

New chiral member B₄₄ containing nonagonal holes

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Supplementary Information. The file contains

- Shapes and relative energies of the low-lying isomers of B₄₄ obtained at the PBE0/6-311+G(d) level (Figure S1)
- Born-Oppenheimer molecular simulations of the lowest isomers B₄₄ at 300K and 500K. The root-mean square deviation (RMSD) values are analyzed using VMD code (Figure S2)
- Cartesian coordinates of the low-lying isomers (Table S1)

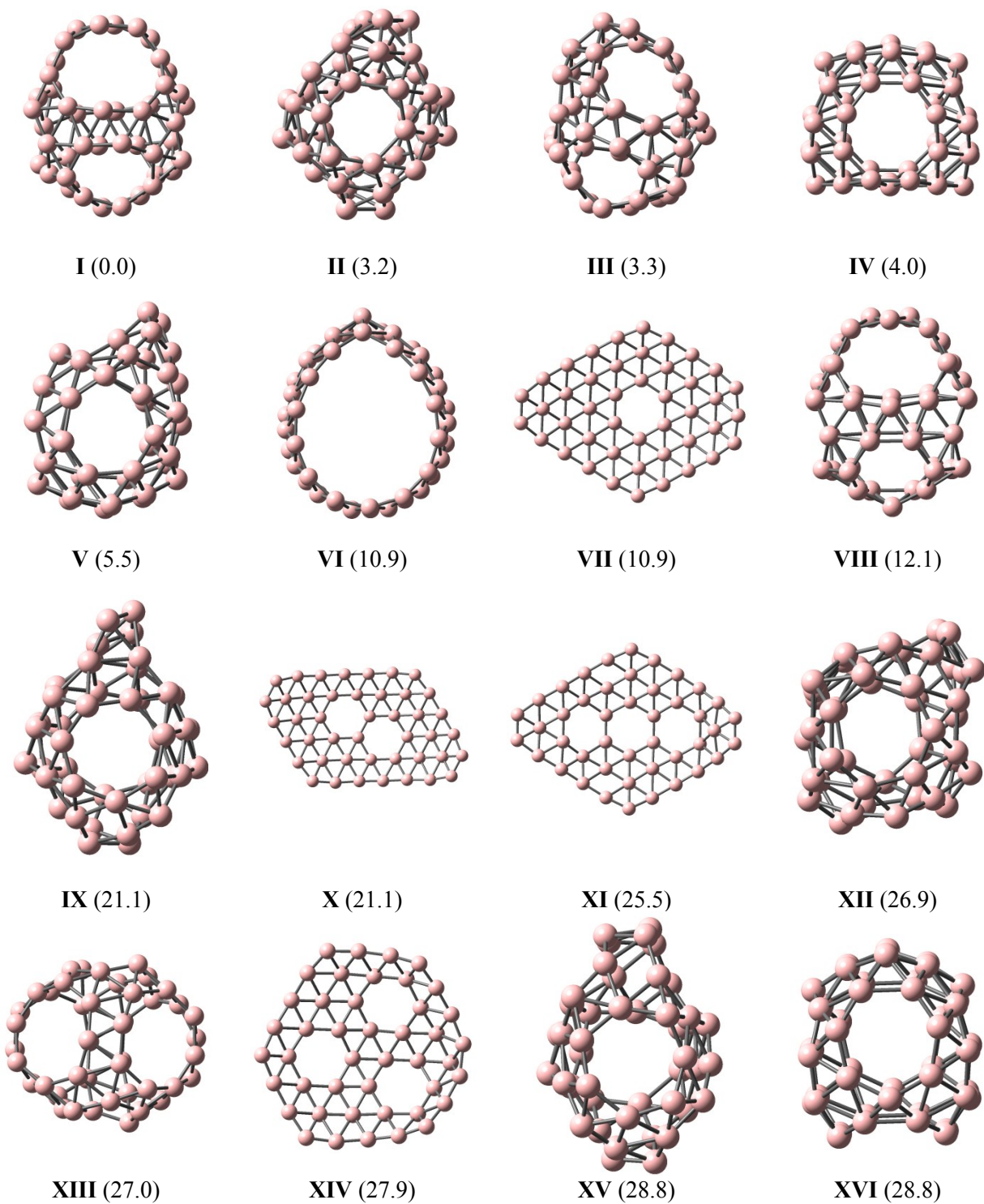
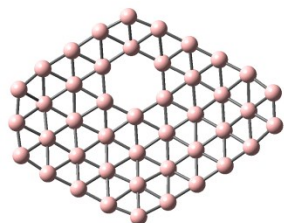
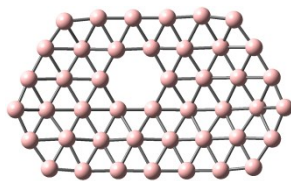


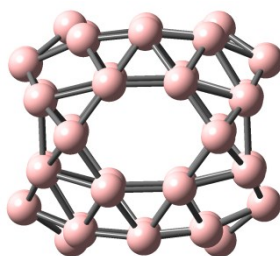
Figure S1 Shapes and relative energies (kcal/mol) of the low-lying isomers of B₄₄ obtained at the PBE0/6-311+G(d) level



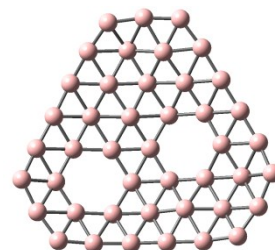
XVII (29.2)



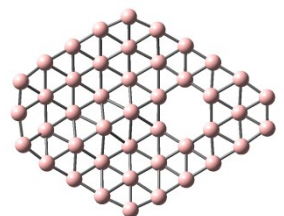
XVIII (36.8)



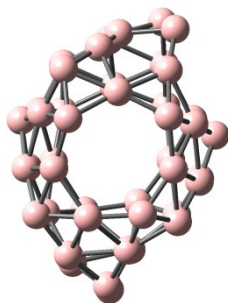
XIX (39.5)



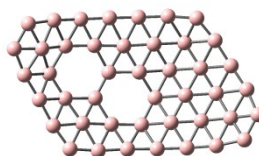
XX (42.9)



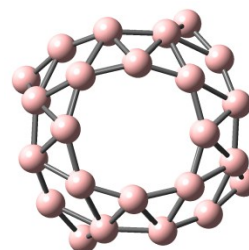
XXI (43.2)



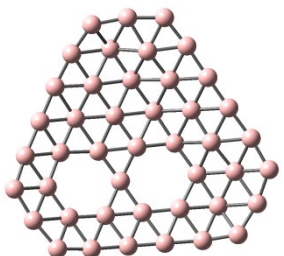
XXII (43.3)



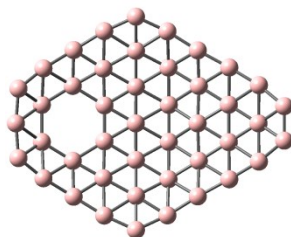
XXIII (43.7)



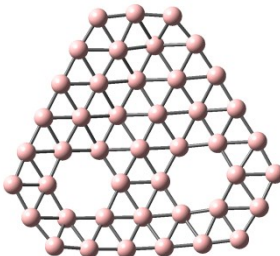
XXIV (48.5)



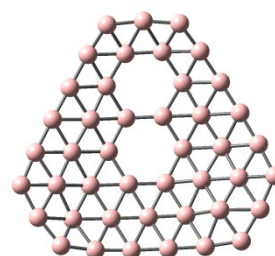
XXV (53.6)



XXVI (54.5)



XXVII (59.6)



XXVIII (60.0)

Figure S1 continued

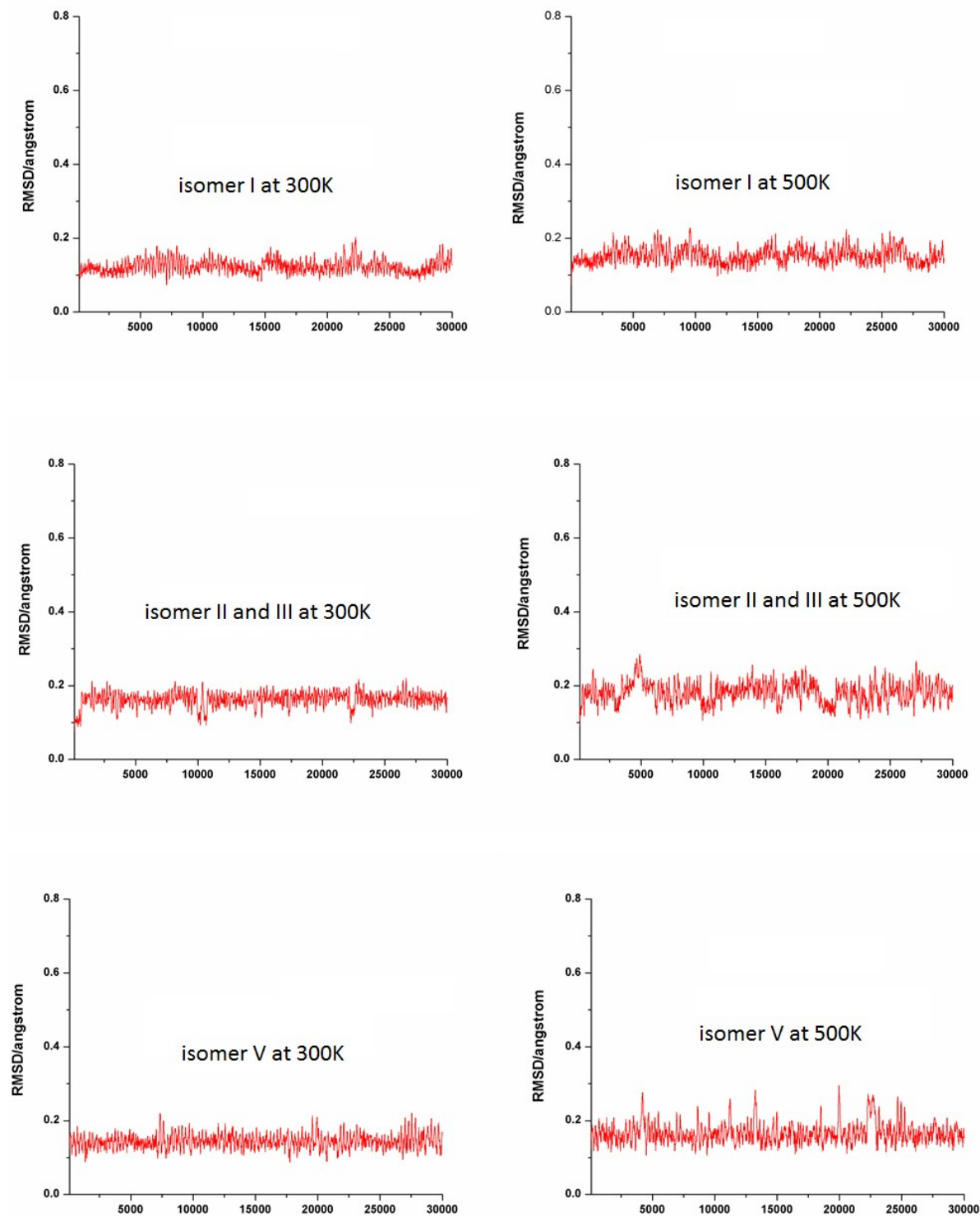


Figure S2 Born-Oppenheimer molecular simulations of the lowest isomers B44 at 300K and 500K. The root-mean square deviation (RMSD) values are analyzed using VMD code

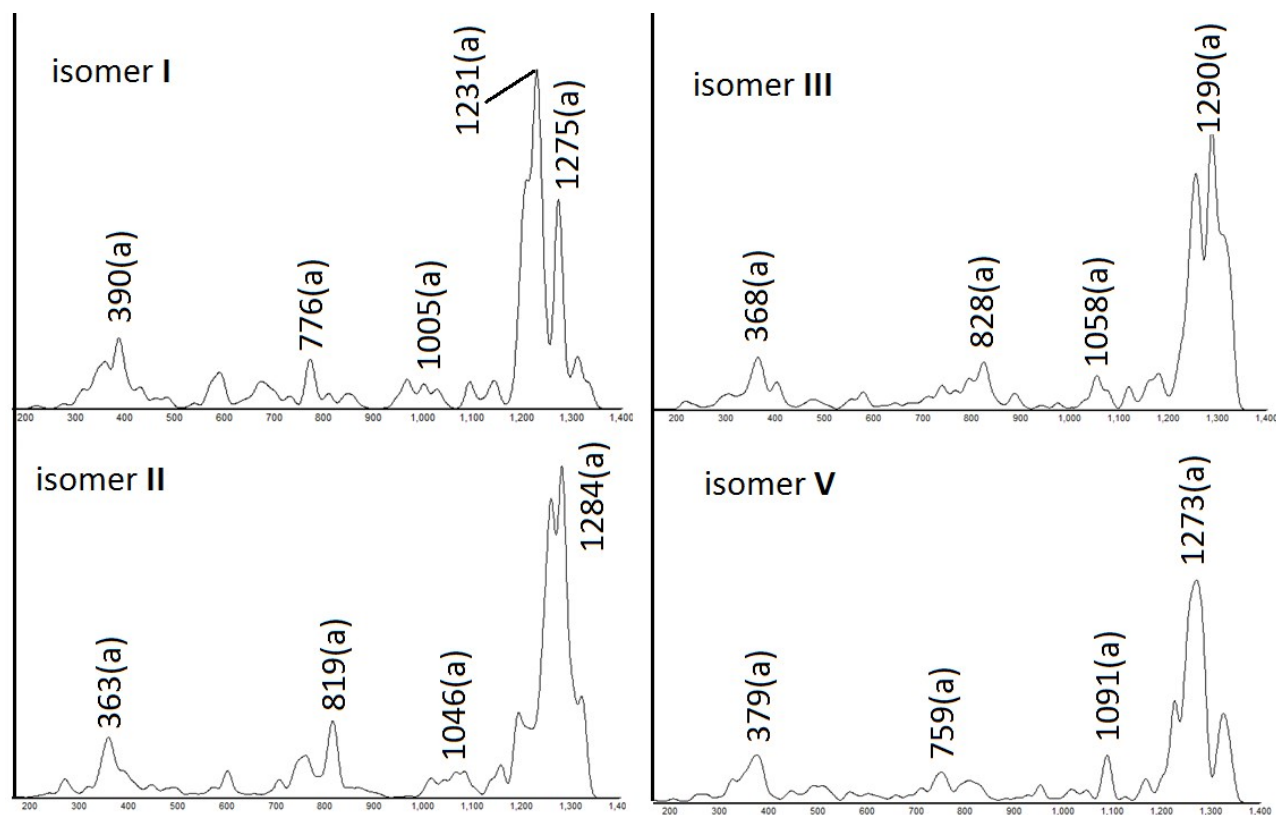


Figure S3. Infrared (IR) spectra of the lowest isomers B₄₄

Table S1 Cartesian coordinates of the low-lying isomers

Isomer I			
5	-2.920362000	-1.244692000	-0.609823000
5	-3.469635000	0.330588000	-0.718954000
5	-1.280976000	1.527828000	-2.323422000
5	-0.804081000	0.146477000	-2.940933000
5	-0.700830000	-2.828008000	-1.407463000
5	0.826168000	-1.987395000	-1.951728000
5	0.528541000	1.076974000	-2.463443000
5	-2.925044000	1.242139000	0.606784000
5	-2.605042000	-1.598301000	1.185379000
5	-0.849825000	-1.391266000	-2.336993000
5	0.598341000	-0.587788000	-2.719236000
5	-2.604249000	1.596407000	-1.187318000
5	-3.471426000	-0.334277000	0.714020000
5	-2.143066000	-2.147800000	-1.689429000
5	0.768258000	-3.355959000	-1.026570000
5	-1.968359000	-2.604423000	-0.139015000
5	0.020743000	2.576091000	-1.704887000
5	-1.584574000	2.834665000	-1.431177000
5	-1.974242000	2.603845000	0.139268000
5	0.522226000	-1.072370000	2.472334000
5	0.587686000	0.592530000	2.728366000
5	3.596158000	1.913900000	0.701861000
5	4.075323000	-1.188553000	0.709817000
5	1.587778000	-2.175700000	1.939964000
5	3.602512000	-1.902918000	-0.682329000
5	2.700764000	2.083508000	-0.767901000
5	-0.860810000	1.393006000	2.341108000
5	-1.285855000	-1.526978000	2.326056000
5	2.702389000	-2.074392000	0.784324000
5	4.075269000	1.200522000	-0.688637000
5	0.815266000	1.992610000	1.961643000
5	-0.813967000	-0.144643000	2.945209000
5	1.199317000	-2.838537000	0.483833000
5	0.020171000	-2.572537000	1.712035000
5	1.195080000	2.844532000	-0.472615000
5	0.757723000	3.361055000	1.036286000
5	2.190728000	2.656956000	0.980159000
5	-0.711577000	2.830055000	1.412094000
5	1.589952000	2.182510000	-1.927391000
5	2.199599000	-2.648891000	-0.965486000
5	-1.583649000	-2.834440000	1.432770000
5	-2.153368000	2.146857000	1.689071000
5	4.185760000	0.392433000	0.777684000
5	4.189218000	-0.380231000	-0.756117000

Isomer II

5	9.788285000	5.557729000	8.612732000
5	10.984437000	6.583636000	8.071730000
5	9.846139000	9.199184000	8.860017000
5	8.999335000	8.624053000	10.074917000
5	7.217768000	5.791953000	9.783877000
5	6.412192000	7.428908000	10.012652000
5	8.094158000	9.752355000	9.188288000
5	10.698657000	6.959317000	6.445268000
5	9.129109000	4.629576000	7.164465000
5	8.179548000	7.161269000	10.191143000
5	7.429613000	8.659541000	10.262863000
5	10.801248000	8.159590000	7.839987000
5	10.515171000	5.432197000	7.095426000
5	8.837536000	5.714028000	9.907911000
5	5.628190000	5.975294000	9.516160000
5	8.256853000	4.755700000	8.728517000
5	8.940714000	10.305823000	7.783288000
5	10.415948000	9.679827000	7.423027000
5	10.433549000	8.640288000	6.156297000
5	6.450428000	5.652907000	5.312086000
5	7.075932000	6.849245000	4.338965000
5	5.058593000	9.315930000	6.315385000
5	4.174379000	8.256861000	7.266127000
5	5.070585000	5.595524000	6.127213000
5	3.951913000	8.807724000	8.896745000
5	6.169737000	10.171858000	7.226423000
5	8.745414000	7.069970000	4.575068000
5	7.878565000	4.654560000	5.943640000
5	3.383053000	7.386455000	8.456337000
5	4.723282000	9.745827000	7.866730000
5	7.418339000	8.395558000	4.589428000
5	7.999743000	5.593634000	4.651397000
5	4.138927000	5.982984000	8.782764000
5	6.281318000	4.641027000	6.713865000
5	7.707110000	10.417032000	6.525998000
5	7.980850000	9.848918000	5.030080000
5	6.466226000	9.513649000	5.575781000
5	9.134745000	8.705611000	4.935633000
5	7.412358000	10.739061000	8.096856000
5	4.788561000	7.444363000	9.491568000
5	7.643727000	4.020872000	7.413338000
5	10.237670000	7.511080000	5.000462000
5	5.293423000	5.464522000	7.785406000
5	4.095249000	6.456247000	7.126405000

Isomer III

5	2.826383000	-1.159436000	0.616129000
5	3.438353000	0.388612000	0.782799000
5	1.264919000	1.590378000	2.373394000
5	0.831990000	0.238643000	3.099766000
5	0.518767000	-2.627051000	1.364547000
5	-0.956710000	-1.810456000	2.172615000
5	-0.513005000	1.139805000	2.607221000
5	2.957256000	1.307811000	-0.554380000
5	2.576148000	-1.483825000	-1.170074000
5	0.787662000	-1.303188000	2.477714000
5	-0.572724000	-0.482290000	3.011164000
5	2.565903000	1.662558000	1.212339000
5	3.483199000	-0.268193000	-0.654432000
5	1.992424000	-2.034390000	1.683648000
5	-0.999604000	-3.115231000	1.160104000
5	1.785529000	-2.446080000	0.114087000
5	-0.081167000	2.565531000	1.723593000
5	1.499286000	2.872154000	1.412121000
5	1.930657000	2.628229000	-0.148870000
5	-0.311349000	-0.960034000	-3.048012000
5	-0.278423000	0.709049000	-3.199105000
5	-3.092986000	0.780487000	-0.707973000
5	-3.311336000	-0.855948000	-0.484968000
5	-1.444072000	-2.005366000	-2.643538000
5	-3.784365000	-1.289762000	1.123864000
5	-2.484848000	1.493267000	0.680809000
5	1.094225000	1.437902000	-2.539367000
5	1.471246000	-1.444875000	-2.533818000
5	-3.570934000	-2.444319000	0.062949000
5	-3.567297000	0.247531000	0.774152000
5	-0.690412000	1.915052000	-2.222115000
5	1.114090000	-0.050827000	-3.253179000
5	-2.095832000	-3.237562000	-0.121313000
5	0.085735000	-2.469611000	-2.297609000
5	-1.287183000	2.697361000	0.433500000
5	-0.839914000	3.058682000	-1.084987000
5	-1.984512000	1.885639000	-1.013686000
5	0.710197000	2.695072000	-1.438712000
5	-1.621381000	2.093997000	1.909295000
5	-2.326366000	-2.188727000	1.309429000
5	1.502683000	-2.667131000	-1.476699000
5	2.237523000	2.194653000	-1.692912000
5	-1.159654000	-2.991144000	-1.405308000
5	-2.569073000	-2.148197000	-1.362302000

Isomer IV

5	1.743358000	-3.148092000	-0.075077000
5	1.645811000	0.000000000	-3.026551000
5	1.338387000	-2.519656000	-1.554189000
5	-1.743358000	3.148092000	-0.075077000
5	0.000000000	3.016482000	2.609931000
5	2.293983000	-0.796714000	2.200205000
5	-2.254510000	0.863040000	-1.801840000
5	-2.154762000	-1.940896000	1.028022000
5	-1.743358000	-3.148092000	-0.075077000
5	-1.645811000	0.000000000	-3.026551000
5	-1.338387000	-2.519656000	-1.554189000
5	2.539540000	1.834206000	-0.554722000
5	1.338387000	2.519656000	-1.554189000
5	-1.338387000	2.519656000	-1.554189000
5	-0.868035000	3.233698000	1.258947000
5	0.868035000	-3.233698000	1.258947000
5	-2.254510000	-0.863040000	-1.801840000
5	0.868035000	3.233698000	1.258947000
5	0.000000000	2.724130000	-2.441274000
5	2.539540000	-1.834206000	-0.554722000
5	2.254510000	-0.863040000	-1.801840000
5	2.254510000	0.863040000	-1.801840000
5	-2.154762000	1.940896000	1.028022000
5	2.154762000	-1.940896000	1.028022000
5	2.154762000	1.940896000	1.028022000
5	-0.878630000	1.420780000	-2.823165000
5	0.878630000	1.420780000	-2.823165000
5	1.743358000	3.148092000	-0.075077000
5	1.197979000	1.920144000	2.469747000
5	-2.293983000	-0.796714000	2.200205000
5	-0.868035000	-3.233698000	1.258947000
5	-0.878630000	-1.420780000	-2.823165000
5	0.878630000	-1.420780000	-2.823165000
5	1.197979000	-1.920144000	2.469747000
5	-2.539540000	1.834206000	-0.554722000
5	0.000000000	-2.724130000	-2.441274000
5	-1.197979000	1.920144000	2.469747000
5	0.000000000	-3.016482000	2.609931000
5	-2.539540000	-1.834206000	-0.554722000
5	-1.197979000	-1.920144000	2.469747000
5	0.852241000	0.000000000	2.567228000
5	2.293983000	0.796714000	2.200205000
5	-0.852241000	0.000000000	2.567228000
5	-2.293983000	0.796714000	2.200205000

Isomer V

5	2.912832000	-1.263238000	0.652247000
5	3.375025000	0.333642000	0.724660000
5	1.093095000	1.497343000	2.225421000
5	0.751520000	0.145559000	3.011535000
5	0.671620000	-2.795374000	1.454370000
5	-0.814884000	-2.022460000	2.099432000
5	-0.669756000	0.906608000	2.474203000
5	2.918923000	1.199852000	-0.648995000
5	2.639646000	-1.680128000	-1.142239000
5	0.866321000	-1.420159000	2.481398000
5	-0.583866000	-0.692484000	2.955558000
5	2.425518000	1.568435000	1.080875000
5	3.462375000	-0.384586000	-0.683069000
5	2.126135000	-2.133556000	1.752470000
5	-0.837012000	-3.219669000	1.001221000
5	1.931643000	-2.610941000	0.208886000
5	-0.290697000	2.353216000	1.552571000
5	1.291112000	2.722495000	1.213879000
5	1.826732000	2.523004000	-0.307740000
5	-0.394911000	-1.139157000	-2.629859000
5	-0.444889000	0.500967000	-3.005578000
5	-3.029426000	1.358844000	-0.873719000
5	-3.318628000	-0.208736000	-0.737680000
5	-1.522727000	-2.111433000	-1.991116000
5	-3.125574000	-1.008880000	0.647336000
5	-3.164109000	2.257865000	0.822794000
5	1.001810000	1.263535000	-2.543526000
5	1.357505000	-1.599750000	-2.335958000
5	-2.457673000	-1.615414000	-0.772893000
5	-2.990042000	0.657659000	0.699538000
5	-0.766126000	1.940854000	-2.334980000
5	0.954914000	-0.266235000	-3.113449000
5	-1.238858000	-2.794761000	-0.538661000
5	0.012726000	-2.595558000	-1.737322000
5	-1.607839000	3.075429000	0.783907000
5	-0.678254000	3.476172000	-1.663669000
5	-3.048424000	3.595057000	-0.065317000
5	0.757906000	2.714043000	-1.699798000
5	-1.850403000	1.707751000	1.749121000
5	-2.083633000	-2.185522000	0.917509000
5	1.576015000	-2.880978000	-1.362949000
5	2.229241000	2.051754000	-1.821099000
5	-1.714122000	4.127239000	-0.620775000
5	-2.077222000	2.600967000	-1.386234000