	0.0192	-23.26	-10.32	-17.73	0.2419	-0.1696	0.010	0.322
-0.0125	0.632	-0.229	0.0226	-23.00	-9.88	-16.81	0.2409	-0.1682	0.006	0.363
-0.0100	0.591	-0.247	0.0261	-22.68	-9.46	-15.81	0.2397	-0.1667	0.003	0.406
-0.0075	0.548	-0.267	0.0298	-22.32	-8.97	-14.76	0.2385	-0.1651	0.001	0.451
-0.0050	0.502	-0.287	0.0337	-21.89	-8.46	-13.64	0.2373	-0.1635	0.000	0.498
-0.0025	0.452	-0.308	0.0375	-21.41	-7.91	-12.45	0.2360	-0.1618	0.001	0.547
0.0000	0.400	-0.246	0.0414	-20.86	-7.34	-11.17	0.2347	-0.1602	0.004	0.597
0.0025	0.343	-0.349	0.0453	-20.25	-6.73	-9.79	0.2332	-0.1583	0.009	0.648
0.0050	0.283	-0.369	0.0492	-19.55	-6.08	-8.31	0.2318	-0.1565	0.016	0.701
0.0075	0.22	-0.388	0.0530	-18.78	-5.38	-6.69	0.2303	-0.1547	0.026	0.753
0.0100	0.155	-0.406	0.0566	-17.92	-4.63	-4.91	0.2288	-0.1529	0.039	0.806
0.0125	0.087	-0.422	0.0601	-16.96	-3.81	-2.95	0.2273	-0.1511	0.054	0.859
0.0150	0.016	-0.437	0.0635	-15.89	-2.91	-0.74	0.2258	-0.1493	0.073	0.911
0.0175	-0.056	-0.449	0.0665	-14.71	-1.90	1.77	0.2243	-0.1475	0.094	0.962
0.0200	-0.127	-0.458	0.0692	-13.45	-0.75	4.67	0.2227	-0.1457	0.118	1.009

Table S14. Values of aromaticity descriptors for three-membered ring of calicene molecule in the presence of electric field $\vec{F}$ (QTAIM parameters values given in au).

$\vec{F}$ [au]	HOMA	EL	FLU	NICS	NICS(1)	NICS(1)$_{zz}$	ρ_{RCP}	H_{RCP}	EN	GEO
-0.0250	0.631	0.637	0.0087	-9.79	-8.45	-25.55	0.0478	0.00469	0.239	0.130
-0.0225	0.612	0.658	0.0101	-9.26	-8.20	-24.67	0.0479	0.00467	0.233	0.155
-0.0200	0.588	0.646	0.0116	-8.80	-7.93	-23.72	0.0480	0.00465	0.230	0.183
-0.0175	0.558	0.601	0.0133	-8.31	-7.64	-22.71	0.0480	0.00464	0.228	0.214
-0.0150	0.524	0.555	0.0152	-7.81	-7.33	-21.63	0.0481	0.00462	0.228	0.248
-0.0125	0.485	0.508	0.0171	-7.28	-7.01	-20.49	0.0481	0.00461	0.230	0.286
-0.0100	0.442	0.461	0.0192	-6.68	-6.76	-19.26	0.0481	0.00464	0.232	0.326
-0.0075	0.395	0.415	0.0214	-6.11	-6.41	-18.02	0.0481	0.00464	0.237	0.368
-0.0050	0.345	0.370	0.0236	-5.52	-6.06	-16.72	0.0481	0.00464	0.243	0.412
-0.0025	0.293	0.326	0.0259	-4.91	-5.69	-15.38	0.0480	0.00464	0.249	0.458
0.0000	0.246	0.285	0.0281	-4.29	-5.31	-14.02	0.0480	0.00464	0.256	0.498
0.0025	0.182	0.243	0.0304	-3.65	-4.91	-12.57	0.0479	0.00465	0.267	0.551
0.0050	0.124	0.204	0.0326	-2.99	-4.50	-11.09	0.0479	0.00466	0.278	0.598
0.0075	0.066	0.168	0.0348	-2.31	-4.07	-9.55	0.0478	0.00468	0.289	0.644
0.0100	0.008	0.135	0.0369	-1.60	-3.61	-7.94	0.0477	0.00469	0.302	0.690
0.0125	-0.05	0.104	0.0388	-0.85	-3.13	-6.24	0.0476	0.00471	0.316	0.734
0.0150	-0.107	0.077	0.0407	-0.05	-2.61	-4.40	0.0475	0.00473	0.734	0.776
0.0175	-0.162	0.053	0.0423	0.83	-2.02	-2.37	0.0474	0.00475	0.347	0.815
0.0200	-0.214	0.034	0.0438	1.85	-1.35	-0.06	0.0473	0.00477	0.364	0.850