

Exploring the Potential Energy Surface of Medium-Sized Aromatic Polycyclic Systems with Embedded Planar Tetracoordinate Carbons: A Guided Approach

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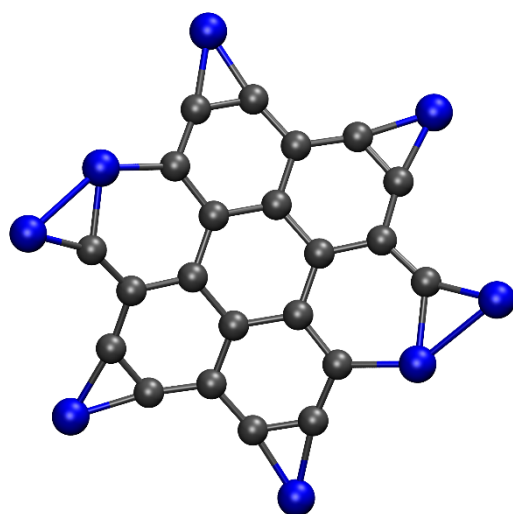
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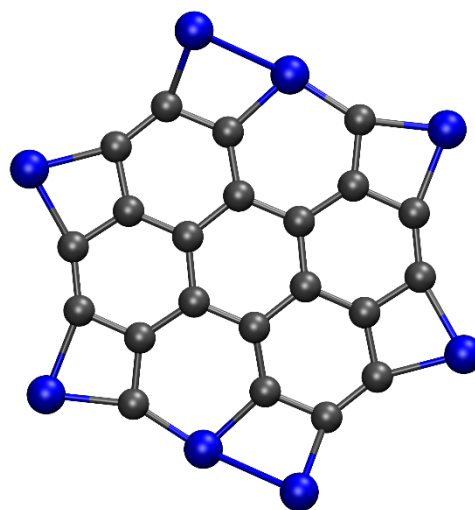
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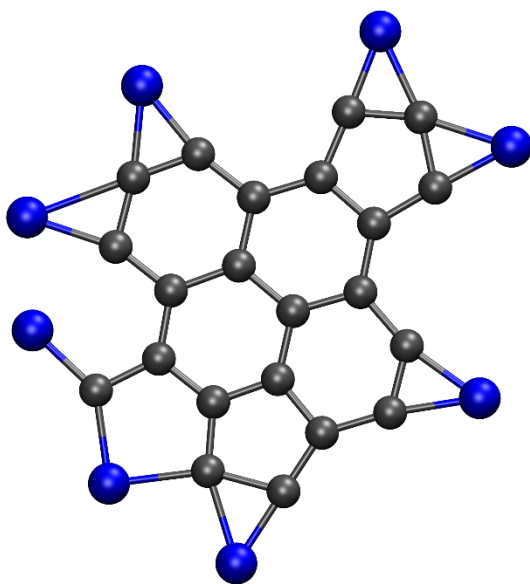
Figures S1. Minimum energy isomers of Si_8C_{22} with their respective point group symmetries and spectroscopic states. Relative energies are shown in $\text{kcal}\cdot\text{mol}^{-1}$ at PBE0-D3/def2-TZVP levels including zero-point energy (ZPE) corrections. To facilitate the connection of the structures with their Cartesian coordinates (at end of the ESI), a number-letter label was assigned to each structure.



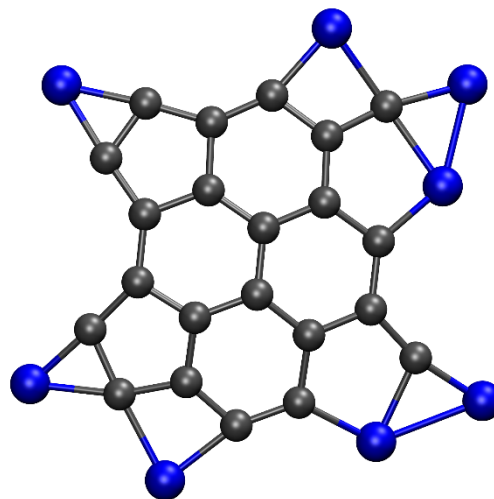
1a. $C_2 (^1A)$
0.0



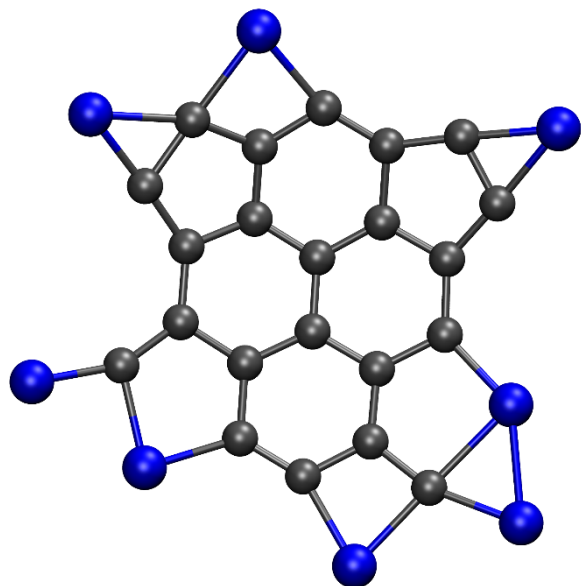
1b. $C_2 (^1A)$
13.8



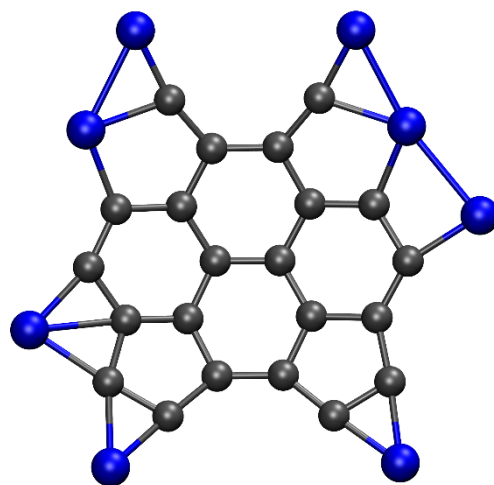
1c. $C_s (^1A')$
20.0



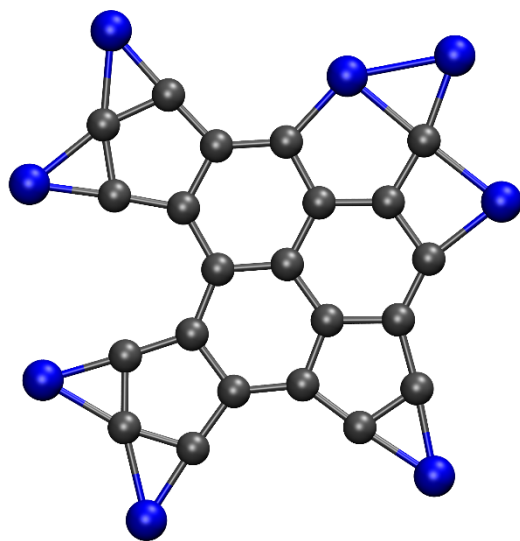
1d. $C_1 (^1A)$
22.2



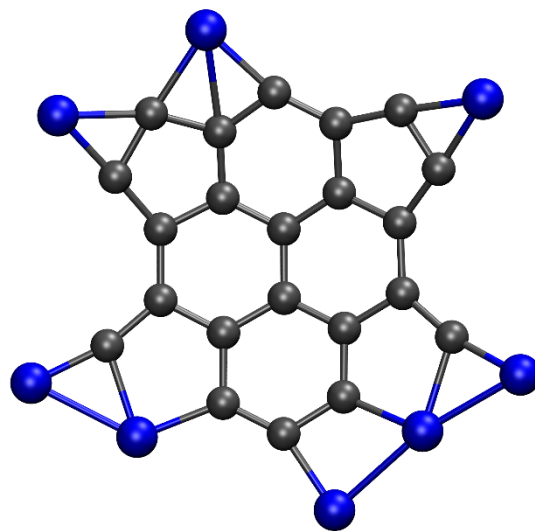
1e. $C_1(^1A)$
22.6



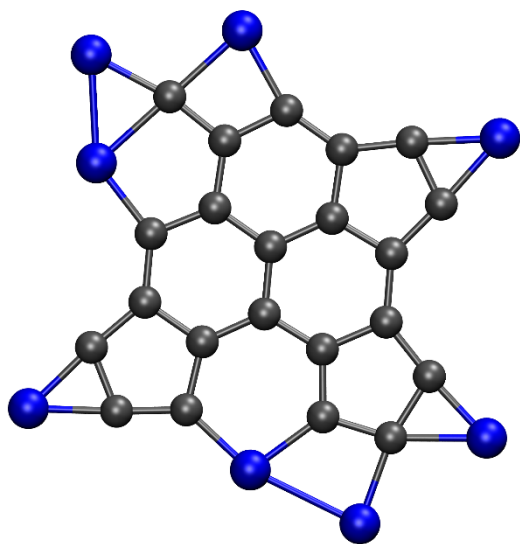
1f. $C_1(^1A)$
22.2



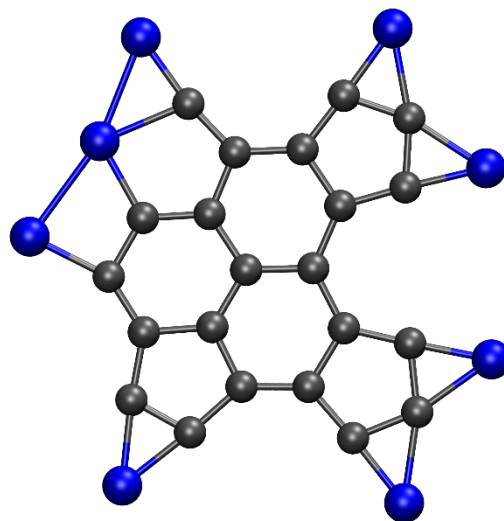
1g. $C_s(^1A')$
24.4



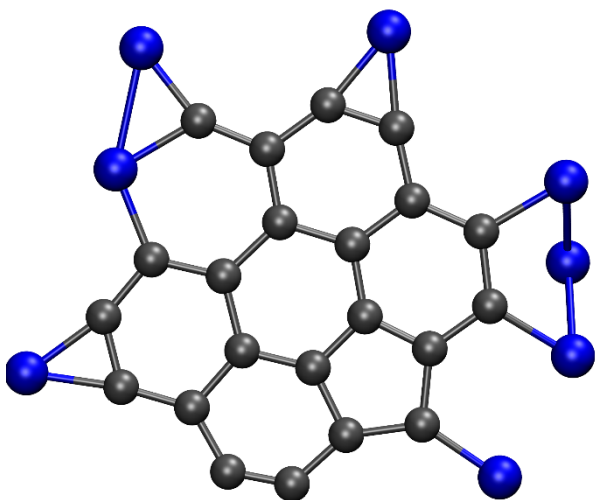
1h. $C_1(^1A)$
24.9



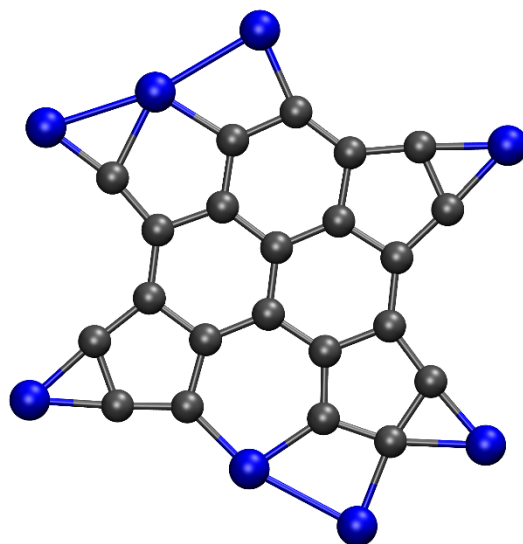
1i. $C_1(^1A)$
26.4



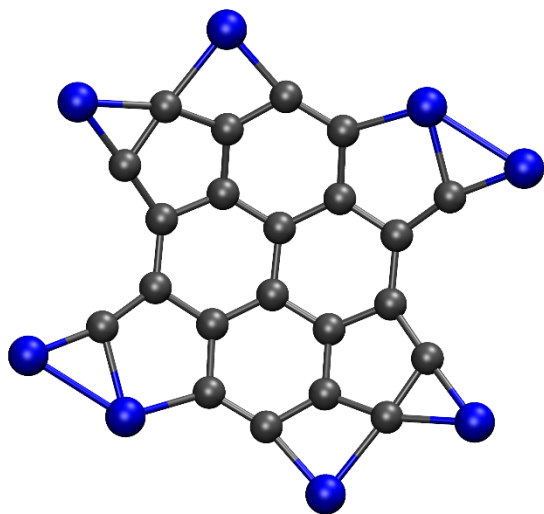
1j. $C_s(^1A')$
27.2



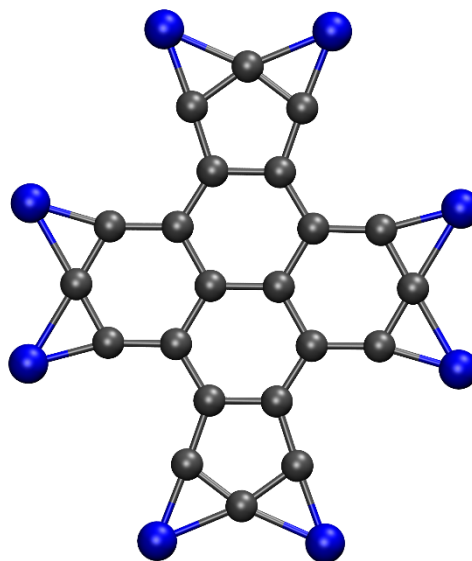
1k. $C_1(^1A)$
28.3



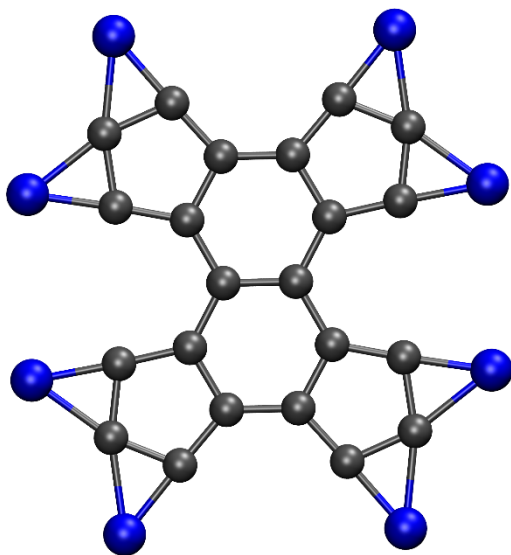
1l. $C_1(^1A)$
28.7



1m. $C_1(^1A)$
29.8

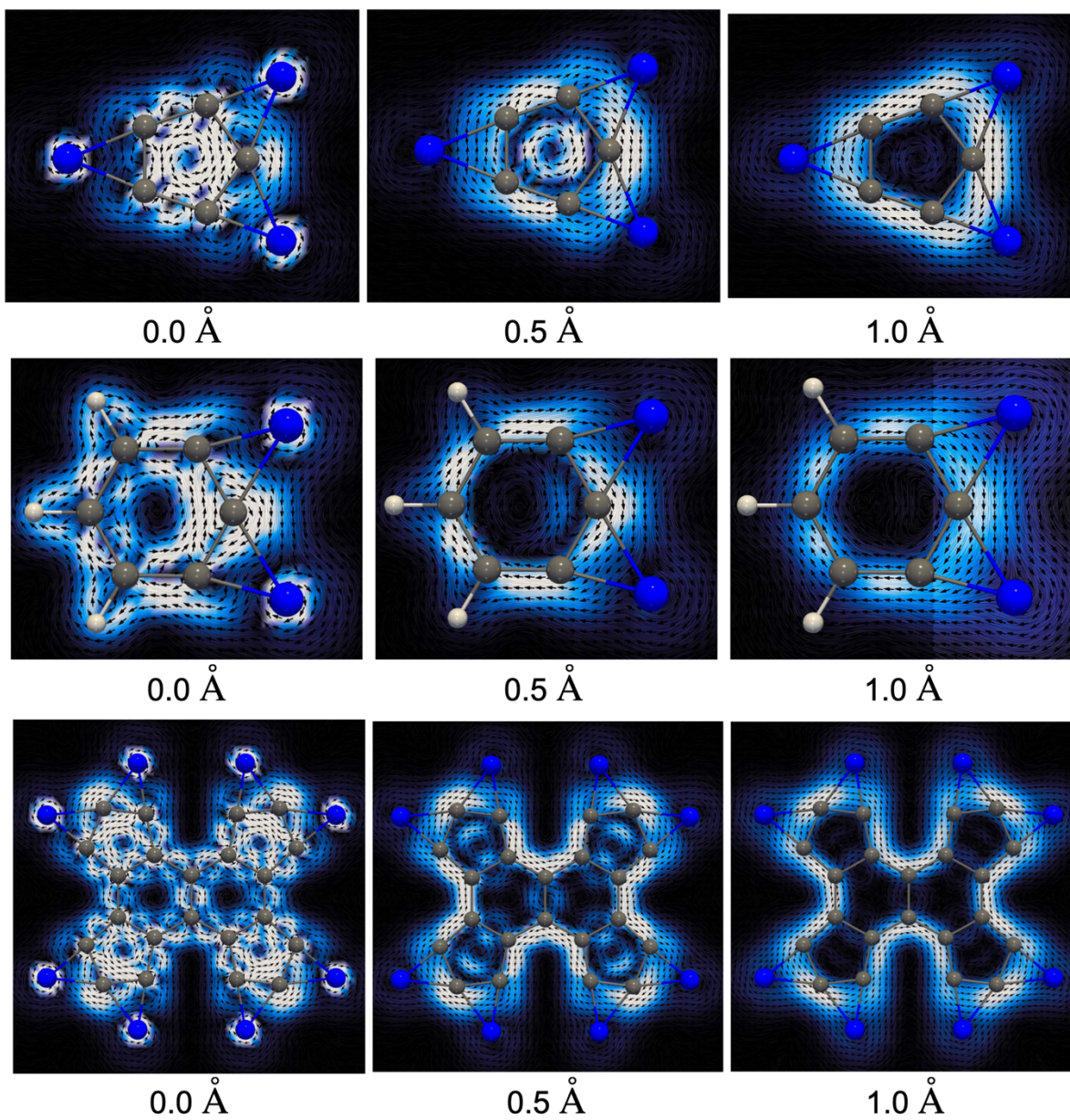


1n. $D_{2h}(^1A_g)$
30.2

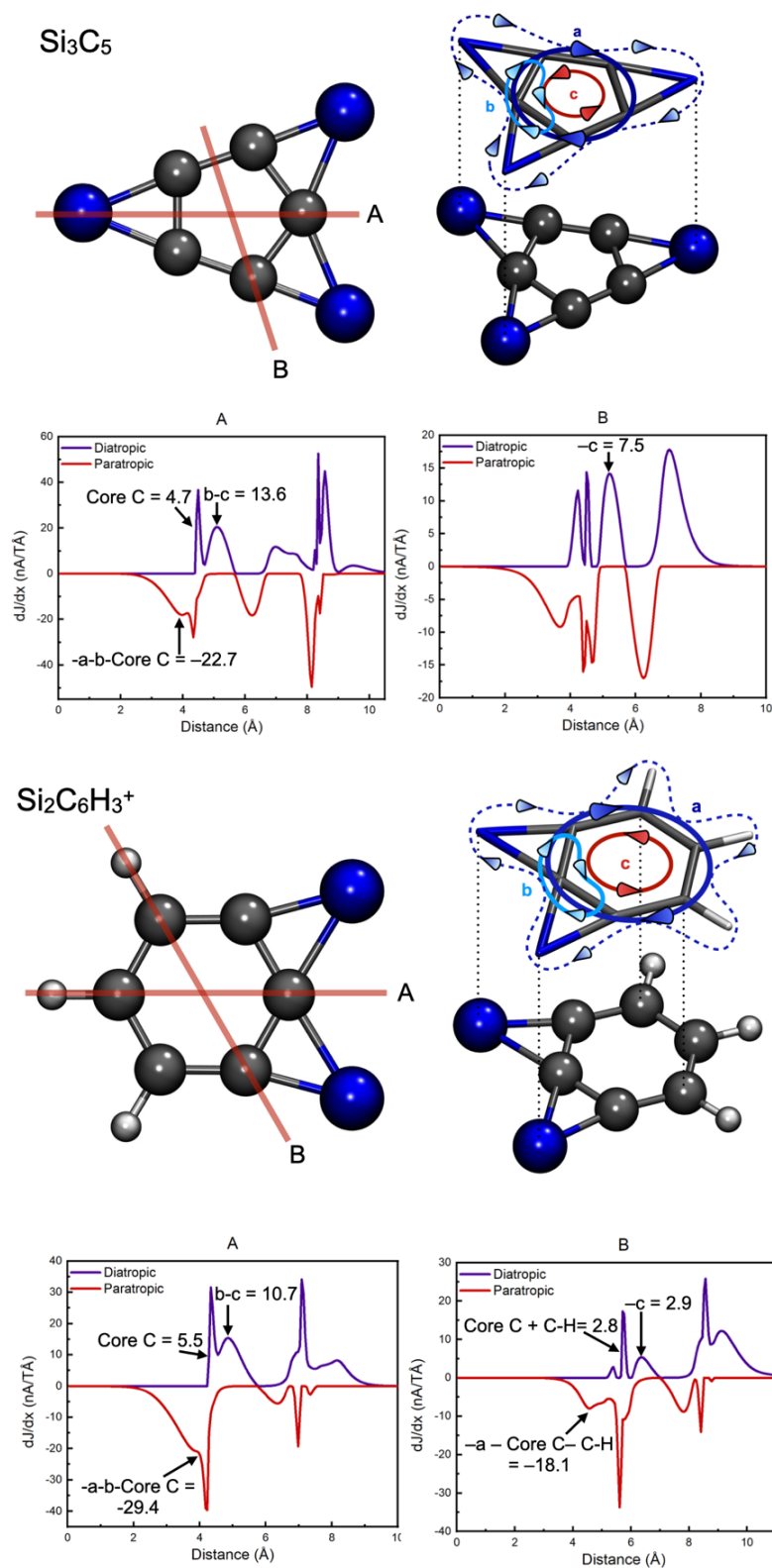


1o. $D_{2h}(^1A_g)$
41.7

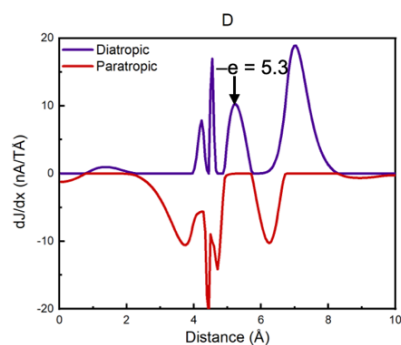
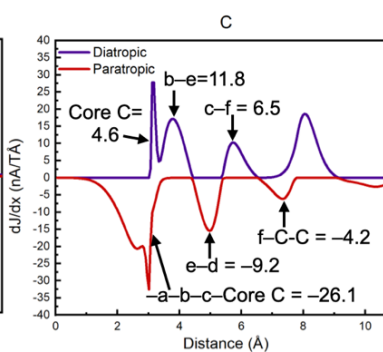
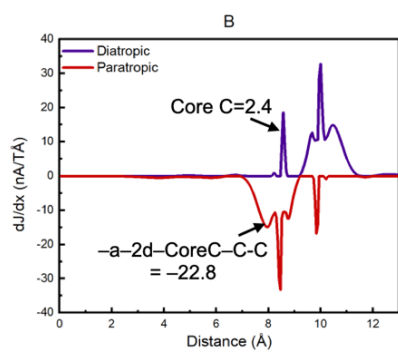
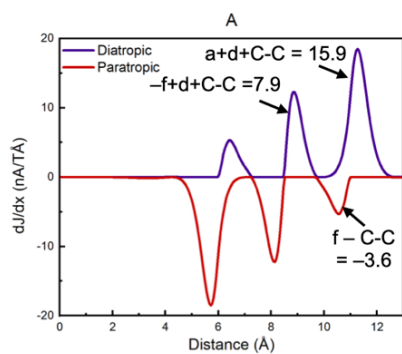
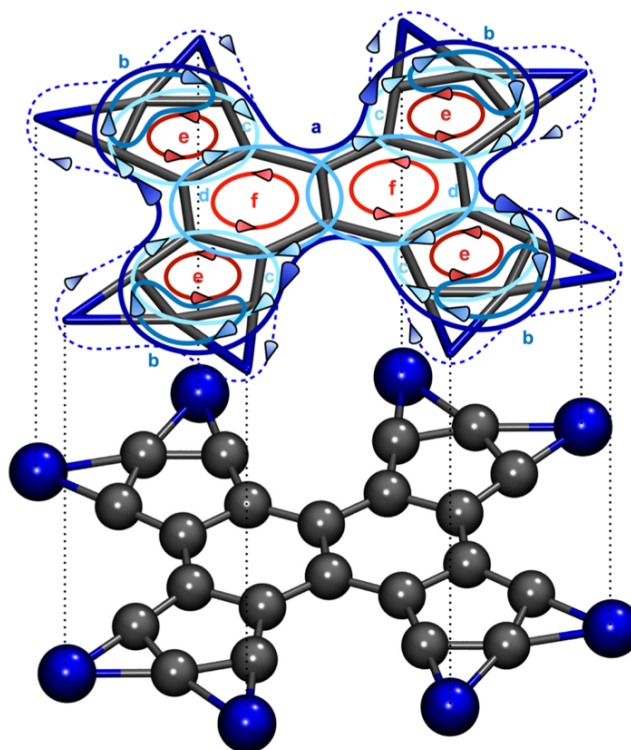
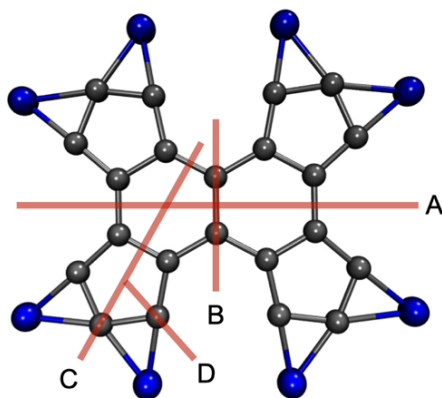
Figures S2. Vector plots visualization of the current density in diverse planes of the Si_3C_5 , $\text{Si}_2\text{C}_6\text{H}_3^+$ and C_{22}Si_8 cluster. Diatropic currents are assumed to circle clockwise.



Figures S3. Top view of integration planes considered to average the profile RCS for Si_3C_5 , $\text{Si}_2\text{C}_6\text{H}_3^+$ and Si_8C_{22} cluster (up) and the RCS profiles along the different integration planes (down).



Si_8C_{22}



Figures S4. Bond length in (black), natural charges (red and blue) and Wiberg bond indices (green) for Si_8C_{22} at the PBE0-D3/Def2-TZVP level of theory.

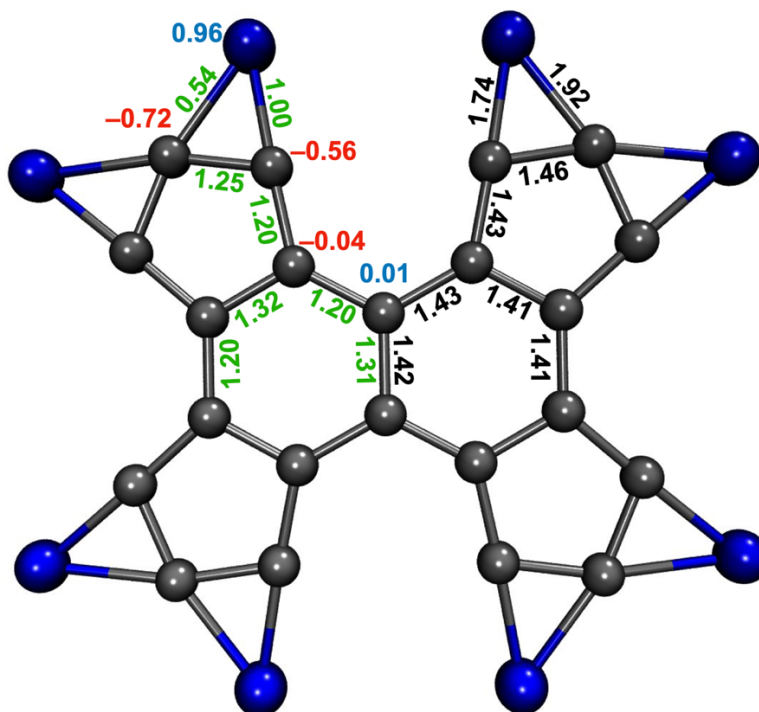


Table S1. Cartesian coordinates of the $\text{Li}_4\text{C}_{22}\text{Si}_8$ and Si_8C_{22} structures with their label for easier identification.

$\text{Li}_4\text{C}_{22}\text{Si}_8$							
6	1.262087000	0.090083000	1.408315000				
6	2.511255000	0.068297000	0.711351000				
6	2.511255000	-0.068297000	-0.711351000				
6	1.262087000	-0.090083000	-1.408315000				
6	0.000000000	0.000000000	-0.702021000				
6	0.000000000	0.000000000	0.702021000				
6	-1.262087000	-0.090083000	1.408315000				
6	-2.511255000	-0.068297000	0.711351000				
6	-2.511255000	0.068297000	-0.711351000				
6	-1.262087000	0.090083000	-1.408315000				
6	-1.573782000	-0.246847000	2.795330000				
6	-3.562011000	-0.188269000	1.652248000				
6	-3.562011000	0.188269000	-1.652248000				
6	-1.573782000	0.246847000	-2.795330000				
6	1.573782000	-0.246847000	-2.795330000				
6	3.562011000	-0.188269000	-1.652248000				
6	3.562011000	0.188269000	1.652248000				
6	1.573782000	0.246847000	2.795330000				
6	-2.974005000	-0.319842000	2.927853000				
6	-2.974005000	0.319842000	-2.927853000				
6	2.974005000	-0.319842000	-2.927853000				
6	2.974005000	0.319842000	2.927853000				
1	-4.619063000	0.219694000	-1.426805000				
1	-3.507238000	0.461020000	-3.858719000				
1	-0.879530000	0.360953000	-3.610156000				
1	0.879530000	-0.360953000	-3.610156000				
1	3.507238000	-0.461020000	-3.858719000				
1	4.619063000	-0.219694000	-1.426805000				
1	-0.879530000	-0.360953000	3.610156000				
1	0.879530000	0.360953000	3.610156000				
1	3.507238000	0.461020000	3.858719000				
1	4.619063000	0.219694000	1.426805000				
1	-3.507238000	-0.461020000	3.858719000				
1	-4.619063000	-0.219694000	1.426805000				
3	2.425823000	1.519503000	-2.091288000				
3	-2.425823000	1.519503000	2.091288000				
3	2.425823000	-1.519503000	2.091288000				
3	-2.425823000	-1.519503000	-2.091288000				
1a				1b			
14	1.120413799	4.020518320	0.722255923	14	0.932486000	4.022134000	-0.304545000
14	4.725136689	2.397351485	-0.785010086	14	-1.131802000	4.957624000	0.605978000
14	-1.120413799	-4.020518320	0.722255923	14	-0.932486000	-4.022134000	-0.304545000
14	-0.743721980	5.255311339	1.438836934	14	4.675314000	-1.990844000	0.090950000
14	0.743721980	-5.255311339	1.438836934	14	-4.315540000	-2.849104000	-0.377889000
14	-4.382358410	2.969862196	-0.758198583	14	-4.675314000	1.990844000	0.090950000
14	-4.725136689	-2.397351485	-0.785010086	14	4.315540000	2.849104000	-0.377889000
14	4.382358410	-2.969862196	-0.758198583	14	1.131802000	-4.957624000	0.605978000
6	0.800022908	1.215785723	0.008584921	6	-0.167458000	1.413440000	0.227018000
6	1.426487823	-0.084993440	-0.169833581	6	-1.267654000	0.537407000	0.224444000
6	-0.647798607	1.291731761	0.021117421	6	1.131802000	0.862664000	0.206746000
6	0.647798607	-1.291731761	0.021117421	6	-1.131802000	-0.862664000	0.206746000
6	-1.426487823	0.084993440	-0.169833581	6	1.267654000	-0.537407000	0.224444000
6	-0.800022908	-1.215785723	0.008584921	6	0.167458000	-1.413440000	0.227018000
6	1.621283254	2.368951658	0.079504922	6	-0.400075000	2.788401000	-0.000798000
6	2.814697447	-0.170687547	-0.465515584	6	-2.540230000	1.090638000	0.006629000

6	-1.316194754	2.539407416	0.145472921	6	2.299344000	1.632637000	-0.009120000
6	1.316194754	-2.539407416	0.145472921	6	-2.299344000	-1.632637000	-0.009120000
6	-2.814697447	0.170687547	-0.465515584	6	2.540230000	-1.090638000	0.006629000
6	-1.621283254	-2.368951658	0.079504922	6	0.400075000	-2.788401000	-0.000798000
6	3.546203804	1.023410964	-0.594005585	6	-2.813258000	2.472753000	-0.119406000
6	2.973144407	2.231702973	-0.292268081	6	-1.722719000	3.340203000	-0.101437000
6	0.693564708	-3.703043629	0.636197426	6	-2.439042000	-3.052466000	-0.155247000
6	-3.546203804	-1.023410964	-0.594005585	6	2.813258000	-2.472753000	-0.119406000
6	-2.677015127	2.578080879	-0.244751082	6	3.604907000	1.047582000	-0.163107000
6	-3.386567893	1.455770443	-0.565045585	6	3.736610000	-0.324114000	-0.149544000
6	-0.693564708	3.703043629	0.636197426	6	2.439042000	3.052466000	-0.155247000
6	-2.973144407	-2.231702973	-0.292268081	6	1.722719000	-3.340203000	-0.101437000
6	3.386567893	-1.455770443	-0.565045585	6	-3.736610000	0.324114000	-0.149544000
6	2.677015127	-2.578080879	-0.244751082	6	-3.604907000	-1.047582000	-0.163107000
1c				1d			
6	0.715317000	0.000000000	1.069410000	6	0.136737000	0.810551000	-0.561896000
6	-0.714260000	0.000000000	1.009796000	6	0.032388000	-0.576057000	-0.588789000
6	3.555088000	0.000000000	0.879566000	6	2.456797000	-3.124239000	0.208259000
6	-3.495925000	0.000000000	0.884468000	6	2.973183000	2.934913000	0.171600000
14	0.334152000	0.000000000	-3.980633000	14	-3.002580000	-3.177411000	0.298132000
6	-0.035047000	0.000000000	5.669669000	6	-1.997958000	3.740069000	0.224334000
6	1.421038000	0.000000000	-0.144566000	14	1.203619000	-4.729644000	0.282581000
6	1.460067000	0.000000000	2.263526000	14	4.305151000	-3.242957000	0.653603000
6	-1.386685000	0.000000000	-0.278435000	6	1.149453000	-2.628433000	-0.188315000
6	-1.428220000	0.000000000	2.220902000	6	3.294787000	-1.901080000	0.152081000
6	0.772726000	0.000000000	-1.358391000	6	1.222331000	-1.275775000	-0.488102000
6	0.722429000	0.000000000	3.461327000	6	2.511539000	-0.756294000	-0.236909000
6	-0.632364000	0.000000000	-1.455664000	6	0.405931000	3.554378000	0.002884000
6	-0.702180000	0.000000000	3.430885000	14	4.744980000	2.998403000	0.546065000
6	2.815891000	0.000000000	-0.342480000	6	3.590622000	1.669636000	0.116103000
6	2.890777000	0.000000000	2.094833000	6	1.562336000	2.787439000	-0.104500000
6	-2.810961000	0.000000000	-0.379475000	6	2.612633000	0.662221000	-0.218458000
6	-2.851708000	0.000000000	2.110356000	6	1.396954000	1.387334000	-0.382067000
6	1.637997000	0.000000000	-2.453365000	6	-0.049946000	-3.341571000	0.020723000
6	1.145408000	0.000000000	4.822838000	14	-5.053778000	-1.957171000	0.460919000
6	-1.137390000	0.000000000	-2.773153000	6	-1.250420000	-2.643917000	-0.097092000
6	-1.180609000	0.000000000	4.774463000	6	-3.501973000	-1.310880000	0.099764000
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14	-4.536915000	0.000000000	-1.141438000	14	-0.576744000	5.144600000	-0.032391000
14	-4.627235000	0.000000000	2.363385000	14	-3.612953000	4.475218000	0.682426000
14	3.329283000	0.000000000	-3.438163000	6	-0.864823000	2.921502000	-0.130199000
14	-2.905719000	0.000000000	-2.745460000	14	-3.444635000	2.304652000	0.236686000
14	1.722769000	0.000000000	6.463978000	6	-1.031680000	1.555558000	-0.409865000
14	-1.816502000	0.000000000	6.395405000	6	-2.298911000	0.949644000	-0.225147000
1e				1f			
6	0.215847000	0.856567000	-0.706060000	6	0.204730000	0.859619000	-0.606432000
6	0.127874000	-0.532091000	-0.564764000	6	0.056807000	-0.523266000	-0.623094000
6	2.318917000	-3.468827000	0.260090000	6	2.400645000	-3.128734000	0.233731000
6	2.934087000	3.125522000	0.120078000	6	3.082155000	2.910563000	0.133533000
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14	3.856386000	-1.913413000	0.166113000	6	3.274273000	-1.931701000	0.155193000
6	1.336823000	-1.237506000	-0.377500000	6	1.226419000	-1.257362000	-0.510806000
6	2.612961000	-0.594307000	-0.248857000	6	2.529933000	-0.774228000	-0.262973000
6	0.336690000	3.661890000	-0.076935000	6	0.537417000	3.595644000	-0.040408000
14	4.751656000	3.272446000	0.585472000	14	4.852712000	2.926846000	0.521735000
6	3.599345000	1.872910000	0.067335000	6	3.669960000	1.628311000	0.081264000
6	1.528366000	2.954543000	-0.214910000	6	1.673237000	2.795138000	-0.154117000

6	2.654723000	0.826868000	-0.297489000	6	2.672929000	0.644876000	-0.261635000
6	1.432320000	1.518018000	-0.522471000	6	1.479381000	1.399412000	-0.435965000
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6	-3.464696000	-1.171330000	0.132880000	6	-3.492738000	-1.119668000	0.136346000
6	-1.140360000	-1.128303000	-0.356825000	6	-1.189355000	-1.122097000	-0.386094000
6	-2.349314000	-0.357215000	-0.220033000	6	-2.357257000	-0.328431000	-0.214119000
14	-0.880904000	5.107616000	0.466270000	14	-0.258580000	5.244540000	0.202652000
14	-4.042798000	3.544222000	0.773941000	14	-4.526922000	3.036842000	0.601612000
6	-0.865159000	2.937896000	-0.318119000	6	-0.757539000	3.007722000	-0.179104000
6	-3.018801000	2.199174000	0.147787000	6	-3.166684000	2.094825000	0.125839000
6	-0.961107000	1.585395000	-0.624244000	6	-0.932228000	1.643252000	-0.440921000
6	-2.239723000	1.062526000	-0.293382000	6	-2.223658000	1.091316000	-0.229975000
lg				lh			
6	0.499217000	0.000000000	1.004440000	6	0.184581000	0.799072000	-0.703684000
6	-0.911844000	0.000000000	0.970985000	6	0.044991000	-0.580860000	-0.586986000
6	-2.965168000	0.000000000	-2.141569000	14	2.677320000	-3.538035000	0.384646000
6	3.011093000	0.000000000	-1.641602000	6	2.976922000	2.932828000	0.140145000
6	-3.092969000	0.000000000	4.013673000	14	-3.125784000	-2.999834000	0.356054000
6	3.398312000	0.000000000	3.375585000	6	-2.083141000	3.443263000	0.194147000
14	-4.571164000	0.000000000	-1.100743000	14	0.659126000	-4.927605000	0.102618000
14	-2.609752000	0.000000000	-4.041882000	14	4.837183000	-2.627871000	0.669902000
6	-2.876797000	0.000000000	-0.692789000	6	1.083633000	-2.682174000	-0.102959000
6	-1.595363000	0.000000000	-2.632041000	6	3.461312000	-1.726103000	0.164175000
6	-1.501638000	0.000000000	-0.315935000	6	1.217015000	-1.321892000	-0.415051000
6	-0.707431000	0.000000000	-1.516082000	6	2.508521000	-0.747848000	-0.233926000
6	3.377972000	0.000000000	0.972706000	6	0.421904000	3.574444000	-0.055746000
14	3.276928000	0.000000000	-3.434520000	14	4.731541000	2.981047000	0.592087000
6	1.812005000	0.000000000	-2.371437000	6	3.589177000	1.667367000	0.091134000
6	2.699738000	0.000000000	-0.228350000	6	1.575418000	2.806452000	-0.201968000
6	0.694572000	0.000000000	-1.450419000	6	2.612598000	0.669146000	-0.288582000
6	1.258154000	0.000000000	-0.169947000	6	1.424347000	1.402293000	-0.518168000
14	-4.650023000	0.000000000	2.883170000	6	-0.195139000	-3.281619000	0.051397000
14	-2.841756000	0.000000000	5.911406000	14	-5.108430000	-1.669542000	0.570638000
6	-2.937899000	0.000000000	2.566858000	6	-1.362579000	-2.528568000	-0.048550000
6	-1.743657000	0.000000000	4.554537000	6	-3.538970000	-1.108220000	0.159943000
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14	4.106514000	0.000000000	5.066220000	14	-3.890982000	3.632461000	0.747935000
6	2.611707000	0.000000000	2.166303000	6	-0.811690000	2.912420000	-0.275274000
14	1.904511000	0.000000000	4.758254000	6	-2.968456000	2.255683000	0.169720000
6	1.210019000	0.000000000	2.221279000	6	-0.958922000	1.564904000	-0.584483000
6	0.601855000	0.000000000	3.487449000	6	-2.242903000	1.091464000	-0.262773000
li				lj			
6	0.087958000	0.771422000	-0.002968000	6	0.862362000	0.000000000	1.044351000
6	-0.038251000	-0.609512000	-0.006805000	6	-0.547635000	0.000000000	1.052731000
6	2.563857000	-3.157081000	0.006482000	14	-3.573081000	0.000000000	-1.707963000
6	2.999463000	2.924330000	0.022137000	6	2.933180000	0.000000000	-2.073497000
6	-3.080515000	-2.609736000	-0.030544000	6	-3.001338000	0.000000000	3.743742000
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14	4.534063000	-3.165410000	0.020158000	14	-2.671340000	0.000000000	-3.877522000
6	1.168549000	-2.727498000	-0.002507000	6	-2.696311000	0.000000000	-0.078249000
6	3.355759000	-1.894929000	0.014440000	6	-1.697875000	0.000000000	-2.460426000
6	1.154431000	-1.338457000	-0.000112000	6	-1.295650000	0.000000000	-0.134866000
6	2.468593000	-0.776615000	0.010353000	6	-0.740532000	0.000000000	-1.424654000
6	0.418425000	3.576628000	0.005676000	14	4.528291000	0.000000000	-0.992395000
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6	3.602530000	1.650550000	0.023617000	6	1.567816000	0.000000000	-2.570342000
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14	-0.326106000	-3.820289000	-0.014310000	6	-3.433522000	0.000000000	1.142281000
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6	-3.596040000	-1.297016000	-0.031653000	6	-1.785676000	0.000000000	4.449510000
6	-1.315600000	-1.183809000	-0.016494000	6	-1.277833000	0.000000000	2.242526000
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1k				1l			
14	-4.847873000	-0.890606000	-0.045279000	6	0.161351000	0.828372000	-0.011288000
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14	-3.831806000	3.387136000	-0.124988000	6	-3.119623000	-2.434371000	0.029535000
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6	-0.377407000	0.554700000	-0.168972000	6	3.342838000	-1.934046000	0.010958000
6	0.000756000	-1.875944000	-0.149366000	6	1.160809000	-1.311008000	0.008052000
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6	1.383291000	-1.764646000	-0.062592000	6	0.560636000	3.624964000	-0.038307000
6	1.952362000	-0.419396000	-0.032835000	14	4.930738000	2.933614000	-0.038870000
6	-2.137100000	-1.170718000	-0.282064000	6	3.690922000	1.612840000	-0.024625000
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6	0.491380000	3.102803000	-0.102058000	6	-2.288288000	1.188498000	-0.008879000
1m				1n			
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14	3.239935000	3.401494000	0.320913000	6	-3.557546000	0.000000000	1.000000000
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6	3.250048000	-1.815627000	0.192200000	6	-1.434674000	0.000000000	2.239629000
6	1.209009000	-1.231376000	-0.575717000	6	0.711523000	0.000000000	-1.426340000
6	2.483228000	-0.700431000	-0.293840000	6	0.711523000	0.000000000	3.426340000
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6	1.501235000	2.893813000	-0.162611000	6	2.865897000	0.000000000	2.230680000

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6	-3.494170000	-1.161836000	0.163334000	6	-1.164617000	0.000000000	4.782632000
6	-1.211639000	-1.125509000	-0.454529000	14	4.547305000	0.000000000	-0.698791000
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lo							
6	0.711231000	0.000000000	1.000000000				
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6	-1.640915000	0.000000000	-2.549437000				
6	-1.395662000	0.000000000	-0.251516000				
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