

Diatropicity (Aromaticity) in cyclopropenium and cyclopropene derivatives containing second and third row elements.

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Supporting information

Table of contents

Topic	pages
B3LYP/6-311G(d) optimized structures (Cartesian coordinates) of all the systems that are discussed	S2-S44
M06-2X/def2-qzvp optimized structures (Cartesian coordinates) of the parent 1-15	S45-S51
Optimized structures of the 6π electrons systems	S51-S60
Figure S1: NICS _{zz} scans of benzene and its planar hexasila and hexagerma derivatives.	S60
Figure S2: Current density plots of 4-9 at 1 a.u. and 2 a.u. above the molecular plane.	S60-S63
Figure S3: Plots of VRE of 1-15 against the VRE of Model-I and Model-II .	S63
Results and discussion of the per-methylated systems. Tables S1-S2, Figures S4-S5.	S64-S66
Table S3: NICS (ppm), MCI (a.u.) and BLW-VRE (kcal mol ⁻¹) for 1-15 at M06-2X/def2-qzvp.	S66
Table S4: Summary of all the results for the parent 1-15 at B3LYP/6-311G+(d) (NICS) and B3LYP/6-311G(d) for BLW and MCI.	S67
Explanation of the NICS methods that are used here	S67-S68
Table S5: Energy differences (kcal mol ⁻¹) between geometrically optimized and D _{nh} 6π electrons systems and the the number of imaginary frequencies of the latter.	S69
Table S6: Experimental and computational E-E (E=Si, Ge) bond lengths (Å) for 2, 3, 12 and 13	S69

1

C,0,1.731562347,-0.3207290048,-0.1927699936
C,0,3.0469599021,0.0051153877,-0.3466564305
C,0,2.3933104626,0.3331808421,0.8045343659
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H,0,2.3970223438,0.7834095042,1.7896031185

2

H,0,0.092301551,-0.9636953076,-0.9239725464
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Si,0,3.5280786813,-0.1083563182,-0.5480577173

3

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H,0,2.2303346057,2.0345462159,2.2184327325
Ge,0,1.3108995932,-0.4196642344,-0.4675093559
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Ge,0,2.3348888065,1.0339955915,1.0515251251

4

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Si,0,1.4073700915,-0.3268095955,-0.4597123693
Si,0,3.5406162425,-0.2129355012,-0.2812753445
C,0,2.3376176362,0.7260155958,0.6243447243

7

H,0,0.1348767615,-1.0312106119,-0.9825400922
H,0,4.8214054815,-0.3048323882,-1.273893848
H,0,2.3168815937,1.7756903346,2.3701623376
Si,0,1.363220667,-0.4035750291,-0.4410533191
Si,0,3.5359398879,-0.0668166201,-0.5761200927
Ge,0,2.3747488586,0.8986396548,1.1145985443

8

H,0,-0.0485007819,0.4550700017,-1.2406922389
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C,0,2.4573575276,0.6279346241,0.7626919375
Ge,0,1.3434588983,0.1807709056,-0.6647734012
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9

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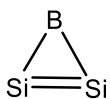
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11



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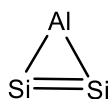
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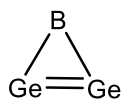
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13



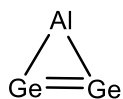
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Al,0,2.8883823879,2.3836152898,-0.5684618704
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14



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B,0,2.874562401,2.0823926342,-0.5284431108
Ge,0,1.7513250111,0.4513967588,-0.293217174
Ge,0,3.9944559032,0.4324843457,-0.5565226576

15



H,0,0.2535418589,-1.1876404914,-1.2348745081
H,0,4.8959613911,-0.5700406801,-1.1970213761
H,0,2.1490915021,2.1014448653,2.3626167135
Ge,0,1.3381940009,-0.39030887,-0.4557808387

Ge,0,3.6282457317,-0.0856551592,-0.4371125887
Al,0,2.2930563053,1.0935014253,1.152322198

1-Me

C,0,0.5002189879,-0.6132609654,0.0311397656
C,0,0.2793888487,0.7427474343,0.0314804854
C,0,-0.7823278165,-0.1261002263,-0.0413102194
C,0,0.8005651018,2.1160631089,0.0617935525
H,0,1.7453815274,2.1684186502,0.6038644047
H,0,0.9940613699,2.4319960688,-0.9705043609
H,0,0.0739078644,2.8073898153,0.4892004545
C,0,1.430300247,-1.7501864908,0.0607706459
H,0,0.9603622015,-2.6370293445,0.4865617865
H,0,1.7150078684,-1.9868951184,-0.9716147477
H,0,2.3424253443,-1.5006287429,0.6039216314
C,0,-2.231041983,-0.3623237418,-0.1069709904
H,0,-2.6132308934,-0.4348361235,0.9184725207
H,0,-2.7462702706,0.465962699,-0.5940571211
H,0,-2.4562005479,-1.3033271929,-0.6098013477

2-Me

Si,0,-0.4406943562,1.2006617413,0.0750958051
Si,0,1.2406258899,-0.2304906766,0.0262385381
Si,0,-0.840107227,-0.9706023984,0.0162402939
C,0,3.0723200488,-0.5790442748,0.0016500919
H,0,3.3561841053,-1.0298512623,-0.9532529835
H,0,3.6414402676,0.3430912793,0.1364979354
H,0,3.3354921589,-1.2764812985,0.8011283404
C,0,-1.0538292672,2.9608221576,0.1305664401
H,0,-0.7263837259,3.4444096882,1.0548967362
H,0,-0.6515520593,3.5275835555,-0.7132493566
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C,0,-2.0585792029,-2.3818183195,-0.015417032
H,0,-2.6731157768,-2.3692319198,0.8887594241
H,0,-2.720605455,-2.289267329,-0.880479632
H,0,-1.5371004779,-3.3395167664,-0.0724168308

3-Me

Ge,0,-1.2631447346,0.4951218603,-0.0277323905
Ge,0,1.0606319745,0.8463530524,0.0069423121
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C,0,-3.0788052773,1.2434883713,-0.0777275699
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H,0,-3.2453866705,1.7044509069,-1.0528668315
H,0,-3.8027127574,0.4439244262,0.0825013113
C,0,2.6168752489,2.0450387841,0.0262634979
H,0,2.2888096531,3.0648683024,-0.1770736618
H,0,3.0893585976,1.9966197358,1.0088942336
H,0,3.3259899909,1.7218232082,-0.7372913091
C,0,0.4620025353,-3.2887624784,0.0520650993
H,0,-0.1866391892,-3.7253065782,0.8129783018
H,0,0.2019738344,-3.6940959938,-0.9273496686
H,0,1.505221128,-3.5102314738,0.2794040656

4-Me

C,0,-0.8261416741,-0.6838162679,0.1352724963
C,0,-0.8281501855,0.6843515503,-0.1436061672
Si,0,0.7811359866,0.0006029365,-0.0145015222
C,0,2.6261501878,0.0002805735,-0.0086112709
H,0,3.0089485854,0.8309690315,-0.6050697712
H,0,2.9815612863,0.1133232374,1.0207331827
H,0,3.0042576816,-0.9455694299,-0.4033784264
C,0,-1.8673878718,1.7162857323,-0.3483550498
H,0,-1.757732711,2.1694439976,-1.3377720447

H,0,-2.8751467672,1.3068624875,-0.2571159283
H,0,-1.7454109372,2.523065093,0.3799666947
C,0,-1.8626919932,-1.7161402198,0.3513164282
H,0,-1.7394357684,-2.1726228493,1.337561893
H,0,-2.8715666786,-1.306456155,0.2748405782
H,0,-1.7508677709,-2.5205797515,-0.3812811224

5-Me

C,0,-0.2939786598,-1.2892314953,0.5435677336
C,0,0.2548992194,-1.1048662021,-0.7112620995
Ge,0,0.0173242077,0.5016077604,0.1818211603
C,0,0.0807735652,2.4180596116,0.4913906901
H,0,1.0482340231,2.640937777,0.9466015232
H,0,-0.0110270513,2.9327176883,-0.464299585
H,0,-0.7251528957,2.6922809571,1.1710358936
C,0,-0.7459744221,-2.4307579661,1.3689111114
H,0,-0.6088110407,-3.3819270135,0.8493319903
H,0,-0.1926058994,-2.4597534134,2.3116354748
H,0,-1.8029461032,-2.3177317492,1.62566442
C,0,0.6619222718,-1.9574708069,-1.8496506944
H,0,1.7237074445,-1.8154024478,-2.0692255172
H,0,0.4820561278,-3.0153052604,-1.6443835059
H,0,0.1115791729,-1.6740467396,-2.7511386853

6-Me

Si,0,1.0705033653,-0.2865419756,-0.0157411684
Si,0,-1.0708681959,-0.2859615438,-0.0151269381
C,0,0.0002162447,1.1498836843,0.0247956035
C,0,0.0006178916,2.6388084114,0.0520105293
H,0,0.8889276416,3.0398201562,0.5444546617
H,0,0.0001853065,3.0220306692,-0.9750421021
H,0,-0.8870150445,3.0402615613,0.5453214816

C,0,2.8621322878,-0.7695035595,-0.0190142332
H,0,2.9745774347,-1.8525731581,0.0562687935
H,0,3.335353515,-0.4285038788,-0.9444601518
H,0,3.3752664836,-0.2982367823,0.8240315105
C,0,-2.8627449842,-0.7680312768,-0.0176304554
H,0,-3.3346459571,-0.4324023622,-0.9457181471
H,0,-2.975795405,-1.8505918928,0.0638895976
H,0,-3.3766965141,-0.2914822325,0.8219245384

7-Me

Si,0,1.0555362679,1.106214315,-0.0426354491
Si,0,1.0510283771,-1.1028471818,-0.0052554402
Ge,0,-0.936847193,0.0074076743,0.0423894577
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H,0,3.076843617,2.5240743442,-0.1231500785
H,0,1.7274907314,3.281320715,-0.9961505396
C,0,1.9957507713,-2.7125102167,-0.0114378173
H,0,3.0717131615,-2.5241365071,-0.0241947857
H,0,1.7516966026,-3.2984764124,0.8786365003
H,0,1.7319502573,-3.3025584894,-0.8932499759
C,0,-2.8933120221,0.000637328,0.1141574796
H,0,-3.2764332225,-0.6438260031,-0.6782602028
H,0,-3.2092624068,-0.3891613798,1.0832663186
H,0,-3.2663851346,1.0161983598,-0.0166273233

8-Me

C,0,0.0004689246,1.351425393,0.0995607094
Ge,0,-1.1445674036,-0.1374395087,-0.0805448144
Ge,0,1.1434114481,-0.1391958561,-0.07976781
C,0,0.0014921165,2.8268724597,0.2648642313
H,0,0.002599976,3.3104738682,-0.7194360855

H,0,-0.8863091246,3.1782701247,0.7967829615
H,0,0.8891967786,3.1768066182,0.7979306884
C,0,3.036139078,-0.6324172932,-0.125844342
H,0,3.3023144109,-0.8965865154,-1.1506174778
H,0,3.6284395537,0.2197535375,0.2092425741
H,0,3.1983303115,-1.4907330272,0.5265121496
C,0,-3.0377353167,-0.6290457178,-0.1258614687
H,0,-3.6314293598,0.2351516741,0.1740551197
H,0,-3.2959693026,-0.929663247,-1.1425133063
H,0,-3.2064323205,-1.4633190698,0.5555378706

9-Me

Ge,0,1.1745916567,-0.3483972385,-0.0044823278
Ge,0,-1.1751439716,-0.3465689551,0.0140950465
Si,0,0.0012244202,1.6037014288,-0.0169527835
C,0,0.0007904197,3.4717629988,-0.0486157664
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H,0,-0.0891922721,3.8320450056,-1.077342237
H,0,-0.8405312866,3.8620728074,0.5296089877
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H,0,3.6942216615,-0.6241797485,-0.1643601032
H,0,2.9979027091,-1.8148734643,0.9699037818
H,0,2.8593716088,-2.0763034869,-0.7872657033
C,0,-2.875941015,-1.3219561127,0.0463462993
H,0,-2.9665136564,-1.8450737969,0.9997387287
H,0,-3.6991006057,-0.6166453568,-0.0699243746
H,0,-2.8872200889,-2.0468405923,-0.7688519984

10-Me

C,0,0.3858263445,-0.677307545,-0.0604391803
C,0,0.3904139708,0.6771028188,-0.0085598214
B,0,-0.9216929812,0.0006701486,0.0608671279

C,0,-2.476300077,0.0008085204,0.1991998523
H,0,-2.9470020509,-0.8680233178,-0.2703077069
H,0,-2.747594759,-0.0364010899,1.2619830759
H,0,-2.940884522,0.9044066962,-0.2064750496
C,0,1.3601123226,1.805425723,-0.0396475829
H,0,1.2813184162,2.4001131914,0.8758573736
H,0,2.3977898056,1.4736474381,-0.1453013203
H,0,1.1298838122,2.4843926997,-0.8665678549
C,0,1.3478697612,-1.8064997989,-0.1779232967
H,0,1.1128361683,-2.4192354594,-1.0537642225
H,0,2.3877348504,-1.4746250588,-0.2588777739
H,0,1.2653329984,-2.4683656966,0.6899158097

11-Me

C,0,0.8860338388,0.6916579195,-0.0392330588
C,0,0.8850969961,-0.6862372923,0.0015928913
Al,0,-0.8497993972,0.0069704164,0.0714545478
C,0,2.0357496518,1.6495986405,-0.1268144795
H,0,3.0138425072,1.155642749,-0.161783794
H,0,1.9450969608,2.2788361931,-1.0184051725
H,0,2.0343288288,2.3317473188,0.7297807012
C,0,2.0339900762,-1.6486529782,-0.0290888215
H,0,1.9425700059,-2.3295998978,-0.881767724
H,0,3.0126166124,-1.1586962882,-0.0932948103
H,0,2.0318858959,-2.2788839265,0.8664029353
C,0,-2.8039307985,0.0000707766,0.1618494764
H,0,-3.2394158655,-0.2983633454,-0.797785388
H,0,-3.1713969711,-0.7098361275,0.9091971102
H,0,-3.2110578015,0.9841930019,0.4098546263

12-Me

Si,0,-1.0654366552,-0.2687932253,-0.0176278717

Si,0,1.065452443,-0.2730936709,0.0128869508
B,0,0.0033307784,1.3479870947,-0.0007473723
C,0,0.0057182355,2.9165736179,0.0218497286
H,0,-0.0193359352,3.2738831916,1.0593909293
H,0,0.9024755623,3.3479825799,-0.4346323741
H,0,-0.8668867296,3.3502610551,-0.4774052301
C,0,2.7597367623,-1.1205891582,0.0180311686
H,0,2.8491276557,-1.8082203934,-0.8269611025
H,0,3.5630697523,-0.3828833426,-0.0477480133
H,0,2.8957839191,-1.6981495497,0.9363984443
C,0,-2.7632992058,-1.1082595706,-0.0557672158
H,0,-2.9718321808,-1.5893907828,0.9038578582
H,0,-3.5524929127,-0.3785666082,-0.2524661614
H,0,-2.7978657391,-1.8773060475,-0.8315048886

13-Me

Al,0,-1.3924320588,-0.0044903146,-0.0035876931
Si,0,0.6840603521,-1.0930343917,-0.0753555601
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H,0,1.7024022295,-3.1378164441,-1.1031183081
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H,0,-3.772806115,-0.9547548797,-0.3439243935

14-Me

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C,0,-0.0007105107,3.0919163528,-0.1041529159
H,0,0.8851169206,3.5303426375,0.367594198
H,0,-0.0013631779,3.4304019484,-1.1480493977
H,0,-0.8848974696,3.5313127983,0.3696441961
C,0,2.9091469323,-1.0293039538,0.0193236064
H,0,3.7040767768,-0.2826298288,-0.0158922833
H,0,3.0085223006,-1.6206398072,0.9311700357
H,0,2.9989811754,-1.6935065548,-0.8419809774
C,0,-2.9085361377,-1.0278011474,0.1015291109
H,0,-2.9728337884,-1.6408053044,1.0020924014
H,0,-3.7029044381,-0.2798308526,0.1153608754
H,0,-3.033546927,-1.6710362423,-0.7712780487

15-Me

Ge,0,1.1605456671,-0.3688017894,-0.0069652028
Ge,0,-1.1609417377,-0.3695807835,-0.0003528948
Al,0,-0.0011572072,1.7269564294,0.0048651002
C,0,-0.0000764488,3.6964560221,0.0055782294
H,0,0.8326095906,4.098554046,0.5921283266
H,0,0.0967263849,4.0956775139,-1.0099392236
H,0,-0.9265768953,4.100409458,0.426645111
C,0,2.7072039102,-1.6286484281,-0.0096765861
H,0,3.6472055218,-1.0745944807,-0.0278338684
H,0,2.6773270609,-2.2520784475,0.886107216
H,0,2.6560827767,-2.274582003,-0.8883541995
C,0,-2.7075075149,-1.6295280403,0.0059148362
H,0,-2.6739536272,-2.2509475181,0.9029652559
H,0,-3.6476062756,-1.075564777,-0.0096372115

H,0,-2.6598803255,-2.2773947019,-0.8715268687

1-S

C,0,-1.172770836,0.0064360663,-0.0844049817

C,0,0.0339344219,0.6622176166,-0.1921614024

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2-S

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3-S

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C,0,-5.0885252405,1.0382779549,2.4264635971
C,0,-5.6273689173,2.1919151411,1.8666759751
H,0,-6.0902517263,3.2482821626,0.0530628815
H,0,-5.0664194894,0.9213501678,3.5052467127
H,0,-6.0209877616,2.9719508036,2.5097997882
C,0,-1.5987878552,-2.7966065417,-2.4846024794
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10-S

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11-S

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12-S

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C,0,5.7895463914,1.9168101581,0.8260734008
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H,0,-3.9235828379,-1.3328230434,4.7586169137
H,0,-2.671111182,-1.0455199607,5.9739093635
C,0,-1.3579754923,-3.8181473038,0.8739214592
H,0,-2.3863966746,-3.8391604406,0.5068729313
H,0,-0.8357243471,-3.0427551233,0.3056630735
H,0,-0.8878395012,-4.7703816875,0.6272364975
C,0,-4.8332335504,2.2350762471,1.6133846401
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H,0,1.0571634114,-0.6756090362,-4.1134748345
H,0,-0.6721676883,-0.8935917999,-4.4259018594
H,0,-0.1183882149,-0.2228993903,-2.891207841
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H,0,2.5321427277,-3.8026010691,0.0214033376
H,0,2.3944740413,-5.47887615,-0.5281116194
H,0,3.4445268363,-4.3360951484,-1.3769573636

C,0,5.6377173717,-0.601969918,0.627289845
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C,0,3.5120615363,-1.8845297858,-2.8556920357
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H,0,-5.8982245165,-1.1051942747,0.7700350667
C,0,-4.3238869056,-2.0623504761,1.9804765638
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13-S

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C,0,0.0002373907,4.3451346578,-0.0003947087
C,0,-1.2194654297,5.0612378296,-0.0453742349
C,0,1.2199969646,5.061146062,0.0444830801
C,0,-1.2030207791,6.4588562375,-0.0455342163
C,0,1.2036689358,6.4587649777,0.0444318106
C,0,0.0003523644,7.1544896837,-0.0006058343
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C,0,0.747974019,-2.4706434447,4.0907997881
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C,0,-4.5618721834,-0.1774190467,-1.3950171609
C,0,-5.5152692401,2.2716638323,-0.4090018738
C,0,-5.1545902488,0.7558340111,-2.2497669018
C,0,-5.6294430748,1.9692929168,-1.7624740974
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C,0,-0.4897318784,-4.3409573426,-2.5953181756
C,0,-1.2089857077,-3.6812747694,-3.5874670306
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Al,0,0.0001472267,2.3772327333,-0.0002568362
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C,0,-3.607487065,-2.4556064182,2.3241400055
H,0,-3.7760937146,-3.2649620137,3.0176425177
C,0,-4.5073059927,-1.7394367216,1.6064645695
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14-S

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C,0,-1.2203380104,4.289836768,0.0643186988
C,0,1.199765886,5.6858458081,-0.0698271641
C,0,-1.1992747818,5.6859326517,0.0710611004
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Ge,0,1.05881546,0.3671296689,0.4051513005
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H,0,1.8897836769,-3.8325239351,-4.1253140431
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H,0,1.0315122708,-5.1177406285,0.6705834251
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H,0,2.4100004709,-0.4996290323,4.4339493003
H,0,1.107408816,0.4161875508,3.6928452537
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H,0,4.0523465091,-1.4796604063,-3.0469896639
C,0,5.3381657662,1.6951570358,1.7979964925
H,0,4.339056365,1.6751407491,2.2416441863
H,0,5.9308545636,0.9508263947,2.3375066497
H,0,5.7756177161,2.6768139874,1.9870309675
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C,0,-3.8338253328,-2.2675543799,-2.3107022568
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15-S

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H,0,-6.0795470992,2.6132222467,2.5826262168
C,0,-1.2551528026,-2.5979572096,-2.6062167819
C,0,-0.5969850526,-1.9351491768,-3.6532886087
C,0,-0.7682856335,-3.8031444476,-2.073329133
C,0,0.5817400233,-2.4971076094,-4.1526062865
C,0,0.4050493558,-4.338177685,-2.6084872189
C,0,1.0811750188,-3.6872754636,-3.6362420394
H,0,1.10884022,-1.9936263442,-4.9574542642
H,0,0.7975916619,-5.266629345,-2.2056005722
H,0,1.9975520349,-4.1101324089,-4.0358013294

C,0,1.4725241112,-4.4700138819,0.9189738254
H,0,1.4467812442,-3.8353413573,0.0285824999
H,0,2.5254974045,-4.6615670472,1.1361366263
H,0,1.0020875843,-5.4215835899,0.6688433825
C,0,1.1284828876,-0.6418909984,4.2147499063
H,0,2.2177221728,-0.6512308654,4.288702858
H,0,0.8598390775,0.2042948289,3.5739520429
H,0,0.7160559383,-0.4477239741,5.2070382091
C,0,4.0360002929,-1.555451566,-1.9791144289
H,0,4.3678617601,-2.4024602041,-1.374015007
H,0,2.9421382269,-1.5523582439,-1.9408199384
H,0,4.3287876798,-1.7380150166,-3.0149765236
C,0,4.8549884712,1.6566008904,1.8331790746
H,0,3.7990616675,1.701710089,2.1169768303
H,0,5.317739963,0.903297202,2.475988547
H,0,5.3078183645,2.6238342322,2.0581955831
C,0,-4.0364955259,-1.5544519789,1.978788909
H,0,-4.3686381761,-2.4012343562,1.3735271498
H,0,-2.9426324195,-1.5517155655,1.9404968657
H,0,-4.3293451238,-1.7371157597,3.0146157425
C,0,-4.854422549,1.65859515,-1.8328943149
H,0,-3.7984818072,1.7034001645,-2.1166884396
H,0,-5.3174323498,0.9055701782,-2.4758443236
H,0,-5.3069256318,2.626024504,-2.0577254989
C,0,-1.4740759246,-4.4693826077,-0.9199130362
H,0,-1.4481411376,-3.8349000097,-0.0293921049
H,0,-2.5271083432,-4.6605429743,-1.1371355501
H,0,-1.0039602827,-5.4211595219,-0.6699673394
C,0,-1.1286680619,-0.6406866845,-4.2148846815
H,0,-2.2179106562,-0.6496277137,-4.2888375364
H,0,-0.8597247581,0.2052762956,-3.5739184308
H,0,-0.7161745716,-0.4464664308,-5.2071349352

Al,0,0.0004149305,2.4047490181,0.0002030933
C,0,3.7205872946,-2.5180631418,2.2589778025
H,0,3.8983227017,-3.3347379637,2.9415331954
C,0,4.6075976897,-1.8111847677,1.5171031374
H,0,5.6790273253,-1.918738148,1.4451982844
C,0,-3.7214379992,-2.5163632366,-2.2594969603
H,0,-3.8994556641,-3.3328429078,-2.9422121864
C,0,-4.6082042298,-1.8093237447,-1.5174843499
H,0,-5.6796708436,-1.9165217339,-1.445599857

M06-2X/def2-qvzp optimized geometries of the parent systems.

1

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	6	0	-0.773787	0.113480	0.000000	
2	6	0	0.485184	0.613373	0.000003	
3	6	0	0.288602	-0.726862	0.000012	
4	1	0	-1.841738	0.270138	-0.000020	
5	1	0	1.154782	1.459908	-0.000027	
6	1	0	0.686968	-1.729990	-0.000050	

2

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	1	0	0.377848	-2.704114	-0.000000	
2	1	0	2.153764	1.678311	0.000001	
3	1	0	-2.530867	1.024923	0.000001	
4	14	0	-1.166294	0.472399	-0.000000	
5	14	0	0.173969	-1.246132	0.000000	
6	14	0	0.992272	0.773796	-0.000000	

3

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	1	0	-1.687531	-2.323604	0.000000	
2	1	0	-1.170136	2.622554	-0.000000	
3	1	0	2.856248	-0.298474	-0.000000	
4	32	0	-0.789006	-1.084702	-0.000000	
5	32	0	-0.544869	1.225640	0.000000	
6	32	0	1.333920	-0.140953	0.000000	

4

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	6	0	0.000000	0.686443	-0.820585	
2	6	0	0.000000	-0.686443	-0.820585	
3	1	0	0.000000	1.453691	-1.581297	
4	1	0	-0.000000	0.000000	2.231264	
5	1	0	0.000000	-1.453691	-1.581297	
6	14	0	-0.000000	0.000000	0.769882	

5

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	0.000000	0.680449	-1.196266
2	6	0	-0.000000	-0.680449	-1.196266
3	1	0	-0.000000	1.469163	-1.935953
4	1	0	-0.000000	0.000000	2.016111
5	1	0	-0.000000	-1.469163	-1.935953
6	32	0	-0.000000	0.000000	0.506593

6

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	1	0	-2.482480	-0.646525	0.000000
2	1	0	2.482480	-0.646525	0.000001
3	1	0	0.000000	2.208844	0.000000
4	14	0	-1.062455	-0.274440	-0.000000
5	14	0	1.062455	-0.274440	-0.000000
6	6	0	0.000000	1.128089	0.000000

7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	1	0	-1.771462	-2.362907	-0.000000
2	1	0	-1.771461	2.362907	0.000000
3	1	0	2.463263	0.000000	0.000000
4	14	0	-1.033347	-1.087693	0.000000
5	14	0	-1.033347	1.087692	-0.000000
6	32	0	0.937918	0.000000	-0.000000

8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	1	0	2.609051	-0.538988	0.000000
2	1	0	-2.609051	-0.538988	0.000000
3	1	0	0.000000	2.401225	0.000000
4	6	0	0.000000	1.319783	-0.000000
5	32	0	1.138054	-0.144405	0.000000
6	32	0	-1.138054	-0.144405	0.000000

9

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	1	0	-2.483948	-1.124562	-0.000000
2	1	0	2.483945	-1.124567	-0.000000
3	1	0	0.000002	3.041193	0.000000
4	32	0	-1.164312	-0.354952	0.000000
5	32	0	1.164312	-0.354953	0.000000
6	14	0	0.000000	1.566064	-0.000000

10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.378215	0.671849	-0.000011
2	6	0	-0.378238	-0.671841	-0.000004
3	1	0	-1.089548	1.481334	0.000039
4	1	0	-1.089611	-1.481290	0.000018
5	1	0	2.098041	-0.000033	0.000001
6	5	0	0.923967	-0.000012	0.000006

11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	-0.852113	-0.683316	-0.000029
2	6	0	-0.852121	0.683315	0.000042
3	1	0	-1.715616	-1.340034	0.000096
4	1	0	-1.715635	1.340021	-0.000120
5	1	0	2.418743	0.000013	0.000045
6	13	0	0.864455	0.000000	-0.000008

12

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	1	0	2.374425	-0.931649	0.000002
2	1	0	-2.374423	-0.931654	0.000006
3	1	0	0.000007	2.511669	-0.000001
4	14	0	1.053512	-0.260973	-0.000000
5	14	0	-1.053513	-0.260970	-0.000001
6	5	0	0.000001	1.331767	0.000001

13

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	1	0	1.605770	2.216543	-0.000110
2	1	0	1.605155	-2.216964	-0.000060
3	1	0	-2.970808	0.000330	0.000175
4	13	0	-1.405032	0.000134	-0.000030
5	14	0	0.643886	1.082463	0.000017
6	14	0	0.643635	-1.082581	0.000010

14

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	2.481128	-0.857667	-0.000000
2	1	0	-2.481130	-0.857665	-0.000000
3	1	0	0.000000	2.678059	0.000000
4	32	0	1.125962	-0.132066	0.000000
5	32	0	-1.125962	-0.132066	0.000000
6	5	0	0.000000	1.497900	-0.000000

15

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-2.320451	-1.369112	-0.000001

2	1	0	2.320452	-1.369112	-0.000001
3	1	0	-0.000000	3.278084	0.000000
4	32	0	-1.153083	-0.356167	0.000000
5	32	0	1.153083	-0.356166	0.000000
6	13	0	-0.000000	1.711908	-0.000000

B3LYP-D3/6-311G(d) optimized structures of 6 π electrons systems

Cyclopentadienyl anion

1	6	0	-0.000000	1.202232	-0.000000
2	6	0	1.143390	0.371510	-0.000000
3	6	0	0.706654	-0.972626	-0.000000
4	6	0	-0.706654	-0.972626	0.000000
5	6	0	-1.143390	0.371510	0.000000
6	1	0	-0.000000	2.291431	-0.000000
7	1	0	2.179280	0.708091	-0.000000
8	1	0	1.346869	-1.853806	-0.000000
9	1	0	-1.346869	-1.853806	0.000000
10	1	0	-2.179280	0.708091	0.000000

D_{5h}-Si₅-cyclopentadienyl anion

1	14	0	0.000000	1.896109	0.000000
2	14	0	1.803306	0.585930	-0.000000
3	14	0	1.114505	-1.533984	0.000000
4	14	0	-1.114505	-1.533984	0.000000
5	14	0	-1.803306	0.585930	-0.000000
6	1	0	0.000000	3.384313	0.000000
7	1	0	3.218673	1.045810	-0.000000

8	1	0	1.989249	-2.737967	0.000000
9	1	0	-1.989249	-2.737967	0.000000
10	1	0	-3.218673	1.045810	-0.000000

Fully optimized Si₅-cyclopentadienyl anion

1	14	0	1.964293	0.124657	0.186532
2	14	0	0.676228	-1.709753	0.004426
3	14	0	-1.511709	-1.207914	-0.281185
4	14	0	-1.621884	1.053550	0.367104
5	14	0	0.456593	1.737973	-0.259783
6	1	0	3.371278	0.214935	-0.319625
7	1	0	1.205544	-3.078517	0.299356
8	1	0	-2.343293	-2.145685	0.561140
9	1	0	-2.605398	1.856030	-0.456953
10	1	0	0.882560	3.174063	-0.323236

D_{5h}-Ge₅-cyclopentadienyl anion

1	32	0	-0.000000	1.976065	-0.000000
2	32	0	1.879349	0.610638	-0.000000
3	32	0	1.161502	-1.598670	-0.000000
4	32	0	-1.161502	-1.598670	0.000000
5	32	0	-1.879349	0.610638	0.000000
6	1	0	-0.000000	3.516752	-0.000000
7	1	0	3.344630	1.086736	-0.000000
8	1	0	2.067095	-2.845112	-0.000000
9	1	0	-2.067095	-2.845112	0.000000
10	1	0	-3.344630	1.086736	0.000000

Fully optimized Ge₅-cyclopentadienyl anion

1	32	0	-1.754005	-1.124122	0.347661
2	32	0	-1.559786	1.299499	-0.478800
3	32	0	0.664471	1.720199	0.402799
4	32	0	2.104362	-0.070188	-0.206474
5	32	0	0.515281	-1.820766	-0.074106
6	1	0	-2.518206	-1.974585	-0.759562
7	1	0	-2.389813	2.164917	0.576255
8	1	0	1.321073	3.144591	0.470076
9	1	0	3.537230	-0.209911	0.402303
10	1	0	0.999386	-3.272933	-0.403670

Benzene

1	6	0	0.000000	1.394294	-0.000000
2	6	0	1.207494	0.697147	-0.000000
3	6	0	1.207494	-0.697147	-0.000000
4	6	0	-0.000000	-1.394294	-0.000000
5	6	0	-1.207494	-0.697147	-0.000000
6	6	0	-1.207494	0.697147	-0.000000
7	1	0	0.000000	2.479840	-0.000000
8	1	0	2.147604	1.239920	-0.000000
9	1	0	2.147604	-1.239920	-0.000000
10	1	0	-0.000000	-2.479840	-0.000000
11	1	0	-2.147604	-1.239920	-0.000000
12	1	0	-2.147604	1.239920	-0.000000

D₆H-Si₆-benzene

1	14	0	0.000000	2.217882	-0.000000
2	14	0	1.920742	1.108941	-0.000000
3	14	0	1.920742	-1.108941	-0.000000
4	14	0	-0.000000	-2.217882	-0.000000
5	14	0	-1.920742	-1.108941	-0.000000
6	14	0	-1.920742	1.108941	-0.000000
7	1	0	0.000000	3.699172	-0.000000
8	1	0	3.203577	1.849586	-0.000000
9	1	0	3.203577	-1.849586	-0.000000
10	1	0	-0.000000	-3.699172	-0.000000
11	1	0	-3.203577	-1.849586	-0.000000
12	1	0	-3.203577	1.849586	-0.000000

Fully optimized Si₆-benzene

1	14	0	-1.909415	1.102401	-0.208528
2	14	0	-0.000000	2.204803	0.208528
3	14	0	1.909415	1.102401	-0.208528
4	14	0	1.909415	-1.102401	0.208528
5	14	0	0.000000	-2.204803	-0.208528
6	14	0	-1.909415	-1.102401	0.208528
7	1	0	-3.176516	1.833962	0.057301
8	1	0	-0.000000	3.667925	-0.057301
9	1	0	3.176516	1.833962	0.057301
10	1	0	3.176516	-1.833962	-0.057301
11	1	0	0.000000	-3.667925	0.057301
12	1	0	-3.176516	-1.833962	-0.057301

D₆H-Ge₆-benzene

1	32	0	0.000000	2.306257	-0.000000
2	32	0	1.997277	1.153129	-0.000000
3	32	0	1.997277	-1.153129	-0.000000
4	32	0	-0.000000	-2.306257	-0.000000
5	32	0	-1.997277	-1.153129	-0.000000
6	32	0	-1.997277	1.153129	-0.000000
7	1	0	0.000000	3.841077	-0.000000
8	1	0	3.326470	1.920538	-0.000000
9	1	0	3.326470	-1.920538	-0.000000
10	1	0	-0.000000	-3.841077	-0.000000
11	1	0	-3.326470	-1.920538	-0.000000
12	1	0	-3.326470	1.920538	-0.000000

Fully optimized Ge₆-benzene

1	32	0	2.223704	0.557531	-0.333140
2	32	0	1.594871	-1.646938	0.332878
3	32	0	-0.629078	-2.204560	-0.332478
4	32	0	-2.224013	-0.557381	0.332364
5	32	0	-1.594546	1.647055	-0.332579
6	32	0	0.629087	2.204293	0.332976
7	1	0	3.675914	0.921589	0.092688
8	1	0	2.635975	-2.723191	-0.092040
9	1	0	-1.040587	-3.644506	0.091899
10	1	0	-3.676383	-0.921104	-0.093180
11	1	0	-2.635702	2.723149	0.092549
12	1	0	1.039993	3.644067	-0.092593

Tropylium cation

1	6	0	0.000000	1.609045	-0.000000
2	6	0	1.258002	1.003223	0.000000
3	6	0	1.568703	-0.358046	0.000000
4	6	0	0.698138	-1.449699	-0.000000
5	6	0	-0.698138	-1.449699	-0.000000
6	6	0	-1.568703	-0.358046	0.000000
7	6	0	-1.258002	1.003223	0.000000
8	1	0	0.000000	2.695032	-0.000000
9	1	0	2.107061	1.680325	0.000000
10	1	0	2.627462	-0.599701	0.000000
11	1	0	1.169331	-2.428140	-0.000000
12	1	0	-1.169331	-2.428140	-0.000000
13	1	0	-2.627462	-0.599701	0.000000
14	1	0	-2.107061	1.680325	0.000000

D_{7h}-Si₇-tropylium cation

1	14	0	0.000000	2.563754	0.000000
2	14	0	2.004424	1.598475	-0.000000
3	14	0	2.499476	-0.570489	-0.000000
4	14	0	1.112371	-2.309863	0.000000
5	14	0	-1.112371	-2.309863	0.000000
6	14	0	-2.499476	-0.570489	-0.000000
7	14	0	-2.004424	1.598475	-0.000000
8	1	0	0.000000	4.041869	0.000000
9	1	0	3.160060	2.520064	-0.000000
10	1	0	3.940531	-0.899400	-0.000000
11	1	0	1.753701	-3.641598	0.000000
12	1	0	-1.753701	-3.641598	0.000000

13	1	0	-3.940531	-0.899400	-0.000000
14	1	0	-3.160060	2.520064	-0.000000

Fully optimized Si₇-tropylium cation

1	14	0	-0.731804	2.452805	-0.108458
2	14	0	-2.374348	0.958775	0.096486
3	14	0	-2.231420	-1.258932	-0.063432
4	14	0	-0.405291	-2.530484	0.008603
5	14	0	1.727150	-1.892741	0.049491
6	14	0	2.555418	0.170372	-0.089132
7	14	0	1.460360	2.102430	0.106405
8	1	0	-1.154993	3.864050	0.022774
9	1	0	-3.744563	1.504329	-0.013078
10	1	0	-3.513866	-1.991576	0.003644
11	1	0	-0.637696	-3.990339	-0.000428
12	1	0	2.718065	-2.988691	-0.001672
13	1	0	4.028088	0.260472	0.010408
14	1	0	2.304066	3.310588	-0.021124

D_{7h}-Ge₇-tropylium cation

1	32	0	0.000000	2.664271	-0.000000
2	32	0	2.083011	1.661146	0.000000
3	32	0	2.597472	-0.592856	-0.000000
4	32	0	1.155984	-2.400425	0.000000
5	32	0	-1.155984	-2.400425	0.000000
6	32	0	-2.597472	-0.592856	-0.000000
7	32	0	-2.083011	1.661146	0.000000
8	1	0	0.000000	4.197334	-0.000000

9	1	0	3.281608	2.616995	0.000000
10	1	0	4.092098	-0.933995	-0.000000
11	1	0	1.821155	-3.781667	0.000000
12	1	0	-1.821155	-3.781667	0.000000
13	1	0	-4.092098	-0.933995	-0.000000
14	1	0	-3.281608	2.616995	0.000000

Fully optimized Ge₇-tropylium cation

1	32	0	-1.790763	1.963047	-0.292275
2	32	0	-2.650667	-0.167088	0.297295
3	32	0	-1.534336	-2.179389	-0.170483
4	32	0	0.769197	-2.555100	-0.066826
5	32	0	2.472473	-0.983143	0.258377
6	32	0	2.310944	1.304410	-0.303598
7	32	0	0.422604	2.628751	0.278349
8	1	0	-2.817875	3.040777	0.132462
9	1	0	-4.158066	-0.342492	0.011337
10	1	0	-2.355308	-3.476637	-0.061403
11	1	0	1.181308	-4.036161	-0.029741
12	1	0	3.855444	-1.632227	0.051399
13	1	0	3.645421	1.995502	0.062816
14	1	0	0.666625	4.083651	-0.193754

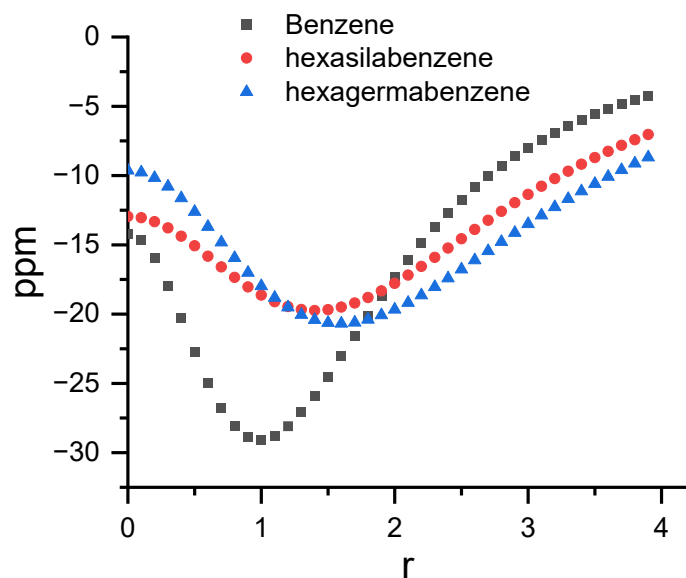
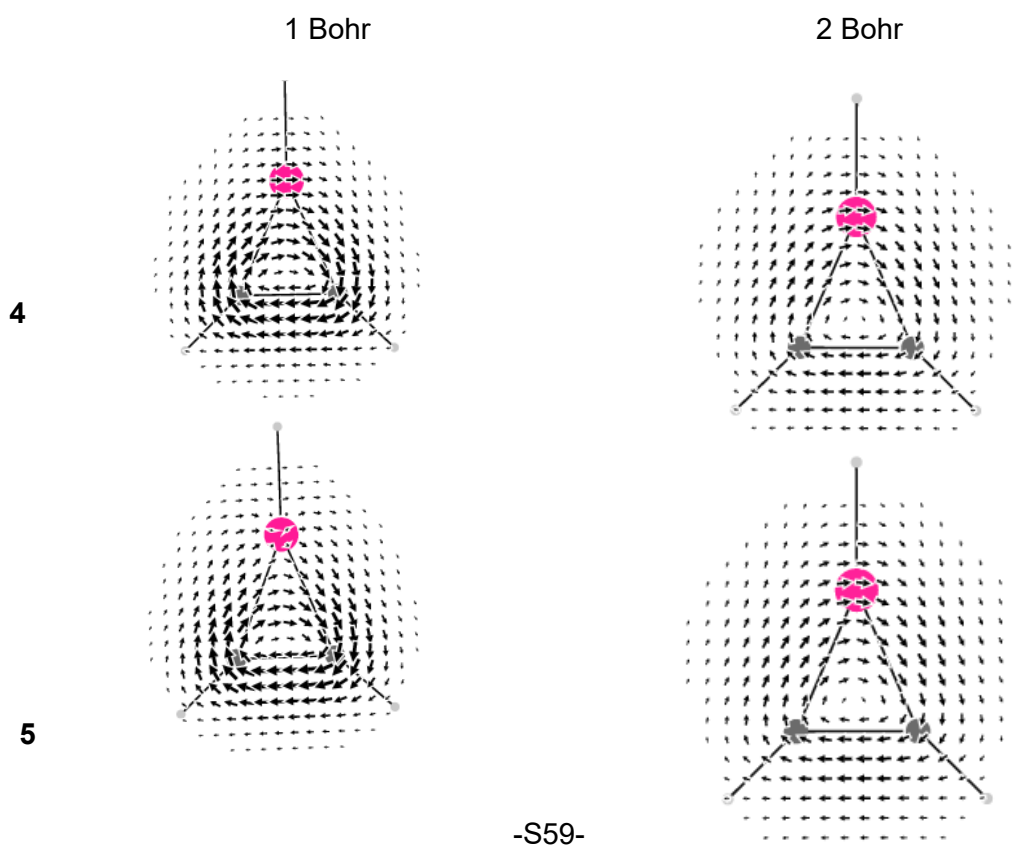
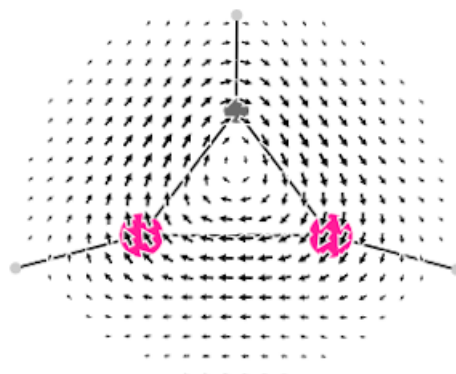
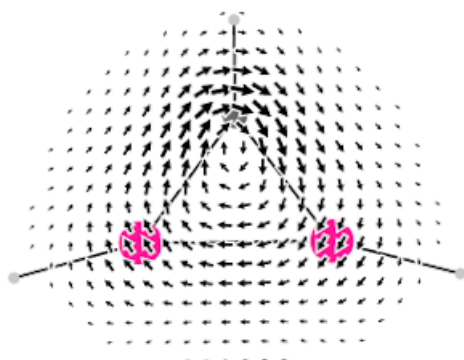


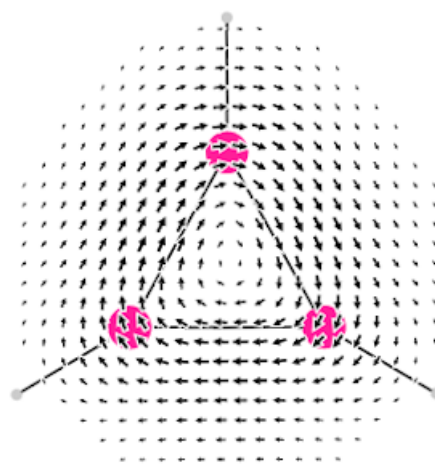
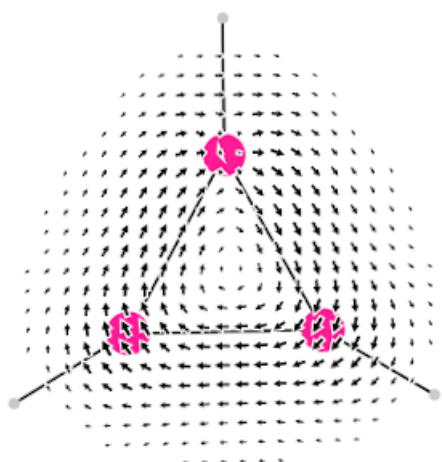
Figure S1: NICS_{zz} scan of benzene (black), hexasilabenzene (red) and hexagermabenzene (blue). Minimum NICS_{zz} values are (ppm@distance, Å) -29.1@1.0 for benzene, -19.7@1.4 for hexasilabenzene and -20.7@1.6 for hexagermabenzene.



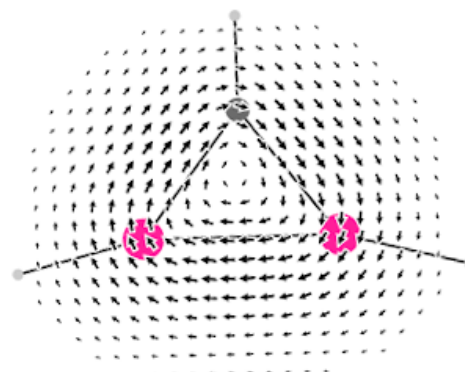
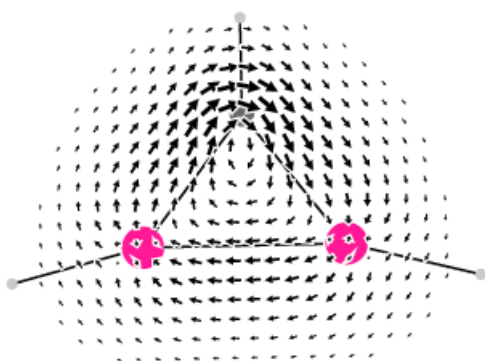
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8



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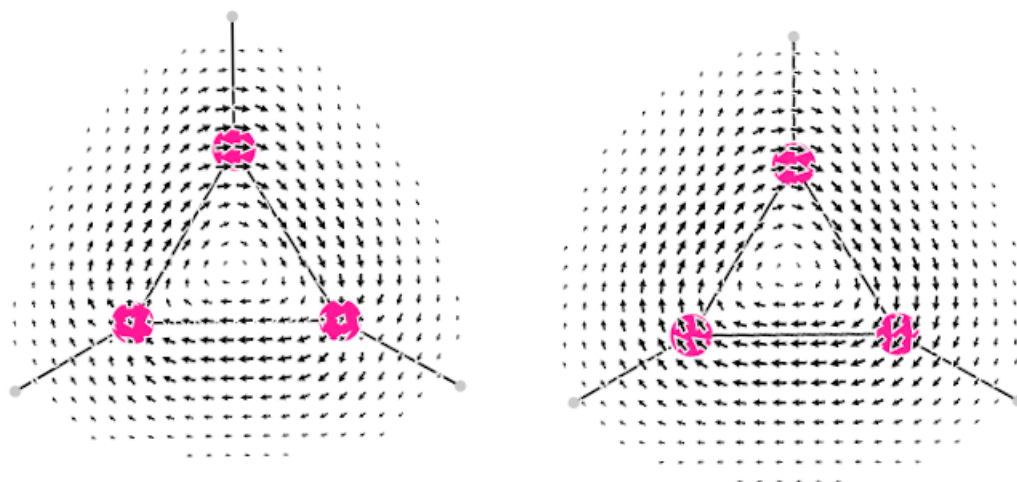
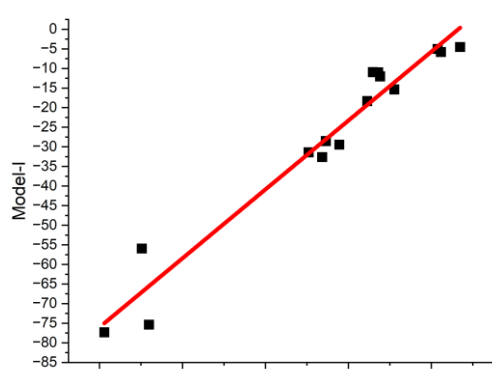
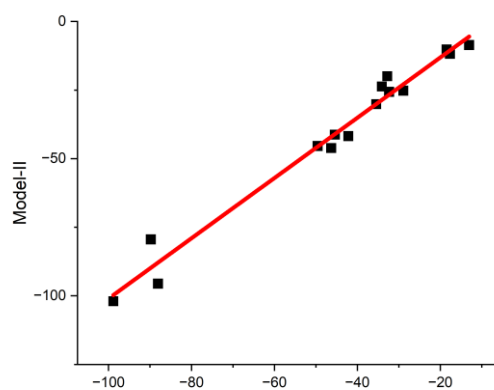


Figure S2: Current density plots of **4-9** at (left) 1 a.u. and (right) 2 a.u. above the molecular plane.



(a)



(b)

Figure S3: Plots of BLW-VRE of the cycles (**1-15**) against VRE of the non-aromatic models. (a, left), **Model-I**; Intercept= 11.83671. Slope= 0.87856. R= 0.95102. (b, right) **Model-II**. Intercept= 8.81649. Slope= 1.09817. R= 0.97568.

In order to get an idea about substitution effect, all the H's were replaced by methyl groups to yield the trimethyl derivatives of systems **1-15** (denoted as **A-Me**, where **A** is **1-15**). Table

Table S1. NICS values (ppm) of the per-methylated systems **1-15**.

5 gives

A-Me	NICS(1) ^s _{π,ZZ}	NICS(1) ^L _{π,ZZ}	∫NICS _{π,ZZ}	A-Me	NICS(1) ^s _{π,ZZ}	NICS(1) ^L _{π,ZZ}	∫NICS _{π,ZZ}
1	-4.7	-4.9	-10.4	9	-12.1	-15.1	-37.5
2	-11.8	-14.7	-36.2	10	-8.4	-9.8	-26.5
3	-12.1	-15.3	-38.0	11	-7.7	-9.9	-24.6
4	-7.5	-8.9	-21.7	12	-11.3	-14.1	-35.1
5	-7.5	-9.3	-23.0	13	-10.7	-13.6	-35.0
6	-10.2	-12.8	-31.0	14	-11.9	-14.5	-36.4
7	-12.0	-15.0	-37.0	15	-11.4	-14.1	-36.5
8	-10.6	-13.1	-31.2				

all the NICS data and figure S4 shows the relations of NICS(1)^L_{π,ZZ} of **A** and **A-Me** (**A** is **1-15**). The relation between the tropicities of the parent and Me substituted systems is (more-or-less)

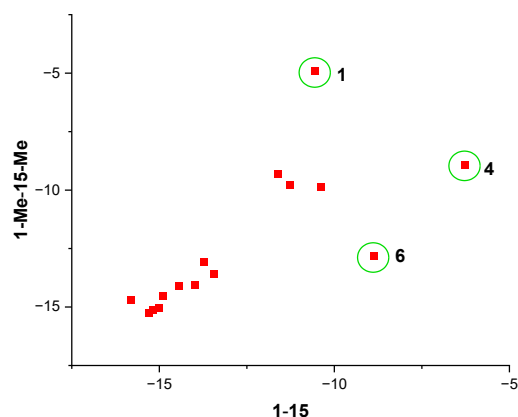


Figure S4: A plot of CMO- NICS(1)^L_{π,ZZ} values (ppm) of **1-15** (X-axis) against Those of **1-Me-15-Me** (Y-axis).

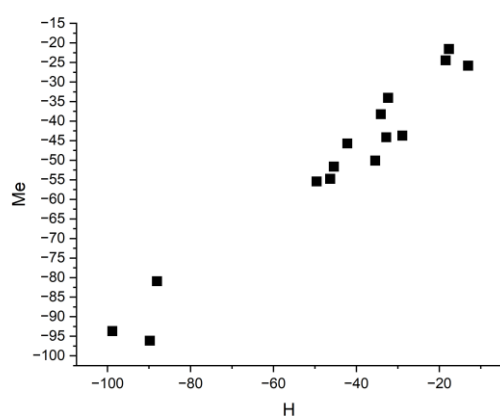
linear, except the points that are circled, which belong to **1**, **4** and **6**, i.e., the carbon and carbon-silicon containing derivatives. For **1**, very effective hyperconjugation transfers electron density into the π system, causing reduction of the diatropic current. In **4**, The C-C bond in the Me derivative is longer than the respective bond in the parent system (1.396 Å and 1.380 Å, respectively), making the C=C bond less localized, allowing better delocalization of the ring's π electrons. In **6** the Me causes elongation of the two C-Si bonds (1.774 Å in **6**, 1.792 in **6-Me**) which allows better overlap between the small

2p(C) and the large 3p(Si), resulting in larger diatropicity. However, except these small and specific effects, the general conclusion is that Me substitution does not influence much the tropicity of **1-15** and that the Si and Ge derivatives are more diatropic than the C derivatives.

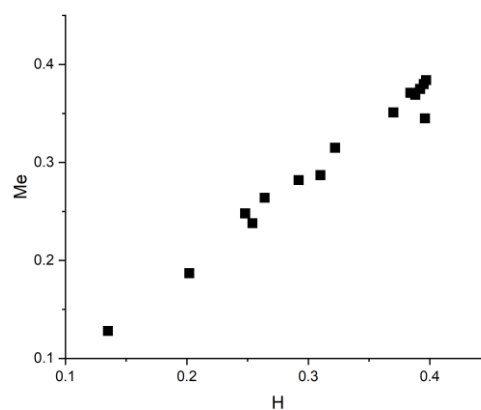
Table S2 lists the VRE and MCI of **1-Me – 15-Me**.

Table S2: BLW's VRE (kcal mol⁻¹) and MCI for **1-Me** – **15-Me**.

	BLW	MCI
1-Me	-96.13	0.345
2-Me	-55.41	0.384
3-Me	-45.71	0.369
4-Me	-50.09	0.238
5-Me	-43.7	0.287
6-Me	-93.68	0.282
7-Me	-51.62	0.380
8-Me	-80.94	0.315
9-Me	-54.74	0.375
10-Me	-44.13	0.187
11-Me	-25.82	0.128
12-Me	-38.23	0.371
13-Me	-24.45	0.248
14-Me	-34.05	0.351
15-Me	-21.56	0.264



(a)



(b)

right) MCI.

Table S3: NICS (ppm), MCI (a.u.) and BLW-VRE (kcal mol⁻¹) for **1-15** at M06-2X/def2-qzvp.

	NICS(1) ^s _{π,ZZ}	NICS(1) ^L _{π,ZZ}	∫NICS _{π,ZZ}	MCI	VRE
1	-11.9	-10.6	-22.8	0.398	-65.7
2	-13.2	-16.3	-38.8	0.397	-28.54
3	-13.1	-16.6	-40.1	0.398	-28.65
4	-11.1	-11.7	-30	0.219	-20.2 ^a
5	-10.4	-11.4	-25.3	0.283	-18.65
6	-11.6	-14.1	-32.2	0.27	-74.04
7	-13.1	-16.4	-39.2	0.397	-30.46
8	-11.8	-14.2	-32.7	0.313	-80.91
9	-13.1	-16.5	-39.6	0.397	-36.81
10	-11.3	-11.2	-24.9	0.17	-23.88 ^b
11	-8.9	-10.3	-23.6	0.116	-9.56 ^b
12	-12.9	-15.6	-37.3	0.381	-25.20 ^b
13	-11.6	-14.7	-36.6	0.207	-10.04 ^b
14	-12	-15.9	-38.4	0.372	-33.11 ^b
15	-11.9	-15.2	-38.3	0.224	-16.49 ^b

(a) convergence problems prevent BLW calculations of some VREs at M06-2X/def2-qzvp.

(a) calculated from the linear regression of the VREs at B3LYP/def2-qzvp and M06-2X/def2-qzvp for **1-3** and **5-9**. (b) at B3LYP/def2-qzvp computational level.

Table S4: Summary of all the results for the parent **1-15** at B3LYP/6-311G+(d) (NICS) and B3LYP/6-311G(d) for BLW and MCI.

	A	B	C	D	E	F	G	H	I
1	-11.6	-10.6	-23.0	-89.79	-33.84	-10.37	0.394	0.286	0.659
2	-11.9	-15.8	-37.1	-49.58	-18.17	-4.19	0.383	0.251	0.631
3	-12.1	-15.3	-37.4	-42.18	-12.72	-0.41	0.389	0.264	0.641
4	-6.2	-6.3	-13.2	-35.46	-17.12	-5.3	0.243	0.163	0.546
5	-14.8	-11.6	-25.9	-28.91	-13.55	-3.68	0.308	0.209	0.593
6	-8.1	-8.9	-20.2	-98.84	-21.52	3.14	0.287	0.173	0.557
7	-12.0	-15.0	-36.2	-45.43	-16.89	-4.19	0.387	0.260	0.638
8	-11.3	-13.7	-32.0	-88.06	-12.7	7.51	0.333	0.232	0.615
9	-12.1	-15.2	-36.8	-46.31	-13.69	-0.19	0.389	0.269	0.646
10	-11.1	-11.3	-25.0	-32.8	-21.83	-12.83	0.185	0.121	0.495
11	-9.0	-10.4	-23.8	-13.05	-8.51	-4.47	0.124	0.072	0.415
12	-11.7	-14.4	-35.0	-34.1	-23.15	-10.39	0.378	0.244	0.625
13	-10.6	-13.4	-34.0	-18.47	-13.44	-8.24	0.230	0.134	0.512
14	-12.3	-14.9	-36.4	-32.34	-20.3	-6.68	0.368	0.246	0.626
15	-11.2	-13.9	-35.7	-17.67	-11.85	-5.89	0.249	0.154	0.536

A= NICS(1)^s_{π,ZZ}. B= NICS(1)^L_{π,ZZ}. C= NICS_{π,ZZ}. D=VRE. E=maximum resonance energy. F=minimum resonance energy. G=MCI. H=MCI^π. I= MCI^π^(1/N)

Explanation of the NICS methods that are used here.

One of the reviewers was worried about the diatropicity of cyclopropane that affects NICS^{S1} and about the effects of core electrons and electron density on NICS.^{S2} The paragraph below explains the NICS methods that we have used and why the above-mentioned NICS problems are neutralized.

Two main principles are applied in our NICS studies. (1) The information that is obtained from a single NICS is limited, sometimes misleading. Therefore, we always use scan procedures, whether from the center of the molecular plane perpendicularly to the molecular plane,^{S3} or parallel to the molecular plane.^{S4} The reported values (e.g., NICS(1)) are always recalculated from the scan's curve (see below), and the shape of the scan matters. (2) Aromaticity is a property of the π system, Therefore, whenever possible (in most cases) we report only the part of the NICS that was formed by the induced (clean) π current (e.g., NICS(1)_{π,ZZ}).

There are two ways to get the clean contribution of the π electrons to NICS. One is named CMO-NICS and can be applied only to planar systems (where the σ and π are orthogonal). Here, the NICS tensor is decomposed according to the contribution of each canonic molecular orbital using the NCS procedure within NBO. Thus, if we look at the ZZ part of the tensor, we can sum up only the contributions made by the π CMOs. This takes care of the first worry of the reviewer: All the NICS numbers that are reported in the paper (except for

the non-planar systems) are CMO-NICS _{π ,zz}, which means that the only the contribution of a single π CMO (for the 3-membered rings systems) or the three π CMOs (for the 6 π electrons systems) were considered. The tropicities of the σ skeletons (diatropicity in the 3-membered rings, paratropicity in the larger systems) are therefore not included in these values.

The second method for obtaining the clean π contribution is using a “chemical” model – the σ -only model.^{S5} Here, the π system is eliminated by binding hydrogen atoms to the atoms that are part of the cyclically conjugated system, using each pair of π electrons to form two σ C-H bonds, keeping all the other geometrical parameters. This means that for each system we have two molecules: one that is studied molecule and one that models only the σ skeleton. NICS-scan^{S3} is performed on each, and subtracting the values of the model from the values of the molecule gives the net π contribution. The advantage of this method is that (a) it can be applied to non-planar systems and (b) most of the σ effects (e.g., tropicity) are the similar in the molecule and in the model, thus cancelling out on the subtraction. Good examples for this are the equality between NICS(1)^s _{π ,zz} and NICS(1)^L _{π ,zz} when calculated by the σ -only model, while they are quite different when calculated using CMO.

There are three NICS-based measures that are used here. NICS^s _{π ,zz} is based on scanning NICS from 1 to 4 Å above the molecular plane. The data of each NICS(r) _{π ,zz} (obtained either by CMO or by the σ -only model) is plotted against the distance (r) and fitted to a 3rd degree polynomial.^{S6} The obtained fit parameters are used to calculate NICS(r) _{π ,zz} at any wished distance (e.g., NICS(1.7) _{π ,zz}).

Few years back we realized that even in system that are built from 2nd row elements, close to the molecular plane, there are pronounced electron density effects on the NICS. Therefore, we suggested scanning at higher elevations, 2-5 Å. Here, the behavior of NICS _{π ,zz} as a function of distance obeys the relation $\text{NICS}(r)_{\pi,zz} = A \cdot B^r + C$. A, B and C are obtained from non-linear regression (correlation coefficients are usually better than 0.9999), allowing calculation of NICS _{π ,zz} at any wished distance.^{S7} Please note that the calculated NICS _{π ,zz} is clean from core electrons and electron density effects, therefore, close to the molecular plane they may become quite different from the directly calculated values.

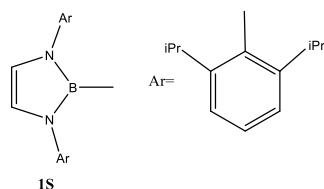
Since NICS generally decays with the distance from the molecular plane, B in the relation $\text{NICS}(r)_{\pi,zz} = A \cdot B^r + C$ must be smaller than 1. This means that when $r \rightarrow \infty$ $A \cdot B^r$ is zero, and C is the NICS value at infinity, which is supposed to be zero. Usually, it is not zero but a very small number. Thus, it is possible to approximate $\text{NICS}(r)_{\pi,zz} = A \cdot B^r + C$ to $\text{NICS}(r)_{\pi,zz} = A \cdot B^r$, which can be integrated and yield $\int \text{NICS}_{\pi,zz} = -A/\ln B$.^{S8} The advantage of this is neutralizing the effect of the current density shape as a function of height, yielding a size that reflects the total induced magnetic field. Please note that the data for $\int \text{NICS}_{\pi,zz}$ are calculated at the range of 2-5 Å, therefore neutralizing the electron density and core electrons effects.^{S9}

Table S5: Energy differences (kcal mol⁻¹) between geometrically optimized and D_{nh} 6 π electrons systems and the the number of imaginary frequencies of the latter.

	$\Delta E(\text{total})$	$\Delta E(\text{ZPE})$	ΔH°	# imag.
Si ₅ CP ⁻	7.98	7.67	6.06	4
Ge ₅ CP ⁻	24.38	24.33	22.76	4
Si ₆ .benzene	2.33	2.13	1.86	1
Ge ₆ .benzene	15.49	15.52	14.18	3
Si ₇ -tropylium ⁺	0.14	-0.07	-1.09	2
Ge ₇ -tropylium ⁺	5.60	5.89	5.37	2

Table S6: Experimental and computational E-E (E=Si, Ge) bond lengths (Å) for **2**, **3**, **12** and **13**.

	R	reference	E ₁ -E ₂	E ₁ -E ₃	E ₂ -E ₃	Av. E-E
2	^t BuMeSi	S10	2.221	2.218	2.211	2.217
2	H	S11	2.201	2.201	2.201	2.201
2	Me	S11	2.208	2.208	2.208	2.208
2	NHB _m R _m	S11	2.212	2.202	2.202	2.205
3	^t Bu ₃ Si	S12	2.325	2.321	2.333	2.326
3	^t Bu ₃ Si	S13	2.325	2.321	2.333	2.326
3	^t Bu ₃ Si	S14	2.329	(i)	2.343	2.335
3	^t Bu ₃ Si	S15	2.333	2.329	2.343	2.335
3	^t Bu ₃ Si	S16	2.3316	2.3284	2.3398	2.3333
3	H	S11	2.3386	2.3386	2.3386	2.3386
3	Me	S11	2.3504	2.3504	2.3504	2.3504
3	NHB _m R _m	S11	2.3426	2.3332	2.3332	2.3363
12	NHB R	S17	2.2035	2.3262	2.3194	
12	H	S11	2.1839	2.3395	2.3395	
12	Me	S11	2.1887	2.3456	2.3461	
12	NHB _m R _m	S11	2.1986	2.3276	2.3276	
13	(ii)	S18	2.1469	1.911 ^(v)	1.952 ^(v)	
13	(iii)	S18	2.133	1.911 ^(v)	1.952 ^(v)	
13	(iv)	S18	2.1452	1.911 ^(v)	1.952 ^(v)	
13	H	S11	2.1273	1.9251	1.9251	
13	Me	S11	2.1311	1.9382	1.9381	
13	NHB _m R _m	S11	2.1435	1.9326	1.9273	



(i) Not reported. (ii) **1S** at the Si, Ph₂N at the B. (iii) **1S** at the Si, 2,4,6-Me₃C₆H₂ at the B. (iv) **1S** at the Si, 2,4,6-ⁱPr₃C₆H₂ at the B. (v) only the range for the three derivatives is reported.

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