# Hybrid Boron-Carbon Chemistry

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**Supplementary Information**

B3LYP/cc-pVTZ optimised geometries, in cartesian coordinates (Å), of the systems included in the work.

**Cyclobutadiene $C_{(4-2k)}B_{(2k)}H_{(4+2k)}$**

$C_4H_4$ (k=0)

| | | | |
|---|---|---|---|
| C | 0.00000000 | 0.66449100 | 0.78749200 |
| C | 0.00000000 | 0.66449100 | -0.78749200 |
| C | 0.00000000 | -0.66449100 | -0.78749200 |
| C | 0.00000000 | -0.66449100 | 0.78749200 |
| H | 0.00000000 | -1.42696700 | 1.55081200 |
| H | 0.00000000 | -1.42696700 | -1.55081200 |
| H | 0.00000000 | 1.42696700 | -1.55081200 |
| H | 0.00000000 | 1.42696700 | 1.55081200 |

$C_2B_2H_6$ (k=1)

| | | | |
|---|---|---|---|
| H | 0.00000000 | 1.78498000 | 1.52627900 |
| H | 0.00000000 | -1.78498000 | 1.52627900 |
| H | 0.00000000 | -1.34894500 | -1.66938200 |
| H | 0.00000000 | 1.34894500 | -1.66938200 |
| B | 0.00000000 | -0.87052800 | 0.77285400 |
| B | 0.00000000 | 0.87052800 | 0.77285400 |
| H | -0.92909800 | 0.00000000 | 1.23502700 |
| H | 0.92909800 | 0.00000000 | 1.23502700 |
| C | 0.00000000 | 0.66904600 | -0.82603200 |
| C | 0.00000000 | -0.66904600 | -0.82603200 |

$B_4H_8$ (k=2)

| | | | |
|---|---|---|---|
| H | -1.71160800 | 1.71397900 | 0.00000000 |
| H | -1.71160800 | -1.71397900 | 0.00000000 |
| H | 1.71160800 | -1.71397900 | 0.00000000 |
| H | 1.71160800 | 1.71397900 | 0.00000000 |
| B | 0.86381500 | -0.87990900 | 0.00000000 |
| B | 0.86381500 | 0.87990900 | 0.00000000 |
| B | -0.86381500 | -0.87990900 | 0.00000000 |
| B | -0.86381500 | 0.87990900 | 0.00000000 |
| H | 1.25257700 | 0.00000000 | 0.92784800 |
| H | 1.25257700 | 0.00000000 | -0.92784800 |
| H | -1.25257700 | 0.00000000 | -0.92784800 |
| H | -1.25257700 | 0.00000000 | 0.92784800 |

**Benzene $C_{(6-2k)}B_{(2k)}H_{(6+2k)}$**

$C_6H_6$ (k=0)

| | | | |
|---|---|---|---|
| C | 0.00000000 | 1.39076500 | 0.00000000 |
| C | -1.20443800 | 0.69538200 | 0.00000000 |
| C | -1.20443800 | -0.69538200 | 0.00000000 |
| C | 0.00000000 | -1.39076500 | 0.00000000 |
| C | 1.20443800 | -0.69538200 | 0.00000000 |
| C | 1.20443800 | 0.69538200 | 0.00000000 |
| H | 0.00000000 | 2.47280200 | 0.00000000 |
| H | -2.14150900 | 1.23640100 | 0.00000000 |
| H | -2.14150900 | -1.23640100 | 0.00000000 |
| H | 0.00000000 | -2.47280200 | 0.00000000 |
| H | 2.14150900 | -1.23640100 | 0.00000000 |
| H | 2.14150900 | 1.23640100 | 0.00000000 |

$C_4B_2H_8$ (k=1)

| | | | |
|---|---|---|---|
| C | 0.00000000 | 1.49120300 | -0.10055000 |
| C | 0.00000000 | -1.49120300 | -0.10055000 |
| C | 0.00000000 | -0.71930100 | -1.21923400 |
| C | 0.00000000 | 0.71930100 | -1.21923400 |
| H | 0.00000000 | 2.56640100 | -0.24278400 |
| H | 0.00000000 | 1.54325200 | 2.31646900 |
| H | 0.00000000 | -1.54325200 | 2.31646900 |
| H | 0.00000000 | -2.56640100 | -0.24278400 |
| H | 0.00000000 | -1.19650700 | -2.19420300 |
| H | 0.00000000 | 1.19650700 | -2.19420300 |
| B | 0.00000000 | -0.89939400 | 1.31987000 |
| B | 0.00000000 | 0.89939400 | 1.31987000 |
| H | -0.96295600 | 0.00000000 | 1.43987600 |
| H | 0.96295600 | 0.00000000 | 1.43987600 |

$C_2B_4H_{10}$ (k=2)

| | | | |
|---|---|---|---|
| B | 0.00000000 | 1.60722500 | -0.12028500 |
| B | 0.00000000 | -1.60722500 | -0.12028500 |
| B | 0.00000000 | -0.84728100 | 1.49972800 |
| B | 0.00000000 | 0.84728100 | 1.49972800 |
| H | 0.00000000 | -1.16961700 | -2.34569700 |
| H | 0.00000000 | -2.79016900 | -0.23829300 |
| H | 0.00000000 | 1.54256800 | 2.46348600 |
| H | 0.00000000 | 2.79016900 | -0.23829300 |
| H | 0.00000000 | 1.16961700 | -2.34569700 |
| H | 0.00000000 | -1.54256800 | 2.46348600 |
| H | 0.96318500 | 1.30844000 | 0.74133900 |
| H | 0.96318500 | -1.30844000 | 0.74133900 |
| H | -0.96318500 | 1.30844000 | 0.74133900 |
| H | -0.96318500 | -1.30844000 | 0.74133900 |
| C | 0.00000000 | 0.67520900 | -1.37656400 |
| C | 0.00000000 | -0.67520900 | -1.37656400 |

$B_6H_{12}$ (k=3)

| | | | |
|---|---|---|---|
| B | -0.85625500 | 1.52943200 | 0.00000000 |
| B | 0.85625500 | 1.52943200 | 0.00000000 |
| B | 1.75265400 | -0.02317800 | 0.00000000 |
| B | 0.89640000 | -1.50625400 | 0.00000000 |
| B | -0.89640000 | -1.50625400 | 0.00000000 |
| B | -1.75265400 | -0.02317800 | 0.00000000 |
| H | 2.94137100 | 0.02759400 | 0.00000000 |
| H | 1.44678800 | -2.56109900 | 0.00000000 |
| H | -2.94137100 | 0.02759400 | 0.00000000 |
| H | -1.49458300 | 2.53350500 | 0.00000000 |
| H | 1.49458300 | 2.53350500 | 0.00000000 |
| H | -1.44678800 | -2.56109900 | 0.00000000 |
| H | -1.35280000 | 0.78103900 | 0.96131800 |
| H | 0.00000000 | -1.56207900 | 0.96131800 |
| H | 1.35280000 | 0.78103900 | 0.96131800 |
| H | -1.35280000 | 0.78103900 | -0.96131800 |
| H | 0.00000000 | -1.56207900 | -0.96131800 |
| H | 1.35280000 | 0.78103900 | -0.96131800 |

**Cyclooctatetraene $C_{(8-2k)}B_{(2k)}H_{(8+2k)}$**

$C_8H_8$ (k=0)

| | | | |
|---|---|---|---|
| C | 0.66759400 | 1.56391900 | 0.37091800 |
| C | -0.66759400 | 1.56391900 | 0.37091800 |
| C | -1.56391900 | 0.66759400 | -0.37091800 |
| C | 1.56391900 | 0.66759400 | -0.37091800 |
| C | -1.56391900 | -0.66759400 | -0.37091800 |
| C | 1.56391900 | -0.66759400 | -0.37091800 |
| C | -0.66759400 | -1.56391900 | 0.37091800 |
| C | 0.66759400 | -1.56391900 | 0.37091800 |
| H | -1.16679300 | 2.35821000 | 0.91903900 |
| H | 1.16679300 | 2.35821000 | 0.91903900 |
| H | 2.35821000 | 1.16679300 | -0.91903900 |
| H | 2.35821000 | -1.16679300 | -0.91903900 |
| H | 1.16679300 | -2.35821000 | 0.91903900 |
| H | -1.16679300 | -2.35821000 | 0.91903900 |
| H | -2.35821000 | -1.16679300 | -0.91903900 |
| H | -2.35821000 | 1.16679300 | -0.91903900 |

$C_6B_2H_{10}$ (k=1)

| | | | |
|---|---|---|---|
| C | -0.71054900 | 0.22540200 | 1.70127100 |
| C | -0.71054900 | 0.22540200 | -1.70127100 |
| C | 0.14155700 | -0.80183400 | 1.60497000 |
| C | 0.14155700 | -0.80183400 | -1.60497000 |
| C | 1.26135300 | -0.98030400 | 0.66963000 |
| C | 1.26135300 | -0.98030400 | -0.66963000 |
| H | -0.73412500 | 2.60664200 | -1.44709900 |
| H | -1.43044400 | 0.16555000 | -2.51463000 |
| H | 0.07450600 | -1.59351300 | -2.34913200 |
| H | 2.20034800 | -1.24373700 | -1.15006700 |
| H | 2.20034800 | -1.24373700 | 1.15006700 |
| H | 0.07450600 | -1.59351300 | 2.34913200 |
| H | -1.43044400 | 0.16555000 | 2.51463000 |
| B | -0.71054900 | 1.55711000 | -0.88501000 |
| B | -0.71054900 | 1.55711000 | 0.88501000 |
| H | 0.26039900 | 1.61318600 | 0.00000000 |
| H | -1.68380300 | 1.62665700 | 0.00000000 |
| H | -0.73412500 | 2.60664200 | 1.44709900 |

$C_4B_4H_{12}$ (k=2) Isomer I

| | | | |
|---|---|---|---|
| C | -1.78272300 | 0.67072000 | -0.40761300 |
| C | 1.78272300 | 0.67072000 | -0.40761300 |
| C | -1.78272300 | -0.67072000 | -0.40761300 |
| C | 1.78272300 | -0.67072000 | -0.40761300 |
| H | 1.40346300 | 2.53506300 | 1.03984000 |
| H | 2.56280200 | 1.15373100 | -0.99685100 |
| H | 2.56280200 | -1.15373100 | -0.99685100 |
| H | 1.40346300 | -2.53506300 | 1.03984000 |
| H | -1.40346300 | -2.53506300 | 1.03984000 |
| H | -2.56280200 | -1.15373100 | -0.99685100 |
| H | -2.56280200 | 1.15373100 | -0.99685100 |
| B | 0.89249700 | 1.67224800 | 0.39857400 |
| B | -0.89249700 | 1.67224800 | 0.39857400 |
| H | 0.00000000 | 1.10144800 | 1.17997200 |
| H | 0.00000000 | 2.28118300 | -0.36033300 |
| H | -1.40346300 | 2.53506300 | 1.03984000 |
| B | 0.89249700 | -1.67224800 | 0.39857400 |
| B | -0.89249700 | -1.67224800 | 0.39857400 |
| H | 0.00000000 | -2.28118300 | -0.36033300 |
| H | 0.00000000 | -1.10144800 | 1.17997200 |

$C_4B_4H_{12}$ (k=2) Isomer II

| | | | |
|---|---|---|---|
| C | -0.95783000 | 1.37512200 | -0.75133900 |
| C | -0.59567000 | 0.43447500 | -1.63469300 |
| H | 0.05706800 | 3.04401900 | 0.61174900 |
| H | -1.84988200 | 1.93896000 | -1.01848300 |
| H | -1.19603600 | 0.33360300 | -2.53774200 |
| H | 1.19603600 | -0.33360300 | -2.53774200 |
| H | 1.84988200 | -1.93896000 | -1.01848300 |
| H | -0.05706800 | -3.04401900 | 0.61174900 |
| H | -0.78903300 | -1.32404500 | 2.79004200 |
| B | -0.20727800 | 1.88614800 | 0.52187200 |
| B | 0.20727800 | 0.82135900 | 1.88100200 |
| H | 0.86386300 | 1.18116500 | 0.80001800 |
| H | -0.83349200 | 1.57429700 | 1.65623800 |
| H | 0.78903300 | 1.32404500 | 2.79004200 |
| B | -0.20727800 | -0.82135900 | 1.88100200 |
| B | 0.20727800 | -1.88614800 | 0.52187200 |
| H | -0.86386300 | -1.18116500 | 0.80001800 |
| H | 0.83349200 | -1.57429700 | 1.65623800 |
| C | 0.59567000 | -0.43447500 | -1.63469300 |
| C | 0.95783000 | -1.37512200 | -0.75133900 |

$C_2B_6H_{14}$ (k=3)

| | | | |
|---|---|---|---|
| C | 0.46566300 | -1.72870900 | 0.67162800 |
| C | 0.46566300 | -1.72870900 | -0.67162800 |
| H | -1.10272600 | -1.57125800 | 2.45972900 |
| H | 1.13708300 | -2.44396000 | 1.14894800 |
| H | 1.13708300 | -2.44396000 | -1.14894800 |
| H | -1.10272600 | -1.57125800 | -2.45972900 |
| H | -1.22717200 | 1.24578400 | -2.66109700 |
| H | 1.17745600 | 2.66404100 | -1.41750900 |
| H | 1.17745600 | 2.66404100 | 1.41750900 |
| B | -0.44068300 | -0.95340900 | 1.68626800 |
| B | -0.48434900 | 0.82652000 | 1.83051900 |
| H | -1.20064700 | -0.03314800 | 1.13771200 |
| H | 0.25057600 | -0.07631300 | 2.41970800 |
| H | -1.22717200 | 1.24578400 | 2.66109700 |
| B | -0.44068300 | -0.95340900 | -1.68626800 |
| B | -0.48434900 | 0.82652000 | -1.83051900 |
| H | 0.25057600 | -0.07631300 | -2.41970800 |
| H | -1.20064700 | -0.03314800 | -1.13771200 |
| B | 0.46566300 | 1.86874500 | 0.88828500 |
| B | 0.46566300 | 1.86874500 | -0.88828500 |
| H | 1.18831300 | 1.22906100 | 0.00000000 |
| H | -0.25172400 | 2.52658400 | 0.00000000 |

$B_8H_{16}$ (k=4)

| | | | |
|---|---|---|---|
| H | -2.63303000 | -1.40454800 | 1.25187700 |
| H | -2.63303000 | 1.40454800 | 1.25187700 |
| H | -1.40454800 | 2.63303000 | -1.25187700 |
| H | 1.40454800 | 2.63303000 | -1.25187700 |
| H | 2.63303000 | 1.40454800 | 1.25187700 |
| H | 2.63303000 | -1.40454800 | 1.25187700 |
| H | 1.40454800 | -2.63303000 | -1.25187700 |
| H | -1.40454800 | -2.63303000 | -1.25187700 |
| B | -0.89295500 | -1.86392500 | -0.49963500 |
| B | -1.86392500 | 0.89295500 | 0.49963500 |
| B | -1.86392500 | -0.89295500 | 0.49963500 |
| B | -0.89295500 | 1.86392500 | -0.49963500 |
| B | 0.89295500 | -1.86392500 | -0.49963500 |
| B | 0.89295500 | 1.86392500 | -0.49963500 |
| B | 1.86392500 | -0.89295500 | 0.49963500 |
| B | 1.86392500 | 0.89295500 | 0.49963500 |
| H | -1.19454700 | 0.00000000 | 1.19208500 |
| H | 0.00000000 | 2.53825200 | 0.19902400 |
| H | 1.19454700 | 0.00000000 | 1.19208500 |
| H | 0.00000000 | -2.53825200 | 0.19902400 |
| H | -2.53825200 | 0.00000000 | -0.19902400 |
| H | 0.00000000 | -1.19454700 | -1.19208500 |
| H | 2.53825200 | 0.00000000 | -0.19902400 |
| H | 0.00000000 | 1.19454700 | -1.19208500 |

**Benzocyclobutadiene Kekulé Structure $K_1$ : $C_{(8-2k)}B_{(2k)}H_{(6+2k)}$**

$C_8H_6$ (k=0) - same energy for Kekulé structures $K_1$, $K_2$ and $K_3$

| | | | |
|---|---|---|---|
| C | 0.00000000 | 0.68599500 | -1.83961000 |
| C | 0.00000000 | 1.43946700 | -0.62161400 |
| C | 0.00000000 | 0.70954000 | 0.52046900 |
| C | 0.00000000 | -0.70954000 | 0.52046900 |
| C | 0.00000000 | -1.43946700 | -0.62161400 |
| C | 0.00000000 | -0.68599500 | -1.83961000 |
| H | 0.00000000 | 1.21700600 | -2.78214600 |
| H | 0.00000000 | 2.52090300 | -0.64319100 |
| C | 0.00000000 | 0.67295800 | 2.04188100 |
| C | 0.00000000 | -0.67295800 | 2.04188100 |
| H | 0.00000000 | -2.52090300 | -0.64319100 |
| H | 0.00000000 | -1.21700600 | -2.78214600 |
| H | 0.00000000 | -1.42183200 | 2.81858700 |
| H | 0.00000000 | 1.42183200 | 2.81858700 |

$C_6B_2H_8$ (k=1) Isomer I

| | | | |
|---|---|---|---|
| H | 0.00000000 | -1.22482500 | -2.82319600 |
| H | 0.00000000 | -2.49922800 | -0.69308100 |
| H | 0.00000000 | 2.49922800 | -0.69308100 |
| H | 0.00000000 | 1.22482500 | -2.82319600 |
| H | 0.00000000 | 1.78527500 | 2.85974600 |
| H | 0.00000000 | -1.78527500 | 2.85974600 |
| B | 0.00000000 | -0.88719300 | 2.08761500 |
| B | 0.00000000 | 0.88719300 | 2.08761500 |
| H | -0.93056700 | 0.00000000 | 2.51413900 |
| H | 0.93056700 | 0.00000000 | 2.51413900 |
| C | 0.00000000 | -0.69263200 | -1.88068500 |
| C | 0.00000000 | -1.41627600 | -0.67422400 |
| C | 0.00000000 | -0.70716500 | 0.50562800 |
| C | 0.00000000 | 0.70716500 | 0.50562800 |
| C | 0.00000000 | 0.69263200 | -1.88068500 |
| C | 0.00000000 | 1.41627600 | -0.67422400 |

$C_6B_2H_8$ (k=1) Isomer II

| | | | |
|---|---|---|---|
| H | 0.00000000 | -1.16780600 | -2.85294600 |
| H | 0.00000000 | -2.63472900 | -0.97016700 |
| H | 0.00000000 | 2.63472900 | -0.97016700 |
| H | 0.00000000 | 1.16780600 | -2.85294600 |
| H | 0.00000000 | 1.32926600 | 3.07776000 |
| H | 0.00000000 | -1.32926600 | 3.07776000 |
| B | 0.00000000 | -0.87467500 | 0.59557200 |
| B | 0.00000000 | 0.87467500 | 0.59557200 |
| H | -0.94191100 | 0.00000000 | 0.29877200 |
| H | 0.94191100 | 0.00000000 | 0.29877200 |
| C | 0.00000000 | -0.67382400 | 2.21624300 |
| C | 0.00000000 | 0.67382400 | 2.21624300 |
| C | 0.00000000 | -1.56874000 | -0.77407700 |
| C | 0.00000000 | -0.72097800 | -1.86404600 |
| C | 0.00000000 | 0.72097800 | -1.86404600 |
| C | 0.00000000 | 1.56874000 | -0.77407700 |

$C_6B_2H_8$ (k=1) Isomer III

| | | | |
|---|---|---|---|
| H | 3.06512000 | -0.57981400 | 0.00000000 |
| H | 2.00847500 | 1.59334400 | 0.00000000 |
| H | -1.38971300 | -2.56271300 | 0.00000000 |
| H | 1.68366000 | -2.94252800 | 0.00000000 |
| H | -3.11956800 | 0.92020700 | 0.00000000 |
| H | -1.14682400 | 2.98085000 | 0.00000000 |
| B | 1.18913700 | -1.86404800 | 0.00000000 |
| B | -0.63574000 | -1.64808800 | 0.00000000 |
| H | 0.27628400 | -1.84702600 | 0.96092000 |
| H | 0.27628400 | -1.84702600 | -0.96092000 |
| C | 0.00000000 | 0.82659100 | 0.00000000 |
| C | -1.11960100 | 1.90192200 | 0.00000000 |
| C | -2.04034100 | 0.93355900 | 0.00000000 |
| C | -0.95326900 | -0.16867100 | 0.00000000 |
| C | 1.98077100 | -0.55058200 | 0.00000000 |
| C | 1.39565500 | 0.69807800 | 0.00000000 |

$C_4B_4H_{10}$ (k=2) Isomer I

| | | | |
|---|---|---|---|
| H | 3.09875100 | -0.58345800 | 0.00000000 |
| H | 2.02925800 | 1.56039300 | 0.00000000 |
| H | -1.32597900 | -2.58722100 | 0.00000000 |
| H | 1.73847600 | -2.96097500 | 0.00000000 |
| H | -3.39005000 | 0.65314500 | 0.00000000 |
| H | -0.94482300 | 3.25628600 | 0.00000000 |
| B | 1.22666800 | -1.88971600 | 0.00000000 |
| B | -0.57467500 | -1.66809700 | 0.00000000 |
| B | -1.02568300 | 2.07364800 | 0.00000000 |
| B | -2.21282200 | 0.78269000 | 0.00000000 |
| H | -1.92940500 | 1.74774100 | 0.93067000 |
| H | -1.92940500 | 1.74774100 | -0.93067000 |
| H | 0.32244800 | -1.89127600 | 0.96189100 |
| H | 0.32244800 | -1.89127600 | -0.96189100 |
| C | 2.01375300 | -0.56401100 | 0.00000000 |
| C | 1.41548800 | 0.66435400 | 0.00000000 |
| C | 0.00000000 | 0.82653200 | 0.00000000 |
| C | -0.93910200 | -0.18416200 | 0.00000000 |

$C_4B_4H_{10}$ (k=2) Isomer II

| | | | |
|---|---|---|---|
| H | 0.00000000 | 1.17118600 | -2.91266800 |
| H | 0.00000000 | 2.62285400 | -1.02418100 |
| H | 0.00000000 | -2.62285400 | -1.02418100 |
| H | 0.00000000 | -1.17118600 | -2.91266800 |
| H | 0.00000000 | -1.70021600 | 3.17603800 |
| H | 0.00000000 | 1.70021600 | 3.17603800 |
| B | 0.00000000 | 0.89615700 | 0.55936200 |
| B | 0.00000000 | -0.89615700 | 0.55936200 |
| B | 0.00000000 | 0.89716100 | 2.29973000 |
| B | 0.00000000 | -0.89716100 | 2.29973000 |
| H | 0.92833400 | 0.00000000 | 2.66537700 |
| H | -0.92833400 | 0.00000000 | 2.66537700 |
| H | 0.93933200 | 0.00000000 | 0.34505900 |
| H | -0.93933200 | 0.00000000 | 0.34505900 |
| C | 0.00000000 | 1.55536300 | -0.83316300 |
| C | 0.00000000 | 0.72173500 | -1.92435100 |
| C | 0.00000000 | -0.72173500 | -1.92435100 |
| C | 0.00000000 | -1.55536300 | -0.83316300 |

$C_4B_4H_{10}$ (k=2) Isomer III

| | | | |
|---|---|---|---|
| H | 3.13307200 | -0.51325900 | 0.00000000 |
| H | 2.24367400 | 1.66982600 | 0.00000000 |
| H | -1.05517700 | -2.98209400 | 0.00000000 |
| H | 1.93169200 | -2.81746400 | 0.00000000 |
| H | -3.28991700 | 0.98362000 | 0.00000000 |
| H | -1.53646200 | 2.99747700 | 0.00000000 |
| B | 1.29112800 | -1.81585000 | 0.00000000 |
| B | -0.53711800 | -1.91451700 | 0.00000000 |
| B | 0.00000000 | 1.01897900 | 0.00000000 |
| B | -1.13217100 | -0.32442800 | 0.00000000 |
| H | -0.33398100 | 0.09340900 | 0.93354800 |
| H | 0.39394300 | -1.97024900 | 0.95706800 |
| H | -0.33398100 | 0.09340900 | -0.93354800 |
| H | 0.39394300 | -1.97024900 | -0.95706800 |
| C | -1.32780500 | 1.93502200 | 0.00000000 |
| C | -2.20831500 | 0.91939000 | 0.00000000 |
| C | 1.54519600 | 0.83802100 | 0.00000000 |
| C | 2.04825800 | -0.42665800 | 0.00000000 |

$C_4B_4H_{10}$ (k=2) Isomer IV

| | | | |
|---|---|---|---|
| H | 0.00000000 | 1.53366700 | -3.14216600 |
| H | 0.00000000 | 2.83761900 | -0.44271200 |
| H | 0.00000000 | -2.83761900 | -0.44271200 |
| H | 0.00000000 | -1.53366700 | -3.14216600 |
| H | 0.00000000 | -1.42802600 | 2.97066400 |
| H | 0.00000000 | 1.42802600 | 2.97066400 |
| B | 0.00000000 | 0.84632000 | -2.17251400 |
| B | 0.00000000 | -0.84632000 | -2.17251400 |
| B | 0.00000000 | 1.65543400 | -0.55446700 |
| B | 0.00000000 | -1.65543400 | -0.55446700 |
| H | 0.96249800 | 1.32109200 | -1.41506800 |
| H | 0.96249800 | -1.32109200 | -1.41506800 |
| H | -0.96249800 | 1.32109200 | -1.41506800 |
| H | -0.96249800 | -1.32109200 | -1.41506800 |
| C | 0.00000000 | 0.68147900 | 0.64137500 |
| C | 0.00000000 | 0.66621700 | 2.20516800 |
| C | 0.00000000 | -0.66621700 | 2.20516800 |
| C | 0.00000000 | -0.68147900 | 0.64137500 |

$C_2B_6H_{12}$ (k=3) Isomer I

0 1

| | | | |
|---|---|---|---|
| H | 0.00000000 | 1.53475500 | -3.18619800 |
| H | 0.00000000 | 2.82092800 | -0.49729900 |
| H | 0.00000000 | -2.82092800 | -0.49729900 |
| H | 0.00000000 | -1.53475500 | -3.18619800 |
| H | 0.00000000 | -1.78308600 | 2.99683100 |
| H | 0.00000000 | 1.78308600 | 2.99683100 |
| B | 0.00000000 | 0.84841600 | -2.21529600 |
| B | 0.00000000 | -0.84841600 | -2.21529600 |
| B | 0.00000000 | 1.63605700 | -0.59800500 |
| B | 0.00000000 | -1.63605700 | -0.59800500 |
| B | 0.00000000 | 0.87233600 | 2.23774800 |
| B | 0.00000000 | -0.87233600 | 2.23774800 |
| H | 0.92940400 | 0.00000000 | 2.68707900 |
| H | -0.92940400 | 0.00000000 | 2.68707900 |
| H | 0.96219600 | 1.31897400 | -1.46112900 |
| H | 0.96219600 | -1.31897400 | -1.46112900 |
| H | -0.96219600 | 1.31897400 | -1.46112900 |
| H | -0.96219600 | -1.31897400 | -1.46112900 |
| C | 0.00000000 | 0.68461600 | 0.63326800 |
| C | 0.00000000 | -0.68461600 | 0.63326800 |

$C_2B_6H_{12}$ (k=3) Isomer II

| | | | |
|---|---|---|---|
| H | 3.20683500 | -0.42527500 | 0.00000000 |
| H | 2.21677100 | 1.70854600 | 0.00000000 |
| H | -0.87874400 | -3.03617000 | 0.00000000 |
| H | 2.08867100 | -2.78049700 | 0.00000000 |
| H | -3.63700100 | 0.60480600 | 0.00000000 |
| H | -1.52678900 | 3.27855100 | 0.00000000 |
| B | 1.41621200 | -1.79940400 | 0.00000000 |
| B | -0.39748400 | -1.95046800 | 0.00000000 |
| B | 0.00000000 | 1.01374500 | 0.00000000 |
| B | -1.10126000 | -0.40153300 | 0.00000000 |
| B | -1.35429800 | 2.10158800 | 0.00000000 |
| B | -2.45161000 | 0.69765000 | 0.00000000 |
| H | -2.19192400 | 1.63782400 | 0.92792000 |
| H | -2.19192400 | 1.63782400 | -0.92792000 |
| H | 0.52072200 | -1.97202000 | 0.95824900 |
| H | -0.36160100 | 0.12776000 | 0.93190500 |
| H | 0.52072200 | -1.97202000 | -0.95824900 |
| H | -0.36160100 | 0.12776000 | -0.93190500 |
| C | 2.11892000 | -0.38777700 | 0.00000000 |
| C | 1.55409000 | 0.84694700 | 0.00000000 |

$C_2B_6H_{12}$ (k=3) Isomer III

| | | | |
|---|---|---|---|
| H | 0.00000000 | 1.45299800 | -3.22415100 |
| H | 0.00000000 | 3.04861400 | -0.76083300 |
| H | 0.00000000 | -3.04861400 | -0.76083300 |
| H | 0.00000000 | -1.45299800 | -3.22415100 |
| H | 0.00000000 | -1.33889700 | 3.19630700 |
| H | 0.00000000 | 1.33889700 | 3.19630700 |
| B | 0.00000000 | 0.86596200 | -2.18830700 |
| B | 0.00000000 | -0.86596200 | -2.18830700 |
| B | 0.00000000 | 1.86415000 | -0.67200600 |
| B | 0.00000000 | -1.86415000 | -0.67200600 |
| B | 0.00000000 | 0.88214000 | 0.73003100 |
| B | 0.00000000 | -0.88214000 | 0.73003100 |
| H | 0.95776200 | 1.42935700 | -1.48555700 |
| H | 0.95776200 | -1.42935700 | -1.48555700 |
| H | 0.92216200 | 0.00000000 | 0.35254100 |
| H | -0.95776200 | 1.42935700 | -1.48555700 |
| H | -0.95776200 | -1.42935700 | -1.48555700 |
| H | -0.92216200 | 0.00000000 | 0.35254100 |
| C | 0.00000000 | 0.67085600 | 2.34311000 |
| C | 0.00000000 | -0.67085600 | 2.34311000 |

$B_8H_{14}$ (k=4) Kekulé Structure $K_1$

| | | | |
|---|---|---|---|
| H | 0.00000000 | 1.46161700 | -3.29102100 |
| H | 0.00000000 | 3.02425400 | -0.82631000 |
| H | 0.00000000 | -3.02425400 | -0.82631000 |
| H | 0.00000000 | -1.46161700 | -3.29102100 |
| H | 0.00000000 | -1.70480500 | 3.30236000 |
| H | 0.00000000 | 1.70480500 | 3.30236000 |
| B | 0.00000000 | 0.86328300 | -2.26137300 |
| B | 0.00000000 | -0.86328300 | -2.26137300 |
| B | 0.00000000 | 1.83875300 | -0.73701000 |
| B | 0.00000000 | -1.83875300 | -0.73701000 |
| B | 0.00000000 | 0.89906900 | 0.69957100 |
| B | 0.00000000 | -0.89906900 | 0.69957100 |
| B | 0.00000000 | 0.88755600 | 2.43746000 |
| B | 0.00000000 | -0.88755600 | 2.43746000 |
| H | 0.92784800 | 0.00000000 | 2.81508300 |
| H | -0.92784800 | 0.00000000 | 2.81508300 |
| H | 0.92264200 | 0.00000000 | 0.40034300 |
| H | 0.95824100 | 1.40859900 | -1.54684600 |
| H | 0.95824100 | -1.40859900 | -1.54684600 |
| H | -0.92264200 | 0.00000000 | 0.40034300 |
| H | -0.95824100 | 1.40859900 | -1.54684600 |
| H | -0.95824100 | -1.40859900 | -1.54684600 |

**Benzocyclobutadiene Kekulé Structure $K_2$ : $C_{(8-2k)}B_{(2k)}H_{(6+2k)}$**

$C_6B_2H_8$ (k=1) Isomer I

| | | | |
|---|---|---|---|
| H | 0.00000000 | 1.22474200 | -2.82314900 |
| H | 0.00000000 | 2.49910000 | -0.69295500 |
| H | 0.00000000 | -2.49910000 | -0.69295500 |
| H | 0.00000000 | -1.22474200 | -2.82314900 |
| H | 0.00000000 | -1.78549500 | 2.85909500 |
| H | 0.00000000 | 1.78549500 | 2.85909500 |
| B | 0.00000000 | 0.88688500 | 2.08756600 |
| B | 0.00000000 | -0.88688500 | 2.08756600 |
| H | 0.93045400 | 0.00000000 | 2.51405600 |
| H | -0.93045400 | 0.00000000 | 2.51405600 |
| C | 0.00000000 | 1.41621100 | -0.67424100 |
| C | 0.00000000 | 0.70728000 | 0.50576000 |
| C | 0.00000000 | -0.70728000 | 0.50576000 |
| C | 0.00000000 | -1.41621100 | -0.67424100 |
| C | 0.00000000 | 0.69267800 | -1.88066600 |
| C | 0.00000000 | -0.69267800 | -1.88066600 |

$C_6B_2H_8$ (k=1) Isomer II

| | | | |
|---|---|---|---|
| H | 0.00000000 | 1.52254600 | -2.95057100 |
| H | 0.00000000 | 2.63321900 | -0.38473200 |
| H | 0.00000000 | -2.63321900 | -0.38473200 |
| H | 0.00000000 | -1.52254600 | -2.95057100 |
| H | 0.00000000 | -1.42294500 | 2.81287300 |
| H | 0.00000000 | 1.42294500 | 2.81287300 |
| B | 0.00000000 | 0.90189700 | -1.93844800 |
| B | 0.00000000 | -0.90189700 | -1.93844800 |
| H | 0.96276900 | 0.00000000 | -2.07417400 |
| H | -0.96276900 | 0.00000000 | -2.07417400 |
| C | 0.00000000 | 0.67637600 | 2.03292400 |
| C | 0.00000000 | -0.67637600 | 2.03292400 |
| C | 0.00000000 | -0.73639600 | 0.53661500 |
| C | 0.00000000 | -1.55778600 | -0.52139900 |
| C | 0.00000000 | 1.55778600 | -0.52139900 |
| C | 0.00000000 | 0.73639600 | 0.53661500 |

$C_6B_2H_8$ (k=1) Isomer III

| | | | |
|---|---|---|---|
| H | 1.80859200 | 2.62397200 | 0.00000000 |
| H | -0.90033700 | 2.89135500 | 0.00000000 |
| H | 2.00767600 | -1.64411500 | 0.00000000 |
| H | 3.00531400 | 0.59334500 | 0.00000000 |
| H | -1.16759600 | -2.92692400 | 0.00000000 |
| H | -3.20968000 | -1.08688700 | 0.00000000 |
| B | -0.33141500 | 1.84883200 | 0.00000000 |
| B | -1.05009200 | 0.24132300 | 0.00000000 |
| H | -0.92759700 | 1.13198300 | 0.96355700 |
| H | -0.92759700 | 1.13198300 | -0.96355700 |
| C | -2.14111600 | -0.92870700 | 0.00000000 |
| C | -1.13791300 | -1.84095900 | 0.00000000 |
| C | 0.00000000 | -0.89228500 | 0.00000000 |
| C | 1.33837400 | -0.79034100 | 0.00000000 |
| C | 1.22327800 | 1.71101000 | 0.00000000 |
| C | 1.92050300 | 0.54703400 | 0.00000000 |

$C_4B_4H_{10}$ (k=2) Isomer I

| | | | |
|---|---|---|---|
| H | 0.00000000 | 1.52856500 | -3.00313300 |
| H | 0.00000000 | 2.60398800 | -0.44239600 |
| H | 0.00000000 | -2.60398800 | -0.44239600 |
| H | 0.00000000 | -1.52856500 | -3.00313300 |
| H | 0.00000000 | -1.78587100 | 2.87516400 |
| H | 0.00000000 | 1.78587100 | 2.87516400 |
| B | 0.00000000 | 0.90123000 | -1.99547900 |
| B | 0.00000000 | -0.90123000 | -1.99547900 |
| B | 0.00000000 | 0.89119200 | 2.09949700 |
| B | 0.00000000 | -0.89119200 | 2.09949700 |
| H | 0.96318700 | 0.00000000 | -2.11238700 |
| H | 0.93146600 | 0.00000000 | 2.50137000 |
| H | -0.96318700 | 0.00000000 | -2.11238700 |
| H | -0.93146600 | 0.00000000 | 2.50137000 |
| C | 0.00000000 | 1.52628800 | -0.57583000 |
| C | 0.00000000 | 0.73496900 | 0.51937900 |
| C | 0.00000000 | -0.73496900 | 0.51937900 |
| C | 0.00000000 | -1.52628800 | -0.57583000 |

$C_4B_4H_{10}$ (k=2) Isomer II

| | | | |
|---|---|---|---|
| H | -1.91475000 | -2.62374500 | 0.00000000 |
| H | 0.78896100 | -2.92075100 | 0.00000000 |
| H | -2.00039700 | 1.62770600 | 0.00000000 |
| H | -3.06143600 | -0.55092200 | 0.00000000 |
| H | 1.06368600 | 3.21193100 | 0.00000000 |
| H | 3.56825800 | 0.78432600 | 0.00000000 |
| B | 0.23491300 | -1.86975100 | 0.00000000 |
| B | 1.02018800 | -0.28489800 | 0.00000000 |
| B | 2.38218300 | 0.76830200 | 0.00000000 |
| B | 1.08610500 | 2.02270900 | 0.00000000 |
| H | 0.84034400 | -1.15370200 | 0.96139900 |
| H | 2.00948600 | 1.64488000 | 0.93094400 |
| H | 0.84034400 | -1.15370200 | -0.96139900 |
| H | 2.00948600 | 1.64488000 | -0.93094400 |
| C | -1.30793100 | -1.72447400 | 0.00000000 |
| C | -1.97570700 | -0.54181500 | 0.00000000 |
| C | -1.34318300 | 0.76176600 | 0.00000000 |
| C | 0.00000000 | 0.88907200 | 0.00000000 |

$C_4B_4H_{10}$ (k=2) Isomer III

| | | | |
|---|---|---|---|
| H | 1.85299400 | 2.94940800 | 0.00000000 |
| H | -1.20888700 | 2.86905200 | 0.00000000 |
| H | 1.86835300 | -1.91209600 | 0.00000000 |
| H | 3.32030200 | 0.42633500 | 0.00000000 |
| H | -1.22414200 | -2.91485500 | 0.00000000 |
| H | -3.22156600 | -1.02795700 | 0.00000000 |
| B | 1.21936500 | 1.94268400 | 0.00000000 |
| B | 2.13259400 | 0.38275000 | 0.00000000 |
| B | -0.49969100 | 1.91400000 | 0.00000000 |
| B | -1.05158200 | 0.24777700 | 0.00000000 |
| H | -0.98804500 | 1.16507100 | 0.96271000 |
| H | 1.71803600 | 1.23270700 | 0.96382800 |
| H | -0.98804500 | 1.16507100 | -0.96271000 |
| H | 1.71803600 | 1.23270700 | -0.96382800 |
| C | -2.14981800 | -0.89131600 | 0.00000000 |
| C | -1.16671800 | -1.82940800 | 0.00000000 |
| C | 0.00000000 | -0.92158500 | 0.00000000 |
| C | 1.34145900 | -0.96127500 | 0.00000000 |

$C_4B_4H_{10}$ (k=2) Isomer IV

| | | | |
|---|---|---|---|
| H | 0.00000000 | 1.15125100 | -3.02622800 |
| H | 0.00000000 | 2.85462700 | -1.00520300 |
| H | 0.00000000 | -2.85462700 | -1.00520300 |
| H | 0.00000000 | -1.15125100 | -3.02622800 |
| H | 0.00000000 | -1.33319800 | 3.14123600 |
| H | 0.00000000 | 1.33319800 | 3.14123600 |
| B | 0.00000000 | 1.67741100 | -0.82175500 |
| B | 0.00000000 | -1.67741100 | -0.82175500 |
| B | 0.00000000 | 0.83247700 | 0.70237500 |
| B | 0.00000000 | -0.83247700 | 0.70237500 |
| H | 0.95981300 | 1.49089300 | 0.06969300 |
| H | 0.95981300 | -1.49089300 | 0.06969300 |
| H | -0.95981300 | 1.49089300 | 0.06969300 |
| H | -0.95981300 | -1.49089300 | 0.06969300 |
| C | 0.00000000 | 0.67987800 | 2.27240300 |
| C | 0.00000000 | -0.67987800 | 2.27240300 |
| C | 0.00000000 | 0.67410400 | -2.04778400 |
| C | 0.00000000 | -0.67410400 | -2.04778400 |

$C_2B_6H_{12}$ (k=3) Isomer I

| | | | |
|---|---|---|---|
| H | -3.37230500 | 0.40083800 | 0.00000000 |
| H | -1.87807200 | -1.86828800 | 0.00000000 |
| H | 1.10471600 | 2.89145200 | 0.00000000 |
| H | -1.95717300 | 2.97047600 | 0.00000000 |
| H | 3.57927500 | -0.75633200 | 0.00000000 |
| H | 1.11301600 | -3.22179100 | 0.00000000 |
| B | -2.18372400 | 0.40669200 | 0.00000000 |
| B | -1.30687400 | 1.97515200 | 0.00000000 |
| B | 0.39787700 | 1.93414200 | 0.00000000 |
| B | 1.02459300 | 0.28476700 | 0.00000000 |
| B | 1.11764000 | -2.03249600 | 0.00000000 |
| B | 2.39321300 | -0.75671200 | 0.00000000 |
| H | -1.79669600 | 1.24349500 | 0.96363000 |
| H | 0.90594200 | 1.17612800 | 0.95932300 |
| H | 2.02681800 | -1.63426700 | 0.93142900 |
| H | -1.79669600 | 1.24349500 | -0.96363000 |
| H | 0.90594200 | 1.17612800 | -0.95932300 |
| H | 2.02681800 | -1.63426700 | -0.93142900 |
| C | -1.34586900 | -0.91760000 | 0.00000000 |
| C | 0.00000000 | -0.92319800 | 0.00000000 |

$C_2B_6H_{12}$ (k=3) Isomer II

| | | | |
|---|---|---|---|
| H | 0.00000000 | 1.15926300 | -3.09763100 |
| H | 0.00000000 | 2.82063900 | -1.05248800 |
| H | 0.00000000 | -2.82063900 | -1.05248800 |
| H | 0.00000000 | -1.15926300 | -3.09763100 |
| H | 0.00000000 | -1.69913200 | 3.27081600 |
| H | 0.00000000 | 1.69913200 | 3.27081600 |
| B | 0.00000000 | 1.64080500 | -0.88315000 |
| B | 0.00000000 | -1.64080500 | -0.88315000 |
| B | 0.00000000 | 0.84661900 | 0.67092500 |
| B | 0.00000000 | -0.84661900 | 0.67092500 |
| B | 0.00000000 | 0.90984200 | 2.37926400 |
| B | 0.00000000 | -0.90984200 | 2.37926400 |
| H | 0.95798700 | 1.45576900 | 0.04157100 |
| H | 0.95798700 | -1.45576900 | 0.04157100 |
| H | 0.93175400 | 0.00000000 | 2.70143800 |
| H | -0.95798700 | 1.45576900 | 0.04157100 |
| H | -0.95798700 | -1.45576900 | 0.04157100 |
| H | -0.93175400 | 0.00000000 | 2.70143800 |
| C | 0.00000000 | 0.67471900 | -2.12341200 |
| C | 0.00000000 | -0.67471900 | -2.12341200 |

$C_2B_6H_{12}$ (k=3) Isomer III

| | | | |
|---|---|---|---|
| H | 0.00000000 | 1.39274300 | -3.24428100 |
| H | 0.00000000 | 3.05048000 | -0.72810000 |
| H | 0.00000000 | -3.05048000 | -0.72810000 |
| H | 0.00000000 | -1.39274300 | -3.24428100 |
| H | 0.00000000 | -1.33081900 | 3.14606300 |
| H | 0.00000000 | 1.33081900 | 3.14606300 |
| B | 0.00000000 | 0.90286700 | -2.15981200 |
| B | 0.00000000 | -0.90286700 | -2.15981200 |
| B | 0.00000000 | 1.85821200 | -0.72477300 |
| B | 0.00000000 | -1.85821200 | -0.72477300 |
| B | 0.00000000 | 0.84072200 | 0.70832700 |
| B | 0.00000000 | -0.84072200 | 0.70832700 |
| H | 0.95963900 | 1.54752400 | 0.10585100 |
| H | 0.96071600 | 0.00000000 | -2.14986200 |
| H | 0.95963900 | -1.54752400 | 0.10585100 |
| H | -0.95963900 | 1.54752400 | 0.10585100 |
| H | -0.96071600 | 0.00000000 | -2.14986200 |
| H | -0.95963900 | -1.54752400 | 0.10585100 |
| C | 0.00000000 | 0.68105900 | 2.27429400 |
| C | 0.00000000 | -0.68105900 | 2.27429400 |

$B_6H_{14}$ (k=4) Kekulé Structure $K_2$

0 1

| | | | |
|---|---|---|---|
| H | 0.00000000 | 1.40891800 | -3.32224500 |
| H | 0.00000000 | 3.00525400 | -0.78689600 |
| H | 0.00000000 | -3.00525400 | -0.78689600 |
| H | 0.00000000 | -1.40891800 | -3.32224500 |
| H | 0.00000000 | -1.69684600 | 3.29075700 |
| H | 0.00000000 | 1.69684600 | 3.29075700 |
| B | 0.00000000 | 0.89935500 | -2.24705500 |
| B | 0.00000000 | -0.89935500 | -2.24705500 |
| B | 0.00000000 | 1.81267600 | -0.79308400 |
| B | 0.00000000 | -1.81267600 | -0.79308400 |
| B | 0.00000000 | 0.85658500 | 0.68542600 |
| B | 0.00000000 | -0.85658500 | 0.68542600 |
| B | 0.00000000 | 0.90969000 | 2.39730200 |
| B | 0.00000000 | -0.90969000 | 2.39730200 |
| H | 0.95715100 | 1.50212100 | 0.07107700 |
| H | 0.96140600 | 0.00000000 | -2.25031100 |
| H | 0.95715100 | -1.50212100 | 0.07107700 |
| H | 0.93205800 | 0.00000000 | 2.71359800 |
| H | -0.95715100 | 1.50212100 | 0.07107700 |
| H | -0.96140600 | 0.00000000 | -2.25031100 |
| H | -0.95715100 | -1.50212100 | 0.07107700 |
| H | -0.93205800 | 0.00000000 | 2.71359800 |

**Benzocyclobutadiene Kekulé Structure $K_3$ : $C_{(8-2k)}B_{(2k)}H_{(6+2k)}$**

$C_6B_2H_8$ (k=1) Isomer I

| | | | |
|---|---|---|---|
| H | -1.54577300 | -2.66444700 | 0.00000000 |
| H | 0.85506800 | -2.67572600 | 0.00000000 |
| H | -2.11706800 | 1.58181700 | 0.00000000 |
| H | -2.95437500 | -0.71753200 | 0.00000000 |
| H | 0.79539800 | 2.97617300 | 0.00000000 |
| H | 3.41442900 | 1.03716000 | 0.00000000 |
| B | 0.95535000 | -0.32084300 | 0.00000000 |
| B | 2.23692000 | 0.89230800 | 0.00000000 |
| H | 1.99624700 | 0.01625200 | 0.93983400 |
| H | 1.99624700 | 0.01625200 | -0.93983400 |
| C | 0.33967600 | -1.72357700 | 0.00000000 |
| C | -1.01758800 | -1.71519200 | 0.00000000 |
| C | -1.88846100 | -0.52910500 | 0.00000000 |
| C | -1.42930400 | 0.74323300 | 0.00000000 |
| C | 0.00000000 | 0.92149500 | 0.00000000 |
| C | 0.92875700 | 1.89860000 | 0.00000000 |

$C_6B_2H_8$ (k=1) Isomer II

| | | | |
|---|---|---|---|
| H | -1.68297400 | -2.94245500 | 0.00000000 |
| H | 1.38917200 | -2.56292800 | 0.00000000 |
| H | -2.00850200 | 1.59363900 | 0.00000000 |
| H | -3.06542300 | -0.57925300 | 0.00000000 |
| H | 1.14784400 | 2.98061100 | 0.00000000 |
| H | 3.11961500 | 0.92043300 | 0.00000000 |
| B | -1.18896600 | -1.86376000 | 0.00000000 |
| B | 0.63516100 | -1.64831500 | 0.00000000 |
| H | -0.27598500 | -1.84682200 | 0.96098500 |
| H | -0.27598500 | -1.84682200 | -0.96098500 |
| C | -1.98100500 | -0.55035400 | 0.00000000 |
| C | -1.39573800 | 0.69822000 | 0.00000000 |
| C | 0.00000000 | 0.82667200 | 0.00000000 |
| C | 0.95338000 | -0.16879000 | 0.00000000 |
| C | 2.04026300 | 0.93332500 | 0.00000000 |
| C | 1.11997800 | 1.90158900 | 0.00000000 |

$C_4B_4H_{10}$ (k=2) Isomer I

| | | | |
|---|---|---|---|
| H | -1.88841500 | -2.79212200 | 0.00000000 |
| H | 1.18054500 | -2.71276400 | 0.00000000 |
| H | -2.21107200 | 1.71266100 | 0.00000000 |
| H | -3.14709700 | -0.46533100 | 0.00000000 |
| H | 1.87239900 | 3.06283900 | 0.00000000 |
| H | 3.15939500 | 0.08447000 | 0.00000000 |
| B | -1.27920800 | -1.77155600 | 0.00000000 |
| B | 0.51721500 | -1.72724200 | 0.00000000 |
| B | 0.00000000 | 0.97548100 | 0.00000000 |
| B | 1.47266500 | 1.94541000 | 0.00000000 |
| H | -0.40084200 | -1.90204700 | 0.96183300 |
| H | -0.40084200 | -1.90204700 | -0.96183300 |
| H | 0.54951400 | 1.89342900 | 0.93575100 |
| H | 0.54951400 | 1.89342900 | -0.93575100 |
| C | -2.06142300 | -0.38514900 | 0.00000000 |
| C | -1.53791800 | 0.85991400 | 0.00000000 |
| C | 0.99257400 | -0.25826200 | 0.00000000 |
| C | 2.13735700 | 0.45299900 | 0.00000000 |

$C_4B_4H_{10}$ (k=2) Isomer II

| | | | |
|---|---|---|---|
| H | 0.00000000 | 1.18065200 | -2.89814100 |
| H | 0.00000000 | 2.63096600 | -1.00542500 |
| H | 0.00000000 | -2.63096600 | -1.00542500 |
| H | 0.00000000 | -1.18065200 | -2.89814100 |
| H | 0.00000000 | -1.72559100 | 3.14100900 |
| H | 0.00000000 | 1.72559100 | 3.14100900 |
| B | 0.00000000 | 0.84515800 | 0.54856000 |
| B | 0.00000000 | -0.84515800 | 0.54856000 |
| B | 0.00000000 | 0.87174700 | 2.30991500 |
| B | 0.00000000 | -0.87174700 | 2.30991500 |
| H | 0.93009600 | 1.26864100 | 1.43989700 |
| H | 0.93009600 | -1.26864100 | 1.43989700 |
| H | -0.93009600 | 1.26864100 | 1.43989700 |
| H | -0.93009600 | -1.26864100 | 1.43989700 |
| C | 0.00000000 | 1.56017500 | -0.83077800 |
| C | 0.00000000 | 0.74232700 | -1.90415700 |
| C | 0.00000000 | -0.74232700 | -1.90415700 |
| C | 0.00000000 | -1.56017500 | -0.83077800 |

$C_4B_4H_{10}$ (k=2) Isomer III

| | | | |
|---|---|---|---|
| H | -1.76816700 | -2.91528300 | 0.00000000 |
| H | 1.25031100 | -2.88469100 | 0.00000000 |
| H | -2.07383900 | 1.59231300 | 0.00000000 |
| H | -3.04688500 | -0.59111300 | 0.00000000 |
| H | 0.57875500 | 3.04746600 | 0.00000000 |
| H | 3.33704700 | 1.34964100 | 0.00000000 |
| B | -1.17634100 | -1.88409200 | 0.00000000 |
| B | 0.62174400 | -1.87721300 | 0.00000000 |
| B | 1.10982800 | -0.25398800 | 0.00000000 |
| B | 2.17226400 | 1.12741900 | 0.00000000 |
| H | -0.24450600 | -2.00523100 | 0.96254600 |
| H | -0.24450600 | -2.00523100 | -0.96254600 |
| H | 1.99566900 | 0.11309200 | 0.92786600 |
| H | 1.99566900 | 0.11309200 | -0.92786600 |
| C | -1.96346500 | -0.52391400 | 0.00000000 |
| C | -1.42718000 | 0.71749400 | 0.00000000 |
| C | 0.00000000 | 0.92051600 | 0.00000000 |
| C | 0.82114000 | 1.99012500 | 0.00000000 |

$C_4B_4H_{10}$ (k=2) Isomer IV

| | | | |
|---|---|---|---|
| H | 0.00000000 | 1.53266300 | -3.14313800 |
| H | 0.00000000 | 2.83740500 | -0.44278900 |
| H | 0.00000000 | -2.83740500 | -0.44278900 |
| H | 0.00000000 | -1.53266300 | -3.14313800 |
| H | 0.00000000 | -1.42767900 | 2.97095500 |
| H | 0.00000000 | 1.42767900 | 2.97095500 |
| B | 0.00000000 | 0.84645700 | -2.17276900 |
| B | 0.00000000 | -0.84645700 | -2.17276900 |
| B | 0.00000000 | 1.65518900 | -0.55439800 |
| B | 0.00000000 | -1.65518900 | -0.55439800 |
| H | 0.96247000 | 1.32063700 | -1.41487300 |
| H | 0.96247000 | -1.32063700 | -1.41487300 |
| H | -0.96247000 | 1.32063700 | -1.41487300 |
| H | -0.96247000 | -1.32063700 | -1.41487300 |
| C | 0.00000000 | 0.68144000 | 0.64145900 |
| C | 0.00000000 | 0.66621800 | 2.20530100 |
| C | 0.00000000 | -0.66621800 | 2.20530100 |
| C | 0.00000000 | -0.68144000 | 0.64145900 |

$C_2B_6H_{12}$ (k=3) Isomer I

| | | | |
|---|---|---|---|
| H | 3.19233100 | -0.45311600 | 0.00000000 |
| H | 2.21909800 | 1.69015600 | 0.00000000 |
| H | -0.93143400 | -3.00584500 | 0.00000000 |
| H | 2.03547100 | -2.79677600 | 0.00000000 |
| H | -3.60444600 | 0.59880500 | 0.00000000 |
| H | -1.46451100 | 3.29737500 | 0.00000000 |
| B | 1.37502700 | -1.80728800 | 0.00000000 |
| B | -0.41871700 | -1.93299800 | 0.00000000 |
| B | 0.00000000 | 0.96750100 | 0.00000000 |
| B | -1.07060000 | -0.36486700 | 0.00000000 |
| B | -1.35261900 | 2.11072400 | 0.00000000 |
| B | -2.42276000 | 0.74962900 | 0.00000000 |
| H | 0.46986400 | -1.97321600 | 0.96221100 |
| H | 0.46986400 | -1.97321600 | -0.96221100 |
| H | -0.44501000 | 1.86283200 | 0.93039400 |
| H | -1.99198500 | -0.15147600 | 0.92463700 |
| H | -0.44501000 | 1.86283200 | -0.93039400 |
| H | -1.99198500 | -0.15147600 | -0.92463700 |
| C | 2.10466800 | -0.40059600 | 0.00000000 |
| C | 1.55134800 | 0.83053300 | 0.00000000 |

$C_2B_6H_{12}$ (k=3) Isomer II

| | | | |
|---|---|---|---|
| H | 3.33292500 | -0.96794600 | 0.00000000 |
| H | 2.29969900 | 1.81944000 | 0.00000000 |
| H | -1.48058100 | -2.75151100 | 0.00000000 |
| H | 1.42152300 | -3.24478100 | 0.00000000 |
| H | -3.38354800 | 1.36424400 | 0.00000000 |
| H | -0.66235100 | 3.12002900 | 0.00000000 |
| B | 2.15576100 | -0.79443500 | 0.00000000 |
| B | 1.04782500 | -2.11468400 | 0.00000000 |
| B | 1.54277100 | 0.90231000 | 0.00000000 |
| B | -0.72919800 | -1.83028300 | 0.00000000 |
| B | -1.09264600 | -0.17301000 | 0.00000000 |
| B | -2.21365000 | 1.16658100 | 0.00000000 |
| H | 1.94239200 | 0.05347900 | 0.96254300 |
| H | 0.13892800 | -2.04545200 | 0.96095000 |
| H | 1.94239200 | 0.05347900 | -0.96254300 |
| H | 0.13892800 | -2.04545200 | -0.96095000 |
| H | -2.00417800 | 0.18402800 | 0.92632600 |
| H | -2.00417800 | 0.18402800 | -0.92632600 |
| C | 0.00000000 | 1.02783000 | 0.00000000 |
| C | -0.87271000 | 2.05450600 | 0.00000000 |

$B_6H_{14}$ (k=4) Kekulé structure $K_3$

| | | | |
|---|---|---|---|
| H | 0.00000000 | 1.47425900 | -3.27108400 |
| H | 0.00000000 | 3.01087300 | -0.81413200 |
| H | 0.00000000 | -3.01087300 | -0.81413200 |
| H | 0.00000000 | -1.47425900 | -3.27108400 |
| H | 0.00000000 | -1.72363900 | 3.26614000 |
| H | 0.00000000 | 1.72363900 | 3.26614000 |
| B | 0.00000000 | 0.86260200 | -2.24984200 |
| B | 0.00000000 | -0.86260200 | -2.24984200 |
| B | 0.00000000 | 1.82424000 | -0.72503000 |
| B | 0.00000000 | -1.82424000 | -0.72503000 |
| B | 0.00000000 | 0.86383300 | 0.68228100 |
| B | 0.00000000 | -0.86383300 | 0.68228100 |
| B | 0.00000000 | 0.86244800 | 2.44256200 |
| B | 0.00000000 | -0.86244800 | 2.44256200 |
| H | 0.96066100 | 1.38043100 | -1.51276200 |
| H | 0.96066100 | -1.38043100 | -1.51276200 |
| H | -0.96066100 | 1.38043100 | -1.51276200 |
| H | -0.96066100 | -1.38043100 | -1.51276200 |
| H | 0.92350000 | 1.27443200 | 1.54736900 |
| H | 0.92350000 | -1.27443200 | 1.54736900 |
| H | -0.92350000 | 1.27443200 | 1.54736900 |
| H | -0.92350000 | -1.27443200 | 1.54736900 |

**Naphthalene Kekulé Structure $K_1$ : $C_{(10-2k)}B_{(2k)}H_{(8+2k)}$**

$C_{10}H_8$ (k=0) - same energy for Kekulé structures $K_1$ and $K_2$

| | | | |
|---|---|---|---|
| C | 0.00000000 | 2.42389600 | 0.70584800 |
| C | 0.00000000 | 1.24066100 | 1.39693200 |
| C | 0.00000000 | 0.00000000 | 0.71398700 |
| C | 0.00000000 | 0.00000000 | -0.71398700 |
| C | 0.00000000 | 1.24066100 | -1.39693200 |
| C | 0.00000000 | 2.42389600 | -0.70584800 |
| H | 0.00000000 | -1.23924000 | 2.47981200 |
| H | 0.00000000 | 3.36455500 | 1.24026300 |
| H | 0.00000000 | 1.23924000 | 2.47981200 |
| C | 0.00000000 | -1.24066100 | 1.39693200 |
| C | 0.00000000 | -1.24066100 | -1.39693200 |
| H | 0.00000000 | 1.23924000 | -2.47981200 |
| H | 0.00000000 | 3.36455500 | -1.24026300 |
| C | 0.00000000 | -2.42389600 | -0.70584800 |
| C | 0.00000000 | -2.42389600 | 0.70584800 |
| H | 0.00000000 | -1.23924000 | -2.47981200 |
| H | 0.00000000 | -3.36455500 | -1.24026300 |
| H | 0.00000000 | -3.36455500 | 1.24026300 |

$C_8B_2H_{10}$ (k=1) Isomer I

| | | | |
|---|---|---|---|
| H | 1.49004800 | 2.39485100 | 0.00000000 |
| H | 3.30821500 | -1.47668400 | 0.00000000 |
| H | 1.08035200 | -2.52341000 | 0.00000000 |
| H | 3.51507100 | 0.99519800 | 0.00000000 |
| B | -1.14146100 | 1.66970900 | 0.00000000 |
| H | -1.22671200 | -2.42721200 | 0.00000000 |
| H | -1.06085600 | 2.85467800 | 0.00000000 |
| B | -2.68815700 | 0.78478500 | 0.00000000 |
| H | -1.98060600 | 1.35551400 | 0.96419800 |
| H | -1.98060600 | 1.35551400 | -0.96419800 |
| H | -3.36466100 | -1.39906200 | 0.00000000 |
| H | -3.74551300 | 1.32391200 | 0.00000000 |
| C | 0.00000000 | -0.66386300 | 0.00000000 |
| C | 0.11099400 | 0.75267300 | 0.00000000 |
| C | 1.39581600 | 1.31625300 | 0.00000000 |
| C | 2.53686400 | 0.53283300 | 0.00000000 |
| C | 2.42045100 | -0.85798900 | 0.00000000 |
| C | 1.17012300 | -1.44413700 | 0.00000000 |
| C | -2.49772500 | -0.74780600 | 0.00000000 |
| C | -1.28429700 | -1.34225900 | 0.00000000 |

$C_8B_2H_{10}$ (k=1) Isomer II

| | | | |
|---|---|---|---|
| B | 0.00000000 | 0.90794800 | 0.00000000 |
| B | 0.00000000 | -0.90794800 | 0.00000000 |
| H | -1.58085300 | -2.59166800 | 0.00000000 |
| H | -3.50357000 | 1.18683200 | 0.00000000 |
| H | -1.58085300 | 2.59166800 | 0.00000000 |
| H | -3.50357000 | -1.18683200 | 0.00000000 |
| H | 0.00000000 | 0.00000000 | 0.96098100 |
| H | 0.00000000 | 0.00000000 | -0.96098100 |
| H | 1.58085300 | 2.59166800 | 0.00000000 |
| H | 1.58085300 | -2.59166800 | 0.00000000 |
| H | 3.50357000 | 1.18683200 | 0.00000000 |
| H | 3.50357000 | -1.18683200 | 0.00000000 |
| C | -2.52153300 | -0.72374800 | 0.00000000 |
| C | -1.41936300 | -1.51853700 | 0.00000000 |
| C | 1.41936300 | 1.51853700 | 0.00000000 |
| C | 2.52153300 | 0.72374800 | 0.00000000 |
| C | 1.41936300 | -1.51853700 | 0.00000000 |
| C | 2.52153300 | -0.72374800 | 0.00000000 |
| C | -2.52153300 | 0.72374800 | 0.00000000 |
| C | -1.41936300 | 1.51853700 | 0.00000000 |

$C_6B_4H_{12}$ (k=2) Isomer I

| | | | |
|---|---|---|---|
| H | 0.00000000 | 2.46254700 | 1.34749600 |
| H | 0.00000000 | -1.24031600 | 3.48143200 |
| H | 0.00000000 | -2.46254700 | 1.34749600 |
| H | 0.00000000 | 1.24031600 | 3.48143200 |
| B | 0.00000000 | -1.60483700 | -1.18028900 |
| B | 0.00000000 | 1.60483700 | -1.18028900 |
| H | 0.00000000 | -2.78904600 | -1.06917600 |
| H | 0.00000000 | 2.78904600 | -1.06917600 |
| B | 0.00000000 | -0.84833200 | -2.79535700 |
| B | 0.00000000 | 0.84833200 | -2.79535700 |
| H | -0.96400700 | -1.30777900 | -2.04309100 |
| H | -0.96400700 | 1.30777900 | -2.04309100 |
| H | 0.96400700 | -1.30777900 | -2.04309100 |
| H | 0.96400700 | 1.30777900 | -2.04309100 |
| H | 0.00000000 | -1.54215400 | -3.76019500 |
| H | 0.00000000 | 1.54215400 | -3.76019500 |
| C | 0.00000000 | -0.71171700 | 0.10719000 |
| C | 0.00000000 | 0.71171700 | 0.10719000 |
| C | 0.00000000 | 1.38018400 | 1.33985400 |
| C | 0.00000000 | 0.69460000 | 2.54709900 |
| C | 0.00000000 | -0.69460000 | 2.54709900 |
| C | 0.00000000 | -1.38018400 | 1.33985400 |

$C_6B_4H_{12}$ (k=2) Isomer II

| | | | |
|---|---|---|---|
| B | 1.48973000 | 1.35489400 | 0.00000000 |
| B | 0.46942200 | 2.81795500 | 0.00000000 |
| H | -2.56378900 | 1.04044000 | 0.00000000 |
| H | 0.91590100 | 3.91688000 | 0.00000000 |
| H | 2.67680800 | 1.39249100 | 0.00000000 |
| H | -1.76968900 | 3.26760800 | 0.00000000 |
| H | 1.09003800 | 2.14808200 | 0.96492700 |
| H | 1.09003800 | 2.14808200 | -0.96492700 |
| B | -1.48973000 | -1.35489400 | 0.00000000 |
| H | 2.56378900 | -1.04044000 | 0.00000000 |
| H | -2.67680800 | -1.39249100 | 0.00000000 |
| B | -0.46942200 | -2.81795500 | 0.00000000 |
| H | -1.09003800 | -2.14808200 | 0.96492700 |
| H | -1.09003800 | -2.14808200 | -0.96492700 |
| H | 1.76968900 | -3.26760800 | 0.00000000 |
| H | -0.91590100 | -3.91688000 | 0.00000000 |
| C | -1.02773400 | 2.47660200 | 0.00000000 |
| C | -1.48973000 | 1.19903400 | 0.00000000 |
| C | -0.69883300 | -0.01434300 | 0.00000000 |
| C | 0.69883300 | 0.01434300 | 0.00000000 |
| C | 1.48973000 | -1.19903400 | 0.00000000 |
| C | 1.02773400 | -2.47660200 | 0.00000000 |

$C_6B_4H_{12}$ (k=2) Isomer III

| | | | |
|---|---|---|---|
| B | 0.00000000 | 1.32569000 | -1.59795000 |
| B | 0.00000000 | 2.80942400 | -0.60277800 |
| H | 0.00000000 | 1.07707900 | 2.46310900 |
| H | 0.00000000 | 3.90729200 | -1.05310400 |
| H | 0.00000000 | 1.36032000 | -2.78425500 |
| H | 0.00000000 | 3.28997300 | 1.63529200 |
| H | 0.96377000 | 2.14548700 | -1.20826100 |
| H | -0.96377000 | 2.14548700 | -1.20826100 |
| B | 0.00000000 | -1.32569000 | -1.59795000 |
| H | 0.00000000 | -1.36032000 | -2.78425500 |
| H | 0.00000000 | -1.07707900 | 2.46310900 |
| B | 0.00000000 | -2.80942400 | -0.60277800 |
| H | 0.96377000 | -2.14548700 | -1.20826100 |
| H | -0.96377000 | -2.14548700 | -1.20826100 |
| H | 0.00000000 | -3.90729200 | -1.05310400 |
| H | 0.00000000 | -3.28997300 | 1.63529200 |
| C | 0.00000000 | 0.00000000 | -0.79575100 |
| C | 0.00000000 | 0.00000000 | 0.59805600 |
| C | 0.00000000 | 1.22394200 | 1.38696800 |
| C | 0.00000000 | 2.48798600 | 0.90506600 |
| C | 0.00000000 | -1.22394200 | 1.38696800 |
| C | 0.00000000 | -2.48798600 | 0.90506600 |

$C_6B_4H_{12}$ (k=2) Isomer IV

| | | | |
|---|---|---|---|
| B | 1.37677200 | -1.79904500 | 0.00000000 |
| B | -0.10819900 | -0.98135400 | 0.00000000 |
| B | 0.00000000 | 0.84106900 | 0.00000000 |
| B | 2.80530500 | -0.70986400 | 0.00000000 |
| H | 1.46002300 | 2.59693500 | 0.00000000 |
| H | 3.90469600 | -1.16396800 | 0.00000000 |
| H | 1.54625900 | -2.97636200 | 0.00000000 |
| H | 3.49900900 | 1.44471700 | 0.00000000 |
| H | 2.14244100 | -1.33894800 | 0.96211000 |
| H | -0.03279500 | -0.08232100 | 0.95747900 |
| H | 2.14244100 | -1.33894800 | -0.96211000 |
| H | -0.03279500 | -0.08232100 | -0.95747900 |
| H | -1.80416100 | -2.53249500 | 0.00000000 |
| H | -1.45750000 | 2.61832000 | 0.00000000 |
| H | -3.63844200 | -1.01647000 | 0.00000000 |
| H | -3.47919600 | 1.35806600 | 0.00000000 |
| C | 2.59213700 | 0.84344500 | 0.00000000 |
| C | 1.41682200 | 1.50868800 | 0.00000000 |
| C | -1.57410600 | -1.47189900 | 0.00000000 |
| C | -2.63026800 | -0.61356200 | 0.00000000 |
| C | -1.37399700 | 1.53583200 | 0.00000000 |
| C | -2.53381600 | 0.82412300 | 0.00000000 |

$C_4B_6H_{14}$ (k=3) Isomer I

| | | | |
|---|---|---|---|
| B | 1.08861000 | -1.73475300 | 0.00000000 |
| B | 1.38120300 | 1.42342000 | 0.00000000 |
| B | 2.92667700 | 0.54007600 | 0.00000000 |
| B | 2.77599400 | -1.14373100 | 0.00000000 |
| H | 1.37890300 | 2.61273600 | 0.00000000 |
| H | 3.66747000 | -1.92916700 | 0.00000000 |
| H | 0.88823700 | -2.90595000 | 0.00000000 |
| H | 3.93752900 | 1.16373700 | 0.00000000 |
| H | 1.97861400 | -1.51612500 | 0.96330600 |
| H | 2.19785800 | 1.05289700 | 0.96443100 |
| H | 1.97861400 | -1.51612500 | -0.96330600 |
| H | 2.19785800 | 1.05289700 | -0.96443100 |
| B | -1.52533000 | -1.41729500 | 0.00000000 |
| H | -1.67242300 | -2.59488300 | 0.00000000 |
| H | -0.91676100 | 2.59340800 | 0.00000000 |
| B | -2.91666600 | -0.29562000 | 0.00000000 |
| H | -2.29699600 | -0.95169400 | 0.96416600 |
| H | -2.29699600 | -0.95169400 | -0.96416600 |
| H | -4.04791000 | -0.65355000 | 0.00000000 |
| H | -3.19190800 | 1.97453200 | 0.00000000 |
| C | -0.12721300 | -0.73645900 | 0.00000000 |
| C | 0.00000000 | 0.64807400 | 0.00000000 |
| C | -1.15333300 | 1.53432200 | 0.00000000 |
| C | -2.46187600 | 1.17214600 | 0.00000000 |

$C_4B_6H_{14}$ (k=3) Isomer II

| | | | |
|---|---|---|---|
| B | 0.00000000 | 1.54851300 | -1.75496300 |
| B | 0.00000000 | 0.00000000 | -1.05654700 |
| B | 0.00000000 | 0.00000000 | 0.76651100 |
| B | 0.00000000 | 2.91190800 | -0.59000800 |
| H | 0.00000000 | 1.33556700 | 2.60904500 |
| H | 0.00000000 | 4.03881100 | -0.97036600 |
| H | 0.00000000 | 1.79471300 | -2.91834600 |
| H | 0.00000000 | 3.45327900 | 1.61168200 |
| H | 0.96214100 | 2.28935900 | -1.24997300 |
| H | 0.95676700 | 0.00000000 | -0.17258000 |
| H | -0.96214100 | 2.28935900 | -1.24997300 |
| H | -0.95676700 | 0.00000000 | -0.17258000 |
| B | 0.00000000 | -1.54851300 | -1.75496300 |
| H | 0.00000000 | -1.79471300 | -2.91834600 |
| H | 0.00000000 | -1.33556700 | 2.60904500 |
| B | 0.00000000 | -2.91190800 | -0.59000800 |
| H | 0.96214100 | -2.28935900 | -1.24997300 |
| H | -0.96214100 | -2.28935900 | -1.24997300 |
| H | 0.00000000 | -4.03881100 | -0.97036600 |
| H | 0.00000000 | -3.45327900 | 1.61168200 |
| C | 0.00000000 | 2.59360200 | 0.94476700 |
| C | 0.00000000 | 1.37193200 | 1.52030800 |
| C | 0.00000000 | -1.37193200 | 1.52030800 |
| C | 0.00000000 | -2.59360200 | 0.94476700 |

$C_4B_6H_{14}$ (k=3) Isomer III

| | | | |
|---|---|---|---|
| B | -1.46182900 | 1.70556400 | 0.00000000 |
| B | 0.03834100 | 0.91255000 | 0.00000000 |
| B | -0.03834100 | -0.91255000 | 0.00000000 |
| B | -2.88450900 | 0.61331700 | 0.00000000 |
| H | -1.49135000 | -2.66341400 | 0.00000000 |
| H | -3.98523600 | 1.06277200 | 0.00000000 |
| H | -1.63753200 | 2.88215600 | 0.00000000 |
| H | -3.54602500 | -1.55151500 | 0.00000000 |
| H | -2.21678000 | 1.23935000 | 0.96288200 |
| H | 0.00000000 | 0.00000000 | 0.95474700 |
| H | -2.21678000 | 1.23935000 | -0.96288200 |
| H | 0.00000000 | 0.00000000 | -0.95474700 |
| B | 1.46182900 | -1.70556400 | 0.00000000 |
| H | 1.49135000 | 2.66341400 | 0.00000000 |
| H | 1.63753200 | -2.88215600 | 0.00000000 |
| B | 2.88450900 | -0.61331700 | 0.00000000 |
| H | 2.21678000 | -1.23935000 | 0.96288200 |
| H | 2.21678000 | -1.23935000 | -0.96288200 |
| H | 3.54602500 | 1.55151500 | 0.00000000 |
| H | 3.98523600 | -1.06277200 | 0.00000000 |
| C | -2.65098200 | -0.93280500 | 0.00000000 |
| C | -1.46182900 | -1.57532500 | 0.00000000 |
| C | 1.46182900 | 1.57532500 | 0.00000000 |
| C | 2.65098200 | 0.93280500 | 0.00000000 |

$C_4B_6H_{14}$ (k=3) Isomer IV

| | | | |
|---|---|---|---|
| B | 0.00000000 | 0.92971600 | 0.11218700 |
| B | 0.00000000 | -0.92971600 | 0.11218700 |
| H | 0.00000000 | -2.59310900 | 1.70524000 |
| H | 0.00000000 | 1.19753500 | 3.65645300 |
| H | 0.00000000 | 2.59310900 | 1.70524000 |
| H | 0.00000000 | -1.19753500 | 3.65645300 |
| H | 0.96356600 | 0.00000000 | 0.06030700 |
| H | -0.96356600 | 0.00000000 | 0.06030700 |
| B | 0.00000000 | 1.79303600 | -1.36831600 |
| B | 0.00000000 | -1.79303600 | -1.36831600 |
| H | 0.00000000 | 2.99720200 | -1.43773000 |
| H | 0.00000000 | -2.99720200 | -1.43773000 |
| B | 0.00000000 | 0.86208300 | -2.93286200 |
| B | 0.00000000 | -0.86208300 | -2.93286200 |
| H | 0.97301700 | 1.37700600 | -2.18721300 |
| H | 0.97301700 | -1.37700600 | -2.18721300 |
| H | -0.97301700 | 1.37700600 | -2.18721300 |
| H | -0.97301700 | -1.37700600 | -2.18721300 |
| H | 0.00000000 | 1.50156300 | -3.95498100 |
| H | 0.00000000 | -1.50156300 | -3.95498100 |
| C | 0.00000000 | 1.50876600 | 1.54614400 |
| C | 0.00000000 | 0.72115400 | 2.66887200 |
| C | 0.00000000 | -0.72115400 | 2.66887200 |
| C | 0.00000000 | -1.50876600 | 1.54614400 |

$C_2B_8H_{16}$ (k=4) Isomer I

| | | | |
|---|---|---|---|
| B | -1.31383300 | 1.57914000 | 0.00000000 |
| B | -1.31383300 | -1.57914000 | 0.00000000 |
| B | -2.94094300 | -0.84403200 | 0.00000000 |
| B | -2.94094300 | 0.84403200 | 0.00000000 |
| H | -1.22430700 | -2.76381600 | 0.00000000 |
| H | -3.89109600 | 1.55706200 | 0.00000000 |
| H | -1.22430700 | 2.76381600 | 0.00000000 |
| H | -3.89109600 | -1.55706200 | 0.00000000 |
| H | -2.16862100 | 1.28048100 | 0.96337800 |
| H | -2.16862100 | -1.28048100 | 0.96337800 |
| H | -2.16862100 | 1.28048100 | -0.96337800 |
| H | -2.16862100 | -1.28048100 | -0.96337800 |
| B | 1.31383300 | 1.57914000 | 0.00000000 |
| B | 1.31383300 | -1.57914000 | 0.00000000 |
| H | 1.22430700 | 2.76381600 | 0.00000000 |
| H | 1.22430700 | -2.76381600 | 0.00000000 |
| B | 2.94094300 | 0.84403200 | 0.00000000 |
| B | 2.94094300 | -0.84403200 | 0.00000000 |
| H | 2.16862100 | 1.28048100 | 0.96337800 |
| H | 2.16862100 | -1.28048100 | 0.96337800 |
| H | 2.16862100 | 1.28048100 | -0.96337800 |
| H | 2.16862100 | -1.28048100 | -0.96337800 |
| H | 3.89109600 | 1.55706200 | 0.00000000 |
| H | 3.89109600 | -1.55706200 | 0.00000000 |
| C | 0.00000000 | 0.69064800 | 0.00000000 |
| C | 0.00000000 | -0.69064800 | 0.00000000 |

$C_2B_8H_{16}$ (k=4) Isomer II

| | | | |
|---|---|---|---|
| B | 1.30210600 | -1.91797500 | 0.00000000 |
| B | -0.13466900 | -0.98084000 | 0.00000000 |
| B | 0.00000000 | 0.84542700 | 0.00000000 |
| B | 1.54410600 | 1.59292800 | 0.00000000 |
| B | 3.02813000 | 0.58741800 | 0.00000000 |
| B | 2.91159200 | -1.12201100 | 0.00000000 |
| H | 1.67846400 | 2.77675400 | 0.00000000 |
| H | 3.87398300 | -1.82248100 | 0.00000000 |
| H | 1.28854100 | -3.10852000 | 0.00000000 |
| H | 4.07352900 | 1.15600600 | 0.00000000 |
| H | 2.13733100 | -1.56699000 | 0.96060500 |
| H | 2.31510200 | 1.13481000 | 0.96139600 |
| H | -0.03897100 | -0.08578700 | 0.95230300 |
| H | 2.13733100 | -1.56699000 | -0.96060500 |
| H | 2.31510200 | 1.13481000 | -0.96139600 |
| H | -0.03897100 | -0.08578700 | -0.95230300 |
| B | -1.72993400 | -1.56763600 | 0.00000000 |
| H | -2.05077500 | -2.71294600 | 0.00000000 |
| H | -1.22682300 | 2.75646900 | 0.00000000 |
| B | -3.01594300 | -0.32019600 | 0.00000000 |
| H | -2.42952200 | -1.01546300 | 0.96267900 |
| H | -2.42952200 | -1.01546300 | -0.96267900 |
| H | -4.16418800 | -0.62952200 | 0.00000000 |
| H | -3.40367500 | 1.91315900 | 0.00000000 |
| C | -1.33320900 | 1.67286100 | 0.00000000 |
| C | -2.59410500 | 1.18586700 | 0.00000000 |

$B_{10}H_{18}$ (k=5) - Kekulé Structure $K_1$

| | | | |
|---|---|---|---|
| B | -1.50496200 | 1.74986000 | 0.00000000 |
| B | 0.00000000 | 0.91728300 | 0.00000000 |
| B | 0.00000000 | -0.91728300 | 0.00000000 |
| B | -1.50496200 | -1.74986000 | 0.00000000 |
| B | -3.06005500 | -0.85558400 | 0.00000000 |
| B | -3.06005500 | 0.85558400 | 0.00000000 |
| H | -1.56750400 | -2.93907600 | 0.00000000 |
| H | -4.06214000 | 1.49753800 | 0.00000000 |
| H | -1.56750400 | 2.93907600 | 0.00000000 |
| H | -4.06214000 | -1.49753800 | 0.00000000 |
| H | -2.30830000 | 1.34504700 | 0.96095200 |
| H | -2.30830000 | -1.34504700 | 0.96095200 |
| H | 0.00000000 | 0.00000000 | 0.94969300 |
| H | -2.30830000 | 1.34504700 | -0.96095200 |
| H | -2.30830000 | -1.34504700 | -0.96095200 |
| H | 0.00000000 | 0.00000000 | -0.94969300 |
| B | 1.50496200 | 1.74986000 | 0.00000000 |
| B | 1.50496200 | -1.74986000 | 0.00000000 |
| H | 1.56750400 | 2.93907600 | 0.00000000 |
| H | 1.56750400 | -2.93907600 | 0.00000000 |
| B | 3.06005500 | 0.85558400 | 0.00000000 |
| B | 3.06005500 | -0.85558400 | 0.00000000 |
| H | 2.30830000 | 1.34504700 | 0.96095200 |
| H | 2.30830000 | -1.34504700 | 0.96095200 |
| H | 2.30830000 | 1.34504700 | -0.96095200 |
| H | 2.30830000 | -1.34504700 | -0.96095200 |
| H | 4.06214000 | 1.49753800 | 0.00000000 |
| H | 4.06214000 | -1.49753800 | 0.00000000 |

**Naphthalene Kekulé Structure $K_2$ : $C_{(10-2k)}B_{(2k)}H_{(8+2k)}$**

$C_8B_2H_{10}$ (k=1) Isomer I – same structure and energy as Isomer I in $K_1$ (see above)

$C_8B_2H_{10}$ (k=1) Isomer II – same structure and energy as Isomer II in $K_1$ (see above)

$C_8B_2H_{10}$ (k=1) Isomer III

| | | | |
|---|---|---|---|
| B | 0.00000000 | 0.90248800 | 2.56883400 |
| B | 0.00000000 | -0.90248800 | 2.56883400 |
| H | 0.00000000 | 2.55899500 | 1.02215600 |
| H | 0.00000000 | -1.55065600 | 3.56256800 |
| H | 0.00000000 | -2.55899500 | 1.02215600 |
| H | 0.00000000 | 1.55065600 | 3.56256800 |
| H | -0.96347100 | 0.00000000 | 2.67912500 |
| H | 0.96347100 | 0.00000000 | 2.67912500 |
| H | 0.00000000 | -2.48291200 | -1.28134400 |
| H | 0.00000000 | 2.48291200 | -1.28134400 |
| H | 0.00000000 | -1.24532100 | -3.39212800 |
| H | 0.00000000 | 1.24532100 | -3.39212800 |
| C | 0.00000000 | -1.48198200 | 1.15863700 |
| C | 0.00000000 | -0.73472900 | -0.00096400 |
| C | 0.00000000 | -1.40050000 | -1.28138200 |
| C | 0.00000000 | -0.71564700 | -2.44871500 |
| C | 0.00000000 | 0.71564700 | -2.44871500 |
| C | 0.00000000 | 1.40050000 | -1.28138200 |
| C | 0.00000000 | 0.73472900 | -0.00096400 |
| C | 0.00000000 | 1.48198200 | 1.15863700 |

$C_6B_4H_{12}$ (k=2) Isomer I

| | | | |
|---|---|---|---|
| H | 0.00000000 | 2.46275800 | 1.34701600 |
| H | 0.00000000 | -1.24006100 | 3.48173600 |
| H | 0.00000000 | -2.46275800 | 1.34701600 |
| H | 0.00000000 | 1.24006100 | 3.48173600 |
| B | 0.00000000 | -1.60447300 | -1.18051500 |
| B | 0.00000000 | 1.60447300 | -1.18051500 |
| H | 0.00000000 | -2.78867400 | -1.06896500 |
| H | 0.00000000 | 2.78867400 | -1.06896500 |
| B | 0.00000000 | -0.84853600 | -2.79571400 |
| B | 0.00000000 | 0.84853600 | -2.79571400 |
| H | -0.96405300 | -1.30631300 | -2.04264900 |
| H | -0.96405300 | 1.30631300 | -2.04264900 |
| H | 0.96405300 | -1.30631300 | -2.04264900 |
| H | 0.96405300 | 1.30631300 | -2.04264900 |
| H | 0.00000000 | -1.54364800 | -3.75959600 |
| H | 0.00000000 | 1.54364800 | -3.75959600 |
| C | 0.00000000 | -0.71175600 | 0.10752700 |
| C | 0.00000000 | -1.38013600 | 1.33978400 |
| C | 0.00000000 | -0.69450700 | 2.54706600 |
| C | 0.00000000 | 0.69450700 | 2.54706600 |
| C | 0.00000000 | 1.38013600 | 1.33978400 |
| C | 0.00000000 | 0.71175600 | 0.10752700 |

$C_6B_4H_{12}$ (k=2) Isomer II

| | | | |
|---|---|---|---|
| B | 0.00000000 | 0.76700900 | 0.00000000 |
| B | 1.67420600 | 1.46367700 | 0.00000000 |
| H | 1.89244900 | 2.63137700 | 0.00000000 |
| H | 3.29438100 | -1.67367200 | 0.00000000 |
| H | 1.09369900 | -2.58789600 | 0.00000000 |
| H | 3.81325600 | 0.65405800 | 0.00000000 |
| H | 0.82584700 | 1.22634200 | 0.96340000 |
| H | 0.82584700 | 1.22634200 | -0.96340000 |
| B | -1.37751100 | -1.53546300 | 0.00000000 |
| H | -1.46645600 | -2.72157500 | 0.00000000 |
| H | -1.23911400 | 2.70175900 | 0.00000000 |
| B | -2.81791900 | -0.47703100 | 0.00000000 |
| H | -2.17238000 | -1.10752500 | 0.96419700 |
| H | -2.17238000 | -1.10752500 | -0.96419700 |
| H | -3.91699800 | -0.92744500 | 0.00000000 |
| H | -3.39803700 | 1.72855900 | 0.00000000 |
| C | -2.53915700 | 1.06153700 | 0.00000000 |
| C | -1.31027100 | 1.61550400 | 0.00000000 |
| C | -0.01203000 | -0.78312800 | 0.00000000 |
| C | 1.15389000 | -1.50237300 | 0.00000000 |
| C | 2.48035100 | -0.95550400 | 0.00000000 |
| C | 2.76488500 | 0.37500400 | 0.00000000 |

$C_6B_4H_{12}$ (k=2) Isomer III

| | | | |
|---|---|---|---|
| B | 2.55897500 | 1.04723100 | 0.00000000 |
| B | 2.68998200 | -0.73811500 | 0.00000000 |
| H | 0.89925700 | 2.58531400 | 0.00000000 |
| H | 3.71986200 | -1.32750000 | 0.00000000 |
| H | 1.26250000 | -2.49700100 | 0.00000000 |
| H | 3.49422500 | 1.77744900 | 0.00000000 |
| H | 2.75731500 | 0.15919700 | 0.96373600 |
| H | 2.75731500 | 0.15919700 | -0.96373600 |
| B | -1.19068400 | -1.66371900 | 0.00000000 |
| H | -1.10882300 | -2.84799500 | 0.00000000 |
| H | -1.26580600 | 2.43652700 | 0.00000000 |
| B | -2.72259600 | -0.78193200 | 0.00000000 |
| H | -2.02868100 | -1.36648600 | 0.96474500 |
| H | -2.02868100 | -1.36648600 | -0.96474500 |
| H | -3.78665100 | -1.30712100 | 0.00000000 |
| H | -3.38861200 | 1.40694800 | 0.00000000 |
| C | -2.52120300 | 0.75596800 | 0.00000000 |
| C | -1.31461300 | 1.35178800 | 0.00000000 |
| C | 0.00000000 | 0.69871800 | 0.00000000 |
| C | 1.10285700 | 1.51898300 | 0.00000000 |
| C | 0.09801900 | -0.76776200 | 0.00000000 |
| C | 1.30800500 | -1.41259000 | 0.00000000 |

$C_6B_4H_{12}$ (k=2) Isomer IV

| | | | |
|---|---|---|---|
| B | 1.66509800 | -1.56612900 | 0.00000000 |
| B | -0.00680500 | -0.88228500 | 0.00000000 |
| H | 1.11486200 | 2.48058700 | 0.00000000 |
| H | 3.81160900 | -0.78399200 | 0.00000000 |
| H | 1.86822200 | -2.73563200 | 0.00000000 |
| H | 3.30759600 | 1.55021600 | 0.00000000 |
| H | 0.78251700 | -1.33395600 | 0.96044700 |
| H | 0.78251700 | -1.33395600 | -0.96044700 |
| B | -1.46566200 | -1.73396400 | 0.00000000 |
| H | -1.61211700 | -2.91403100 | 0.00000000 |
| H | -1.14157900 | 2.51162800 | 0.00000000 |
| B | -2.85015200 | -0.61130600 | 0.00000000 |
| H | -2.22937700 | -1.29436700 | 0.96223400 |
| H | -2.22937700 | -1.29436700 | -0.96223400 |
| H | -3.97984900 | -0.98200800 | 0.00000000 |
| H | -3.31279200 | 1.61505600 | 0.00000000 |
| C | -2.49343400 | 0.90325900 | 0.00000000 |
| C | -1.24772800 | 1.42825900 | 0.00000000 |
| C | 0.00000000 | 0.67986200 | 0.00000000 |
| C | 1.17464200 | 1.39496700 | 0.00000000 |
| C | 2.48841100 | 0.83793800 | 0.00000000 |
| C | 2.76567100 | -0.49707900 | 0.00000000 |

$C_6B_4H_{12}$ (k=2) Isomer V

| | | | |
|---|---|---|---|
| B | 0.00000000 | 1.62639500 | -1.49998100 |
| B | 0.00000000 | 0.84483600 | 0.11349700 |
| B | 0.00000000 | -0.84483600 | 0.11349700 |
| B | 0.00000000 | -1.62639500 | -1.49998100 |
| H | 0.00000000 | -2.80999900 | -1.62934200 |
| H | 0.00000000 | 1.16349700 | -3.71405800 |
| H | 0.00000000 | 2.80999900 | -1.62934200 |
| H | 0.00000000 | -1.16349700 | -3.71405800 |
| H | -0.96298100 | -1.34350100 | -0.64874200 |
| H | -0.96298100 | 1.34350100 | -0.64874200 |
| H | 0.96298100 | -1.34350100 | -0.64874200 |
| H | 0.96298100 | 1.34350100 | -0.64874200 |
| H | 0.00000000 | 2.59479100 | 1.66422600 |
| H | 0.00000000 | -2.59479100 | 1.66422600 |
| H | 0.00000000 | 1.19271600 | 3.59597000 |
| H | 0.00000000 | -1.19271600 | 3.59597000 |
| C | 0.00000000 | 1.51944800 | 1.51455500 |
| C | 0.00000000 | 0.73360800 | 2.61180000 |
| C | 0.00000000 | -0.73360800 | 2.61180000 |
| C | 0.00000000 | -1.51944800 | 1.51455500 |
| C | 0.00000000 | 0.67674800 | -2.74083700 |
| C | 0.00000000 | -0.67674800 | -2.74083700 |

$C_4B_6H_{14}$ (k=3) Isomer I

| | | | |
|---|---|---|---|
| B | 0.00000000 | 0.89167000 | 2.69335600 |
| B | 0.00000000 | -0.89167000 | 2.69335600 |
| H | 0.00000000 | 2.54333400 | 1.14865300 |
| H | 0.00000000 | -1.55840300 | 3.67509200 |
| H | 0.00000000 | -2.54333400 | 1.14865300 |
| H | 0.00000000 | 1.55840300 | 3.67509200 |
| H | -0.96379600 | 0.00000000 | 2.83319500 |
| H | 0.96379600 | 0.00000000 | 2.83319500 |
| B | 0.00000000 | -1.60508600 | -1.21949600 |
| B | 0.00000000 | 1.60508600 | -1.21949600 |
| H | 0.00000000 | -2.78943500 | -1.12090300 |
| H | 0.00000000 | 2.78943500 | -1.12090300 |
| B | 0.00000000 | -0.84948700 | -2.83005800 |
| B | 0.00000000 | 0.84948700 | -2.83005800 |
| H | -0.96437500 | -1.30551900 | -2.07704200 |
| H | -0.96437500 | 1.30551900 | -2.07704200 |
| H | 0.96437500 | -1.30551900 | -2.07704200 |
| H | 0.96437500 | 1.30551900 | -2.07704200 |
| H | 0.00000000 | -1.54387000 | -3.79411700 |
| H | 0.00000000 | 1.54387000 | -3.79411700 |
| C | 0.00000000 | -0.73752200 | 0.10087100 |
| C | 0.00000000 | -1.46440100 | 1.26465500 |
| C | 0.00000000 | 0.73752200 | 0.10087100 |
| C | 0.00000000 | 1.46440100 | 1.26465500 |

$C_4B_6H_{14}$ (k=3) Isomer II

| | | | |
|---|---|---|---|
| B | 1.82814100 | -1.38039700 | 0.00000000 |
| B | 0.10709600 | -0.81196200 | 0.00000000 |
| H | 0.99890200 | 2.61153500 | 0.00000000 |
| H | 3.91908500 | -0.44867700 | 0.00000000 |
| H | 2.11605800 | -2.53225600 | 0.00000000 |
| H | 3.24834600 | 1.84409200 | 0.00000000 |
| H | 0.93904500 | -1.20679800 | 0.95893100 |
| H | 0.93904500 | -1.20679800 | -0.95893100 |
| B | -1.22317600 | -1.87829400 | 0.00000000 |
| B | -1.37596800 | 1.49406600 | 0.00000000 |
| H | -1.11814000 | -3.06485600 | 0.00000000 |
| H | -1.42069800 | 2.68384500 | 0.00000000 |
| B | -2.84794500 | -1.13425600 | 0.00000000 |
| B | -2.91451500 | 0.57186300 | 0.00000000 |
| H | -2.07427200 | -1.59279200 | 0.96086600 |
| H | -2.19416100 | 1.07151800 | 0.96403500 |
| H | -2.07427200 | -1.59279200 | -0.96086600 |
| H | -2.19416100 | 1.07151800 | -0.96403500 |
| H | -3.81240100 | -1.83151700 | 0.00000000 |
| H | -3.92382500 | 1.20047500 | 0.00000000 |
| C | 0.00000000 | 0.74582500 | 0.00000000 |
| C | 1.12391400 | 1.53161400 | 0.00000000 |
| C | 2.48448900 | 1.07253000 | 0.00000000 |
| C | 2.85547900 | -0.23523600 | 0.00000000 |

$C_4B_6H_{14}$ (k=3) Isomer III

| | | | |
|---|---|---|---|
| B | 1.54087600 | -1.73470900 | 0.00000000 |
| B | -0.03952600 | -0.86570000 | 0.00000000 |
| B | 2.62650700 | 0.97182000 | 0.00000000 |
| B | 2.94021900 | -0.78802000 | 0.00000000 |
| H | 1.01468100 | 2.54430800 | 0.00000000 |
| H | 4.06059900 | -1.18394700 | 0.00000000 |
| H | 1.50459100 | -2.92284600 | 0.00000000 |
| H | 3.51786300 | 1.75857600 | 0.00000000 |
| H | 2.88614200 | 0.09816900 | 0.96302100 |
| H | 0.72788500 | -1.36545200 | 0.95990700 |
| H | 2.88614200 | 0.09816900 | -0.96302100 |
| H | 0.72788500 | -1.36545200 | -0.95990700 |
| B | -1.52951000 | -1.68529600 | 0.00000000 |
| H | -1.67725600 | -2.86509700 | 0.00000000 |
| H | -1.15179600 | 2.54938300 | 0.00000000 |
| B | -2.89564300 | -0.55372400 | 0.00000000 |
| H | -2.28939600 | -1.25225500 | 0.96254200 |
| H | -2.28939600 | -1.25225500 | -0.96254200 |
| H | -4.03165400 | -0.90370900 | 0.00000000 |
| H | -3.32305400 | 1.67858200 | 0.00000000 |
| C | -2.51282400 | 0.95630400 | 0.00000000 |
| C | -1.26491800 | 1.46719700 | 0.00000000 |
| C | 0.00000000 | 0.72414900 | 0.00000000 |
| C | 1.14810000 | 1.46267900 | 0.00000000 |

$C_4B_6H_{14}$ (k=3) Isomer IV

| | | | |
|---|---|---|---|
| B | 1.39799100 | -1.80072300 | 0.00000000 |
| B | -0.15421200 | -0.91024600 | 0.00000000 |
| B | 0.00000000 | 0.78026000 | 0.00000000 |
| B | 1.68673800 | 1.41141000 | 0.00000000 |
| H | 1.91057500 | 2.58099900 | 0.00000000 |
| H | 3.64991200 | -1.55892900 | 0.00000000 |
| H | 1.42268400 | -2.99067300 | 0.00000000 |
| H | 3.86150600 | 0.76651800 | 0.00000000 |
| H | 0.82500400 | 1.18722600 | 0.96193600 |
| H | 0.54071300 | -1.45773000 | 0.96045900 |
| H | 0.82500400 | 1.18722600 | -0.96193600 |
| H | 0.54071300 | -1.45773000 | -0.96045900 |
| B | -1.72702600 | -1.55613300 | 0.00000000 |
| H | -2.05851100 | -2.69902200 | 0.00000000 |
| H | -1.13382200 | 2.79133600 | 0.00000000 |
| B | -2.97258400 | -0.27211200 | 0.00000000 |
| H | -2.41517900 | -1.00058000 | 0.96264400 |
| H | -2.41517900 | -1.00058000 | -0.96264400 |
| H | -4.12919900 | -0.55018900 | 0.00000000 |
| H | -3.32920400 | 1.96805800 | 0.00000000 |
| C | -2.52411500 | 1.23570200 | 0.00000000 |
| C | -1.26218600 | 1.70937100 | 0.00000000 |
| C | 2.72776900 | -0.98122500 | 0.00000000 |
| C | 2.85027300 | 0.36478400 | 0.00000000 |

$C_4B_6H_{14}$ (k=3) Isomer V

| | | | |
|---|---|---|---|
| B | 0.00000000 | 1.76960100 | -1.42031100 |
| B | 0.00000000 | 0.85617100 | 0.13087200 |
| B | 0.00000000 | -0.85617100 | 0.13087200 |
| B | 0.00000000 | -1.76960100 | -1.42031100 |
| B | 0.00000000 | -0.89878300 | -2.89117500 |
| B | 0.00000000 | 0.89878300 | -2.89117500 |
| H | 0.00000000 | -2.96038100 | -1.36730800 |
| H | 0.00000000 | 1.43612900 | -3.95297800 |
| H | 0.00000000 | 2.96038100 | -1.36730800 |
| H | 0.00000000 | -1.43612900 | -3.95297800 |
| H | -0.96111600 | 0.00000000 | -2.93305000 |
| H | -0.96162000 | -1.37610100 | -0.63168900 |
| H | -0.96162000 | 1.37610100 | -0.63168900 |
| H | 0.96111600 | 0.00000000 | -2.93305000 |
| H | 0.96162000 | -1.37610100 | -0.63168900 |
| H | 0.96162000 | 1.37610100 | -0.63168900 |
| H | 0.00000000 | 2.59175100 | 1.68801800 |
| H | 0.00000000 | -2.59175100 | 1.68801800 |
| H | 0.00000000 | 1.19485100 | 3.62463400 |
| H | 0.00000000 | -1.19485100 | 3.62463400 |
| C | 0.00000000 | 1.51579300 | 1.54342300 |
| C | 0.00000000 | 0.73515800 | 2.64109900 |
| C | 0.00000000 | -0.73515800 | 2.64109900 |
| C | 0.00000000 | -1.51579300 | 1.54342300 |

$C_2B_8H_{16}$ (k=4) Isomer I

| | | | |
|---|---|---|---|
| B | -0.07326800 | -0.80584200 | 0.00000000 |
| B | -1.71810600 | -1.56638100 | 0.00000000 |
| B | -3.05102300 | -0.52628600 | 0.00000000 |
| B | -2.61842600 | 1.20390200 | 0.00000000 |
| H | -1.76779200 | -2.75411400 | 0.00000000 |
| H | -3.45048100 | 2.05348500 | 0.00000000 |
| H | -0.90344400 | 2.66154500 | 0.00000000 |
| H | -4.19549700 | -0.84616800 | 0.00000000 |
| H | -2.93938600 | 0.35886700 | 0.96292700 |
| H | -0.88520600 | -1.25093800 | 0.95814700 |
| H | -2.93938600 | 0.35886700 | -0.96292700 |
| H | -0.88520600 | -1.25093800 | -0.95814700 |
| B | 1.38545600 | 1.53467100 | 0.00000000 |
| B | 1.30267100 | -1.82896900 | 0.00000000 |
| H | 1.41650200 | 2.72419400 | 0.00000000 |
| H | 1.21614200 | -3.01669800 | 0.00000000 |
| B | 2.94062500 | 0.64633700 | 0.00000000 |
| B | 2.91202500 | -1.06060000 | 0.00000000 |
| H | 2.20672900 | 1.12578100 | 0.96423800 |
| H | 2.14505600 | -1.53332300 | 0.96112800 |
| H | 2.20672900 | 1.12578100 | -0.96423800 |
| H | 2.14505600 | -1.53332300 | -0.96112800 |
| H | 3.93479800 | 1.29816200 | 0.00000000 |
| H | 3.88897300 | -1.73959200 | 0.00000000 |
| C | 0.00000000 | 0.78270300 | 0.00000000 |
| C | -1.09889300 | 1.58967300 | 0.00000000 |

$C_2B_8H_{16}$ (k=4) Isomer II

| | | | |
|---|---|---|---|
| B | 0.00000000 | 1.60448100 | 1.61992900 |
| B | 0.00000000 | 0.85403000 | -0.01387300 |
| B | 0.00000000 | -0.85403000 | -0.01387300 |
| B | 0.00000000 | -1.60448100 | 1.61992900 |
| H | 0.00000000 | -2.78821300 | 1.74382600 |
| H | 0.00000000 | 1.16973400 | 3.84585800 |
| H | 0.00000000 | 2.78821300 | 1.74382600 |
| H | 0.00000000 | -1.16973400 | 3.84585800 |
| H | 0.95906100 | -1.32425500 | 0.74507500 |
| H | 0.95906100 | 1.32425500 | 0.74507500 |
| H | -0.95906100 | -1.32425500 | 0.74507500 |
| H | -0.95906100 | 1.32425500 | 0.74507500 |
| B | 0.00000000 | 1.76864100 | -1.45812500 |
| B | 0.00000000 | -1.76864100 | -1.45812500 |
| H | 0.00000000 | 2.95842700 | -1.51854200 |
| H | 0.00000000 | -2.95842700 | -1.51854200 |
| B | 0.00000000 | 0.85849300 | -3.00549200 |
| B | 0.00000000 | -0.85849300 | -3.00549200 |
| H | 0.96107400 | 1.35526000 | -2.25920100 |
| H | 0.96107400 | -1.35526000 | -2.25920100 |
| H | -0.96107400 | 1.35526000 | -2.25920100 |
| H | -0.96107400 | -1.35526000 | -2.25920100 |
| H | 0.00000000 | 1.49076200 | -4.01399600 |
| H | 0.00000000 | -1.49076200 | -4.01399600 |
| C | 0.00000000 | 0.67543500 | 2.87648500 |
| C | 0.00000000 | -0.67543500 | 2.87648500 |

$C_2B_8H_{16}$ (k=4) Isomer III

| | | | |
|---|---|---|---|
| B | -1.65614900 | 1.52667800 | 0.00000000 |
| B | 0.00000000 | 0.79694000 | 0.00000000 |
| B | 0.19333000 | -0.91119600 | 0.00000000 |
| B | -1.27017300 | -1.95735800 | 0.00000000 |
| B | -2.83680500 | -1.26719700 | 0.00000000 |
| B | -3.03454400 | 0.51565700 | 0.00000000 |
| H | -1.09730800 | -3.13584700 | 0.00000000 |
| H | -4.14514500 | 0.94304300 | 0.00000000 |
| H | -1.72479100 | 2.71667300 | 0.00000000 |
| H | -3.82531200 | -1.93017500 | 0.00000000 |
| H | -2.98896500 | -0.38531700 | 0.96110600 |
| H | -0.49404000 | -1.49007900 | 0.95855700 |
| H | -0.83982300 | 1.20338000 | 0.96001200 |
| H | -2.98896500 | -0.38531700 | -0.96110600 |
| H | -0.49404000 | -1.49007900 | -0.95855700 |
| H | -0.83982300 | 1.20338000 | -0.96001200 |
| B | 1.78947400 | -1.51468000 | 0.00000000 |
| H | 1.11366300 | 2.81009400 | 0.00000000 |
| H | 2.13301400 | -2.65395400 | 0.00000000 |
| B | 3.01275200 | -0.21602300 | 0.00000000 |
| H | 2.47028100 | -0.95522600 | 0.96298500 |
| H | 2.47028100 | -0.95522600 | -0.96298500 |
| H | 3.32196600 | 2.03141000 | 0.00000000 |
| H | 4.17461700 | -0.47025600 | 0.00000000 |
| C | 2.53226900 | 1.28254600 | 0.00000000 |
| C | 1.26189200 | 1.73068600 | 0.00000000 |

$B_{10}H_{18}$ (k=5) – Kekulé structure $K_2$

| | | | |
|---|---|---|---|
| B | 0.00000000 | 1.74417700 | 1.54761600 |
| B | 0.00000000 | 0.86509000 | -0.03241200 |
| B | 0.00000000 | -0.86509000 | -0.03241200 |
| B | 0.00000000 | -1.74417700 | 1.54761600 |
| B | 0.00000000 | -0.89571900 | 3.03332000 |
| B | 0.00000000 | 0.89571900 | 3.03332000 |
| H | 0.00000000 | -2.93407300 | 1.49697700 |
| H | 0.00000000 | 1.44856000 | 4.08729300 |
| H | 0.00000000 | 2.93407300 | 1.49697700 |
| H | 0.00000000 | -1.44856000 | 4.08729300 |
| H | 0.96123500 | 0.00000000 | 3.08978900 |
| H | 0.95681700 | -1.34991800 | 0.73359200 |
| H | 0.95681700 | 1.34991800 | 0.73359200 |
| H | -0.96123500 | 0.00000000 | 3.08978900 |
| H | -0.95681700 | -1.34991800 | 0.73359200 |
| H | -0.95681700 | 1.34991800 | 0.73359200 |
| B | 0.00000000 | 1.76159100 | -1.49488700 |
| B | 0.00000000 | -1.76159100 | -1.49488700 |
| H | 0.00000000 | 2.95131300 | -1.55332800 |
| H | 0.00000000 | -2.95131300 | -1.55332800 |
| B | 0.00000000 | 0.85796800 | -3.04383800 |
| B | 0.00000000 | -0.85796800 | -3.04383800 |
| H | 0.96130600 | 1.35008000 | -2.29347500 |
| H | 0.96130600 | -1.35008000 | -2.29347500 |
| H | -0.96130600 | 1.35008000 | -2.29347500 |
| H | -0.96130600 | -1.35008000 | -2.29347500 |
| H | 0.00000000 | 1.49355800 | -4.04995300 |
| H | 0.00000000 | -1.49355800 | -4.04995300 |

**Azulene $C_{(10-2k)}B_{(2k)}H_{(8+2k)}$**

$C_{10}H_8$ (k=0)

| | | | |
|---|---|---|---|
| C | 0.00000000 | 0.00000000 | -2.49343800 |
| C | 0.00000000 | 1.26113200 | -1.90366000 |
| C | 0.00000000 | 1.58900700 | -0.55026500 |
| C | 0.00000000 | -1.26113200 | -1.90366000 |
| C | 0.00000000 | 0.74773500 | 0.55154300 |
| C | 0.00000000 | -1.58900700 | -0.55026500 |
| C | 0.00000000 | -0.74773500 | 0.55154300 |
| H | 0.00000000 | 0.00000000 | -3.57782100 |
| H | 0.00000000 | 2.09910300 | -2.58997200 |
| H | 0.00000000 | 2.65050500 | -0.32290000 |
| H | 0.00000000 | -2.09910300 | -2.58997200 |
| H | 0.00000000 | -2.65050500 | -0.32290000 |
| C | 0.00000000 | 1.14577400 | 1.89503400 |
| H | 0.00000000 | 2.16779100 | 2.24004300 |
| C | 0.00000000 | 0.00000000 | 2.69888800 |
| H | 0.00000000 | 0.00000000 | 3.77895200 |
| C | 0.00000000 | -1.14577400 | 1.89503400 |
| H | 0.00000000 | -2.16779100 | 2.24004300 |

$C_8B_2H_{10}$ (k=1) Isomer I

| | | | |
|---|---|---|---|
| H | -2.99402400 | 2.08304200 | 0.00000000 |
| H | -3.33631300 | -0.17340500 | 0.00000000 |
| H | -1.82808200 | -1.93161200 | 0.00000000 |
| H | -1.05491900 | 3.32366200 | 0.00000000 |
| H | 1.15022400 | 2.62225900 | 0.00000000 |
| H | 0.34730700 | -3.07735700 | 0.00000000 |
| H | 2.84488800 | -2.70912100 | 0.00000000 |
| H | 3.62616000 | 0.10938500 | 0.00000000 |
| B | 0.89436600 | 0.38168400 | 0.00000000 |
| B | 2.54159000 | -0.37236100 | 0.00000000 |
| H | 1.87423800 | 0.22782300 | 0.95154400 |
| H | 1.87423800 | 0.22782300 | -0.95154400 |
| C | 0.40923000 | 1.82695700 | 0.00000000 |
| C | -0.88774800 | 2.25047300 | 0.00000000 |
| C | -2.08884800 | 1.48575200 | 0.00000000 |
| C | -2.29518300 | 0.13001100 | 0.00000000 |
| C | -1.37116500 | -0.94449200 | 0.00000000 |
| C | 0.00000000 | -0.89890600 | 0.00000000 |
| C | 0.80627100 | -2.09337700 | 0.00000000 |
| C | 2.14686200 | -1.88127100 | 0.00000000 |

$C_8B_2H_{10}$ (k=1) Isomer II

| | | | |
|---|---|---|---|
| H | -2.88976800 | -2.21037600 | 0.00000000 |
| H | -0.82515100 | -3.27297800 | 0.00000000 |
| H | 1.30574500 | -2.31511500 | 0.00000000 |
| H | -3.35501600 | 0.08472700 | 0.00000000 |
| H | -1.89694900 | 1.86780000 | 0.00000000 |
| H | 3.30594300 | -0.60885400 | 0.00000000 |
| H | 3.07248700 | 2.74454800 | 0.00000000 |
| H | 0.17831700 | 3.03677700 | 0.00000000 |
| B | 2.22454500 | 1.91657600 | 0.00000000 |
| B | 2.37676200 | 0.12827000 | 0.00000000 |
| H | 2.57156300 | 1.00303700 | 0.95099600 |
| H | 2.57156300 | 1.00303700 | -0.95099600 |
| C | 0.70110000 | 2.08887700 | 0.00000000 |
| C | 0.00000000 | 0.90821900 | 0.00000000 |
| C | 0.86750900 | -0.28688100 | 0.00000000 |
| C | 0.49205800 | -1.59720900 | 0.00000000 |
| C | -0.80970400 | -2.18947200 | 0.00000000 |
| C | -2.01767100 | -1.56652100 | 0.00000000 |
| C | -2.30081400 | -0.16652100 | 0.00000000 |
| C | -1.44002200 | 0.88337000 | 0.00000000 |

$C_8B_2H_{10}$ (k=1) Isomer III

| | | | |
|---|---|---|---|
| H | -3.06463300 | 2.13633700 | 0.00000000 |
| H | -3.34118600 | -0.12582400 | 0.00000000 |
| H | -1.83417200 | -1.83584100 | 0.00000000 |
| H | -0.90675200 | 3.61158500 | 0.00000000 |
| H | 1.71437600 | 2.45782800 | 0.00000000 |
| H | 0.26815700 | -3.12752900 | 0.00000000 |
| H | 2.86531300 | -2.59370600 | 0.00000000 |
| H | 3.18707100 | 0.06907600 | 0.00000000 |
| B | -0.83548400 | 2.42600900 | 0.00000000 |
| B | 0.79862600 | 1.70202200 | 0.00000000 |
| H | -0.03512700 | 2.09167700 | 0.97115400 |
| H | -0.03512700 | 2.09167700 | -0.97115400 |
| C | -2.13785300 | 1.56931900 | 0.00000000 |
| C | -2.31397800 | 0.22701100 | 0.00000000 |
| C | -1.36072500 | -0.85828000 | 0.00000000 |
| C | 0.00000000 | -0.90074600 | 0.00000000 |
| C | 0.73098900 | -2.15282700 | 0.00000000 |
| C | 2.06113900 | -1.87340000 | 0.00000000 |
| C | 2.23221100 | -0.43552100 | 0.00000000 |
| C | 1.01594400 | 0.18853700 | 0.00000000 |

$C_8B_2H_{10}$ (k=1) Isomer IV

| | | | |
|---|---|---|---|
| C | 0.68822000 | -1.60188100 | 0.00000000 |
| C | -2.38754200 | 0.01237700 | 0.00000000 |
| C | 0.94006000 | -0.27311500 | 0.00000000 |
| C | -1.43059100 | 0.97626100 | 0.00000000 |
| C | 0.00000000 | 0.90124800 | 0.00000000 |
| H | -3.20132600 | -2.22445400 | 0.00000000 |
| H | -0.69157500 | -3.54853200 | 0.00000000 |
| H | 1.58031700 | -2.22410000 | 0.00000000 |
| H | -3.40521400 | 0.39042700 | 0.00000000 |
| H | -1.78065600 | 2.00610700 | 0.00000000 |
| C | 2.27679100 | 0.29167900 | 0.00000000 |
| H | 3.17788800 | -0.30119100 | 0.00000000 |
| C | 2.18314300 | 1.64710300 | 0.00000000 |
| H | 3.00776100 | 2.34376100 | 0.00000000 |
| C | 0.79148700 | 2.02044200 | 0.00000000 |
| H | 0.42290200 | 3.03549000 | 0.00000000 |
| B | -2.24660000 | -1.51840200 | 0.00000000 |
| B | -0.67188100 | -2.36124700 | 0.00000000 |
| H | -1.44354900 | -1.96197100 | 0.97106000 |
| H | -1.44354900 | -1.96197100 | -0.97106000 |

$C_8B_2H_{10}$ (k=1) Isomer V

| | | | |
|---|---|---|---|
| H | -3.03937500 | -2.05358400 | 0.00000000 |
| H | -1.19681800 | -3.36886100 | 0.00000000 |
| H | 1.34856000 | -2.79631100 | 0.00000000 |
| H | -3.33552900 | 0.18895300 | 0.00000000 |
| H | -1.88573200 | 1.94402700 | 0.00000000 |
| H | 3.43129200 | -0.00293800 | 0.00000000 |
| H | 2.96404300 | 2.52886600 | 0.00000000 |
| H | 0.40511300 | 3.10172800 | 0.00000000 |
| B | 0.51653500 | -1.94776200 | 0.00000000 |
| B | 1.03827700 | -0.25510500 | 0.00000000 |
| H | 0.85779300 | -1.09827400 | 0.97434600 |
| H | 0.85779300 | -1.09827400 | -0.97434600 |
| C | -0.98109800 | -2.30430900 | 0.00000000 |
| C | -2.09343700 | -1.51825300 | 0.00000000 |
| C | -2.28839700 | -0.09298200 | 0.00000000 |
| C | -1.41806000 | 0.96210900 | 0.00000000 |
| C | 0.00000000 | 0.96288500 | 0.00000000 |
| C | 0.77859100 | 2.08441600 | 0.00000000 |
| C | 2.19977400 | 1.76044000 | 0.00000000 |
| C | 2.43909400 | 0.42386100 | 0.00000000 |

$C_6B_4H_{12}$ (k=2) Isomer I

| | | | |
|---|---|---|---|
| H | -3.42634900 | -1.98938200 | 0.00000000 |
| H | -1.08492900 | -3.45584600 | 0.00000000 |
| H | 1.31780800 | -2.41894400 | 0.00000000 |
| H | -3.54661600 | 0.62219500 | 0.00000000 |
| H | -1.85251900 | 2.18076700 | 0.00000000 |
| H | 3.07624600 | -0.79576400 | 0.00000000 |
| H | 3.59808200 | 1.67615100 | 0.00000000 |
| H | 1.20365600 | 3.36503200 | 0.00000000 |
| B | -2.43951300 | -1.32883800 | 0.00000000 |
| B | -0.92621100 | -2.27913600 | 0.00000000 |
| H | -1.66788800 | -1.78496300 | 0.97030800 |
| H | -1.66788800 | -1.78496300 | -0.97030800 |
| B | 0.00000000 | 0.92025300 | 0.00000000 |
| B | 1.29294800 | 2.18216700 | 0.00000000 |
| H | 0.48823000 | 1.74622700 | 0.95008000 |
| H | 0.48823000 | 1.74622700 | -0.95008000 |
| C | -2.53366200 | 0.22430500 | 0.00000000 |
| C | -1.53978500 | 1.13633600 | 0.00000000 |
| C | 0.51137200 | -1.68548300 | 0.00000000 |
| C | 0.90310800 | -0.38629000 | 0.00000000 |
| C | 2.31609500 | -0.02057500 | 0.00000000 |
| C | 2.58250700 | 1.30187800 | 0.00000000 |

$C_6B_4H_{12}$ (k=2) Isomer II

| | | | |
|---|---|---|---|
| H | -3.14866900 | 1.94872900 | 0.00000000 |
| H | -3.37607200 | -0.32441100 | 0.00000000 |
| H | -1.78892000 | -1.99714200 | 0.00000000 |
| H | -1.25755100 | 3.27814600 | 0.00000000 |
| H | 0.97071600 | 2.66735400 | 0.00000000 |
| H | 0.38740300 | -3.31509400 | 0.00000000 |
| H | 3.49393800 | -2.52882700 | 0.00000000 |
| H | 3.50775500 | 0.69554800 | 0.00000000 |
| B | 0.82594300 | 0.41082400 | 0.00000000 |
| B | 2.59132400 | -0.06354200 | 0.00000000 |
| H | 1.82764400 | 0.33296300 | 0.95586200 |
| H | 1.82764400 | 0.33296300 | -0.95586200 |
| B | 2.58629100 | -1.76224700 | 0.00000000 |
| B | 0.85604000 | -2.22070100 | 0.00000000 |
| H | 1.77837100 | -2.20279400 | 0.95145600 |
| H | 1.77837100 | -2.20279400 | -0.95145600 |
| C | 0.00000000 | -0.90662600 | 0.00000000 |
| C | -1.36318200 | -0.99618100 | 0.00000000 |
| C | -2.35337200 | 0.03658800 | 0.00000000 |
| C | -2.21770700 | 1.39242100 | 0.00000000 |
| C | -1.04390000 | 2.21320300 | 0.00000000 |
| C | 0.26172500 | 1.84287900 | 0.00000000 |

$C_6B_4H_{12}$ (k=2) Isomer III

| | | | |
|---|---|---|---|
| H | -3.18348100 | 2.07253200 | 0.00000000 |
| H | -3.37321900 | -0.20517600 | 0.00000000 |
| H | -1.82476500 | -1.85170900 | 0.00000000 |
| H | -1.04105300 | 3.59881600 | 0.00000000 |
| H | 1.57758100 | 2.51502800 | 0.00000000 |
| H | 0.19720300 | -3.35862300 | 0.00000000 |
| H | 3.42440400 | -2.43837600 | 0.00000000 |
| H | 3.09441700 | 0.44973500 | 0.00000000 |
| B | -0.95591500 | 2.41460100 | 0.00000000 |
| B | 0.68389600 | 1.73327400 | 0.00000000 |
| H | -0.13611600 | 2.08782800 | 0.97185800 |
| H | -0.13611600 | 2.08782800 | -0.97185800 |
| B | 2.42714700 | -1.79815300 | 0.00000000 |
| B | 0.72579600 | -2.29737600 | 0.00000000 |
| H | 1.63906400 | -2.32655800 | 0.94979200 |
| H | 1.63906400 | -2.32655800 | -0.94979200 |
| C | 0.98240800 | 0.20313400 | 0.00000000 |
| C | 2.26794400 | -0.25014200 | 0.00000000 |
| C | 0.00000000 | -0.90099500 | 0.00000000 |
| C | -1.36246300 | -0.86935400 | 0.00000000 |
| C | -2.36084200 | 0.18944100 | 0.00000000 |
| C | -2.24064700 | 1.53349900 | 0.00000000 |

$C_6B_4H_{12}$ (k=2) Isomer IV

| | | | |
|---|---|---|---|
| H | -3.22805500 | -2.29037000 | 0.00000000 |
| H | -0.67485700 | -3.59341600 | 0.00000000 |
| H | 1.54465200 | -2.23833600 | 0.00000000 |
| H | -3.42222900 | 0.31876000 | 0.00000000 |
| H | -1.83074900 | 1.93762000 | 0.00000000 |
| H | 3.37886300 | -0.49512600 | 0.00000000 |
| H | 3.01313800 | 2.84478300 | 0.00000000 |
| H | 0.12655800 | 3.00636100 | 0.00000000 |
| B | -2.26386200 | -1.59711600 | 0.00000000 |
| B | -0.68807400 | -2.40569500 | 0.00000000 |
| H | -1.48449000 | -2.04524600 | 0.97190100 |
| H | -1.48449000 | -2.04524600 | -0.97190100 |
| B | 2.22027400 | 1.96421000 | 0.00000000 |
| B | 2.42580400 | 0.20927700 | 0.00000000 |
| H | 2.61611200 | 1.09878500 | 0.94995100 |
| H | 2.61611200 | 1.09878500 | -0.94995100 |
| C | -2.40140500 | -0.05278800 | 0.00000000 |
| C | -1.46339300 | 0.91444400 | 0.00000000 |
| C | 0.00000000 | 0.88388100 | 0.00000000 |
| C | 0.67335700 | 2.07144200 | 0.00000000 |
| C | 0.92695600 | -0.28262500 | 0.00000000 |
| C | 0.65760600 | -1.60947700 | 0.00000000 |

$C_6B_4H_{12}$ (k=2) Isomer V

| | | | |
|---|---|---|---|
| H | -3.15445900 | 2.10010500 | 0.00000000 |
| H | -3.34664800 | -0.14555900 | 0.00000000 |
| H | -1.84753000 | -1.82655100 | 0.00000000 |
| H | -1.13226900 | 3.69416100 | 0.00000000 |
| H | 1.55013100 | 2.80213200 | 0.00000000 |
| H | 0.10911800 | -3.09706500 | 0.00000000 |
| H | 2.63501000 | -3.01448600 | 0.00000000 |
| H | 3.69605800 | -0.28764200 | 0.00000000 |
| B | -0.96350000 | 2.51795700 | 0.00000000 |
| B | 0.72503200 | 1.94625100 | 0.00000000 |
| H | -0.10978900 | 2.21696100 | 0.96859600 |
| H | -0.10978900 | 2.21696100 | -0.96859600 |
| B | 1.05062400 | 0.30010800 | 0.00000000 |
| B | 2.56883800 | -0.65612200 | 0.00000000 |
| H | 1.94783100 | 0.06232600 | 0.94586400 |
| H | 1.94783100 | 0.06232600 | -0.94586400 |
| C | 2.02977500 | -2.11714800 | 0.00000000 |
| C | 0.67930400 | -2.17260000 | 0.00000000 |
| C | 0.00000000 | -0.88667300 | 0.00000000 |
| C | -1.36376600 | -0.85134400 | 0.00000000 |
| C | -2.32613200 | 0.22825800 | 0.00000000 |
| C | -2.20092400 | 1.57873200 | 0.00000000 |

$C_6B_4H_{12}$ (k=2) Isomer VI

| | | | |
|---|---|---|---|
| H | -2.89335600 | 2.57113000 | 0.00000000 |
| H | -3.61428400 | 0.42252800 | 0.00000000 |
| H | -2.38477200 | -1.83239700 | 0.00000000 |
| H | -0.59224900 | 3.65961700 | 0.00000000 |
| H | 1.86072900 | 2.39804900 | 0.00000000 |
| H | 0.47551100 | -3.40556900 | 0.00000000 |
| H | 2.95469600 | -2.69369200 | 0.00000000 |
| H | 3.25409300 | -0.07788700 | 0.00000000 |
| B | -0.66599200 | 2.47319800 | 0.00000000 |
| B | 0.93566800 | 1.65161200 | 0.00000000 |
| H | 0.10009900 | 2.05107700 | 0.96878700 |
| H | 0.10009900 | 2.05107700 | -0.96878700 |
| B | -1.76459300 | -0.81816000 | 0.00000000 |
| B | 0.00000000 | -1.02960300 | 0.00000000 |
| H | -0.87207000 | -0.92446400 | 0.97403300 |
| H | -0.87207000 | -0.92446400 | -0.97403300 |
| C | 1.09756700 | 0.12347900 | 0.00000000 |
| C | 2.27467200 | -0.54432400 | 0.00000000 |
| C | 2.10884300 | -2.01629300 | 0.00000000 |
| C | 0.81222500 | -2.37894700 | 0.00000000 |
| C | -2.53246100 | 0.54575000 | 0.00000000 |
| C | -2.10115200 | 1.82362700 | 0.00000000 |

$C_6B_4H_{12}$ (k=2) Isomer VII

| | | | |
|---|---|---|---|
| H | -3.26440300 | -1.85304000 | 0.00000000 |
| H | -1.52351100 | -3.25984300 | 0.00000000 |
| H | 1.03363400 | -2.93299000 | 0.00000000 |
| H | -3.48043000 | 0.37454000 | 0.00000000 |
| H | -2.00419000 | 2.08878000 | 0.00000000 |
| H | 3.37007600 | -0.56210100 | 0.00000000 |
| H | 3.60511100 | 1.90537000 | 0.00000000 |
| H | 1.20587700 | 3.45513500 | 0.00000000 |
| B | 0.30702700 | -1.99038600 | 0.00000000 |
| B | 1.00129500 | -0.35385500 | 0.00000000 |
| H | 0.70082100 | -1.18742400 | 0.97002000 |
| H | 0.70082100 | -1.18742400 | -0.97002000 |
| B | 0.00000000 | 1.01582500 | 0.00000000 |
| B | 1.28454100 | 2.26794700 | 0.00000000 |
| H | 0.46525800 | 1.85462400 | 0.94720500 |
| H | 0.46525800 | 1.85462400 | -0.94720500 |
| C | -1.54305800 | 1.10314200 | 0.00000000 |
| C | -2.43347700 | 0.08183600 | 0.00000000 |
| C | -2.29166600 | -1.36796100 | 0.00000000 |
| C | -1.23194200 | -2.21261800 | 0.00000000 |
| C | 2.50023100 | 0.08859900 | 0.00000000 |
| C | 2.62680700 | 1.43235200 | 0.00000000 |

$C_6B_4H_{12}$ (k=2) Isomer VIII

| | | | |
|---|---|---|---|
| H | -3.06405300 | -2.12788100 | 0.00000000 |
| H | -1.19823300 | -3.43584300 | 0.00000000 |
| H | 1.33637600 | -2.79542500 | 0.00000000 |
| H | -3.35058400 | 0.12211200 | 0.00000000 |
| H | -1.92671400 | 1.86912200 | 0.00000000 |
| H | 3.67945800 | -0.18115100 | 0.00000000 |
| H | 2.94616200 | 3.02076900 | 0.00000000 |
| H | 0.09936000 | 3.07637500 | 0.00000000 |
| B | 0.49150200 | -1.96010000 | 0.00000000 |
| B | 1.02549100 | -0.26784400 | 0.00000000 |
| H | 0.82083100 | -1.11047500 | 0.97112100 |
| H | 0.82083100 | -1.11047500 | -0.97112100 |
| B | 2.21490700 | 2.08449000 | 0.00000000 |
| B | 2.61689000 | 0.34816500 | 0.00000000 |
| H | 2.68866600 | 1.24258100 | 0.94891400 |
| H | 2.68866600 | 1.24258100 | -0.94891400 |
| C | 0.65480500 | 2.14183900 | 0.00000000 |
| C | 0.00000000 | 0.94757700 | 0.00000000 |
| C | -1.44610100 | 0.89356800 | 0.00000000 |
| C | -2.30256600 | -0.15813600 | 0.00000000 |
| C | -2.11584400 | -1.59698300 | 0.00000000 |
| C | -1.00441200 | -2.36717200 | 0.00000000 |

$C_6B_4H_{12}$ (k=2) Isomer IX

| | | | |
|---|---|---|---|
| H | -3.25808300 | 2.45866600 | 0.00000000 |
| H | -3.59908400 | -0.28153100 | 0.00000000 |
| H | -1.75462400 | -2.02729900 | 0.00000000 |
| H | -0.58306100 | 3.78961700 | 0.00000000 |
| H | 1.81684700 | 2.34432200 | 0.00000000 |
| H | 0.37829200 | -3.20109300 | 0.00000000 |
| H | 2.95033400 | -2.55583000 | 0.00000000 |
| H | 3.14237300 | 0.12222400 | 0.00000000 |
| B | -2.23459800 | 1.85495600 | 0.00000000 |
| B | -2.46951200 | 0.08768600 | 0.00000000 |
| H | -2.33096700 | 0.97168900 | 0.96755500 |
| H | -2.33096700 | 0.97168900 | -0.96755500 |
| B | -0.71111500 | 2.60770500 | 0.00000000 |
| B | 0.82413600 | 1.69035200 | 0.00000000 |
| H | 0.02326800 | 2.16074600 | 0.96817200 |
| H | 0.02326800 | 2.16074600 | -0.96817200 |
| C | 0.97407800 | 0.15456400 | 0.00000000 |
| C | 2.21023600 | -0.42397300 | 0.00000000 |
| C | 2.11121400 | -1.87693800 | 0.00000000 |
| C | 0.80327300 | -2.20917200 | 0.00000000 |
| C | 0.00000000 | -0.98138700 | 0.00000000 |
| C | -1.35249200 | -1.01600100 | 0.00000000 |

$C_6B_4H_{12}$ (k=2) Isomer X

| | | | |
|---|---|---|---|
| H | -3.36078200 | -2.09131500 | 0.00000000 |
| H | -1.14986800 | -3.71472700 | 0.00000000 |
| H | 1.66717100 | -2.70282700 | 0.00000000 |
| H | -3.40202100 | 0.44441500 | 0.00000000 |
| H | -1.80626100 | 2.05154200 | 0.00000000 |
| H | 3.46316700 | 0.04116200 | 0.00000000 |
| H | 2.95267100 | 2.57223300 | 0.00000000 |
| H | 0.37632200 | 3.08127600 | 0.00000000 |
| B | -2.33233800 | -1.49546900 | 0.00000000 |
| B | -0.88662800 | -2.55557500 | 0.00000000 |
| H | -1.56179000 | -2.01579500 | 0.96698800 |
| H | -1.56179000 | -2.01579500 | -0.96698800 |
| B | 0.71541600 | -1.98981600 | 0.00000000 |
| B | 1.06816000 | -0.25527500 | 0.00000000 |
| H | 0.91605100 | -1.12478500 | 0.97097000 |
| H | 0.91605100 | -1.12478500 | -0.97097000 |
| C | -2.38701800 | 0.05612500 | 0.00000000 |
| C | -1.43816700 | 1.02631600 | 0.00000000 |
| C | 0.00000000 | 0.94935500 | 0.00000000 |
| C | 0.76836300 | 2.07049100 | 0.00000000 |
| C | 2.21021300 | 1.78340200 | 0.00000000 |
| C | 2.46794900 | 0.46099100 | 0.00000000 |

$C_4B_6H_{14}$ (k=3) Isomer I

| | | | |
|---|---|---|---|
| H | -3.48744700 | -1.99421700 | 0.00000000 |
| H | -1.15101800 | -3.48596200 | 0.00000000 |
| H | 1.24414800 | -2.47780500 | 0.00000000 |
| H | -3.56312200 | 0.62204800 | 0.00000000 |
| H | -1.84475900 | 2.14803700 | 0.00000000 |
| H | 3.25039600 | -1.03606100 | 0.00000000 |
| H | 3.78793600 | 2.13063700 | 0.00000000 |
| H | 0.83769000 | 3.41658000 | 0.00000000 |
| B | -2.48970800 | -1.35047500 | 0.00000000 |
| B | -0.98930400 | -2.30940100 | 0.00000000 |
| H | -1.72597400 | -1.81925800 | 0.97099300 |
| H | -1.72597400 | -1.81925800 | -0.97099300 |
| B | 0.00000000 | 0.87351000 | 0.00000000 |
| B | 1.16884100 | 2.27439900 | 0.00000000 |
| H | 0.49045800 | 1.71893600 | 0.95359100 |
| H | 0.49045800 | 1.71893600 | -0.95359100 |
| B | 2.72839500 | 1.59413200 | 0.00000000 |
| B | 2.44279500 | -0.16227100 | 0.00000000 |
| H | 2.81648100 | 0.68545700 | 0.95112400 |
| H | 2.81648100 | 0.68545700 | -0.95112400 |
| C | -2.55716800 | 0.20647100 | 0.00000000 |
| C | -1.54850400 | 1.09867000 | 0.00000000 |
| C | 0.46004800 | -1.72052500 | 0.00000000 |
| C | 0.88881500 | -0.43345000 | 0.00000000 |

$C_4B_6H_{14}$ (k=3) Isomer II

| | | | |
|---|---|---|---|
| H | -2.95985700 | -2.91157100 | 0.00000000 |
| H | -0.26827900 | -3.63431100 | 0.00000000 |
| H | 1.68991900 | -2.07331600 | 0.00000000 |
| H | -3.84383600 | -0.04883500 | 0.00000000 |
| H | -2.08709700 | 2.07355300 | 0.00000000 |
| H | 3.42856600 | -0.29977000 | 0.00000000 |
| H | 2.96505600 | 3.02434100 | 0.00000000 |
| H | 0.07111200 | 3.09149700 | 0.00000000 |
| B | -2.20090600 | -1.99729200 | 0.00000000 |
| B | -0.48474100 | -2.46529500 | 0.00000000 |
| H | -1.35305400 | -2.22700300 | 0.96779300 |
| H | -1.35305400 | -2.22700300 | -0.96779300 |
| B | -2.70025100 | -0.37161300 | 0.00000000 |
| B | -1.56961900 | 1.00414500 | 0.00000000 |
| H | -2.12641200 | 0.28387500 | 0.96770600 |
| H | -2.12641200 | 0.28387500 | -0.96770600 |
| B | 2.20436500 | 2.11580300 | 0.00000000 |
| B | 2.45295300 | 0.37279700 | 0.00000000 |
| H | 2.62208900 | 1.27657800 | 0.94942600 |
| H | 2.62208900 | 1.27657800 | -0.94942600 |
| C | 0.00000000 | 0.96877900 | 0.00000000 |
| C | 0.64147900 | 2.17096600 | 0.00000000 |
| C | 0.96570400 | -0.16354000 | 0.00000000 |
| C | 0.76117900 | -1.50640700 | 0.00000000 |

$C_4B_6H_{14}$ (k=3) Isomer III

| | | | |
|---|---|---|---|
| H | -3.01117700 | 2.54092600 | 0.00000000 |
| H | -3.67512000 | 0.36119000 | 0.00000000 |
| H | -2.37560400 | -1.84405100 | 0.00000000 |
| H | -0.70584200 | 3.65483800 | 0.00000000 |
| H | 1.73417600 | 2.44931900 | 0.00000000 |
| H | 0.39598100 | -3.66147400 | 0.00000000 |
| H | 3.48833000 | -2.55662600 | 0.00000000 |
| H | 3.19708900 | 0.27833700 | 0.00000000 |
| B | -0.77730700 | 2.46882800 | 0.00000000 |
| B | 0.83104100 | 1.67647400 | 0.00000000 |
| H | -0.00235600 | 2.03947000 | 0.96893000 |
| H | -0.00235600 | 2.03947000 | -0.96893000 |
| B | -1.77740100 | -0.81710300 | 0.00000000 |
| B | 0.00000000 | -1.02876400 | 0.00000000 |
| H | -0.87992500 | -0.91024600 | 0.96922700 |
| H | -0.87992500 | -0.91024600 | -0.96922700 |
| B | 2.46652800 | -1.95028900 | 0.00000000 |
| B | 0.79728500 | -2.54459000 | 0.00000000 |
| H | 1.70534000 | -2.51881000 | 0.94776300 |
| H | 1.70534000 | -2.51881000 | -0.94776300 |
| C | -2.20524100 | 1.80862300 | 0.00000000 |
| C | -2.59793600 | 0.52072900 | 0.00000000 |
| C | 1.07471500 | 0.13701400 | 0.00000000 |
| C | 2.32934800 | -0.37737700 | 0.00000000 |

$C_4B_6H_{14}$ (k=3) Isomer IV

| | | | |
|---|---|---|---|
| H | -3.38157100 | 2.36615000 | 0.00000000 |
| H | -3.60254400 | -0.31502300 | 0.00000000 |
| H | -1.76619100 | -2.05323400 | 0.00000000 |
| H | -0.85868100 | 3.91652200 | 0.00000000 |
| H | 1.66821000 | 2.69164800 | 0.00000000 |
| H | 0.25716600 | -3.19037700 | 0.00000000 |
| H | 2.77425400 | -2.95522600 | 0.00000000 |
| H | 3.65678100 | -0.16442200 | 0.00000000 |
| B | -2.31752500 | 1.83727000 | 0.00000000 |
| B | -2.47367600 | 0.05568800 | 0.00000000 |
| H | -2.33053100 | 0.95676800 | 0.96633700 |
| H | -2.33053100 | 0.95676800 | -0.96633700 |
| B | -0.86613500 | 2.72736500 | 0.00000000 |
| B | 0.73681500 | 1.94961800 | 0.00000000 |
| H | -0.06786900 | 2.32939000 | 0.96516800 |
| H | -0.06786900 | 2.32939000 | -0.96516800 |
| B | 0.98523400 | 0.26988200 | 0.00000000 |
| B | 2.55615200 | -0.60561000 | 0.00000000 |
| H | 1.88357100 | 0.07685200 | 0.94511200 |
| H | 1.88357100 | 0.07685200 | -0.94511200 |
| C | -1.35628500 | -1.04222600 | 0.00000000 |
| C | 0.00000000 | -0.99038800 | 0.00000000 |
| C | 0.77259400 | -2.23451700 | 0.00000000 |
| C | 2.11334100 | -2.09839000 | 0.00000000 |

$C_4B_6H_{14}$ (k=3) Isomer V

| | | | |
|---|---|---|---|
| H | -3.30719000 | 1.96821000 | 0.00000000 |
| H | -3.38322700 | -0.28580100 | 0.00000000 |
| H | -1.82165700 | -1.88416300 | 0.00000000 |
| H | -1.34941400 | 3.65491600 | 0.00000000 |
| H | 1.36239700 | 2.86872400 | 0.00000000 |
| H | 0.12117500 | -3.33087500 | 0.00000000 |
| H | 3.29985100 | -2.90016800 | 0.00000000 |
| H | 3.64993300 | 0.29830300 | 0.00000000 |
| B | -1.13228800 | 2.48688600 | 0.00000000 |
| B | 0.57166700 | 1.98064600 | 0.00000000 |
| H | -0.26738600 | 2.21853400 | 0.96914500 |
| H | -0.26738600 | 2.21853400 | -0.96914500 |
| B | 0.98265200 | 0.34070900 | 0.00000000 |
| B | 2.65632900 | -0.35402500 | 0.00000000 |
| H | 1.91768500 | 0.16597000 | 0.94819400 |
| H | 1.91768500 | 0.16597000 | -0.94819400 |
| B | 2.47470400 | -2.04585500 | 0.00000000 |
| B | 0.70954100 | -2.29630600 | 0.00000000 |
| H | 1.63520600 | -2.39196800 | 0.95170100 |
| H | 1.63520600 | -2.39196800 | -0.95170100 |
| C | -2.32967900 | 1.49322500 | 0.00000000 |
| C | -2.38393500 | 0.14206100 | 0.00000000 |
| C | -1.36237000 | -0.89747100 | 0.00000000 |
| C | 0.00000000 | -0.89356500 | 0.00000000 |

$C_4B_6H_{14}$ (k=3) Isomer VI

| | | | |
|---|---|---|---|
| H | -2.97967300 | 2.58417800 | 0.00000000 |
| H | -3.63098400 | 0.43083000 | 0.00000000 |
| H | -2.40502300 | -1.79545500 | 0.00000000 |
| H | -0.76608900 | 3.77559100 | 0.00000000 |
| H | 1.72446800 | 2.74601400 | 0.00000000 |
| H | 0.21961300 | -3.38835800 | 0.00000000 |
| H | 2.69595900 | -3.17050600 | 0.00000000 |
| H | 3.75691000 | -0.52437700 | 0.00000000 |
| B | -0.76250800 | 2.58698800 | 0.00000000 |
| B | 0.89295000 | 1.89604000 | 0.00000000 |
| H | 0.04951500 | 2.17176000 | 0.96544000 |
| H | 0.04951500 | 2.17176000 | -0.96544000 |
| B | -1.77121500 | -0.78796400 | 0.00000000 |
| B | 0.00000000 | -1.01583100 | 0.00000000 |
| H | -0.87943800 | -0.86625100 | 0.96881600 |
| H | -0.87943800 | -0.86625100 | -0.96881600 |
| B | 1.17461900 | 0.22856700 | 0.00000000 |
| B | 2.60520800 | -0.82155800 | 0.00000000 |
| H | 2.04670900 | -0.03096800 | 0.94309700 |
| H | 2.04670900 | -0.03096800 | -0.94309700 |
| C | -2.15987000 | 1.86682400 | 0.00000000 |
| C | -2.55133800 | 0.57506400 | 0.00000000 |
| C | 2.04809400 | -2.29823100 | 0.00000000 |
| C | 0.70577700 | -2.41669300 | 0.00000000 |

$C_4B_6H_{14}$ (k=3) Isomer VII

| | | | |
|---|---|---|---|
| H | -3.58810400 | -1.84411700 | 0.00000000 |
| H | -1.55850100 | -3.57718700 | 0.00000000 |
| H | 1.34048300 | -2.92288500 | 0.00000000 |
| H | -3.54572300 | 0.68197900 | 0.00000000 |
| H | -1.88344400 | 2.22938000 | 0.00000000 |
| H | 3.41342700 | -0.53246100 | 0.00000000 |
| H | 3.60611000 | 1.94260700 | 0.00000000 |
| H | 1.16325300 | 3.43318600 | 0.00000000 |
| B | -2.53235500 | -1.29838100 | 0.00000000 |
| B | -1.16540700 | -2.45569300 | 0.00000000 |
| H | -1.78843900 | -1.83091900 | 0.96550800 |
| H | -1.78843900 | -1.83091900 | -0.96550800 |
| B | 0.49620400 | -2.08305100 | 0.00000000 |
| B | 1.04492100 | -0.38720900 | 0.00000000 |
| H | 0.78612400 | -1.24975400 | 0.96612500 |
| H | 0.78612400 | -1.24975400 | -0.96612500 |
| B | 0.00000000 | 0.98222800 | 0.00000000 |
| B | 1.27613400 | 2.24924900 | 0.00000000 |
| H | 0.46863300 | 1.80418700 | 0.94764900 |
| H | 0.46863300 | 1.80418700 | -0.94764900 |
| C | -2.53655200 | 0.27185400 | 0.00000000 |
| C | -1.54932700 | 1.19103100 | 0.00000000 |
| C | 2.53437100 | 0.10611400 | 0.00000000 |
| C | 2.63857100 | 1.44879300 | 0.00000000 |

$C_4B_6H_{14}$ (k=3) Isomer VIII

| | | | |
|---|---|---|---|
| H | -3.39552900 | -2.15214800 | 0.00000000 |
| H | -1.14861700 | -3.78504900 | 0.00000000 |
| H | 1.63391800 | -2.70556800 | 0.00000000 |
| H | -3.41221800 | 0.37174700 | 0.00000000 |
| H | -1.85103300 | 1.98002500 | 0.00000000 |
| H | 3.70411300 | -0.14640800 | 0.00000000 |
| H | 2.93261200 | 3.05772000 | 0.00000000 |
| H | 0.10073700 | 3.06206200 | 0.00000000 |
| B | -2.35656100 | -1.57419400 | 0.00000000 |
| B | -0.91204800 | -2.62005200 | 0.00000000 |
| H | -1.60921500 | -2.10487600 | 0.96782100 |
| H | -1.60921500 | -2.10487600 | -0.96782100 |
| B | 0.67416400 | -2.00397900 | 0.00000000 |
| B | 1.05338400 | -0.26249000 | 0.00000000 |
| H | 0.86696500 | -1.13361900 | 0.96631500 |
| H | 0.86696500 | -1.13361900 | -0.96631500 |
| B | 2.22959600 | 2.10013300 | 0.00000000 |
| B | 2.64237100 | 0.38382800 | 0.00000000 |
| H | 2.72522200 | 1.28385600 | 0.94760200 |
| H | 2.72522200 | 1.28385600 | -0.94760200 |
| C | -2.39564100 | -0.01427400 | 0.00000000 |
| C | -1.46255100 | 0.96258600 | 0.00000000 |
| C | 0.00000000 | 0.94037200 | 0.00000000 |
| C | 0.66078100 | 2.12975900 | 0.00000000 |

$C_4B_6H_{14}$ (k=3) Isomer IX

| | | | |
|---|---|---|---|
| H | -3.17437600 | -2.73476100 | 0.00000000 |
| H | -0.69733700 | -3.87288700 | 0.00000000 |
| H | 1.85741700 | -2.47063400 | 0.00000000 |
| H | -3.81071600 | 0.08694100 | 0.00000000 |
| H | -2.08816100 | 2.19744200 | 0.00000000 |
| H | 3.48536400 | 0.20987600 | 0.00000000 |
| H | 2.94607600 | 2.73810700 | 0.00000000 |
| H | 0.35471400 | 3.20341600 | 0.00000000 |
| B | -2.29714700 | -1.93149100 | 0.00000000 |
| B | -0.67288000 | -2.68382900 | 0.00000000 |
| H | -1.45843300 | -2.26718800 | 0.96290900 |
| H | -1.45843300 | -2.26718800 | -0.96290900 |
| B | -2.67303600 | -0.26048600 | 0.00000000 |
| B | -1.54280800 | 1.14031300 | 0.00000000 |
| H | -2.09178800 | 0.37569400 | 0.96599300 |
| H | -2.09178800 | 0.37569400 | -0.96599300 |
| B | 0.83245100 | -1.86701600 | 0.00000000 |
| B | 1.08260900 | -0.10602200 | 0.00000000 |
| H | 0.91455700 | -0.99027500 | 0.96963500 |
| H | 0.91455700 | -0.99027500 | -0.96963500 |
| C | 0.00000000 | 1.07069700 | 0.00000000 |
| C | 0.75584500 | 2.19538300 | 0.00000000 |
| C | 2.21654800 | 1.93713200 | 0.00000000 |
| C | 2.48634100 | 0.62157000 | 0.00000000 |

$C_4B_6H_{14}$ (k=3) Isomer X

| | | | |
|---|---|---|---|
| H | -3.31619800 | -1.88050500 | 0.00000000 |
| H | -1.57754100 | -3.30285400 | 0.00000000 |
| H | 0.97102400 | -2.97770100 | 0.00000000 |
| H | -3.50072400 | 0.35630600 | 0.00000000 |
| H | -1.99793400 | 2.04403800 | 0.00000000 |
| H | 3.60559500 | -0.76137700 | 0.00000000 |
| H | 3.75523600 | 2.38033400 | 0.00000000 |
| H | 0.81242600 | 3.52206800 | 0.00000000 |
| B | 0.25354600 | -2.02861000 | 0.00000000 |
| B | 0.99358500 | -0.41069300 | 0.00000000 |
| H | 0.67980400 | -1.21934400 | 0.96777100 |
| H | 0.67980400 | -1.21934400 | -0.96777100 |
| B | 0.00000000 | 0.96623600 | 0.00000000 |
| B | 1.14361500 | 2.37694000 | 0.00000000 |
| H | 0.45526100 | 1.81987300 | 0.95145000 |
| H | 0.45526100 | 1.81987300 | -0.95145000 |
| B | 2.74184500 | 1.75565700 | 0.00000000 |
| B | 2.66055000 | -0.03667300 | 0.00000000 |
| H | 2.90467100 | 0.84475200 | 0.95012900 |
| H | 2.90467100 | 0.84475200 | -0.95012900 |
| C | -1.55150700 | 1.05094300 | 0.00000000 |
| C | -2.45845500 | 0.04711000 | 0.00000000 |
| C | -2.33802000 | -1.40637300 | 0.00000000 |
| C | -1.28486100 | -2.25587300 | 0.00000000 |

$C_2B_8H_{16}$ (k=4) Isomer I

| | | | |
|---|---|---|---|
| H | -3.23006700 | -2.66795500 | 0.00000000 |
| H | -0.69788800 | -3.59260500 | 0.00000000 |
| H | 1.45198200 | -2.30613300 | 0.00000000 |
| H | -4.02966100 | 0.19246000 | 0.00000000 |
| H | -2.15870100 | 2.27353200 | 0.00000000 |
| H | 3.33734400 | -0.80866100 | 0.00000000 |
| H | 3.74524400 | 2.37667700 | 0.00000000 |
| H | 0.74670100 | 3.53044300 | 0.00000000 |
| B | -2.43326600 | -1.78671000 | 0.00000000 |
| B | -0.75911300 | -2.40573100 | 0.00000000 |
| H | -1.58745600 | -2.03558000 | 0.96638400 |
| H | -1.58745600 | -2.03558000 | -0.96638400 |
| B | -2.89003800 | -0.14602700 | 0.00000000 |
| B | -1.69834100 | 1.17537900 | 0.00000000 |
| H | -2.27892000 | 0.50643800 | 0.96512800 |
| H | -2.27892000 | 0.50643800 | -0.96512800 |
| B | 0.00000000 | 0.97277300 | 0.00000000 |
| B | 1.12147300 | 2.40287800 | 0.00000000 |
| H | 0.42415700 | 1.81607100 | 0.94689500 |
| H | 0.42415700 | 1.81607100 | -0.94689500 |
| B | 2.71087900 | 1.79319400 | 0.00000000 |
| B | 2.49291700 | 0.02936300 | 0.00000000 |
| H | 2.83326100 | 0.89556500 | 0.95143800 |
| H | 2.83326100 | 0.89556500 | -0.95143800 |
| C | 0.60540600 | -1.61840100 | 0.00000000 |
| C | 0.94966100 | -0.30465600 | 0.00000000 |

$C_2B_8H_{16}$ (k=4) Isomer II

| | | | |
|---|---|---|---|
| H | -3.20461000 | -2.81558500 | 0.00000000 |
| H | -0.68213800 | -3.93342100 | 0.00000000 |
| H | 1.82135700 | -2.48183100 | 0.00000000 |
| H | -3.81318000 | 0.01673100 | 0.00000000 |
| H | -2.13975300 | 2.10206200 | 0.00000000 |
| H | 3.73195800 | 0.05466700 | 0.00000000 |
| H | 2.89952800 | 3.24008000 | 0.00000000 |
| H | 0.06177700 | 3.18371900 | 0.00000000 |
| B | -2.32107200 | -2.01911800 | 0.00000000 |
| B | -0.68880600 | -2.74376800 | 0.00000000 |
| H | -1.49174700 | -2.35806800 | 0.96352900 |
| H | -1.49174700 | -2.35806800 | -0.96352900 |
| B | -2.68046500 | -0.34457500 | 0.00000000 |
| B | -1.56577200 | 1.06076100 | 0.00000000 |
| H | -2.07925700 | 0.28732100 | 0.96501000 |
| H | -2.07925700 | 0.28732100 | -0.96501000 |
| B | 0.79352100 | -1.88389600 | 0.00000000 |
| B | 1.07759400 | -0.11212100 | 0.00000000 |
| H | 0.87429000 | -1.00106400 | 0.96411100 |
| H | 0.87429000 | -1.00106400 | -0.96411100 |
| B | 2.21810700 | 2.26687900 | 0.00000000 |
| B | 2.65818800 | 0.55966100 | 0.00000000 |
| H | 2.72317600 | 1.46938600 | 0.94702000 |
| H | 2.72317600 | 1.46938600 | -0.94702000 |
| C | 0.00000000 | 1.05984000 | 0.00000000 |
| C | 0.63594300 | 2.26004500 | 0.00000000 |

$C_2B_8H_{16}$ (k=4) Isomer III

| | | | |
|---|---|---|---|
| H | -3.16452600 | 2.84456200 | 0.00000000 |
| H | -3.93805600 | 0.29216000 | 0.00000000 |
| H | -2.30201300 | -2.09892300 | 0.00000000 |
| H | -0.52063900 | 3.95305200 | 0.00000000 |
| H | 1.85107400 | 2.66253500 | 0.00000000 |
| H | 0.35579100 | -3.44619100 | 0.00000000 |
| H | 2.81972000 | -3.10311400 | 0.00000000 |
| H | 3.73408600 | -0.39919200 | 0.00000000 |
| B | -2.23286800 | 2.10556600 | 0.00000000 |
| B | -2.75324500 | 0.39111300 | 0.00000000 |
| H | -2.41046000 | 1.22540100 | 0.96152100 |
| H | -2.41046000 | 1.22540100 | -0.96152100 |
| B | -0.64981100 | 2.77073600 | 0.00000000 |
| B | 0.92433200 | 1.91574800 | 0.00000000 |
| H | 0.09770900 | 2.27884600 | 0.96216300 |
| H | 0.09770900 | 2.27884600 | -0.96216300 |
| B | -1.78780200 | -1.02466900 | 0.00000000 |
| B | 0.00000000 | -1.09556000 | 0.00000000 |
| H | -0.90610900 | -1.00015500 | 0.96442800 |
| H | -0.90610900 | -1.00015500 | -0.96442800 |
| B | 1.11589800 | 0.22305400 | 0.00000000 |
| B | 2.60200200 | -0.76306500 | 0.00000000 |
| H | 1.99284100 | -0.00979900 | 0.94287700 |
| H | 1.99284100 | -0.00979900 | -0.94287700 |
| C | 2.12702500 | -2.26629300 | 0.00000000 |
| C | 0.79365400 | -2.45172300 | 0.00000000 |

$C_2B_8H_{16}$ (k=4) Isomer IV

| | | | |
|---|---|---|---|
| H | 3.64815000 | 1.86011300 | 0.00000000 |
| H | 1.62218300 | 3.61798500 | 0.00000000 |
| H | -1.26486600 | 2.97555400 | 0.00000000 |
| H | 3.56074000 | -0.66768300 | 0.00000000 |
| H | 1.87566300 | -2.18377100 | 0.00000000 |
| H | -3.64736000 | 0.73744000 | 0.00000000 |
| H | -3.75508200 | -2.41623800 | 0.00000000 |
| H | -0.78531500 | -3.48591500 | 0.00000000 |
| B | 2.58418800 | 1.33073700 | 0.00000000 |
| B | 1.22882100 | 2.49638300 | 0.00000000 |
| H | 1.84831400 | 1.87395700 | 0.96605400 |
| H | 1.84831400 | 1.87395700 | -0.96605400 |
| B | -0.43409100 | 2.12307100 | 0.00000000 |
| B | -1.03534100 | 0.44096300 | 0.00000000 |
| H | -0.76055300 | 1.28137700 | 0.96294400 |
| H | -0.76055300 | 1.28137700 | -0.96294400 |
| B | 0.00000000 | -0.93444100 | 0.00000000 |
| B | -1.14589200 | -2.35028400 | 0.00000000 |
| H | -0.47192800 | -1.76548900 | 0.95096700 |
| H | -0.47192800 | -1.76548900 | -0.95096700 |
| B | -2.75759500 | -1.76717100 | 0.00000000 |
| B | -2.69833300 | 0.01795900 | 0.00000000 |
| H | -2.94372200 | -0.86271800 | 0.94973100 |
| H | -2.94372200 | -0.86271800 | -0.94973100 |
| C | 2.55906300 | -0.23933900 | 0.00000000 |
| C | 1.55641500 | -1.14029900 | 0.00000000 |

$C_2B_8H_{16}$ (k=4) Isomer V

| | | | |
|---|---|---|---|
| H | -3.16196800 | 2.46374400 | 0.00000000 |
| H | -3.70296900 | 0.27466600 | 0.00000000 |
| H | -2.37559700 | -1.87348200 | 0.00000000 |
| H | -0.99284300 | 3.75160100 | 0.00000000 |
| H | 1.52947200 | 2.82092900 | 0.00000000 |
| H | 0.27384400 | -3.65063300 | 0.00000000 |
| H | 3.36563300 | -3.04764700 | 0.00000000 |
| H | 3.76055500 | 0.07407700 | 0.00000000 |
| B | -0.94301200 | 2.56431900 | 0.00000000 |
| B | 0.73399300 | 1.93655900 | 0.00000000 |
| H | -0.11769600 | 2.17336300 | 0.96555300 |
| H | -0.11769600 | 2.17336300 | -0.96555300 |
| B | -1.78109700 | -0.84332500 | 0.00000000 |
| B | 0.00000000 | -1.02654800 | 0.00000000 |
| H | -0.86772500 | -0.89726700 | 0.96599900 |
| H | -0.86772500 | -0.89726700 | -0.96599900 |
| B | 1.10941200 | 0.27844200 | 0.00000000 |
| B | 2.72431700 | -0.51367400 | 0.00000000 |
| H | 2.01368500 | 0.07821600 | 0.94603200 |
| H | 2.01368500 | 0.07821600 | -0.94603200 |
| B | 2.51183700 | -2.21811200 | 0.00000000 |
| B | 0.75455500 | -2.56131300 | 0.00000000 |
| H | 1.67317400 | -2.59157000 | 0.95019300 |
| H | 1.67317400 | -2.59157000 | -0.95019300 |
| C | -2.30894300 | 1.78636700 | 0.00000000 |
| C | -2.63256200 | 0.47688600 | 0.00000000 |

$B_{10}H_{18}$ (k=5)

| | | | |
|---|---|---|---|
| H | 3.46622500 | 2.58460500 | 0.00000000 |
| H | 1.10734900 | 3.85080300 | 0.00000000 |
| H | -1.54187900 | 2.72761600 | 0.00000000 |
| H | 4.00036100 | -0.24075000 | 0.00000000 |
| H | 2.25063000 | -2.28100500 | 0.00000000 |
| H | -3.69586600 | 0.50611300 | 0.00000000 |
| H | -3.72423500 | -2.64979600 | 0.00000000 |
| H | -0.73704700 | -3.64092900 | 0.00000000 |
| B | 2.55346800 | 1.82255000 | 0.00000000 |
| B | 0.97657200 | 2.66885700 | 0.00000000 |
| H | 1.72687300 | 2.17446600 | 0.96178300 |
| H | 1.72687300 | 2.17446600 | -0.96178300 |
| B | 2.87272000 | 0.13652800 | 0.00000000 |
| B | 1.70748200 | -1.22174800 | 0.00000000 |
| H | 2.22709600 | -0.48675000 | 0.96180200 |
| H | 2.22709600 | -0.48675000 | -0.96180200 |
| B | -0.60247400 | 1.99714400 | 0.00000000 |
| B | -1.07347500 | 0.26497200 | 0.00000000 |
| H | -0.77787300 | 1.11267100 | 0.96074500 |
| H | -0.77787300 | 1.11267100 | -0.96074500 |
| B | 0.00000000 | -1.08826900 | 0.00000000 |
| B | -1.11591700 | -2.51190700 | 0.00000000 |
| H | -0.40254200 | -1.91950300 | 0.94579400 |
| H | -0.40254200 | -1.91950300 | -0.94579400 |
| B | -2.74506700 | -1.97305600 | 0.00000000 |
| B | -2.72787300 | -0.18730500 | 0.00000000 |
| H | -2.94991000 | -1.07863000 | 0.94984200 |
| H | -2.94991000 | -1.07863000 | -0.94984200 |