

## Supplementary Information

### Theoretical Studies on Boron Dimesityl-based Thermally Activated Delayed Fluorescence Organic Emitters: Excited-State Properties and Mechanism

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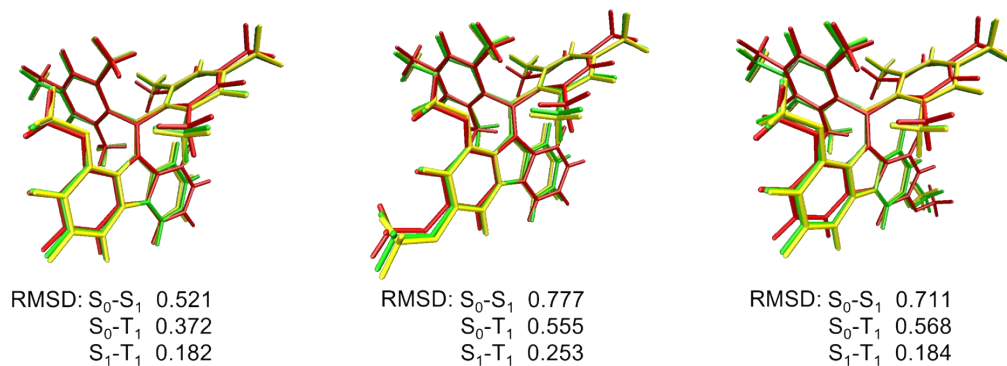
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**Table S1** Partial geometric parameters at the  $S_0$ ,  $S_1$ , and  $T_1$  minima for **CzBM-1**, **-2** and **-3** in cyclohexane.

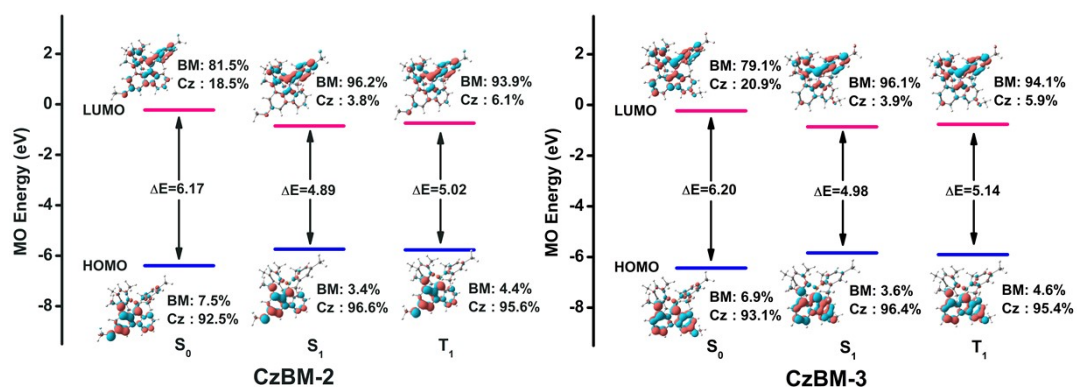
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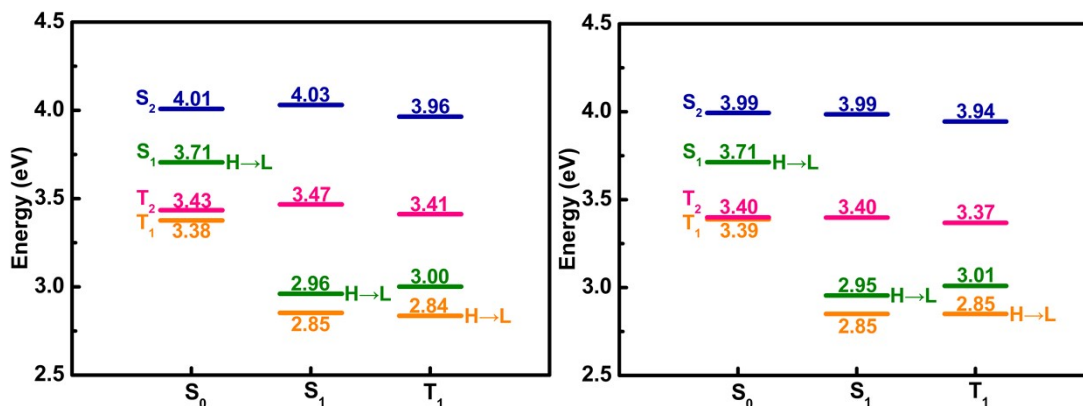
## **III Cartesian Coordinates of Optimized Structures**



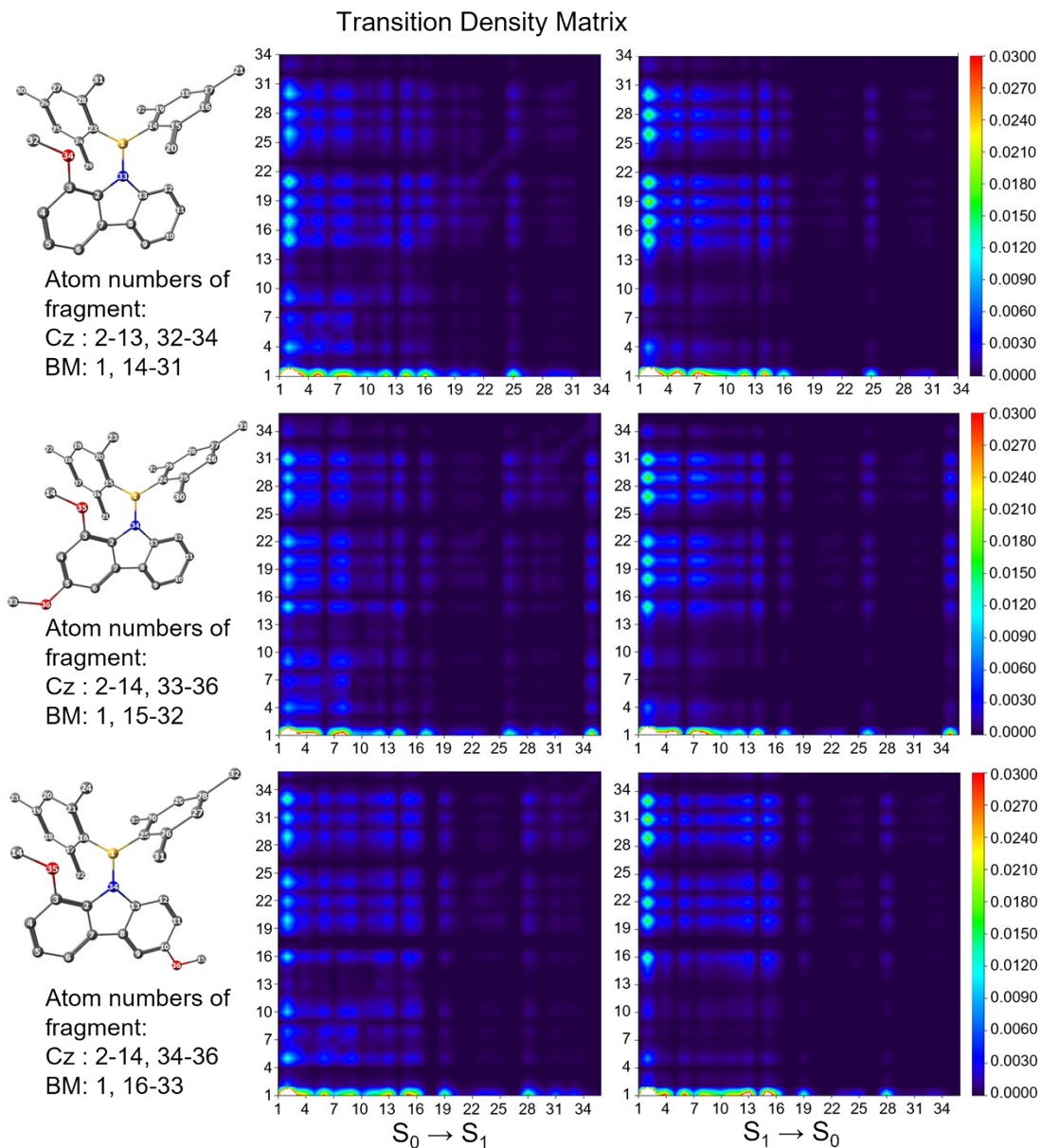
**Fig. S1** The spatial overlap and root-mean-square deviation (RMSD) of S<sub>0</sub> (red), S<sub>1</sub> (yellow) and T<sub>1</sub> (green) minima for **CzBM-1** (left), **-2** (middle) and **-3** (right) in cyclohexane.



**Fig. S2** Frontier molecular orbitals and corresponding energy levels at the S<sub>0</sub>, S<sub>1</sub> and T<sub>1</sub> minima for **CzBM-2** (left) and **-3** (right).



**Fig. S3** The calculated the adiabatic energies (eV) at the S<sub>0</sub>, S<sub>1</sub> and T<sub>1</sub> minima for **CzBM-2** (left) and **-3** (right).



**Fig. S4** Transition density matrix of non-H atoms during vertical excitation and emission process of CzBM-1 (top), -2 (middle) and -3 (bottom). The electrons transition mainly originate from the Cz fragment to the BM fragment, which is consistent with HOMO  $\rightarrow$  LUMO, showing CT characteristic.

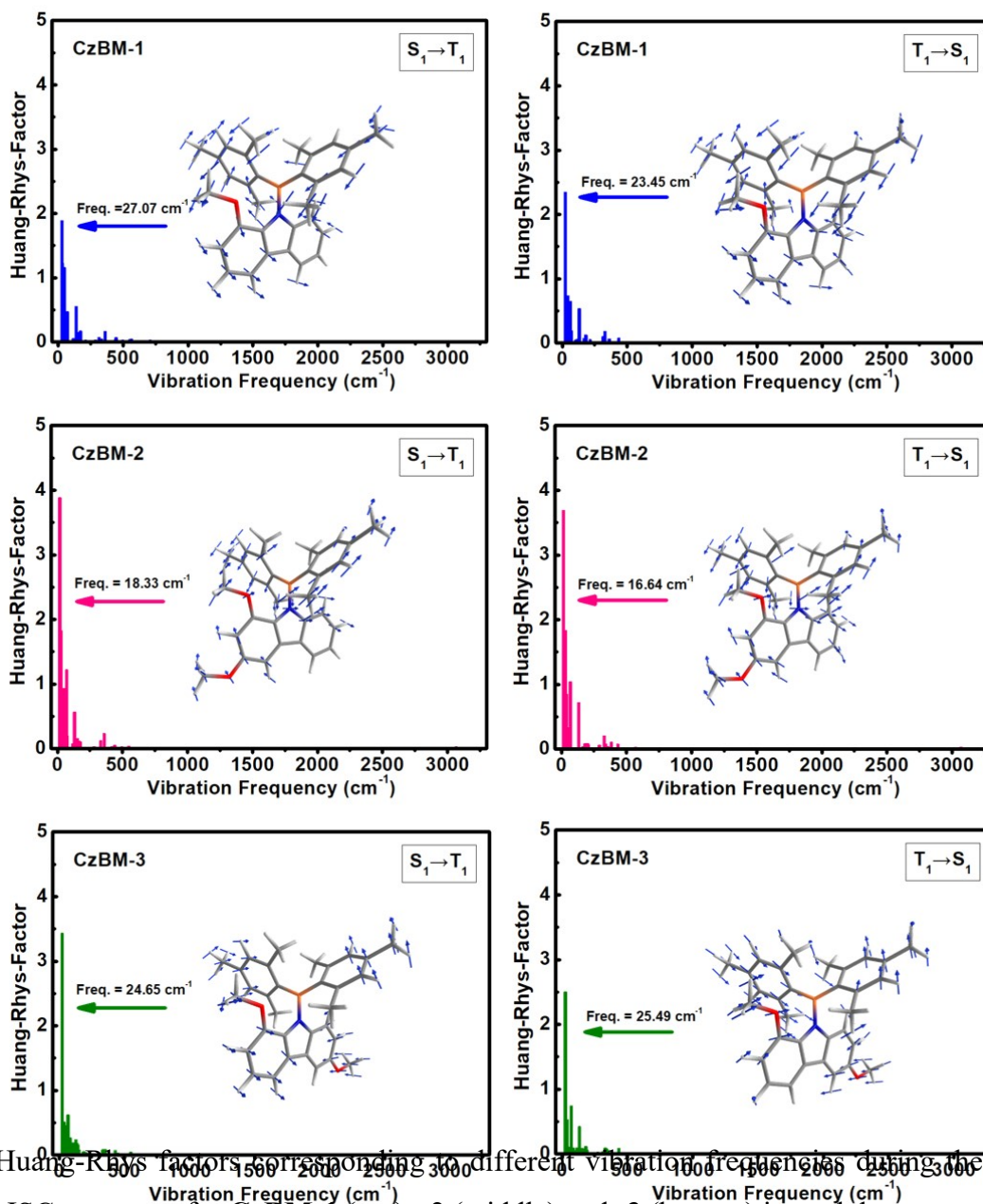
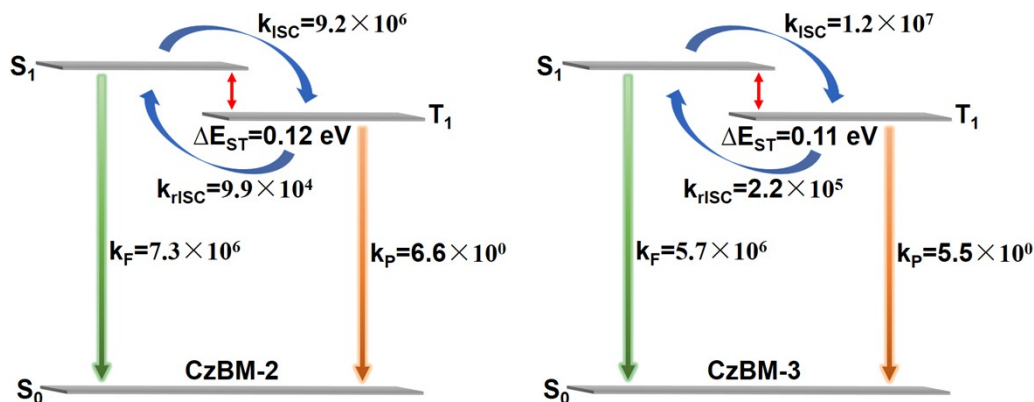


Fig. S5 Huang-Rhys factors corresponding to different vibration frequencies during the ISC and rISC processes for **CzBM-1** (top), **-2** (middle) and **-3** (bottom) in cyclohexane.



**Fig. S6** Schematic of the luminescence mechanism for **CzBM-2** (left) and **-3** (right) in cyclohexane at 300K.

**Table S1** Partial geometric parameters at the  $S_0$ ,  $S_1$ , and  $T_1$  minima for **CzBM-1**, **-2** and **-3** in cyclohexane. (Bond length unit: angstrom; torsion angle unit: degree)

|             | <b>CzBM-1</b> |       |       | <b>CzBM-2</b> |       |       | <b>CzBM-3</b> |       |       |
|-------------|---------------|-------|-------|---------------|-------|-------|---------------|-------|-------|
|             | $S_0$         | $S_1$ | $T_1$ | $S_0$         | $S_1$ | $T_1$ | $S_0$         | $S_1$ | $T_1$ |
| B3-C1       | 1.573         | 1.565 | 1.570 | 1.576         | 1.563 | 1.569 | 1.576         | 1.564 | 1.570 |
| B3-C2       | 1.570         | 1.554 | 1.563 | 1.571         | 1.554 | 1.564 | 1.572         | 1.552 | 1.561 |
| B3-N4       | 1.459         | 1.555 | 1.543 | 1.453         | 1.557 | 1.545 | 1.453         | 1.557 | 1.544 |
| N4-C5       | 1.405         | 1.367 | 1.364 | 1.409         | 1.358 | 1.355 | 1.406         | 1.386 | 1.386 |
| C1-B3-N4-C5 | 28.6          | 59.9  | 48.4  | 22.9          | 62.9  | 48.9  | 22.2          | 57.2  | 49.3  |
| B3-N4-C5-C6 | 29.2          | 3.8   | 9.2   | 32.3          | 1.5   | 9.0   | 32.3          | 7.0   | 9.6   |
| N4-C5-C6-O7 | 4.4           | 8.8   | 8.3   | 5.7           | 7.9   | 8.0   | 6.4           | 8.0   | 6.7   |

**Table S2** The temperature (K) dependence of ISC and rISC rates ( $k_{\text{ISC}}$ ,  $k_{\text{rISC}}$ ,  $\text{s}^{-1}$ ) for **CzBM-1, -2 and -3** in cyclohexane.

|     | <b>CzBM-1</b>     |                      | <b>CzBM-2</b>     |                      | <b>CzBM-3</b>     |                      |
|-----|-------------------|----------------------|-------------------|----------------------|-------------------|----------------------|
|     | at $S_1$          | at $T_1$             | at $S_1$          | at $T_1$             | at $S_1$          | at $T_1$             |
| 300 | $3.1 \times 10^7$ | $8.4 \times 10^4$    | $9.2 \times 10^6$ | $9.9 \times 10^4$    | $1.2 \times 10^7$ | $2.2 \times 10^5$    |
| 250 | $3.5 \times 10^7$ | $3.3 \times 10^4$    | $1.2 \times 10^7$ | $4.7 \times 10^4$    | $1.4 \times 10^7$ | $1.1 \times 10^5$    |
| 200 | $4.0 \times 10^7$ | $7.4 \times 10^3$    | $1.5 \times 10^7$ | $1.3 \times 10^4$    | $1.5 \times 10^7$ | $3.3 \times 10^4$    |
| 150 | $4.6 \times 10^7$ | $5.5 \times 10^2$    | $1.9 \times 10^7$ | $1.4 \times 10^3$    | $2.1 \times 10^7$ | $4.1 \times 10^3$    |
| 100 | $5.2 \times 10^7$ | $2.6 \times 10^0$    | $2.4 \times 10^7$ | $1.1 \times 10^1$    | $2.7 \times 10^7$ | $5.3 \times 10^1$    |
| 77  | $5.5 \times 10^7$ | $2.0 \times 10^{-2}$ | $2.5 \times 10^7$ | $5.2 \times 10^{-2}$ | $3.0 \times 10^7$ | $9.6 \times 10^{-1}$ |

**Table S3** Calculated vertical excitation energies (eV) of **CzBM-1, -2 and -3** in cyclohexane by different functionals. The experimental data are also shown in this table.

|               | B3LYP | M06  | MN15 | CAM-B3LYP | Exp. |
|---------------|-------|------|------|-----------|------|
| <b>CzBM-1</b> | 3.42  | 3.56 | 3.64 | 4.06      | 3.72 |
| <b>CzBM-2</b> | 3.29  | 3.44 | 3.62 | 3.98      | 3.63 |
| <b>CzBM-3</b> | 3.30  | 3.45 | 3.64 | 3.99      | 3.65 |

### III Cartesian Coordinates of Optimized Structures

#### CzBM-1

S<sub>0</sub>

66

symmetry c1

|   |              |              |              |
|---|--------------|--------------|--------------|
| B | 18.944728000 | 9.220343000  | 11.744493000 |
| N | 19.093352000 | 10.670205000 | 11.814631000 |
| O | 21.720397000 | 9.844714000  | 10.898205000 |
| C | 19.995247000 | 11.450873000 | 11.072389000 |
| C | 21.254198000 | 11.079034000 | 10.572654000 |
| C | 21.966528000 | 12.023702000 | 9.835110000  |
| H | 22.928594000 | 11.758682000 | 9.407001000  |
| C | 21.478305000 | 13.332778000 | 9.675823000  |
| H | 22.066797000 | 14.043325000 | 9.101344000  |
| C | 20.291830000 | 13.736558000 | 10.271717000 |
| H | 19.943957000 | 14.763446000 | 10.193621000 |
| C | 19.556926000 | 12.782749000 | 10.987355000 |
| C | 18.338694000 | 12.854076000 | 11.773071000 |
| C | 17.468742000 | 13.908667000 | 12.064556000 |
| H | 17.655796000 | 14.900857000 | 11.659463000 |
| C | 16.367925000 | 13.664729000 | 12.877121000 |
| H | 15.681318000 | 14.471431000 | 13.119679000 |
| C | 16.136839000 | 12.377295000 | 13.386396000 |



|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 15.271260000 | 12.201475000 | 14.020231000 |
| C | 16.988085000 | 11.312251000 | 13.101517000 |
| H | 16.787757000 | 10.323130000 | 13.499133000 |
| C | 18.105664000 | 11.563217000 | 12.297424000 |
| C | 18.387597000 | 8.462859000  | 13.001424000 |
| C | 19.004839000 | 8.660235000  | 14.260329000 |
| C | 18.569830000 | 7.927847000  | 15.368022000 |
| H | 19.062794000 | 8.078816000  | 16.328865000 |
| C | 17.516905000 | 7.015384000  | 15.280249000 |
| C | 16.900206000 | 6.840034000  | 14.038591000 |
| H | 16.065438000 | 6.143780000  | 13.952811000 |
| C | 17.327811000 | 7.530856000  | 12.903116000 |
| C | 20.139026000 | 9.643630000  | 14.455626000 |
| H | 20.664059000 | 9.436318000  | 15.394204000 |
| H | 20.868381000 | 9.610195000  | 13.637206000 |
| H | 19.762457000 | 10.673427000 | 14.502975000 |
| C | 17.072763000 | 6.224287000  | 16.483783000 |
| H | 17.287632000 | 6.760867000  | 17.413792000 |
| H | 15.998744000 | 6.013297000  | 16.446613000 |
| H | 17.593097000 | 5.259407000  | 16.534099000 |
| C | 16.620230000 | 7.271738000  | 11.591852000 |
| H | 15.684222000 | 6.728815000  | 11.761293000 |
| H | 16.380308000 | 8.203642000  | 11.065504000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 17.242048000 | 6.674604000  | 10.913995000 |
| C | 19.286209000 | 8.477655000  | 10.400871000 |
| C | 18.734099000 | 8.928256000  | 9.181601000  |
| C | 19.016866000 | 8.239612000  | 7.994923000  |
| H | 18.576829000 | 8.593804000  | 7.062024000  |
| C | 19.837337000 | 7.113440000  | 7.973231000  |
| C | 20.372433000 | 6.667986000  | 9.187550000  |
| H | 21.020752000 | 5.790660000  | 9.193688000  |
| C | 20.098147000 | 7.317741000  | 10.389966000 |
| C | 17.803347000 | 10.120505000 | 9.099248000  |
| H | 17.202411000 | 10.068769000 | 8.185019000  |
| H | 17.113356000 | 10.173117000 | 9.950464000  |
| H | 18.355902000 | 11.068551000 | 9.077485000  |
| C | 20.116607000 | 6.374864000  | 6.689046000  |
| H | 19.495664000 | 5.473800000  | 6.607987000  |
| H | 19.904450000 | 7.001427000  | 5.816606000  |
| H | 21.162240000 | 6.051908000  | 6.634513000  |
| C | 20.719504000 | 6.787122000  | 11.661852000 |
| H | 21.486562000 | 6.038159000  | 11.433401000 |
| H | 21.188546000 | 7.593597000  | 12.240332000 |
| H | 19.971464000 | 6.317439000  | 12.311838000 |
| C | 22.737782000 | 9.289329000  | 10.090216000 |
| H | 23.689637000 | 9.820604000  | 10.220191000 |

H 22.858500000 8.251929000 10.409315000

H 22.443230000 9.310436000 9.032581000

S<sub>1</sub>

66

symmetry c1

B 18.839776000 9.090137000 11.647235000

N 18.992191000 10.637927000 11.666275000

O 21.653314000 9.685098000 11.005701000

C 20.066967000 11.405230000 11.311687000

C 21.356272000 10.979360000 10.899654000

C 22.250398000 11.961518000 10.431607000

H 23.241566000 11.668265000 10.102346000

C 21.892434000 13.304685000 10.429609000

H 22.613278000 14.038367000 10.080992000

C 20.625735000 13.739588000 10.874868000

H 20.366636000 14.794275000 10.852666000

C 19.724991000 12.790028000 11.313887000

C 18.343221000 12.847945000 11.773527000

C 17.445119000 13.875357000 12.022248000

H 17.729472000 14.915612000 11.884501000

C 16.155544000 13.540534000 12.462922000

H 15.440733000 14.332884000 12.666344000

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 15.776389000 | 12.206695000 | 12.654591000 |
| H | 14.772949000 | 11.982613000 | 13.004600000 |
| C | 16.668072000 | 11.158769000 | 12.415885000 |
| H | 16.403822000 | 10.118628000 | 12.582073000 |
| C | 17.946704000 | 11.502560000 | 11.964691000 |
| C | 18.536669000 | 8.420270000  | 13.016284000 |
| C | 19.106967000 | 8.851459000  | 14.250185000 |
| C | 18.744845000 | 8.252039000  | 15.456111000 |
| H | 19.213432000 | 8.601209000  | 16.377991000 |
| C | 17.817231000 | 7.209199000  | 15.519973000 |
| C | 17.244830000 | 6.788119000  | 14.316621000 |
| H | 16.495835000 | 5.994436000  | 14.337509000 |
| C | 17.578419000 | 7.361138000  | 13.088678000 |
| C | 20.158457000 | 9.933558000  | 14.286151000 |
| H | 20.674565000 | 9.941657000  | 15.252806000 |
| H | 20.906412000 | 9.776179000  | 13.497265000 |
| H | 19.731883000 | 10.935592000 | 14.135769000 |
| C | 17.465137000 | 6.549495000  | 16.828580000 |
| H | 17.570203000 | 7.246574000  | 17.667616000 |
| H | 16.434316000 | 6.177167000  | 16.821825000 |
| H | 18.117239000 | 5.690595000  | 17.037083000 |
| C | 16.843322000 | 6.877289000  | 11.861364000 |
| H | 16.008870000 | 6.225877000  | 12.145455000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 16.450400000 | 7.726368000  | 11.282553000 |
| H | 17.490138000 | 6.319683000  | 11.172462000 |
| C | 19.019528000 | 8.419770000  | 10.244863000 |
| C | 18.526568000 | 8.966795000  | 9.029220000  |
| C | 18.820393000 | 8.368556000  | 7.800907000  |
| H | 18.413660000 | 8.811923000  | 6.890200000  |
| C | 19.597240000 | 7.213952000  | 7.703980000  |
| C | 20.079918000 | 6.666703000  | 8.896979000  |
| H | 20.702974000 | 5.771074000  | 8.853390000  |
| C | 19.808151000 | 7.233775000  | 10.143151000 |
| C | 17.618666000 | 10.172076000 | 9.026042000  |
| H | 17.117263000 | 10.278474000 | 8.057595000  |
| H | 16.847902000 | 10.077823000 | 9.804269000  |
| H | 18.154222000 | 11.111868000 | 9.220359000  |
| C | 19.879802000 | 6.563166000  | 6.373699000  |
| H | 19.168834000 | 5.753917000  | 6.160409000  |
| H | 19.804901000 | 7.285777000  | 5.553413000  |
| H | 20.883479000 | 6.122674000  | 6.349204000  |
| C | 20.424246000 | 6.585891000  | 11.361118000 |
| H | 21.164552000 | 5.833356000  | 11.062133000 |
| H | 20.910233000 | 7.335664000  | 12.000005000 |
| H | 19.678472000 | 6.089005000  | 11.995030000 |
| C | 22.764134000 | 9.161434000  | 10.289514000 |

|   |              |             |              |
|---|--------------|-------------|--------------|
| H | 23.707031000 | 9.470406000 | 10.755012000 |
| H | 22.662935000 | 8.076830000 | 10.335598000 |
| H | 22.733343000 | 9.489400000 | 9.244948000  |

T<sub>1</sub>

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symmetry c1

|   |              |              |              |
|---|--------------|--------------|--------------|
| B | 18.838718000 | 9.091901000  | 11.669083000 |
| N | 19.005696000 | 10.626000000 | 11.694411000 |
| O | 21.633974000 | 9.695115000  | 10.872187000 |
| C | 20.029096000 | 11.391459000 | 11.218922000 |
| C | 21.300408000 | 10.973245000 | 10.729633000 |
| C | 22.136879000 | 11.952979000 | 10.161219000 |
| H | 23.100808000 | 11.664639000 | 9.756300000  |
| C | 21.760830000 | 13.290466000 | 10.154638000 |
| H | 22.438312000 | 14.023306000 | 9.726842000  |
| C | 20.530738000 | 13.725730000 | 10.706294000 |
| H | 20.268883000 | 14.779805000 | 10.702292000 |
| C | 19.682031000 | 12.778829000 | 11.231163000 |
| C | 18.353912000 | 12.840354000 | 11.832914000 |
| C | 17.479105000 | 13.874156000 | 12.132051000 |
| H | 17.742991000 | 14.909658000 | 11.932480000 |
| C | 16.236769000 | 13.548207000 | 12.696634000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 15.538785000 | 14.343154000 | 12.943736000 |
| C | 15.879190000 | 12.218074000 | 12.941108000 |
| H | 14.907717000 | 11.997613000 | 13.373836000 |
| C | 16.746413000 | 11.164930000 | 12.637258000 |
| H | 16.484096000 | 10.127161000 | 12.817505000 |
| C | 17.986708000 | 11.502350000 | 12.091830000 |
| C | 18.452987000 | 8.419931000  | 13.025961000 |
| C | 19.042494000 | 8.801842000  | 14.261431000 |
| C | 18.644170000 | 8.202940000  | 15.459056000 |
| H | 19.121847000 | 8.515474000  | 16.389511000 |
| C | 17.671198000 | 7.202456000  | 15.499756000 |
| C | 17.093170000 | 6.817549000  | 14.286283000 |
| H | 16.319251000 | 6.047755000  | 14.288427000 |
| C | 17.460275000 | 7.400074000  | 13.072180000 |
| C | 20.150171000 | 9.828131000  | 14.307678000 |
| H | 20.694008000 | 9.772042000  | 15.257549000 |
| H | 20.864016000 | 9.662939000  | 13.487607000 |
| H | 19.776426000 | 10.857361000 | 14.207039000 |
| C | 17.279257000 | 6.539982000  | 16.796543000 |
| H | 17.462887000 | 7.199841000  | 17.651845000 |
| H | 16.217799000 | 6.266421000  | 16.799583000 |
| H | 17.850075000 | 5.617725000  | 16.968565000 |
| C | 16.754271000 | 6.957496000  | 11.813291000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 15.893208000 | 6.322085000  | 12.050622000 |
| H | 16.407190000 | 7.827642000  | 11.236086000 |
| H | 17.417560000 | 6.397101000  | 11.141699000 |
| C | 19.109598000 | 8.420462000  | 10.276259000 |
| C | 18.622210000 | 8.959926000  | 9.057994000  |
| C | 18.953975000 | 8.371754000  | 7.832546000  |
| H | 18.556495000 | 8.807420000  | 6.913973000  |
| C | 19.752998000 | 7.231240000  | 7.750021000  |
| C | 20.219263000 | 6.683675000  | 8.950583000  |
| H | 20.850258000 | 5.793106000  | 8.917389000  |
| C | 19.917432000 | 7.251300000  | 10.188759000 |
| C | 17.683799000 | 10.143774000 | 9.047212000  |
| H | 17.142462000 | 10.201773000 | 8.096194000  |
| H | 16.948288000 | 10.056493000 | 9.860193000  |
| H | 18.198188000 | 11.105828000 | 9.185985000  |
| C | 20.072392000 | 6.588646000  | 6.423680000  |
| H | 19.404991000 | 5.742300000  | 6.214359000  |
| H | 19.961875000 | 7.302112000  | 5.599550000  |
| H | 21.097605000 | 6.200406000  | 6.403201000  |
| C | 20.501775000 | 6.626948000  | 11.432630000 |
| H | 21.248724000 | 5.866041000  | 11.173939000 |
| H | 20.970998000 | 7.392952000  | 12.066456000 |
| H | 19.733696000 | 6.149641000  | 12.055039000 |



|   |              |             |              |
|---|--------------|-------------|--------------|
| C | 22.743521000 | 9.172580000 | 10.153134000 |
| H | 23.684405000 | 9.582833000 | 10.536924000 |
| H | 22.714891000 | 8.093908000 | 10.306910000 |
| H | 22.639042000 | 9.393249000 | 9.085252000  |

### **CzBM-2**

S<sub>0</sub>

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symmetry c1

|   |              |             |              |
|---|--------------|-------------|--------------|
| B | 7.098506000  | 2.911037000 | 8.210105000  |
| N | 6.772042000  | 2.052395000 | 9.335764000  |
| O | 9.566957000  | 1.339929000 | 8.901066000  |
| C | 7.683905000  | 1.592369000 | 10.306650000 |
| C | 9.041969000  | 1.293464000 | 10.153360000 |
| C | 9.766888000  | 0.897325000 | 11.280973000 |
| H | 10.825981000 | 0.688866000 | 11.181785000 |
| C | 9.120918000  | 0.710704000 | 12.518185000 |
| C | 7.742456000  | 0.879259000 | 12.640899000 |
| H | 7.259829000  | 0.668560000 | 13.590796000 |
| C | 7.034047000  | 1.308340000 | 11.519067000 |
| C | 5.619329000  | 1.526470000 | 11.271539000 |
| C | 4.495106000  | 1.382052000 | 12.088500000 |
| H | 4.607974000  | 1.065333000 | 13.123080000 |

|   |              |             |              |
|---|--------------|-------------|--------------|
| C | 3.239575000  | 1.647083000 | 11.554172000 |
| C | 3.114446000  | 2.057053000 | 10.218176000 |
| H | 2.126374000  | 2.258540000 | 9.811934000  |
| C | 4.224472000  | 2.213778000 | 9.390745000  |
| H | 4.103776000  | 2.537043000 | 8.362728000  |
| C | 5.486975000  | 1.934171000 | 9.925288000  |
| C | 10.954635000 | 1.578603000 | 8.774404000  |
| H | 11.241834000 | 2.474909000 | 9.340611000  |
| H | 11.146296000 | 1.748013000 | 7.712825000  |
| H | 11.544886000 | 0.716695000 | 9.112156000  |
| C | 8.377545000  | 3.830165000 | 8.267412000  |
| C | 8.603759000  | 4.679951000 | 9.372566000  |
| C | 9.714064000  | 5.535888000 | 9.377061000  |
| H | 9.868158000  | 6.192855000 | 10.234030000 |
| C | 10.616879000 | 5.580756000 | 8.317344000  |
| C | 10.384721000 | 4.737373000 | 7.224544000  |
| H | 11.084233000 | 4.745940000 | 6.387481000  |
| C | 9.285598000  | 3.881450000 | 7.180689000  |
| C | 7.677581000  | 4.741581000 | 10.569601000 |
| H | 7.700997000  | 5.742550000 | 11.014306000 |
| H | 7.980863000  | 4.029003000 | 11.347616000 |
| H | 6.636700000  | 4.512408000 | 10.313412000 |
| C | 11.790816000 | 6.526511000 | 8.328780000  |

|   |              |              |             |
|---|--------------|--------------|-------------|
| H | 12.008639000 | 6.876526000  | 9.343102000 |
| H | 11.592592000 | 7.410313000  | 7.709428000 |
| H | 12.692008000 | 6.048368000  | 7.928828000 |
| C | 9.124936000  | 2.973238000  | 5.982847000 |
| H | 10.030220000 | 2.987549000  | 5.365078000 |
| H | 8.279904000  | 3.273405000  | 5.352168000 |
| H | 8.942887000  | 1.937139000  | 6.297211000 |
| C | 6.127769000  | 2.944855000  | 6.975048000 |
| C | 5.797017000  | 1.736653000  | 6.316055000 |
| C | 5.014143000  | 1.769790000  | 5.159378000 |
| H | 4.777684000  | 0.833450000  | 4.652917000 |
| C | 4.519095000  | 2.968046000  | 4.639970000 |
| C | 4.829630000  | 4.153703000  | 5.310423000 |
| H | 4.435827000  | 5.097604000  | 4.932218000 |
| C | 5.634217000  | 4.161676000  | 6.452096000 |
| C | 6.263202000  | 0.391468000  | 6.829644000 |
| H | 6.159855000  | -0.371586000 | 6.050775000 |
| H | 5.663816000  | 0.073061000  | 7.692470000 |
| H | 7.308412000  | 0.407842000  | 7.161546000 |
| C | 3.691177000  | 2.983934000  | 3.380483000 |
| H | 4.326306000  | 3.102233000  | 2.493373000 |
| H | 2.978130000  | 3.815130000  | 3.383938000 |
| H | 3.132435000  | 2.049873000  | 3.259805000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 5.937206000  | 5.486220000  | 7.116226000  |
| H | 6.967806000  | 5.805592000  | 6.919763000  |
| H | 5.822974000  | 5.430531000  | 8.205907000  |
| H | 5.263222000  | 6.265886000  | 6.745324000  |
| H | 2.351142000  | 1.536222000  | 12.170088000 |
| O | 9.781244000  | 0.323116000  | 13.645699000 |
| C | 11.172413000 | 0.113702000  | 13.570306000 |
| H | 11.499704000 | -0.166733000 | 14.572943000 |
| H | 11.421057000 | -0.696713000 | 12.871385000 |
| H | 11.700142000 | 1.026142000  | 13.260729000 |

S<sub>1</sub>

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symmetry c1

|   |              |             |              |
|---|--------------|-------------|--------------|
| B | 7.141221000  | 3.211248000 | 8.202613000  |
| N | 6.829673000  | 2.419123000 | 9.506177000  |
| O | 9.513546000  | 1.581652000 | 8.796572000  |
| C | 7.638567000  | 1.598287000 | 10.224940000 |
| C | 8.985159000  | 1.217614000 | 9.964353000  |
| C | 9.669363000  | 0.472573000 | 10.931532000 |
| H | 10.694716000 | 0.176472000 | 10.746857000 |
| C | 9.017159000  | 0.072060000 | 12.106125000 |
| C | 7.663609000  | 0.412213000 | 12.361609000 |

|   |              |             |              |
|---|--------------|-------------|--------------|
| H | 7.212856000  | 0.087600000 | 13.294296000 |
| C | 6.991400000  | 1.161740000 | 11.425585000 |
| C | 5.653942000  | 1.733737000 | 11.372600000 |
| C | 4.538345000  | 1.666984000 | 12.198876000 |
| H | 4.554226000  | 1.081421000 | 13.115006000 |
| C | 3.387807000  | 2.368436000 | 11.819465000 |
| C | 3.355046000  | 3.114237000 | 10.634262000 |
| H | 2.444484000  | 3.640311000 | 10.361474000 |
| C | 4.463825000  | 3.186007000 | 9.787826000  |
| H | 4.447087000  | 3.736145000 | 8.851273000  |
| C | 5.611337000  | 2.497004000 | 10.184454000 |
| C | 10.921432000 | 1.536714000 | 8.619073000  |
| H | 11.428492000 | 2.025520000 | 9.458358000  |
| H | 11.123070000 | 2.086464000 | 7.699255000  |
| H | 11.268362000 | 0.501320000 | 8.520687000  |
| C | 8.259180000  | 4.295795000 | 8.332167000  |
| C | 8.426804000  | 5.137164000 | 9.466139000  |
| C | 9.519662000  | 6.002081000 | 9.564989000  |
| H | 9.605771000  | 6.641005000 | 10.445865000 |
| C | 10.490477000 | 6.089935000 | 8.566796000  |
| C | 10.328884000 | 5.270218000 | 7.445249000  |
| H | 11.078885000 | 5.305955000 | 6.652390000  |
| C | 9.250095000  | 4.395328000 | 7.308038000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 7.398419000  | 5.173509000  | 10.569820000 |
| H | 7.537322000  | 6.057878000  | 11.201817000 |
| H | 7.442459000  | 4.292870000  | 11.225577000 |
| H | 6.382417000  | 5.206051000  | 10.151168000 |
| C | 11.647673000 | 7.050275000  | 8.674427000  |
| H | 11.871065000 | 7.288925000  | 9.720359000  |
| H | 11.435486000 | 7.998645000  | 8.162969000  |
| H | 12.554586000 | 6.636187000  | 8.218202000  |
| C | 9.204729000  | 3.522701000  | 6.075319000  |
| H | 10.152226000 | 3.585937000  | 5.525620000  |
| H | 8.398534000  | 3.809242000  | 5.387795000  |
| H | 9.012477000  | 2.474986000  | 6.343286000  |
| C | 6.299903000  | 2.827418000  | 6.953948000  |
| C | 5.904465000  | 1.493130000  | 6.639457000  |
| C | 5.101451000  | 1.224054000  | 5.531804000  |
| H | 4.833566000  | 0.187894000  | 5.317009000  |
| C | 4.642110000  | 2.232864000  | 4.681169000  |
| C | 5.009151000  | 3.544723000  | 4.991450000  |
| H | 4.640365000  | 4.358314000  | 4.364141000  |
| C | 5.811512000  | 3.857727000  | 6.089746000  |
| C | 6.381094000  | 0.321446000  | 7.462859000  |
| H | 6.208268000  | -0.621297000 | 6.931543000  |
| H | 5.861233000  | 0.252424000  | 8.428850000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 7.455428000  | 0.405215000  | 7.675924000  |
| C | 3.803389000  | 1.917856000  | 3.469218000  |
| H | 4.425493000  | 1.729781000  | 2.583663000  |
| H | 3.133708000  | 2.749506000  | 3.221955000  |
| H | 3.190776000  | 1.023293000  | 3.629352000  |
| C | 6.078206000  | 5.317983000  | 6.370156000  |
| H | 7.124315000  | 5.599976000  | 6.197067000  |
| H | 5.874536000  | 5.556431000  | 7.424625000  |
| H | 5.447078000  | 5.951302000  | 5.736005000  |
| H | 2.503810000  | 2.326431000  | 12.449506000 |
| O | 9.607109000  | -0.659181000 | 13.065880000 |
| C | 10.964529000 | -1.034416000 | 12.910802000 |
| H | 11.230724000 | -1.596866000 | 13.805566000 |
| H | 11.096435000 | -1.668964000 | 12.026221000 |
| H | 11.607374000 | -0.149951000 | 12.827645000 |

T<sub>1</sub>

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symmetry c1

|   |             |             |              |
|---|-------------|-------------|--------------|
| B | 7.115299000 | 3.172992000 | 8.179258000  |
| N | 6.810813000 | 2.337852000 | 9.442986000  |
| O | 9.552629000 | 1.602184000 | 8.821692000  |
| C | 7.655990000 | 1.623566000 | 10.224321000 |

|   |              |             |              |
|---|--------------|-------------|--------------|
| C | 9.030673000  | 1.300261000 | 10.005575000 |
| C | 9.736983000  | 0.657326000 | 11.028273000 |
| H | 10.783031000 | 0.417844000 | 10.883034000 |
| C | 9.082495000  | 0.277225000 | 12.208238000 |
| C | 7.694232000  | 0.521779000 | 12.407802000 |
| H | 7.236057000  | 0.189561000 | 13.334062000 |
| C | 7.004509000  | 1.179830000 | 11.424488000 |
| C | 5.622171000  | 1.625391000 | 11.299199000 |
| C | 4.497262000  | 1.508464000 | 12.105659000 |
| H | 4.537977000  | 0.973615000 | 13.051381000 |
| C | 3.307294000  | 2.103044000 | 11.669502000 |
| C | 3.254417000  | 2.806827000 | 10.460610000 |
| H | 2.318434000  | 3.262638000 | 10.150329000 |
| C | 4.379994000  | 2.938304000 | 9.642646000  |
| H | 4.353778000  | 3.481552000 | 8.703108000  |
| C | 5.555022000  | 2.328651000 | 10.079635000 |
| C | 10.959858000 | 1.559123000 | 8.639633000  |
| H | 11.459278000 | 2.161258000 | 9.406980000  |
| H | 11.145990000 | 1.993689000 | 7.657445000  |
| H | 11.325823000 | 0.526032000 | 8.669735000  |
| C | 8.316170000  | 4.173638000 | 8.315021000  |
| C | 8.508715000  | 4.986928000 | 9.461295000  |
| C | 9.637858000  | 5.805547000 | 9.577438000  |



|   |              |             |              |
|---|--------------|-------------|--------------|
| H | 9.751365000  | 6.423524000 | 10.470277000 |
| C | 10.607088000 | 5.877426000 | 8.577135000  |
| C | 10.410862000 | 5.093354000 | 7.434681000  |
| H | 11.154289000 | 5.125748000 | 6.635334000  |
| C | 9.301691000  | 4.259007000 | 7.291511000  |
| C | 7.475683000  | 5.040354000 | 10.562592000 |
| H | 7.601073000  | 5.943802000 | 11.170202000 |
| H | 7.525653000  | 4.180554000 | 11.246404000 |
| H | 6.461598000  | 5.046334000 | 10.136548000 |
| C | 11.799931000 | 6.792130000 | 8.700585000  |
| H | 12.004348000 | 7.039644000 | 9.748275000  |
| H | 11.640539000 | 7.738649000 | 8.167312000  |
| H | 12.701736000 | 6.334375000 | 8.276706000  |
| C | 9.190782000  | 3.410490000 | 6.047741000  |
| H | 10.119192000 | 3.448912000 | 5.464069000  |
| H | 8.368249000  | 3.735398000 | 5.397344000  |
| H | 8.971928000  | 2.365575000 | 6.310857000  |
| C | 6.207192000  | 2.892096000 | 6.937876000  |
| C | 5.832285000  | 1.578752000 | 6.545654000  |
| C | 4.992093000  | 1.371241000 | 5.448687000  |
| H | 4.729928000  | 0.348466000 | 5.171242000  |
| C | 4.496562000  | 2.428536000 | 4.683786000  |
| C | 4.866625000  | 3.723024000 | 5.060978000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 4.483286000  | 4.571389000  | 4.490824000  |
| C | 5.696075000  | 3.967509000  | 6.156619000  |
| C | 6.372414000  | 0.368733000  | 7.271416000  |
| H | 6.248174000  | -0.536374000 | 6.665825000  |
| H | 5.866123000  | 0.190879000  | 8.231210000  |
| H | 7.442267000  | 0.497701000  | 7.490853000  |
| C | 3.620957000  | 2.185398000  | 3.480168000  |
| H | 4.204004000  | 2.178480000  | 2.549533000  |
| H | 2.859240000  | 2.966917000  | 3.375878000  |
| H | 3.108805000  | 1.219202000  | 3.550118000  |
| C | 6.010044000  | 5.398298000  | 6.521921000  |
| H | 7.061309000  | 5.652366000  | 6.334036000  |
| H | 5.847563000  | 5.569059000  | 7.596765000  |
| H | 5.383422000  | 6.094268000  | 5.952115000  |
| H | 2.412706000  | 2.020565000  | 12.280324000 |
| O | 9.692941000  | -0.352572000 | 13.222844000 |
| C | 11.080900000 | -0.626601000 | 13.131074000 |
| H | 11.359634000 | -1.109651000 | 14.067306000 |
| H | 11.290971000 | -1.301700000 | 12.293142000 |
| H | 11.653622000 | 0.300283000  | 13.009708000 |

### **CzBM-3**

S<sub>0</sub>

## symmetry c1

|   |              |             |              |
|---|--------------|-------------|--------------|
| B | 7.099553000  | 2.896620000 | 8.196295000  |
| N | 6.768629000  | 2.022446000 | 9.308565000  |
| O | 9.556384000  | 1.332635000 | 8.873467000  |
| O | 2.154550000  | 1.407356000 | 12.344896000 |
| C | 7.670192000  | 1.560399000 | 10.282923000 |
| C | 9.036521000  | 1.276610000 | 10.128213000 |
| C | 9.750759000  | 0.891234000 | 11.262316000 |
| H | 10.817038000 | 0.699777000 | 11.186990000 |
| C | 9.101436000  | 0.697739000 | 12.494279000 |
| H | 9.691127000  | 0.387372000 | 13.352838000 |
| C | 7.726619000  | 0.849046000 | 12.615054000 |
| H | 7.217559000  | 0.642788000 | 13.553084000 |
| C | 7.011365000  | 1.271735000 | 11.488434000 |
| C | 5.596856000  | 1.482112000 | 11.233468000 |
| C | 4.475493000  | 1.325808000 | 12.043565000 |
| H | 4.555379000  | 1.006112000 | 13.079342000 |
| C | 3.214637000  | 1.584069000 | 11.505048000 |
| C | 3.090999000  | 1.998829000 | 10.168430000 |
| H | 2.112035000  | 2.197953000 | 9.744434000  |
| C | 4.213855000  | 2.163605000 | 9.355005000  |
| H | 4.088589000  | 2.490175000 | 8.328497000  |

|   |              |             |              |
|---|--------------|-------------|--------------|
| C | 5.474169000  | 1.894136000 | 9.886970000  |
| C | 10.945348000 | 1.565788000 | 8.750655000  |
| H | 11.234847000 | 2.458357000 | 9.321860000  |
| H | 11.140382000 | 1.739016000 | 7.690249000  |
| H | 11.530575000 | 0.700405000 | 9.087765000  |
| C | 0.861968000  | 1.650924000 | 11.839389000 |
| H | 0.747333000  | 2.693350000 | 11.512026000 |
| H | 0.165475000  | 1.453316000 | 12.656102000 |
| H | 0.627512000  | 0.986310000 | 10.996647000 |
| C | 8.376622000  | 3.817451000 | 8.264940000  |
| C | 8.608276000  | 4.648725000 | 9.382577000  |
| C | 9.718569000  | 5.505217000 | 9.395628000  |
| H | 9.876595000  | 6.147657000 | 10.262841000 |
| C | 10.616140000 | 5.568010000 | 8.332979000  |
| C | 10.379051000 | 4.742174000 | 7.227503000  |
| H | 11.074916000 | 4.764174000 | 6.387675000  |
| C | 9.280545000  | 3.886636000 | 7.175050000  |
| C | 7.691171000  | 4.691773000 | 10.587616000 |
| H | 7.690900000  | 5.695948000 | 11.025911000 |
| H | 8.023972000  | 3.993872000 | 11.367035000 |
| H | 6.654732000  | 4.431170000 | 10.344339000 |
| C | 11.791227000 | 6.512077000 | 8.354635000  |
| H | 11.994179000 | 6.869576000 | 9.369375000  |

|   |              |              |             |
|---|--------------|--------------|-------------|
| H | 11.604347000 | 7.390784000  | 7.724663000 |
| H | 12.697710000 | 6.029028000  | 7.972777000 |
| C | 9.116822000  | 2.995515000  | 5.964926000 |
| H | 10.018495000 | 3.022762000  | 5.342434000 |
| H | 8.266793000  | 3.300579000  | 5.343477000 |
| H | 8.941774000  | 1.954139000  | 6.265593000 |
| C | 6.123116000  | 2.950160000  | 6.966105000 |
| C | 5.791731000  | 1.753731000  | 6.286587000 |
| C | 4.997026000  | 1.805862000  | 5.138683000 |
| H | 4.760121000  | 0.878625000  | 4.615909000 |
| C | 4.490783000  | 3.011817000  | 4.648511000 |
| C | 4.802178000  | 4.185410000  | 5.339479000 |
| H | 4.400021000  | 5.134690000  | 4.984165000 |
| C | 5.618416000  | 4.174639000  | 6.472927000 |
| C | 6.267590000  | 0.401260000  | 6.771047000 |
| H | 6.164662000  | -0.347080000 | 5.977987000 |
| H | 5.673759000  | 0.063330000  | 7.630366000 |
| H | 7.314003000  | 0.416743000  | 7.098876000 |
| C | 3.650278000  | 3.048765000  | 3.397793000 |
| H | 4.275933000  | 3.188663000  | 2.507127000 |
| H | 2.932892000  | 3.875802000  | 3.425137000 |
| H | 3.095406000  | 2.114248000  | 3.263427000 |
| C | 5.921431000  | 5.486742000  | 7.161376000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 6.949256000 | 5.813948000 | 6.963462000 |
| H | 5.816200000 | 5.408430000 | 8.250638000 |
| H | 5.241632000 | 6.271126000 | 6.811588000 |

S<sub>1</sub>

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symmetry c1

|   |              |              |              |
|---|--------------|--------------|--------------|
| B | 7.081650000  | 3.076584000  | 8.122707000  |
| N | 6.774431000  | 2.134275000  | 9.323519000  |
| O | 9.489857000  | 1.398269000  | 8.578394000  |
| O | 2.334233000  | 1.785469000  | 12.479370000 |
| C | 7.625732000  | 1.292764000  | 10.023028000 |
| C | 8.967601000  | 0.973761000  | 9.738234000  |
| C | 9.664342000  | 0.199285000  | 10.682877000 |
| H | 10.701856000 | -0.059552000 | 10.496772000 |
| C | 9.034422000  | -0.269291000 | 11.834883000 |
| H | 9.602693000  | -0.876496000 | 12.533504000 |
| C | 7.687767000  | 0.019790000  | 12.104903000 |
| H | 7.211011000  | -0.345273000 | 13.010399000 |
| C | 6.994464000  | 0.800556000  | 11.192980000 |
| C | 5.641640000  | 1.344413000  | 11.162026000 |
| C | 4.542457000  | 1.237575000  | 11.982975000 |
| H | 4.534930000  | 0.635695000  | 12.887258000 |

|   |              |             |              |
|---|--------------|-------------|--------------|
| C | 3.365730000  | 1.943944000 | 11.631008000 |
| C | 3.305751000  | 2.736197000 | 10.466660000 |
| H | 2.390233000  | 3.255787000 | 10.207025000 |
| C | 4.409483000  | 2.844140000 | 9.630210000  |
| H | 4.378238000  | 3.425414000 | 8.713839000  |
| C | 5.581995000  | 2.153880000 | 9.988054000  |
| C | 10.900769000 | 1.473517000 | 8.448571000  |
| H | 11.339547000 | 1.976610000 | 9.317908000  |
| H | 11.089340000 | 2.066728000 | 7.552764000  |
| H | 11.339989000 | 0.475385000 | 8.332406000  |
| C | 1.115426000  | 2.457348000 | 12.212179000 |
| H | 1.262201000  | 3.543749000 | 12.193576000 |
| H | 0.437378000  | 2.194556000 | 13.024176000 |
| H | 0.688106000  | 2.129734000 | 11.257048000 |
| C | 8.197128000  | 4.143971000 | 8.375265000  |
| C | 8.357908000  | 4.864265000 | 9.590186000  |
| C | 9.437900000  | 5.731544000 | 9.774195000  |
| H | 9.519749000  | 6.275488000 | 10.717014000 |
| C | 10.401581000 | 5.938307000 | 8.786808000  |
| C | 10.249260000 | 5.234183000 | 7.588600000  |
| H | 10.996223000 | 5.361158000 | 6.802399000  |
| C | 9.184588000  | 4.358866000 | 7.366678000  |
| C | 7.339916000  | 4.766106000 | 10.699799000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 7.475915000  | 5.576913000  | 11.424237000 |
| H | 7.404143000  | 3.819270000  | 11.253934000 |
| H | 6.319543000  | 4.832358000  | 10.295307000 |
| C | 11.543317000 | 6.901881000  | 8.989241000  |
| H | 11.774868000 | 7.027145000  | 10.052951000 |
| H | 11.308634000 | 7.896949000  | 8.588268000  |
| H | 12.451570000 | 6.557310000  | 8.481085000  |
| C | 9.152532000  | 3.608416000  | 6.055644000  |
| H | 10.096348000 | 3.744725000  | 5.513106000  |
| H | 8.337537000  | 3.941307000  | 5.400144000  |
| H | 8.986412000  | 2.535725000  | 6.224100000  |
| C | 6.253579000  | 2.812219000  | 6.836385000  |
| C | 5.893958000  | 1.506682000  | 6.388187000  |
| C | 5.076465000  | 1.332100000  | 5.271788000  |
| H | 4.835412000  | 0.317043000  | 4.950633000  |
| C | 4.575629000  | 2.411490000  | 4.539301000  |
| C | 4.918783000  | 3.694738000  | 4.974935000  |
| H | 4.523335000  | 4.558452000  | 4.437210000  |
| C | 5.732581000  | 3.913472000  | 6.086975000  |
| C | 6.436956000  | 0.273617000  | 7.069509000  |
| H | 6.315043000  | -0.608201000 | 6.430195000  |
| H | 5.927757000  | 0.060370000  | 8.019937000  |
| H | 7.505451000  | 0.392153000  | 7.294250000  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.723879000 | 2.201789000 | 3.313559000 |
| H | 4.332848000 | 2.152185000 | 2.400773000 |
| H | 3.009743000 | 3.022493000 | 3.179563000 |
| H | 3.158528000 | 1.265028000 | 3.376173000 |
| C | 5.983677000 | 5.340391000 | 6.512000000 |
| H | 7.027925000 | 5.645992000 | 6.370209000 |
| H | 5.778961000 | 5.468089000 | 7.585788000 |
| H | 5.347593000 | 6.029406000 | 5.944389000 |

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symmetry c1

|   |              |              |              |
|---|--------------|--------------|--------------|
| B | 7.082205000  | 3.100761000  | 8.135255000  |
| N | 6.785880000  | 2.187081000  | 9.343663000  |
| O | 9.549343000  | 1.511947000  | 8.675033000  |
| O | 2.259930000  | 1.586904000  | 12.354964000 |
| C | 7.661859000  | 1.417027000  | 10.092387000 |
| C | 9.019314000  | 1.121615000  | 9.837414000  |
| C | 9.719290000  | 0.392162000  | 10.817876000 |
| H | 10.769808000 | 0.167854000  | 10.665405000 |
| C | 9.077442000  | -0.076897000 | 11.959906000 |
| H | 9.648485000  | -0.648845000 | 12.685399000 |
| C | 7.707199000  | 0.155792000  | 12.183939000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 7.214321000  | -0.233803000 | 13.070146000 |
| C | 7.016648000  | 0.898670000  | 11.246027000 |
| C | 5.629068000  | 1.346076000  | 11.149937000 |
| C | 4.517002000  | 1.180842000  | 11.941911000 |
| H | 4.524437000  | 0.603809000  | 12.862082000 |
| C | 3.307877000  | 1.802714000  | 11.539159000 |
| C | 3.242251000  | 2.584577000  | 10.370251000 |
| H | 2.310014000  | 3.056817000  | 10.081138000 |
| C | 4.368162000  | 2.760508000  | 9.572776000  |
| H | 4.337054000  | 3.359154000  | 8.668168000  |
| C | 5.559924000  | 2.127158000  | 9.963450000  |
| C | 10.959629000 | 1.525112000  | 8.521906000  |
| H | 11.428139000 | 2.080621000  | 9.342447000  |
| H | 11.152829000 | 2.039380000  | 7.579859000  |
| H | 11.361279000 | 0.505622000  | 8.479658000  |
| C | 1.010728000  | 2.173967000  | 12.034682000 |
| H | 1.084554000  | 3.267838000  | 12.014733000 |
| H | 0.319259000  | 1.869601000  | 12.820511000 |
| H | 0.645426000  | 1.814819000  | 11.065223000 |
| C | 8.269439000  | 4.106366000  | 8.342761000  |
| C | 8.442628000  | 4.851900000  | 9.536866000  |
| C | 9.559280000  | 5.677318000  | 9.709058000  |
| H | 9.659510000  | 6.242069000  | 10.637853000 |

|   |              |             |              |
|---|--------------|-------------|--------------|
| C | 10.533647000 | 5.820384000 | 8.721395000  |
| C | 10.356578000 | 5.102442000 | 7.533336000  |
| H | 11.105300000 | 5.191370000 | 6.743446000  |
| C | 9.260723000  | 4.262317000 | 7.333516000  |
| C | 7.402545000  | 4.826948000 | 10.632548000 |
| H | 7.525350000  | 5.684171000 | 11.304185000 |
| H | 7.450035000  | 3.919638000 | 11.251920000 |
| H | 6.391412000  | 4.865719000 | 10.201259000 |
| C | 11.713136000 | 6.741561000 | 8.907507000  |
| H | 11.913292000 | 6.921620000 | 9.969603000  |
| H | 11.540086000 | 7.718883000 | 8.437848000  |
| H | 12.621214000 | 6.325373000 | 8.455475000  |
| C | 9.169429000  | 3.486005000 | 6.042140000  |
| H | 10.098730000 | 3.575671000 | 5.465743000  |
| H | 8.342936000  | 3.834101000 | 5.408953000  |
| H | 8.970491000  | 2.423876000 | 6.243564000  |
| C | 6.181648000  | 2.883152000 | 6.878828000  |
| C | 5.817829000  | 1.588117000 | 6.417340000  |
| C | 4.973012000  | 1.432925000 | 5.315360000  |
| H | 4.720223000  | 0.424243000 | 4.983062000  |
| C | 4.462815000  | 2.525332000 | 4.611577000  |
| C | 4.825103000  | 3.801473000 | 5.054740000  |
| H | 4.431521000  | 4.675512000 | 4.532336000  |

|   |             |              |             |
|---|-------------|--------------|-------------|
| C | 5.659655000 | 3.994911000  | 6.156155000 |
| C | 6.379828000 | 0.346248000  | 7.068795000 |
| H | 6.270543000 | -0.522592000 | 6.409646000 |
| H | 5.879756000 | 0.100706000  | 8.016838000 |
| H | 7.447699000 | 0.479843000  | 7.295347000 |
| C | 3.581608000 | 2.339554000  | 3.401946000 |
| H | 4.157959000 | 2.392160000  | 2.468634000 |
| H | 2.809998000 | 3.116422000  | 3.346530000 |
| H | 3.081507000 | 1.364736000  | 3.420567000 |
| C | 5.964003000 | 5.406610000  | 6.595466000 |
| H | 7.014567000 | 5.675796000  | 6.426187000 |
| H | 5.796039000 | 5.520894000  | 7.677111000 |
| H | 5.336024000 | 6.127548000  | 6.059225000 |