

THE HIDDEN AROMATICITY IN BORAZINE

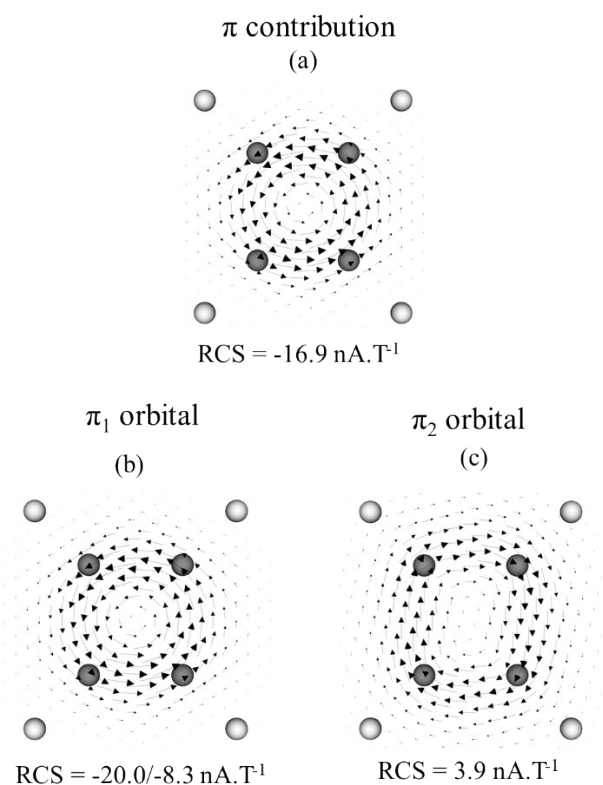
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SUPPORTING INFORMATION

Fig. S1. Dissected Magnetically Induced Current Density maps and their π -contributions for cyclobutadiene at the PBE0/def2-TZVP level.



Cartesian Coordinates

Singlet state							
Benzene			Borazine				
1	-2.472353000	0.000008000	-0.000012000	1	-2.410000000	0.004272000	0.000018000
1	-1.235740000	2.140918000	-0.000019000	1	-1.316858000	2.290636000	0.000061000
1	-1.235755000	-2.140909000	-0.000019000	1	-1.324970000	-2.285953000	0.000061000
1	1.235780000	2.140956000	0.000069000	1	1.208464000	2.084984000	0.000028000
1	1.235765000	-2.140964000	0.000069000	1	1.201066000	-2.089255000	0.000028000
6	-1.388074000	0.000005000	0.000016000	7	-1.403964000	0.002489000	-0.000007000
6	0.693925000	1.201851000	-0.000009000	7	0.704090000	1.214497000	0.000002000
6	0.693916000	-1.201855000	-0.000009000	7	0.699779000	-1.216985000	0.000002000
6	-0.693863000	1.201771000	0.000000000	5	-0.720227000	1.252563000	-0.000016000
6	1.387939000	-0.000005000	-0.000020000	5	1.445026000	-0.002561000	0.000003000
6	-0.693871000	-1.201766000	0.000000000	5	-0.724663000	-1.250002000	-0.000015000
1	2.472468000	-0.000009000	0.000052000	1	2.642277000	-0.004684000	-0.000034000
Figure 3(a) C ₇ H ₈ ⁻			Figure 3(a) C ₇ H ₈ ⁻				
6	-0.274788000	1.254897000	0.112236000	6	0.193657000	1.194578000	-0.008784000
6	-1.024626000	0.013350000	0.028648000	6	0.909114000	0.000138000	-0.011092000
6	-0.239100000	-1.265337000	0.198545000	6	0.193818000	-1.194489000	-0.008827000
6	1.223646000	-1.141338000	-0.087620000	6	-1.192898000	-1.197635000	0.001895000
6	1.827054000	0.047781000	-0.132390000	6	-1.892713000	-0.000092000	0.008402000
6	1.065783000	1.272869000	0.040510000	6	-1.193134000	1.197510000	0.001935000
1	-0.836289000	2.181336000	0.177465000	1	0.732569000	2.136922000	-0.017984000
1	-0.340637000	-1.595896000	1.244536000	1	0.732874000	-2.136761000	-0.018069000
1	1.793979000	-2.056595000	-0.207176000	1	-1.729141000	-2.140195000	0.001201000
1	2.895998000	0.116615000	-0.301169000	1	-2.976680000	-0.000196000	0.013746000
1	1.598127000	2.217244000	0.069664000	1	-1.729507000	2.139995000	0.001269000
6	-2.347091000	0.012995000	-0.172321000	6	2.408405000	0.000064000	0.009149000
1	-2.903202000	0.941766000	-0.232526000	1	2.785529000	-0.008397000	1.036725000
1	-2.908408000	-0.908508000	-0.279450000	1	2.813498000	-0.880172000	-0.493659000
1	-0.684834000	-2.067259000	-0.396996000	1	2.813368000	0.888359000	-0.479291000
Figure 3(b) B ₄ N ₃ H ₈ ⁻			Figure 3(b) B ₄ N ₃ H ₈ ⁻				
1	0.946115000	2.311183000	0.004511000	1	0.802259000	2.289758000	-0.011679000
1	-1.762176000	-1.982801000	-0.019610000	1	-1.670387000	-2.086751000	0.001239000
1	-3.075274000	0.153922000	-0.023518000	1	-3.147854000	-0.000921000	0.007065000
1	0.648282000	-2.003779000	1.035281000	1	0.803893000	-2.288747000	-0.011669000
1	-1.537222000	2.175768000	0.005284000	1	-1.671834000	2.085921000	0.001251000
7	-1.204361000	-1.145781000	-0.008276000	7	-1.191121000	-1.203217000	0.002771000
7	-1.072195000	1.285840000	0.006842000	7	-1.191963000	1.202716000	0.002783000
7	1.069828000	0.019638000	0.001959000	7	0.981837000	0.000556000	-0.010129000
5	-1.863669000	0.066460000	-0.008903000	5	-1.939433000	-0.000478000	0.005141000
5	0.348702000	1.258423000	0.005226000	5	0.259541000	1.213138000	-0.006683000
5	0.329219000	-1.377943000	0.016533000	5	0.260289000	-1.212562000	-0.006696000
5	2.463139000	0.069245000	-0.012629000	5	2.568330000	0.000071000	0.007976000
1	3.044654000	1.132517000	-0.016974000	1	2.974570000	-0.010457000	1.175278000
1	3.120750000	-0.945206000	-0.020943000	1	2.987062000	-1.001044000	-0.572935000
1	0.675013000	-2.040407000	-0.968846000	1	2.987383000	1.011014000	-0.555213000
Figure 3(c) B ₃ N ₄ H ₈ ⁺			Figure 3(c) B ₃ N ₄ H ₈ ⁺				
1	-2.922044000	0.069078000	0.000074000	1	-2.948412000	-0.000079000	0.008449000
1	-1.800858000	2.322152000	0.000593000	1	-1.858726000	2.293902000	0.003967000
1	-1.871127000	-2.264211000	0.000091000	1	-1.858575000	-2.293986000	0.003983000
1	0.684750000	2.157297000	-0.000174000	1	0.642504000	2.115033000	-0.004923000
1	0.520684000	-1.812618000	0.802235000	1	0.642651000	-2.114949000	-0.004932000
7	-1.912017000	0.030310000	0.000018000	7	-1.939485000	-0.000044000	0.004591000
7	0.216589000	1.262509000	-0.000278000	7	0.168333000	1.225554000	-0.005956000
7	0.227927000	-1.247141000	-0.000084000	7	0.168411000	-1.225506000	-0.005962000
5	-1.203171000	1.296906000	0.000128000	5	-1.281199000	1.255386000	0.001346000
5	1.015289000	0.095769000	-0.000051000	5	0.837022000	0.000050000	-0.009908000
5	-1.321607000	-1.213001000	0.000063000	5	-1.281112000	-1.255434000	0.001350000
7	2.396472000	0.017382000	0.000191000	7	2.408683000	0.000023000	0.005015000
1	2.982878000	0.836696000	0.000031000	1	2.766767000	-0.001972000	0.963101000
1	2.929945000	-0.835786000	0.000185000	1	2.799255000	-0.820389000	-0.460372000
1	0.520421000	-1.812396000	-0.802664000	1	2.799387000	0.822246000	-0.457033000
Triplet state							
Benzene			Borazine				
1	-2.518979000	0.000014000	0.000142000	1	-2.441885000	0.000083000	-0.001699000
1	-1.283610000	2.145989000	-0.001079000	1	-1.338283000	2.338607000	-0.004631000
1	-1.283636000	-2.145974000	-0.001070000	1	-1.338443000	-2.338523000	-0.004610000
1	1.283607000	2.146140000	0.001215000	1	1.244014000	2.078928000	0.003386000
1	1.283582000	-2.146154000	0.001206000	1	1.243878000	-2.079010000	0.003370000
6	-1.433949000	0.000007000	0.000302000	7	-1.433367000	0.000046000	0.000448000
6	0.755221000	1.202162000	-0.000023000	7	0.751044000	1.195375000	0.000603000
6	0.755206000	-1.202171000	-0.000026000	7	0.750962000	-1.195427000	0.000597000
6	-0.755152000	1.202130000	-0.000007000	5	-0.815030000	1.271121000	0.000497000

6	1.433811000	-0.000008000	-0.000300000	5	1.517964000	-0.000044000	-0.001818000
6	-0.755167000	-1.202121000	-0.000004000	5	-0.815123000	-1.271070000	0.000503000
1	2.519220000	-0.000014000	-0.000062000	1	2.711189000	-0.000089000	-0.003267000
Figure 3(a) C ₇ H ₈ ⁻				Figure 3(a) C ₇ H ₈ ⁻			
6	0.215084000	1.246557000	-0.031736000	6	-0.264168000	1.232105000	-0.000055000
6	0.899453000	0.000160000	-0.030767000	6	-0.999265000	0.075710000	0.000037000
6	0.215881000	-1.246430000	-0.031856000	6	-0.299316000	-1.255822000	-0.000119000
6	-1.202065000	-1.246744000	0.004544000	6	1.179460000	-1.180998000	0.000022000
6	-1.861649000	-0.000268000	0.020561000	6	1.862954000	0.036438000	0.000013000
6	-1.202851000	1.246410000	0.004458000	6	1.188727000	1.228037000	0.000025000
1	0.790687000	2.162288000	-0.038864000	1	-0.784899000	2.184085000	-0.000517000
1	0.791807000	-2.161955000	-0.039091000	1	-0.654252000	-1.841690000	0.865308000
1	-1.773797000	-2.163198000	0.025753000	1	1.735566000	-2.111523000	0.000412000
1	-2.948699000	-0.000623000	0.047711000	1	2.947832000	0.030818000	0.000035000
1	-1.774914000	2.162650000	0.025530000	1	1.722403000	2.169823000	0.000259000
6	2.375888000	0.000491000	0.024772000	6	-2.400731000	0.074484000	0.000095000
1	2.678601000	-0.006109000	1.081613000	1	-2.958648000	1.002814000	0.000208000
1	2.798911000	-0.893916000	-0.436251000	1	-2.959872000	-0.852909000	0.000196000
1	2.798965000	0.899805000	-0.426260000	1	-0.654102000	-1.841146000	-0.866010000
Figure 3(b) B ₄ N ₃ H ₈ ⁻				Figure 3(b) B ₄ N ₃ H ₈ ⁻			
1	0.716417000	2.389089000	-0.001276000	1	0.751703000	2.329311000	-0.017437000
1	-1.492712000	-2.127534000	-0.000079000	1	-1.558595000	-2.136005000	0.022660000
1	-3.093567000	-0.142151000	-0.002669000	1	-3.131308000	-0.095064000	0.041892000
1	0.942580000	-1.985193000	0.792737000	1	0.911893000	-2.154316000	-0.415891000
1	-1.749958000	2.034498000	-0.000553000	1	-1.730313000	2.037634000	-0.016325000
7	-1.064925000	-1.217993000	0.000909000	7	-1.124288000	-1.231834000	0.027994000
7	-1.216738000	1.182999000	0.000851000	7	-1.222963000	1.171419000	-0.018030000
7	1.028086000	0.119619000	0.000357000	7	0.997710000	0.058908000	0.005076000
5	-1.887296000	-0.064743000	-0.000867000	5	-1.920934000	-0.061016000	0.002830000
5	0.231322000	1.284499000	-0.000406000	5	0.227018000	1.240882000	-0.018952000
5	0.384325000	-1.136579000	-0.000099000	5	0.326481000	-1.182674000	0.027195000
5	2.531539000	0.116929000	0.000318000	5	2.427447000	0.118603000	0.011349000
1	3.116702000	1.172890000	-0.000368000	1	2.879557000	-0.844899000	0.765026000
1	3.095489000	-0.950425000	-0.002128000	1	2.973863000	-0.851066000	-0.611331000
1	0.940642000	-1.984075000	-0.795211000	1	3.049926000	1.145974000	0.014015000
Figure 3(c) B ₃ N ₄ H ₈ ⁺				Figure 3(c) B ₃ N ₄ H ₈ ⁺			
1	-2.875486000	-0.156430000	0.169917000	1	-2.921827000	-0.000162000	-0.257387000
1	-1.976798000	2.166836000	0.030182000	1	-1.877171000	2.230891000	0.327838000
1	-1.478129000	-1.537653000	-1.153984000	1	-1.876911000	-2.231111000	0.327467000
1	0.602635000	2.162321000	-0.008832000	1	0.636880000	2.118078000	-0.041403000
1	0.695017000	-1.657872000	0.892471000	1	0.637159000	-2.117915000	-0.039918000
7	-1.870255000	-0.097048000	0.045220000	7	-1.936417000	-0.000083000	0.010644000
7	0.153984000	1.259807000	-0.028193000	7	0.170887000	1.225581000	-0.035358000
7	0.311750000	-1.184194000	0.064320000	7	0.171039000	-1.225479000	-0.035517000
5	-1.294476000	1.196989000	-0.011680000	5	-1.278317000	1.255368000	-0.003620000
5	0.900323000	0.080470000	0.008763000	5	0.839451000	0.000099000	-0.050657000
5	-1.132772000	-1.307144000	0.081098000	5	-1.278154000	-1.255452000	-0.003773000
7	2.298143000	0.112956000	-0.018372000	7	2.401942000	0.000022000	0.031555000
1	2.818785000	0.971301000	-0.096628000	1	2.714429000	-0.000374000	1.005814000
1	2.904659000	-0.689086000	0.035932000	1	2.810013000	-0.822857000	-0.416055000
1	0.688594000	-1.751637000	-0.700791000	1	2.810365000	0.823087000	-0.415384000