

Supplementary Information (ESI)

A topological path to the formation of the quasi-planar **B₇₀** boron cluster and its dianion

Pinaki Saha,¹ Fernando Buendía,² Long Van Duong³ and Minh Tho Nguyen^{4,5*}

1. Department of Chemistry, KU Leuven, Celestijnenlaan 200F, B-3001 Leuven, Belgium
2. Instituto de Física, Universidad Nacional Autónoma de México, C.P. 04510 Cd. de México.
3. Department of Chemistry, Quy Nhon University, Quy Nhon, Vietnam
4. Laboratory for Chemical Computation and Modeling, Institute for Computational Science and Artificial Intelligence, Van Lang University, Ho Chi Minh City, Vietnam.
5. Faculty of Applied Technology, School of Technology, Van Lang University, Ho Chi Minh City, Vietnam

* Corresponding author. Email: minhtho.nguyen@vlu.edu.vn

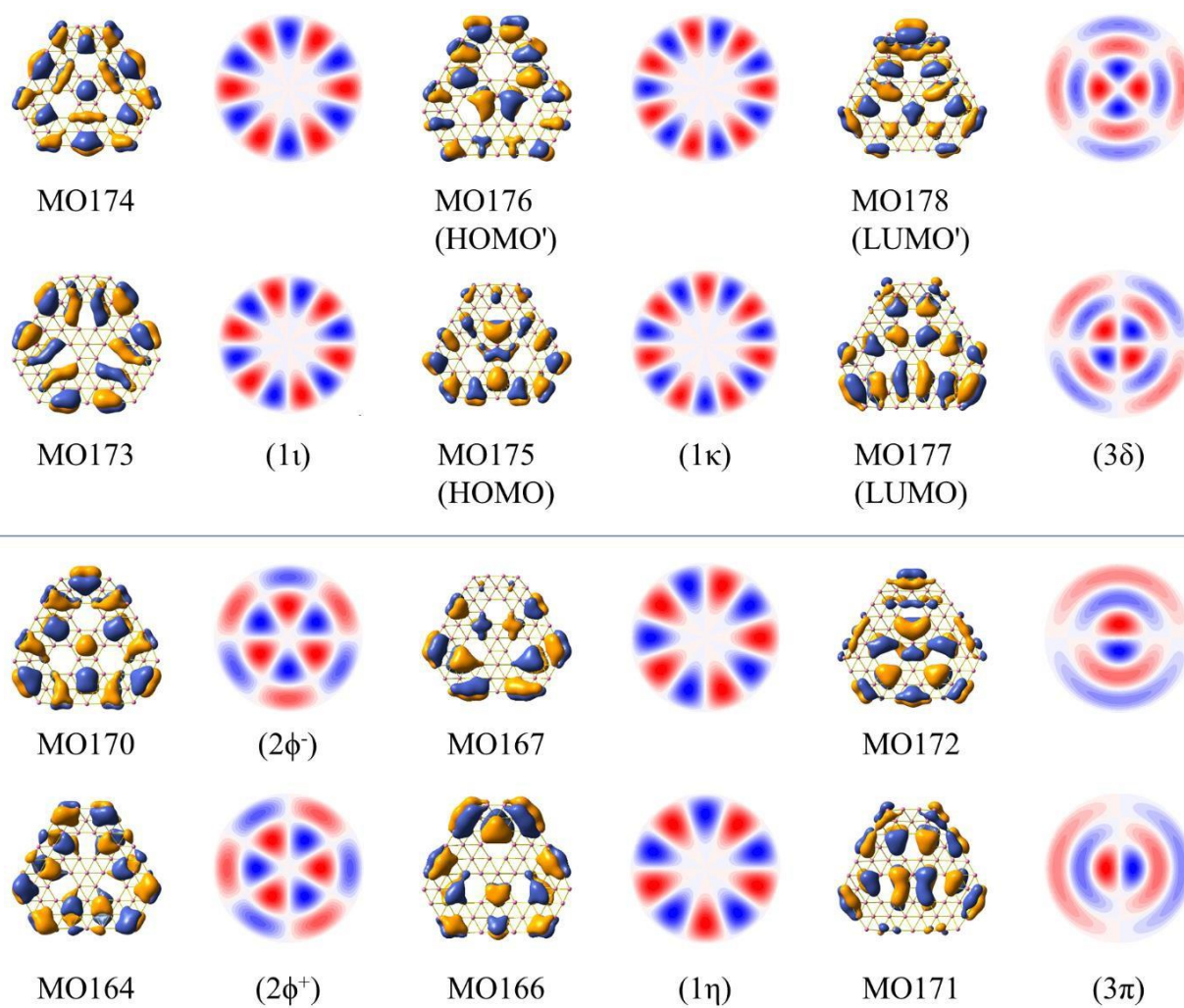


Figure S1b. Correspondence between the π -MO of the B_{70}^{2-} dianion with the energy levels of the Disk Aromaticity Model (DM; continued).

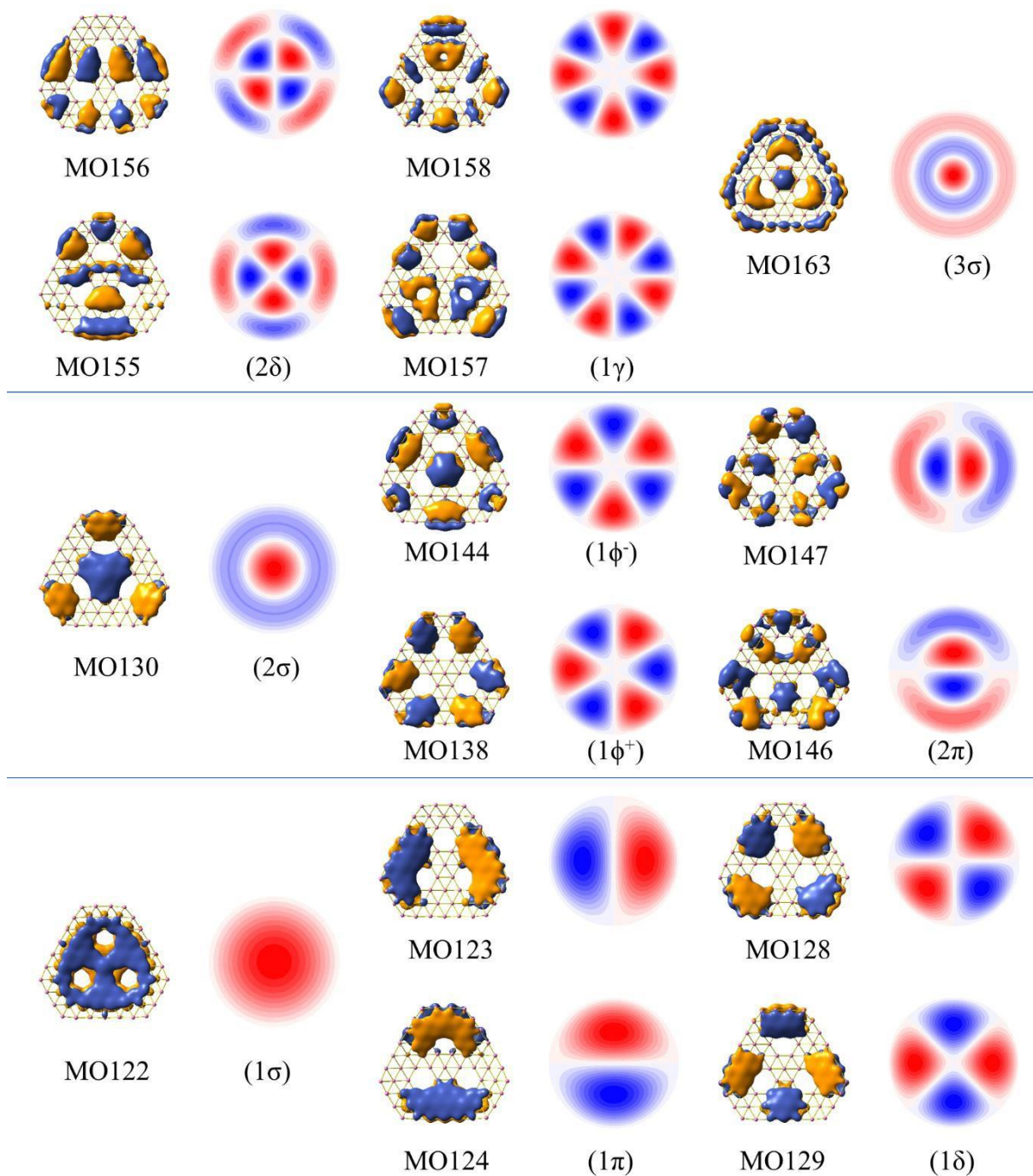
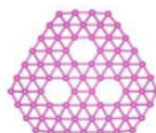


Figure S1a: Correspondence between the π -MO of the B_{70}^{2-} dianion with the energy levels of the Disk Aromaticity Model (DM).

Cartesian coordinates of the main neutral (B_{70}) and dianionic (B_{70}^{2-}) structures of the B_{70} boron cluster (B3PW91/6-311G optimizations).

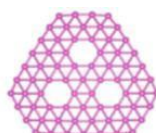
B_{70} Quasiplanar Structure neutral (III)



| | | | |
|---|--------------|--------------|--------------|
| B | -0.565772000 | -4.942010000 | -0.156266000 |
| B | -4.594182000 | -1.936701000 | -0.189295000 |
| B | -0.411915000 | -3.312812000 | -0.731780000 |
| B | 3.075443000 | 1.299352000 | -0.732884000 |
| B | -3.060384000 | -1.326775000 | -0.724797000 |
| B | -4.238038000 | 1.339317000 | -0.390835000 |
| B | 1.155382000 | -2.698220000 | -0.837923000 |
| B | 4.385183000 | 0.326168000 | -0.484979000 |
| B | -2.909720000 | 0.348188000 | -0.828802000 |
| B | 4.186624000 | -1.353328000 | -0.491974000 |
| B | 0.001522000 | -0.000582000 | -1.067556000 |
| B | -4.434647000 | -0.301363000 | -0.391652000 |
| B | -1.910610000 | -3.963449000 | -0.491264000 |
| B | 2.478566000 | -3.689267000 | -0.385201000 |
| B | 0.959159000 | -4.339004000 | -0.382449000 |
| B | 2.682528000 | -1.989119000 | -0.735688000 |
| B | 4.570173000 | 1.984334000 | -0.178413000 |
| B | -0.920806000 | 4.301684000 | -0.489149000 |
| B | -3.260344000 | -2.945272000 | -0.476015000 |
| B | 0.381541000 | 3.315352000 | -0.728846000 |
| B | -2.660463000 | 2.011301000 | -0.723307000 |
| B | 1.758990000 | 2.348167000 | -0.835190000 |
| B | 3.969197000 | -3.003836000 | -0.165687000 |
| B | 3.279753000 | 3.000014000 | -0.387417000 |
| B | -2.472803000 | 3.631379000 | -0.474823000 |
| B | 0.617408000 | 4.936267000 | -0.157627000 |
| B | -4.006399000 | 2.965703000 | -0.186210000 |
| B | 1.956447000 | 3.989582000 | -0.383010000 |
| B | -0.241333000 | -1.684582000 | -0.968037000 |
| B | 1.387219000 | -0.987693000 | -0.969879000 |
| B | 0.163033000 | 1.693008000 | -0.966331000 |
| B | -1.545931000 | -0.707464000 | -0.963438000 |
| B | -1.335229000 | 1.051773000 | -0.962665000 |
| B | 1.581164000 | 0.631372000 | -0.968263000 |
| B | 0.842322000 | 6.485442000 | 0.682433000 |
| B | -0.728678000 | 5.881325000 | 0.163209000 |
| B | -2.232284000 | 5.213322000 | 0.063212000 |
| B | -5.282955000 | 3.871735000 | 0.656871000 |
| B | -5.729515000 | 0.685644000 | 0.267752000 |

| | | | |
|---|--------------|--------------|-------------|
| B | -5.861101000 | -0.925115000 | 0.322987000 |
| B | -6.048756000 | -2.516048000 | 0.653486000 |
| B | -4.732246000 | -3.572094000 | 0.151475000 |
| B | -3.400781000 | -4.539788000 | 0.060126000 |
| B | 2.269482000 | -5.299435000 | 0.289177000 |
| B | 3.728941000 | -4.606990000 | 0.343198000 |
| B | 5.200217000 | -3.973308000 | 0.672112000 |
| B | 5.853496000 | 0.956697000 | 0.148508000 |
| B | 5.994490000 | 2.635445000 | 0.662382000 |
| B | 4.713347000 | 3.597958000 | 0.335637000 |
| B | 3.457664000 | 4.614671000 | 0.284256000 |
| B | 2.127230000 | 5.530802000 | 0.346455000 |
| B | 5.635874000 | -0.674519000 | 0.049878000 |
| B | 5.461885000 | -2.310734000 | 0.151546000 |
| B | -3.754659000 | 4.587573000 | 0.154311000 |
| B | -5.476740000 | 2.281841000 | 0.324758000 |
| B | -0.713412000 | -6.500258000 | 0.684234000 |
| B | 0.760591000 | -5.875740000 | 0.349403000 |
| B | -2.097061000 | -5.543317000 | 0.162493000 |
| B | 6.519239000 | -3.192133000 | 1.081768000 |
| B | 6.850453000 | -1.662444000 | 0.916101000 |
| B | 7.051590000 | 0.000340000 | 0.911902000 |
| B | -0.493681000 | 7.234927000 | 1.097206000 |
| B | -1.984245000 | 6.756414000 | 0.932242000 |
| B | -3.526529000 | 6.101537000 | 0.921504000 |
| B | -2.188887000 | -6.913695000 | 1.097104000 |
| B | -3.524390000 | -6.097377000 | 0.930132000 |
| B | -4.868697000 | -5.097507000 | 0.917667000 |
| B | 7.091659000 | 1.565434000 | 1.073808000 |
| B | -6.030840000 | -4.046743000 | 1.072026000 |
| B | -4.903785000 | 5.354653000 | 1.076288000 |

B₇₀ Quasiplanar Structure dianion (III)

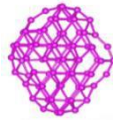


| | | | |
|---|--------------|--------------|--------------|
| B | -0.565772041 | -4.942010380 | -0.156266012 |
| B | -4.594182348 | -1.936701147 | -0.189295014 |
| B | -0.411915031 | -3.312812253 | -0.731780056 |
| B | 3.075443236 | 1.299352099 | -0.732884057 |
| B | -3.060384233 | -1.326775101 | -0.724797054 |
| B | -4.238038323 | 1.339317105 | -0.390835030 |
| B | 1.155382089 | -2.698220208 | -0.837923064 |
| B | 4.385183334 | 0.326168025 | -0.484979037 |
| B | -2.909720220 | 0.348188027 | -0.828802064 |
| B | 4.186624319 | -1.353328104 | -0.491974038 |

| | | | |
|---|--------------|--------------|--------------|
| B | 0.001522000 | -0.000582000 | -1.067556081 |
| B | -4.434647341 | -0.301363023 | -0.391652030 |
| B | -1.910610148 | -3.963449302 | -0.491264038 |
| B | 2.478566188 | -3.689267281 | -0.385201029 |
| B | 0.959159074 | -4.339004332 | -0.382449029 |
| B | 2.682528203 | -1.989119154 | -0.735688057 |
| B | 4.570173349 | 1.984334154 | -0.178413014 |
| B | -0.920806070 | 4.301684328 | -0.489149037 |
| B | -3.260344250 | -2.945272227 | -0.476015036 |
| B | 0.381541029 | 3.315352251 | -0.728846054 |
| B | -2.660463205 | 2.011301153 | -0.723307055 |
| B | 1.758990134 | 2.348167177 | -0.835190064 |
| B | 3.969197304 | -3.003836230 | -0.165687013 |
| B | 3.279753249 | 3.000014227 | -0.387417029 |
| B | -2.472803189 | 3.631379275 | -0.474823036 |
| B | 0.617408046 | 4.936267378 | -0.157627012 |
| B | -4.006399306 | 2.965703226 | -0.186210014 |
| B | 1.956447148 | 3.989582302 | -0.383010029 |
| B | -0.241333019 | -1.684582129 | -0.968037076 |
| B | 1.387219108 | -0.987693074 | -0.969879073 |
| B | 0.163033013 | 1.693008129 | -0.966331072 |
| B | -1.545931118 | -0.707464055 | -0.963438076 |
| B | -1.335229099 | 1.051773078 | -0.962665075 |
| B | 1.581164120 | 0.631372049 | -0.968263072 |
| B | 0.842322067 | 6.485442479 | 0.682433050 |
| B | -0.728678056 | 5.881325423 | 0.163209012 |
| B | -2.232284170 | 5.213322397 | 0.063212005 |
| B | -5.282955402 | 3.871735296 | 0.656871048 |
| B | -5.729515425 | 0.685644050 | 0.267752021 |
| B | -5.861101433 | -0.925115070 | 0.322987024 |
| B | -6.048756470 | -2.516048194 | 0.653486049 |
| B | -4.732246360 | -3.572094272 | 0.151475012 |
| B | -3.400781261 | -4.539788346 | 0.060126004 |
| B | 2.269482171 | -5.299435400 | 0.289177022 |
| B | 3.728941287 | -4.606990353 | 0.343198026 |
| B | 5.200217396 | -3.973308303 | 0.672112051 |
| B | 5.853496468 | 0.956697072 | 0.148508012 |
| B | 5.994490454 | 2.635445202 | 0.662382053 |
| B | 4.713347360 | 3.597958276 | 0.335637026 |
| B | 3.457664264 | 4.614671351 | 0.284256022 |
| B | 2.127230162 | 5.530802435 | 0.346455026 |
| B | 5.635874441 | -0.674519051 | 0.049878004 |
| B | 5.461885407 | -2.310734179 | 0.151546012 |
| B | -3.754659285 | 4.587573348 | 0.154311012 |
| B | -5.476740418 | 2.281841175 | 0.324758025 |
| B | -0.713412055 | -6.500258489 | 0.684234052 |
| B | 0.760591059 | -5.875740434 | 0.349403027 |
| B | -2.097061158 | -5.543317424 | 0.162493013 |

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|---|--------------|--------------|-------------|
| B | 6.519239495 | -3.192133244 | 1.081768083 |
| B | 6.850453546 | -1.662444126 | 0.916101070 |
| B | 7.051590538 | 0.000340000 | 0.911902070 |
| B | -0.493681038 | 7.234927541 | 1.097206083 |
| B | -1.984245151 | 6.756414516 | 0.932242071 |
| B | -3.526529269 | 6.101537456 | 0.921504070 |
| B | -2.188887169 | -6.913695519 | 1.097104084 |
| B | -3.524390272 | -6.097377487 | 0.930132072 |
| B | -4.868697370 | -5.097507389 | 0.917667069 |
| B | 7.091659522 | 1.565434120 | 1.073808082 |
| B | -6.030840486 | -4.046743309 | 1.072026083 |
| B | -4.903785372 | 5.354653405 | 1.076288082 |

B₇₀ Bilayer Structure neutral (I)



| | | | |
|---|--------------|--------------|--------------|
| B | -4.198956000 | -1.101438000 | -1.362531000 |
| B | -3.054886000 | 1.615327000 | -1.649175000 |
| B | -2.761346000 | -0.105061000 | -0.831431000 |
| B | -1.699287000 | 2.539550000 | -1.562681000 |
| B | -1.397190000 | -0.896652000 | -1.691064000 |
| B | -4.351727000 | 0.647840000 | -1.501084000 |
| B | -1.256113000 | -2.610486000 | -1.630036000 |
| B | 0.078786000 | -1.426194000 | -0.804742000 |
| B | 1.593614000 | -2.309451000 | -1.781003000 |
| B | -2.759266000 | -1.905208000 | -1.457608000 |
| B | -0.044737000 | 0.068961000 | -1.783420000 |
| B | 3.079633000 | -1.513951000 | -1.743212000 |
| B | 0.221830000 | -3.223098000 | -1.584220000 |
| B | -0.176125000 | 1.608680000 | -0.865741000 |
| B | 1.320619000 | 1.056312000 | -1.658511000 |
| B | -0.358760000 | 3.507560000 | -1.415303000 |
| B | 2.634918000 | 2.131661000 | -1.422560000 |
| B | 1.462575000 | -0.645033000 | -1.679052000 |
| B | -1.537829000 | 0.823792000 | -1.684476000 |
| B | 4.085296000 | 1.305365000 | -1.301086000 |
| B | 1.109561000 | 2.756604000 | -1.532383000 |
| B | 4.199293000 | -0.383596000 | -1.533535000 |
| B | 2.647419000 | 0.322045000 | -0.800608000 |
| B | -4.189667000 | -0.999540000 | 1.565198000 |
| B | -3.014579000 | 1.773900000 | 1.374521000 |
| B | -2.775087000 | -0.031004000 | 0.867802000 |
| B | -1.595126000 | 2.613951000 | 1.448943000 |
| B | -1.497229000 | -0.748891000 | 1.901681000 |
| B | -4.338246000 | 0.776127000 | 1.352670000 |
| B | -1.596290000 | -2.685274000 | 1.391852000 |
| B | 0.016033000 | -1.433359000 | 0.883322000 |

| | | | |
|---|--------------|--------------|--------------|
| B | 1.438260000 | -2.309231000 | 1.683593000 |
| B | -2.781017000 | -1.708876000 | 2.040063000 |
| B | -0.100209000 | 0.107172000 | 1.801150000 |
| B | 2.943504000 | -1.445020000 | 1.749604000 |
| B | -0.012650000 | -3.220977000 | 1.357115000 |
| B | -0.154180000 | 1.625973000 | 0.790396000 |
| B | 1.277309000 | 1.067184000 | 1.677021000 |
| B | -0.260430000 | 3.570956000 | 1.270182000 |
| B | 2.665690000 | 2.102049000 | 1.565228000 |
| B | 1.394335000 | -0.638459000 | 1.811538000 |
| B | -1.541332000 | 0.943872000 | 1.603980000 |
| B | 4.072020000 | 1.311042000 | 1.534875000 |
| B | 1.177205000 | 2.769542000 | 1.447125000 |
| B | 4.156095000 | -0.386160000 | 1.692796000 |
| B | 2.633272000 | 0.277911000 | 0.899573000 |
| B | 5.029536000 | 1.801437000 | 0.077666000 |
| B | -1.191995000 | -4.030193000 | 0.285837000 |
| B | -5.117339000 | -1.667053000 | 0.084212000 |
| B | -4.388186000 | 2.307446000 | 0.349414000 |
| B | 4.155265000 | -2.416015000 | -0.029499000 |
| B | 0.352403000 | -4.346482000 | -0.042062000 |
| B | 5.041598000 | -1.047095000 | 0.089010000 |
| B | -0.377515000 | 4.792100000 | -0.087388000 |
| B | -5.359557000 | 1.135647000 | -0.048697000 |
| B | 1.100460000 | 4.352907000 | -0.046732000 |
| B | 2.357319000 | 3.292858000 | -0.012575000 |
| B | 3.926999000 | 2.836600000 | -0.414163000 |
| B | -2.450098000 | -3.201657000 | -0.330687000 |
| B | -3.984232000 | -2.654409000 | -0.397571000 |
| B | -5.570244000 | -0.294118000 | -0.824286000 |
| B | -5.549118000 | -0.299772000 | 0.860949000 |
| B | 5.442335000 | 0.353928000 | -0.752435000 |
| B | 5.368630000 | 0.390817000 | 0.909306000 |
| B | 2.872920000 | -3.009614000 | 0.960045000 |
| B | 1.563813000 | -3.924471000 | 1.050097000 |
| B | 1.666216000 | -3.930884000 | -0.966961000 |
| B | 3.020914000 | -3.094682000 | -1.020017000 |
| B | -1.758975000 | 4.117404000 | -0.090099000 |
| B | -2.906155000 | 2.938884000 | -0.038132000 |

B₇₀ Bilayer Structure dianion (I)

| | | | |
|---|--------------|--------------|--------------|
| B | -4.223880000 | -1.113108000 | -1.369873000 |
| B | -3.071074000 | 1.585234000 | -1.636113000 |
| B | -2.764003000 | -0.113201000 | -0.807851000 |
| B | -1.715958000 | 2.525049000 | -1.558537000 |
| B | -1.409392000 | -0.904154000 | -1.680546000 |

| | | | |
|---|--------------|--------------|--------------|
| B | -4.370329000 | 0.622374000 | -1.499307000 |
| B | -1.257646000 | -2.621828000 | -1.577122000 |
| B | 0.069014000 | -1.417421000 | -0.792956000 |
| B | 1.615054000 | -2.309129000 | -1.760155000 |
| B | -2.776802000 | -1.901827000 | -1.457800000 |
| B | -0.054627000 | 0.063104000 | -1.771623000 |
| B | 3.086623000 | -1.444151000 | -1.721230000 |
| B | 0.235203000 | -3.214475000 | -1.544771000 |
| B | -0.185631000 | 1.613927000 | -0.885719000 |
| B | 1.328401000 | 1.047896000 | -1.648841000 |
| B | -0.363626000 | 3.485864000 | -1.463223000 |
| B | 2.638764000 | 2.148333000 | -1.423545000 |
| B | 1.458220000 | -0.645920000 | -1.689351000 |
| B | -1.548676000 | 0.814241000 | -1.705647000 |
| B | 4.083356000 | 1.325470000 | -1.317950000 |
| B | 1.112448000 | 2.742369000 | -1.595503000 |
| B | 4.241091000 | -0.321629000 | -1.639093000 |
| B | 2.653246000 | 0.284010000 | -0.800761000 |
| B | -4.175451000 | -0.999813000 | 1.567707000 |
| B | -3.027179000 | 1.780855000 | 1.362980000 |
| B | -2.764952000 | -0.030720000 | 0.879297000 |
| B | -1.595867000 | 2.625465000 | 1.386069000 |
| B | -1.498575000 | -0.715952000 | 1.990843000 |
| B | -4.347076000 | 0.772942000 | 1.363853000 |
| B | -1.621279000 | -2.707962000 | 1.298802000 |
| B | 0.017431000 | -1.431332000 | 0.894987000 |
| B | 1.446014000 | -2.296027000 | 1.679206000 |
| B | -2.756171000 | -1.698300000 | 2.062339000 |
| B | -0.102587000 | 0.113681000 | 1.804398000 |
| B | 2.955733000 | -1.432087000 | 1.804660000 |
| B | -0.021808000 | -3.225529000 | 1.342905000 |
| B | -0.156447000 | 1.635799000 | 0.767395000 |
| B | 1.281472000 | 1.072479000 | 1.642854000 |
| B | -0.252940000 | 3.587917000 | 1.230497000 |
| B | 2.664193000 | 2.106497000 | 1.572373000 |
| B | 1.401431000 | -0.631995000 | 1.800138000 |
| B | -1.545434000 | 0.965056000 | 1.588932000 |
| B | 4.073402000 | 1.315197000 | 1.543482000 |
| B | 1.184704000 | 2.787513000 | 1.413172000 |
| B | 4.159781000 | -0.368443000 | 1.723042000 |
| B | 2.635393000 | 0.275924000 | 0.887974000 |
| B | 5.074190000 | 1.791049000 | 0.078297000 |
| B | -1.190195000 | -4.070423000 | 0.165322000 |
| B | -5.110301000 | -1.670749000 | 0.095777000 |
| B | -4.414689000 | 2.315690000 | 0.432582000 |
| B | 4.199225000 | -2.450839000 | -0.033641000 |
| B | 0.384580000 | -4.368122000 | -0.059724000 |
| B | 5.028761000 | -1.055492000 | 0.149703000 |

| | | | |
|---|--------------|--------------|--------------|
| B | -0.384685000 | 4.785604000 | -0.144074000 |
| B | -5.352224000 | 1.130350000 | -0.032959000 |
| B | 1.083933000 | 4.335264000 | -0.000442000 |
| B | 2.359176000 | 3.302005000 | -0.006613000 |
| B | 3.922784000 | 2.798258000 | -0.361945000 |
| B | -2.443206000 | -3.197644000 | -0.319546000 |
| B | -4.006998000 | -2.655138000 | -0.425450000 |
| B | -5.619465000 | -0.289609000 | -0.789441000 |
| B | -5.588373000 | -0.309037000 | 0.871055000 |
| B | 5.459201000 | 0.325939000 | -0.728705000 |
| B | 5.396996000 | 0.381224000 | 0.909850000 |
| B | 2.877088000 | -2.996966000 | 0.940702000 |
| B | 1.556193000 | -3.904870000 | 1.071239000 |
| B | 1.685387000 | -3.926018000 | -0.975786000 |
| B | 3.037498000 | -3.067505000 | -0.982653000 |
| B | -1.777197000 | 4.115733000 | -0.072694000 |
| B | -2.911244000 | 2.929107000 | -0.041244000 |

B₇₀ tubular Structure neutral (II)



| | | | |
|---|--------------|--------------|--------------|
| B | 1.702405000 | 3.422315000 | 2.945172000 |
| B | 3.008237000 | 2.488277000 | 2.920756000 |
| B | 3.781936000 | -0.561478000 | 2.945139000 |
| B | 3.297209000 | -2.092233000 | 2.920453000 |
| B | 0.634329000 | -3.769227000 | 2.945227000 |
| B | -0.971324000 | -3.781075000 | 2.920712000 |
| B | -3.390324000 | -1.769294000 | 2.945131000 |
| B | -3.896332000 | -0.245600000 | 2.920854000 |
| B | -2.728693000 | 2.676231000 | 2.945358000 |
| B | -1.437373000 | 3.630396000 | 2.920595000 |
| B | 3.600199000 | 1.887905000 | 1.429993000 |
| B | 3.944145000 | 0.248209000 | 1.462497000 |
| B | 2.907531000 | -2.839757000 | 1.429799000 |
| B | 1.453921000 | -3.672622000 | 1.462504000 |
| B | -1.802714000 | -3.642669000 | 1.429800000 |
| B | -3.046212000 | -2.519739000 | 1.462570000 |
| B | -4.021745000 | 0.588185000 | 1.430016000 |
| B | -3.334993000 | 2.116328000 | 1.462477000 |
| B | -0.683152000 | 4.007458000 | 1.430152000 |
| B | 0.982436000 | 3.826263000 | 1.462538000 |
| B | 4.212511000 | -0.597882000 | -0.000158000 |
| B | 0.732987000 | -4.190681000 | -0.000015000 |
| B | -3.760222000 | -1.992742000 | -0.000323000 |
| B | -3.055825000 | 2.959251000 | 0.000293000 |
| B | 1.870039000 | 3.821113000 | 0.000166000 |
| B | 2.907956000 | -2.840601000 | -1.430091000 |
| B | 1.454735000 | -3.674150000 | -1.462579000 |

| | | | |
|---|--------------|--------------|--------------|
| B | -1.802490000 | -3.643116000 | -1.429974000 |
| B | -3.043005000 | -2.517058000 | -1.462438000 |
| B | -4.021289000 | 0.588597000 | -1.429944000 |
| B | -3.336554000 | 2.117733000 | -1.462466000 |
| B | -0.683223000 | 4.007373000 | -1.429844000 |
| B | 0.982522000 | 3.828265000 | -1.462523000 |
| B | 3.599525000 | 1.887876000 | -1.429924000 |
| B | 3.942365000 | 0.247889000 | -1.462544000 |
| B | 0.634751000 | -3.769998000 | -2.945407000 |
| B | -0.970780000 | -3.781677000 | -2.920632000 |
| B | -3.388703000 | -1.768077000 | -2.945391000 |
| B | -3.896278000 | -0.244737000 | -2.920922000 |
| B | -2.729562000 | 2.677345000 | -2.944986000 |
| B | -1.437453000 | 3.630313000 | -2.920463000 |
| B | 1.702056000 | 3.422704000 | -2.945008000 |
| B | 3.007905000 | 2.488657000 | -2.920675000 |
| B | 3.781393000 | -0.561629000 | -2.945197000 |
| B | 3.296785000 | -2.092479000 | -2.920654000 |
| B | -2.371889000 | -2.997578000 | -2.945256000 |
| B | -3.584218000 | 1.329998000 | -2.945318000 |
| B | 0.156805000 | 3.820123000 | -2.944917000 |
| B | 3.680572000 | 1.030758000 | -2.945237000 |
| B | 2.118608000 | -3.183203000 | -2.945277000 |
| B | -3.916847000 | -1.087729000 | -1.430283000 |
| B | -2.245576000 | 3.389201000 | -1.429922000 |
| B | 2.528389000 | 3.181733000 | -1.429696000 |
| B | 3.808631000 | -1.422121000 | -1.430114000 |
| B | -0.175382000 | -4.060854000 | -1.430095000 |
| B | 0.201819000 | 4.249747000 | 0.000317000 |
| B | 4.105047000 | 1.120998000 | -0.000149000 |
| B | 2.333932000 | -3.555960000 | 0.000103000 |
| B | -2.661176000 | -3.318932000 | -0.000351000 |
| B | -3.978739000 | 1.504704000 | 0.000082000 |
| B | 2.529248000 | 3.182395000 | 1.429972000 |
| B | -2.245226000 | 3.388786000 | 1.430120000 |
| B | -3.916534000 | -1.088119000 | 1.430027000 |
| B | -0.175779000 | -4.060789000 | 1.429990000 |
| B | 3.808518000 | -1.421803000 | 1.429996000 |
| B | 3.682016000 | 1.031005000 | 2.945098000 |
| B | 2.117946000 | -3.182000000 | 2.945306000 |
| B | -2.373253000 | -2.998761000 | 2.944964000 |
| B | -3.583576000 | 1.329109000 | 2.945260000 |
| B | 0.157032000 | 3.819128000 | 2.945334000 |

B₇₀ tubular Structure dianion (II)

| | | | |
|---|-------------|-------------|--------------|
| B | 2.486638000 | 2.862565000 | -2.973222000 |
| B | 1.143127000 | 3.727571000 | -2.932977000 |

| | | | |
|---|--------------|--------------|--------------|
| B | -2.004767000 | 3.297103000 | -2.948668000 |
| B | -3.182272000 | 2.184142000 | -2.975729000 |
| B | -3.801674000 | -0.886894000 | -2.972194000 |
| B | -3.098586000 | -2.313881000 | -2.970753000 |
| B | -0.319415000 | -3.751005000 | -2.962993000 |
| B | 1.293978000 | -3.676565000 | -2.935042000 |
| B | 3.615379000 | -1.509206000 | -2.952567000 |
| B | 3.852294000 | 0.076148000 | -2.988239000 |
| B | 0.356652000 | 3.997221000 | -1.439918000 |
| B | -1.318265000 | 3.729626000 | -1.479791000 |
| B | -3.786169000 | 1.575684000 | -1.469718000 |
| B | -4.058860000 | -0.079836000 | -1.491787000 |
| B | -2.666282000 | -3.036387000 | -1.450016000 |
| B | -1.164478000 | -3.779098000 | -1.479754000 |
| B | 2.102373000 | -3.461184000 | -1.450778000 |
| B | 3.295499000 | -2.259376000 | -1.482341000 |
| B | 3.992049000 | 0.924575000 | -1.459548000 |
| B | 3.199030000 | 2.386732000 | -1.481653000 |
| B | -2.143256000 | 3.556454000 | 0.000079000 |
| B | -3.984907000 | -0.940487000 | 0.000094000 |
| B | -0.377353000 | -4.175238000 | 0.000146000 |
| B | 3.830036000 | -1.609318000 | -0.000122000 |
| B | 2.764346000 | 3.168643000 | -0.000124000 |
| B | -3.786011000 | 1.575569000 | 1.469858000 |
| B | -4.059731000 | -0.079813000 | 1.491983000 |
| B | -2.666350000 | -3.036354000 | 1.450311000 |
| B | -1.164144000 | -3.778150000 | 1.479933000 |
| B | 2.102567000 | -3.461134000 | 1.450740000 |
| B | 3.295714000 | -2.259298000 | 1.482122000 |
| B | 3.992387000 | 0.924656000 | 1.459279000 |
| B | 3.199013000 | 2.386577000 | 1.481299000 |
| B | 0.356853000 | 3.997315000 | 1.439796000 |
| B | -1.317845000 | 3.728598000 | 1.479777000 |
| B | -3.802033000 | -0.886824000 | 2.972393000 |
| B | -3.098497000 | -2.313559000 | 2.971016000 |
| B | -0.319122000 | -3.750435000 | 2.963187000 |
| B | 1.294325000 | -3.676450000 | 2.935053000 |
| B | 3.615759000 | -1.509150000 | 2.952338000 |
| B | 3.852511000 | 0.076210000 | 2.987997000 |
| B | 2.486958000 | 2.862656000 | 2.973001000 |
| B | 1.143481000 | 3.727670000 | 2.932795000 |
| B | -2.004396000 | 3.296642000 | 2.948763000 |
| B | -3.182190000 | 2.183956000 | 2.975887000 |
| B | -1.865872000 | -3.367332000 | 2.949700000 |
| B | 2.605436000 | -2.765887000 | 2.973948000 |
| B | 3.549248000 | 1.652133000 | 2.950900000 |
| B | -0.469429000 | 3.731637000 | 2.964672000 |
| B | -3.842717000 | 0.736155000 | 2.970685000 |

| | | | |
|---|--------------|--------------|--------------|
| B | 0.519136000 | -3.976732000 | 1.439554000 |
| B | 4.029430000 | -0.766694000 | 1.460652000 |
| B | 1.957275000 | 3.540052000 | 1.448320000 |
| B | -2.788655000 | 2.931819000 | 1.452017000 |
| B | -3.720456000 | -1.725902000 | 1.469995000 |
| B | 3.763645000 | 1.763519000 | -0.000153000 |
| B | -0.544758000 | 4.160257000 | 0.000057000 |
| B | -4.014033000 | 0.777715000 | 0.000077000 |
| B | -1.999114000 | -3.643088000 | 0.000156000 |
| B | 2.884661000 | -3.052683000 | -0.000060000 |
| B | 1.957048000 | 3.539932000 | -1.448536000 |
| B | 4.029186000 | -0.766714000 | -1.460900000 |
| B | 0.518938000 | -3.976826000 | -1.439484000 |
| B | -3.720629000 | -1.726091000 | -1.469779000 |
| B | -2.788519000 | 2.931702000 | -1.451836000 |
| B | -0.469757000 | 3.732026000 | -2.964666000 |
| B | -3.842312000 | 0.736093000 | -2.970542000 |
| B | -1.866185000 | -3.367868000 | -2.949450000 |
| B | 2.605100000 | -2.765977000 | -2.974037000 |
| B | 3.548967000 | 1.652082000 | -2.951200000 |