

Supporting Information File (ESI) for:

Aryl-Crowding in the Carborane Cage. Aromatic Characteristics in a Spherical Aromatic Unit Crowned by Aromatic Rings

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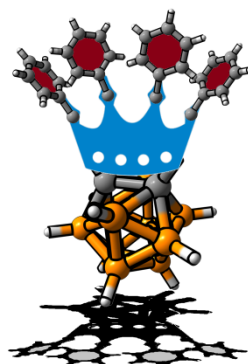


Table S1. Calculated and experimental ^{11}B -NMR patterns for the studied species.
Values in ppm.

	0		1		2		3		3a		4	
	Calc	Exp.	Calc	Exp.	Calc	Exp.	Calc	Exp.	Calc	Exp.	Calc	Exp.
	.	1	.	2	.	3	.	4	.	4	.	4
B1	-14.1	-14.1	-15.4	-10.3	-9.9	-11.4	-3.3	-1.6	-1.4	-0.9	-1.0	1.4
B2	-10.8	-12.8	-13.7	-11.9	-7.2	-10.4	-7.9	-8.0	-15.2	-14.1	-9.5	-9.5
B3	-10.2	-12.8	-11.4	-11.9	-6.8	-10.4	-9.8	-8.6	-15.7	-14.1	-6.9	-9.5
B4	-15.3	-14.1	-11.5	-10.3	-15.8	-11.4	-16.1	-10.2	-1.8	-0.9	-0.2	1.4
B5	-10.1	-12.8	-12.1	-9.9	-6.7	-10.4	-9.4	-8.6	-12.6	-11.0	-11.0	-9.5
B6	-10.6	-12.8	-9.8	-9.9	-8.3	-10.4	-8.7	-8.0	-12.8	-11.0	-6.5	-8.5
B7	-3.1	-8.3	-8.4	-8.1	-6.0	-9.1	-9.3	-8.0	-8.6	-9.8	-2.3	-2.8
B8	4.3	-1.5	-3.6	-3.5	3.1	-2.4	-2.6	-3.0	-2.1	-2.8	-6.7	-8.5
B9	-3.0	-8.3	-8.8	-8.1	-4.9	-9.1	-8.4	-8.0	-8.7	-9.8	-	-9.5
B10	4.6	-1.5	-0.7	-1.2	3.0	-2.4	-2.9	-3.0	-5.8	-4.8	-2.4	-2.8

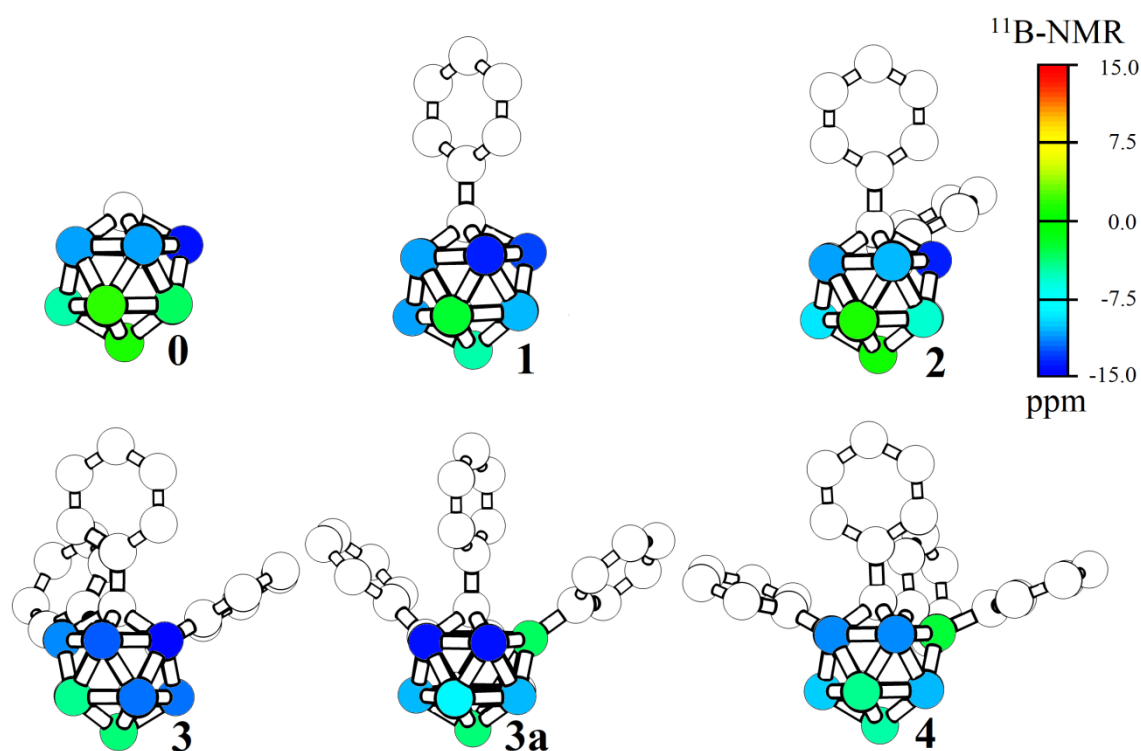


Figure S1. Graphical representation of the calculated values and boron labels in the ^{11}B -NMR calculations.

References for experimental ^{11}B -NMR values.

- 1 R. K. Harris, J. Bowles, I. R. Stephenson and E. H. Wong, *Spectrochim. Acta Part A Mol. Spectrosc.*, 1988, **44**, 273–276.
- 2 P. T. Brain, J. Cowie, D. J. Donohoe, D. Hnyk, D. W. H. Rankin, D. Reed, B. D. Reid, H. E. Robertson, A. J. Welch, M. Hofmann and P. von R. Schleyer, *Inorg. Chem.*, 1996, **35**, 1701–1708.
- 3 T.-J. Ha, D.-K. Im, S.-M. Kim and J.-D. Lee, *Molecules*, 2023, **28**, 4942.
- 4 S.-Y. Kim, S.-Y. Ma, S. O. Kang and J.-D. Lee, *J. Organomet. Chem.*, 2018, **865**, 100–108.

Table S2. Coordinated for the optimized structures related to the current work, in a MultiXYZ format. Values in Angstrom (Å).

24			
0 oB10C2H12 q0			
B	4.261119000	5.092705000	5.100612000
B	5.864386000	4.480473000	5.575223000
H	6.080103000	3.401984000	5.603590000
B	7.083386000	5.671167000	5.058954000
H	8.094943000	5.372210000	4.746112000
B	6.215473000	7.004104000	4.285279000
H	6.653525000	7.564980000	3.446118000
B	5.190428000	7.798886000	5.493366000
H	4.971320000	8.876907000	5.462568000
B	3.977221000	6.602122000	6.002503000
H	2.963098000	6.900457000	6.307078000
B	4.821551000	5.254089000	6.773908000
H	4.359007000	4.676561000	7.587620000
B	6.565816000	5.614364000	6.749432000
H	7.241842000	5.272609000	7.547097000
B	6.793364000	7.186186000	5.947229000
H	7.615850000	7.866894000	6.213063000
B	5.399939000	6.924734000	7.021426000
H	5.318021000	7.432698000	7.994476000
C	5.676059000	5.358826000	4.110866000
C	4.525655000	6.667796000	4.376376000
H	3.861682988	7.022861147	3.602121579
H	5.772841191	4.845403828	3.165651272
H	3.396094090	4.387488037	4.784382747
34			
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B	5.963394	4.484841	5.654293
H	6.226011	3.330514	5.594632
B	7.191878	5.689205	5.210995
H	8.258526	5.336520	4.831657
B	6.380749	6.998713	4.335046
H	6.812551	7.555107	3.386771
B	5.208127	7.765574	5.420622
H	4.887770	8.881443	5.177358
B	3.983707	6.558505	5.862593
H	2.838233	6.862738	5.916871
B	4.790658	5.246408	6.750776
H	4.214587	4.610327	7.572686
B	6.526864	5.656881	6.861163
H	7.199352	5.303967	7.775538
B	6.785487	7.215649	6.034060
H	7.631719	7.993348	6.336623
B	5.301047	6.943603	6.991029
H	5.084279	7.534840	7.999119
C	5.862734	5.351126	4.184732
C	4.726409	6.552640	4.339061
C	6.002710	4.656247	2.860108
C	5.631871	3.308390	2.752186
H	5.246616	2.783918	3.623073
C	5.758400	2.635156	1.539629
H	5.468982	1.586919	1.473406
C	6.249191	3.299084	0.414872
H	6.345633	2.772826	-0.534412
C	6.618957	4.640129	0.514296
H	7.005674	5.168387	-0.356030
C	6.500564	5.314496	1.729176
H	6.804134	6.355948	1.795258
H	4.174936	6.776491	3.430488
H	3.591054	4.342320	4.515616
44			

2 oB10C2H10Ph2 q0			
B	4.261119000	5.092705000	5.100612000
B	5.864386000	4.480473000	5.575223000
H	6.080103000	3.401984000	5.603590000
B	7.083386000	5.671167000	5.058954000
H	8.094943000	5.372210000	4.746112000
B	6.215473000	7.004104000	4.285279000
H	6.653525000	7.564980000	3.446118000
B	5.190428000	7.798886000	5.493366000
H	4.971320000	8.876907000	5.462568000
B	3.977221000	6.602122000	6.002503000
H	2.963098000	6.900457000	6.307078000
B	4.821551000	5.254089000	6.773908000
H	4.359007000	4.676561000	7.587620000
B	6.565816000	5.614364000	6.749432000
H	7.241842000	5.272609000	7.547097000
B	6.793364000	7.186186000	5.947229000
H	7.615850000	7.866894000	6.213063000
B	5.399939000	6.924734000	7.021426000
H	5.318021000	7.432698000	7.994476000
C	5.676059000	5.358826000	4.110866000
C	4.525655000	6.667796000	4.376376000
C	5.861656000	4.638277000	2.787044000
C	5.599602000	3.266901000	2.697893000
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H	5.725127000	1.641854000	1.517200000
C	6.478934000	3.184886000	0.468938000
H	6.679176000	2.703224000	-0.301495000
C	6.751165000	4.533230000	0.534910000
H	7.139239000	4.962913000	-0.192892000
C	6.450800000	5.257980000	1.683995000
H	6.644424000	6.167458000	1.716575000
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C	2.232626000	7.155683000	3.455196000
H	1.872519000	6.783737000	4.227412000
C	1.390281000	7.682944000	2.489764000
H	0.469992000	7.659912000	2.622681000
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H	1.322265000	8.582774000	0.692141000
C	3.257671000	8.276191000	1.157027000
H	3.608509000	8.652806000	0.382542000
C	4.109365000	7.759824000	2.115813000
H	5.028414000	7.801531000	1.980789000
H	3.396094090	4.387488037	4.784382747
54			
3 oB10C2H9Ph3 q0			
B	4.259292000	5.144875000	5.130756000
B	5.858897000	4.521615000	5.652293000
H	6.045787000	3.353560000	5.576691000
B	7.105967000	5.678768000	5.144177000
H	8.134089000	5.312207000	4.679651000
B	6.264528000	7.014746000	4.338981000
H	6.705548000	7.572954000	3.396871000
B	5.241024000	7.840556000	5.525237000
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H	2.889633000	7.015300000	6.237674000
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H	4.269846000	4.702725000	7.682376000
B	6.560507000	5.647358000	6.833350000
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B	6.825391000	7.202530000	6.004770000
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B	5.412586000	6.978191000	7.067231000
H	5.280790000	7.556002000	8.098365000
C	5.724923000	5.384466000	4.197652000
C	4.570323000	6.721818000	4.432990000

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C	5.490726000	3.326935000	2.790211000
H	5.077872000	2.818634000	3.656119000
C	5.640955000	2.633804000	1.593027000
H	5.340427000	1.588394000	1.539167000
C	6.167817000	3.273374000	0.470306000
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C	6.568118000	4.605760000	0.564321000
H	7.005740000	5.109675000	-0.296632000
C	6.425879000	5.297732000	1.764960000
H	6.780418000	6.320981000	1.834950000
C	3.681775000	7.183696000	3.321317000
C	2.289441000	7.133762000	3.490493000
H	1.873230000	6.735946000	4.410997000
C	1.436622000	7.577628000	2.484924000
H	0.359216000	7.527841000	2.636779000
C	1.956776000	8.072203000	1.288087000
H	1.288603000	8.412181000	0.497607000
C	3.338808000	8.137107000	1.115483000
H	3.758861000	8.534715000	0.192394000
C	4.194006000	7.706728000	2.128073000
H	5.266012000	7.794130000	1.990645000
C	3.070903000	4.233446000	4.654397000
C	2.395092000	3.470608000	5.623107000
H	2.713282000	3.530294000	6.663032000
C	1.326762000	2.641086000	5.281074000
H	0.822006000	2.061496000	6.054225000
C	0.906621000	2.554650000	3.953285000
H	0.072110000	1.907836000	3.682071000
C	1.562822000	3.303857000	2.974660000
H	1.244122000	3.244139000	1.934085000
C	2.629614000	4.129832000	3.322096000
H	3.124240000	4.697790000	2.537999000
54			
3a oB10C2H9Ph3 q0			
B	4.076725000	4.925144000	4.332592000
B	5.580519000	5.691669000	3.773119000
H	6.488004000	5.750957000	4.535612000
B	5.889891000	5.245035000	2.081673000
H	7.000223000	5.013373000	1.733582000
B	4.594356000	4.177429000	1.492584000
B	3.080655000	5.100062000	1.606086000
H	2.181849000	4.734103000	0.922032000
B	2.771901000	5.546374000	3.296570000
H	1.667411000	5.474366000	3.726354000
B	4.074466000	6.624311000	3.842500000
H	3.895441000	7.452964000	4.675404000
B	5.197128000	6.831400000	2.470348000
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H	2.793177000	7.671141000	1.809310000
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C	3.563931000	4.110687000	2.885808000
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C	5.869514000	2.921508000	3.619513000
C	7.252915000	2.980265000	3.818128000
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C	7.952727000	1.852660000	4.241203000
H	9.029934000	1.913002000	4.391313000
C	7.279522000	0.652950000	4.471530000
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H	5.362431000	-0.339395000	4.453302000
C	5.199471000	1.717325000	3.852892000
H	4.124536000	1.640794000	3.713091000
C	3.871530000	4.188894000	5.693400000

C	4.908164000	4.117300000	6.637099000
H	5.854482000	4.615545000	6.431337000
C	4.749836000	3.409573000	7.826956000
H	5.568168000	3.365571000	8.545465000
C	3.547292000	2.755807000	8.096821000
H	3.423447000	2.200179000	9.025816000
C	2.501228000	2.822903000	7.175081000
H	1.557413000	2.320087000	7.383147000
C	2.665102000	3.534301000	5.986963000
H	1.835971000	3.586544000	5.279090000
C	4.790761000	2.869331000	0.664794000
C	3.732266000	1.967973000	0.470656000
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C	3.921697000	0.769532000	-0.216343000
H	3.086209000	0.082326000	-0.352247000
C	5.179046000	0.454422000	-0.735319000
H	5.331079000	-0.481388000	-1.273271000
C	6.239515000	1.345755000	-0.566154000
H	7.222026000	1.108136000	-0.975255000
C	6.045286000	2.539172000	0.128119000
H	6.882223000	3.223158000	0.263362000
64			
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B	4.071165000	10.195330000	7.002065000
B	5.049781000	10.883309000	5.694554000
H	5.744660000	11.793406000	6.001517000
B	4.128296000	10.890777000	4.195569000
H	4.166805000	11.821058000	3.460460000
B	2.516795000	10.204615000	4.485891000
B	2.778212000	8.524684000	5.023461000
H	1.893758000	7.746764000	4.885302000
B	3.788825000	9.212872000	3.746896000
H	3.639524000	8.899945000	2.610005000
B	5.355326000	9.641277000	4.470284000
H	6.368136000	9.648575000	3.847555000
B	5.299414000	9.206013000	6.192731000
H	6.251544000	8.897087000	6.833730000
B	3.704665000	8.517615000	6.529932000
H	3.416841000	7.750700000	7.388761000
B	4.514293000	8.163977000	4.986383000
H	4.895495000	7.063443000	4.746636000
C	3.351748000	11.149918000	5.706540000
C	2.552144000	9.730480000	6.207495000
C	2.826094000	12.521821000	6.020855000
C	3.628381000	13.622260000	5.681508000
H	4.596089000	13.457495000	5.216011000
C	3.196549000	14.921572000	5.935083000
H	3.837204000	15.760187000	5.664053000
C	1.954941000	15.146594000	6.530907000
H	1.617779000	16.162573000	6.732954000
C	1.146097000	14.058133000	6.853429000
H	0.165824000	14.215231000	7.301531000
C	1.571909000	12.756603000	6.594948000
H	0.908729000	11.933456000	6.827433000
C	1.263036000	9.704657000	6.987977000
C	0.066817000	9.371795000	6.337654000
H	0.065195000	9.168222000	5.273228000
C	-1.133984000	9.311014000	7.041289000
H	-2.050259000	9.055780000	6.509279000
C	-1.161557000	9.568031000	8.411772000
H	-2.100721000	9.521351000	8.962156000
C	0.028640000	9.874682000	9.071725000
H	0.029874000	10.068363000	10.144229000
C	1.229687000	9.938533000	8.369697000
H	2.139334000	10.189561000	8.902458000
C	4.263043000	10.685830000	8.481816000
C	4.267685000	12.036990000	8.863905000
H	4.076152000	12.813057000	8.127759000

C	4.516396000	12.409896000	10.184272000
H	4.514233000	13.465747000	10.455924000
C	4.776073000	11.440286000	11.152733000
H	4.974004000	11.733262000	12.183955000
C	4.797027000	10.092589000	10.788925000
H	5.012297000	9.326561000	11.533751000
C	4.549219000	9.724507000	9.469071000
H	4.569530000	8.669988000	9.194648000
C	1.267785000	10.699102000	3.672064000
C	0.951473000	12.051877000	3.468929000
H	1.548068000	12.828789000	3.938653000
C	-0.114537000	12.430267000	2.653720000
H	-0.338240000	13.488148000	2.516290000
C	-0.883286000	11.463547000	2.007117000
H	-1.714208000	11.759923000	1.367055000
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H	0.751486000	8.685879000	3.081360000