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Structure and stability of the C-doped boron fullerenes B₆₀C₁₂ and B₈₀C₁₂ with quasi-planar pentacoordinated cage carbon atoms: a quantum-chemical study

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pages **S6-S9**: Structure 5

4 [B3LYP/6-311+G(d,p)]

C₂

B	-0.486465000000	-3.961865000000	1.443204000000
B	1.178976000000	-3.921338000000	0.910324000000
B	2.283992000000	-3.086418000000	1.703466000000
B	1.862291000000	-2.176832000000	3.135563000000
B	0.348927000000	-2.125142000000	3.666452000000
B	-0.921737000000	-3.082185000000	2.713620000000
B	-0.369082000000	-0.705741000000	4.217679000000
B	0.369082000000	0.705741000000	4.217679000000
B	2.159286000000	0.700556000000	3.611244000000
B	2.817784000000	-0.677076000000	3.144359000000
B	3.835844000000	-0.669432000000	1.691435000000
B	3.524899000000	-2.130300000000	0.792282000000
B	3.523065000000	-2.140355000000	-0.804555000000
B	2.268816000000	-3.085910000000	-1.702509000000
B	1.178512000000	-3.932313000000	-0.899853000000
B	-1.529696000000	-3.993293000000	0.016702000000
B	-3.524899000000	2.130300000000	0.792282000000
B	4.051808000000	0.708866000000	0.898083000000
B	-2.817784000000	0.677076000000	3.144359000000
B	2.416240000000	2.175662000000	2.755926000000
B	3.346744000000	2.215405000000	1.428513000000
B	2.880294000000	3.140376000000	0.043902000000
B	3.393750000000	2.169044000000	-1.482162000000
B	4.078058000000	0.719721000000	-0.958791000000
B	-2.268816000000	3.085910000000	-1.702509000000
B	3.830718000000	-0.675583000000	-1.708926000000
B	2.800256000000	-0.688633000000	-3.157914000000
B	1.845646000000	-2.181697000000	-3.136108000000
B	0.313810000000	-2.140816000000	-3.612480000000
B	-0.970431000000	-3.130849000000	-2.706147000000
B	-4.051808000000	-0.708866000000	0.898083000000
B	-3.346744000000	-2.215405000000	1.428513000000
B	2.414234000000	2.262567000000	-2.734663000000
B	2.093592000000	0.653085000000	-3.657932000000
B	0.447767000000	0.676905000000	-4.182310000000
B	-0.313810000000	2.140816000000	-3.612480000000
B	0.970431000000	3.130849000000	-2.706147000000
B	0.486840000000	3.971252000000	-1.428403000000
B	1.529696000000	3.993293000000	0.016702000000
B	0.486465000000	3.961865000000	1.443204000000
B	0.921737000000	3.082185000000	2.713620000000
B	-1.178976000000	3.921338000000	0.910324000000
B	-1.178512000000	3.932313000000	-0.899853000000
B	-1.845646000000	2.181697000000	-3.136108000000
B	-2.800256000000	0.688633000000	-3.157914000000
B	-2.093592000000	-0.653085000000	-3.657932000000
B	-0.447767000000	-0.676905000000	-4.182310000000
B	-2.414234000000	-2.262567000000	-2.734663000000
B	-3.393750000000	-2.169044000000	-1.482162000000
B	-2.880294000000	-3.140376000000	0.043902000000
B	-0.348927000000	2.125142000000	3.666452000000
B	-4.078058000000	-0.719721000000	-0.958791000000
B	-3.835844000000	0.669432000000	1.691435000000
B	-3.830718000000	0.675583000000	-1.708926000000
B	-3.523065000000	2.140355000000	-0.804555000000
B	-2.416240000000	-2.175662000000	2.755926000000
B	-2.159286000000	-0.700556000000	3.611244000000
B	-1.862291000000	2.176832000000	3.135563000000
B	-2.283992000000	3.086418000000	1.703466000000
C	-0.014836000000	-4.170647000000	0.001684000000
C	0.014836000000	4.170647000000	0.001684000000
C	1.178512000000	1.869459000000	-3.553679000000
C	-1.178512000000	-1.869459000000	-3.553679000000

C	-3.738296000000	-1.880484000000	-0.015048000000
C	-1.157801000000	-1.850429000000	3.569701000000
C	3.738296000000	1.880484000000	-0.015048000000
C	1.157801000000	1.850429000000	3.569701000000
C	3.017967000000	-1.858986000000	2.201381000000
B	-0.486840000000	-3.971252000000	-1.428403000000
C	3.015808000000	-1.859580000000	-2.204039000000
C	-3.017967000000	1.858986000000	2.201381000000
C	-3.015808000000	1.859580000000	-2.204039000000

4 [M06/6-311+G(d,p)]

C₁

B	-2.819334000000	1.428568000000	2.797632000000
B	-1.431099000000	0.855038000000	3.861602000000
B	-0.049031000000	1.677564000000	3.890633000000
B	0.180010000000	3.104366000000	2.850736000000
B	-0.993905000000	3.604530000000	1.910224000000
B	-2.532150000000	2.713401000000	1.891090000000
B	-0.657624000000	4.140818000000	0.300970000000
B	0.816793000000	4.189631000000	-0.297593000000
B	2.118923000000	3.544168000000	0.759555000000
B	1.855092000000	3.093073000000	2.265608000000
B	2.625970000000	1.694188000000	2.837037000000
B	1.427803000000	0.767830000000	3.882551000000
B	1.450331000000	-0.840365000000	3.893194000000
B	-0.077751000000	-1.663911000000	3.861372000000
B	-1.481783000000	-0.878971000000	3.872534000000
B	-3.638409000000	0.061373000000	2.217215000000
B	-1.483568000000	0.824840000000	-3.795223000000
B	3.601061000000	0.814742000000	1.925969000000
B	-1.778480000000	3.158687000000	-2.241228000000
B	3.294937000000	2.713410000000	-0.267497000000
B	3.981019000000	1.363344000000	0.290307000000
B	4.196490000000	-0.050112000000	-0.715569000000
B	3.913386000000	-1.504460000000	0.312266000000
B	3.603980000000	-0.963341000000	1.925118000000
B	0.078211000000	-1.701416000000	-3.793835000000
B	2.577855000000	-1.739875000000	2.850907000000
B	1.734279000000	-3.176532000000	2.241534000000
B	0.133353000000	-3.151084000000	2.803070000000
B	-1.109585000000	-3.547575000000	1.879864000000
B	-2.651373000000	-2.661783000000	1.877499000000
B	-3.633440000000	1.003483000000	-1.908588000000
B	-3.992972000000	1.497086000000	-0.322802000000
B	3.223762000000	-2.800060000000	-0.305678000000
B	2.005445000000	-3.617353000000	0.733866000000
B	0.704797000000	-4.205715000000	-0.309269000000
B	0.973733000000	-3.649545000000	-1.892992000000
B	2.643025000000	-2.729315000000	-1.873701000000
B	2.760105000000	-1.477728000000	-2.866507000000
B	3.644476000000	-0.012444000000	-2.216998000000
B	2.851780000000	1.410338000000	-2.852664000000
B	2.699383000000	2.666184000000	-1.858989000000
B	1.486065000000	0.916797000000	-3.776430000000
B	1.472501000000	-0.936727000000	-3.805698000000
B	-0.183344000000	-3.142170000000	-2.888564000000
B	-1.815268000000	-3.123116000000	-2.263532000000
B	-2.136731000000	-3.599074000000	-0.770064000000
B	-0.810826000000	-4.129982000000	0.239679000000
B	-3.261357000000	-2.639150000000	0.259406000000
B	-4.034558000000	-1.387855000000	-0.350569000000
B	-4.140407000000	0.063265000000	0.704078000000
B	1.067483000000	3.650193000000	-1.862058000000
B	-3.670103000000	-0.902922000000	-1.910387000000
B	-2.607124000000	1.761128000000	-2.887903000000
B	-2.638127000000	-1.618870000000	-2.904224000000
B	-1.518502000000	-0.764433000000	-3.825719000000
B	-3.174903000000	2.767196000000	0.245771000000
B	-2.044446000000	3.659304000000	-0.744851000000
B	-0.061728000000	3.126508000000	-2.869540000000
B	0.125746000000	1.739732000000	-3.805411000000
C	-2.543708000000	0.019764000000	3.304210000000
C	2.569137000000	-0.024710000000	-3.276381000000
C	2.011459000000	-3.606729000000	-0.800021000000
C	-2.120316000000	-3.547256000000	0.743492000000

C	-4.123650000000	0.071260000000	-0.829330000000
C	-2.017962000000	3.600980000000	0.768601000000
C	4.121362000000	-0.061732000000	0.797230000000
C	2.129868000000	3.544890000000	-0.774119000000
C	1.264892000000	2.155485000000	3.340062000000
B	-2.818859000000	-1.394870000000	2.815463000000
C	1.211138000000	-2.211688000000	3.327155000000
C	-1.220607000000	2.237336000000	-3.298832000000
C	-1.282453000000	-2.177669000000	-3.312622000000

5 [B3LYP/6-311+G(d,p)]

 C_i

B	0.924341000000	-2.843816000000	-3.912252000000
B	2.416999000000	-2.857569000000	-3.189970000000
B	2.703352000000	-3.745642000000	-1.672340000000
B	3.927017000000	-2.853609000000	-0.734314000000
B	3.910361000000	-2.840772000000	0.923213000000
B	4.389240000000	-1.441303000000	1.671469000000
B	3.633019000000	-0.890857000000	3.187376000000
B	3.633014000000	0.890849000000	3.187376000000
B	2.417380000000	1.755941000000	3.910196000000
B	1.969595000000	3.179033000000	3.187403000000
B	0.275365000000	3.729898000000	3.187677000000
B	-0.014308000000	4.619059000000	1.671541000000
B	-1.493348000000	4.596161000000	0.923689000000
B	-1.499957000000	4.616541000000	-0.733776000000
B	-2.727227000000	3.728770000000	-1.671583000000
B	-1.969593000000	3.179027000000	-3.187400000000
B	-2.417376000000	1.755937000000	-3.910195000000
B	-1.224158000000	0.890592000000	-4.667116000000
B	-1.224155000000	-0.890608000000	-4.667124000000
B	0.469628000000	-1.441422000000	-4.670434000000
B	-0.275365000000	-3.729898000000	-3.187677000000
B	-1.969595000000	-3.179033000000	-3.187403000000
B	-2.417380000000	-1.755941000000	-3.910196000000
B	-3.633014000000	-0.890849000000	-3.187376000000
B	-3.633019000000	0.890857000000	-3.187376000000
B	-4.389240000000	1.441303000000	-1.671469000000
B	-3.910361000000	2.840772000000	-0.923213000000
B	-3.927017000000	2.853609000000	0.734314000000
B	-2.703352000000	3.745642000000	1.672340000000
B	-2.416999000000	2.857569000000	3.189970000000
B	-0.924341000000	2.843816000000	3.912252000000
B	-0.469628000000	1.441422000000	4.670434000000
B	1.224155000000	0.890608000000	4.667124000000
B	1.224158000000	-0.890592000000	4.667116000000
B	2.417376000000	-1.755937000000	3.910195000000
B	1.969593000000	-3.179027000000	3.187400000000
B	2.727227000000	-3.728770000000	1.671583000000
B	1.499957000000	-4.616541000000	0.733776000000
B	1.493348000000	-4.596161000000	-0.923689000000
B	0.014308000000	-4.619059000000	-1.671541000000
B	-1.499962000000	-4.616542000000	-0.733775000000
B	-2.727230000000	-3.728776000000	-1.671585000000
B	-3.910360000000	-2.840772000000	-0.923215000000
B	-4.389235000000	-1.441298000000	-1.671461000000
B	-4.854391000000	0.000004000000	-0.733993000000
B	-4.831057000000	0.000002000000	0.923275000000
B	-4.396307000000	1.413468000000	1.671733000000
B	-3.463063000000	1.415558000000	3.189378000000
B	-2.989877000000	0.000003000000	3.911463000000
B	-1.516603000000	0.000008000000	4.670738000000
B	-0.469631000000	-1.441410000000	4.670420000000
B	-0.924337000000	-2.843811000000	3.912252000000
B	0.275360000000	-3.729906000000	3.187677000000
B	-0.014309000000	-4.619069000000	1.671550000000
B	-1.493348000000	-4.596167000000	0.923690000000
B	-2.703355000000	-3.745651000000	1.672345000000
B	-3.927010000000	-2.853615000000	0.734312000000
B	-4.396291000000	-1.413463000000	1.671722000000
B	-3.463046000000	-1.415554000000	3.189371000000
B	-2.416994000000	-2.857575000000	3.189967000000
B	3.463063000000	-1.415558000000	-3.189378000000
B	4.396307000000	-1.413468000000	-1.671733000000

B	4.831057000000	-0.000002000000	-0.923275000000
B	4.854391000000	-0.000004000000	0.733993000000
B	4.389235000000	1.441298000000	1.671461000000
B	3.910360000000	2.840772000000	0.923215000000
B	2.727230000000	3.728776000000	1.671585000000
B	1.499962000000	4.616542000000	0.733775000000
B	1.493348000000	4.596167000000	-0.923690000000
B	0.014309000000	4.619069000000	-1.671550000000
B	-0.275360000000	3.729906000000	-3.187677000000
B	0.924337000000	2.843811000000	-3.912252000000
B	0.469631000000	1.441410000000	-4.670420000000
B	1.516603000000	-0.000008000000	-4.670738000000
B	2.989877000000	-0.000003000000	-3.911463000000
B	3.463046000000	1.415554000000	-3.189371000000
B	4.396291000000	1.413463000000	-1.671722000000
B	3.927010000000	2.853615000000	-0.734312000000
B	2.703355000000	3.745651000000	-1.672345000000
B	2.416994000000	2.857575000000	-3.189967000000
C	-0.001114000000	0.000002000000	4.913003000000
C	-3.560296000000	2.586890000000	2.201011000000
C	-4.401422000000	0.000000000000	-2.200769000000
C	-1.359980000000	-4.184963000000	-2.200428000000
C	3.560296000000	-2.586890000000	-2.201011000000
C	4.401422000000	0.000000000000	2.200769000000
C	1.359980000000	4.184963000000	2.200428000000
C	-3.560289000000	-2.586883000000	2.201007000000
C	0.001114000000	-0.000002000000	-4.913003000000
C	1.359981000000	-4.184963000000	2.200429000000
C	-1.359981000000	4.184963000000	-2.200429000000
C	3.560289000000	2.586883000000	-2.201007000000

5 [M06/6-311+G(d,p)]

 C_i

B	2.408029000000	-1.750542000000	-3.893313000000
B	3.623272000000	-0.887743000000	-3.177212000000
B	4.377862000000	-1.436202000000	-1.667513000000
B	4.838463000000	0.000016000000	-0.733099000000
B	4.809866000000	-0.000070000000	0.919365000000
B	4.381637000000	1.410673000000	1.665969000000
B	3.452579000000	1.412508000000	3.178602000000
B	2.409565000000	2.849596000000	3.179030000000
B	0.920115000000	2.834008000000	3.896778000000
B	-0.275699000000	3.720968000000	3.177370000000
B	-1.963692000000	3.172081000000	3.176193000000
B	-2.719096000000	3.721333000000	1.667105000000
B	-3.895156000000	2.830065000000	0.920670000000
B	-3.914568000000	2.845243000000	-0.732619000000
B	-4.381677000000	1.410791000000	-1.665997000000
B	-3.452694000000	1.412609000000	-3.178706000000
B	-2.979456000000	0.000016000000	-3.895545000000
B	-1.511163000000	0.000011000000	-4.653283000000
B	-0.467704000000	-1.435813000000	-4.653468000000
B	1.219271000000	-0.886633000000	-4.648130000000
B	1.963692000000	-3.172081000000	-3.176193000000
B	0.275699000000	-3.720968000000	-3.177370000000
B	-0.920115000000	-2.834008000000	-3.896778000000
B	-2.409565000000	-2.849596000000	-3.179030000000
B	-3.452579000000	-1.412508000000	-3.178602000000
B	-4.381637000000	-1.410673000000	-1.665969000000
B	-4.809866000000	0.000070000000	-0.919365000000
B	-4.838463000000	-0.000016000000	0.733099000000
B	-4.377862000000	1.436202000000	1.667513000000
B	-3.623272000000	0.887743000000	3.177212000000
B	-2.408029000000	1.750542000000	3.893313000000
B	-1.219271000000	0.886633000000	4.648130000000
B	0.467704000000	1.435813000000	4.653468000000
B	1.511163000000	-0.000011000000	4.653283000000
B	2.979456000000	-0.000016000000	3.895545000000
B	3.452694000000	-1.412609000000	3.178706000000
B	4.381677000000	-1.410791000000	1.665997000000
B	3.914568000000	-2.845243000000	0.732619000000
B	3.895156000000	-2.830065000000	-0.920670000000
B	2.719096000000	-3.721333000000	-1.667105000000
B	1.494922000000	-4.604120000000	-0.732556000000
B	-0.012967000000	-4.608238000000	-1.667198000000
B	-1.487456000000	-4.580753000000	-0.920483000000
B	-2.695735000000	-3.734455000000	-1.666887000000
B	-3.914392000000	-2.845133000000	-0.732510000000
B	-3.895012000000	-2.830012000000	0.920767000000
B	-4.377926000000	-1.436259000000	1.667646000000
B	-3.623581000000	-0.887892000000	3.177374000000
B	-2.408207000000	-1.750661000000	3.893486000000
B	-1.219339000000	-0.886674000000	4.648087000000
B	0.467711000000	-1.435941000000	4.653548000000
B	0.920213000000	-2.834285000000	3.897105000000
B	2.409656000000	-2.849775000000	3.179207000000
B	2.695771000000	-3.734512000000	1.666985000000
B	1.487522000000	-4.580781000000	0.920507000000
B	0.013005000000	-4.607967000000	1.667125000000
B	-1.494963000000	-4.604180000000	0.732600000000
B	-2.719068000000	-3.721376000000	1.667271000000
B	-1.963846000000	-3.172210000000	3.176268000000
B	-0.275699000000	-3.721030000000	3.177496000000
B	3.623581000000	0.887892000000	-3.177374000000
B	4.377926000000	1.436259000000	-1.667646000000
B	3.895012000000	2.830012000000	-0.920767000000

B	3.914392000000	2.845133000000	0.732510000000
B	2.695735000000	3.734455000000	1.666887000000
B	1.487456000000	4.580753000000	0.920483000000
B	0.012967000000	4.608238000000	1.667198000000
B	-1.494922000000	4.604120000000	0.732556000000
B	-1.487522000000	4.580781000000	-0.920507000000
B	-2.695771000000	3.734512000000	-1.666985000000
B	-2.409656000000	2.849775000000	-3.179207000000
B	-0.920213000000	2.834285000000	-3.897105000000
B	-0.467710000000	1.435941000000	-4.653548000000
B	1.219339000000	0.886674000000	-4.648087000000
B	2.408207000000	1.750661000000	-3.893486000000
B	1.963846000000	3.172210000000	-3.176268000000
B	2.719068000000	3.721376000000	-1.667271000000
B	1.494963000000	4.604180000000	-0.732600000000
B	-0.013005000000	4.607967000000	-1.667125000000
B	0.275659000000	3.721030000000	-3.177496000000
C	0.001551000000	-0.000079000000	4.906964000000
C	-4.401049000000	0.000011000000	2.200851000000
C	-3.557726000000	-2.586031000000	-2.199604000000
C	1.359952000000	-4.186203000000	-2.200065000000
C	4.401049000000	-0.000011000000	-2.200851000000
C	3.557726000000	2.586031000000	2.199604000000
C	-1.359952000000	4.186203000000	2.200065000000
C	-1.359869000000	-4.186156000000	2.200116000000
C	-0.001551000000	0.000079000000	-4.906964000000
C	3.557836000000	-2.586170000000	2.199732000000
C	-3.557836000000	2.586170000000	-2.199732000000
C	1.359869000000	4.186156000000	-2.200116000000