

## Supporting information

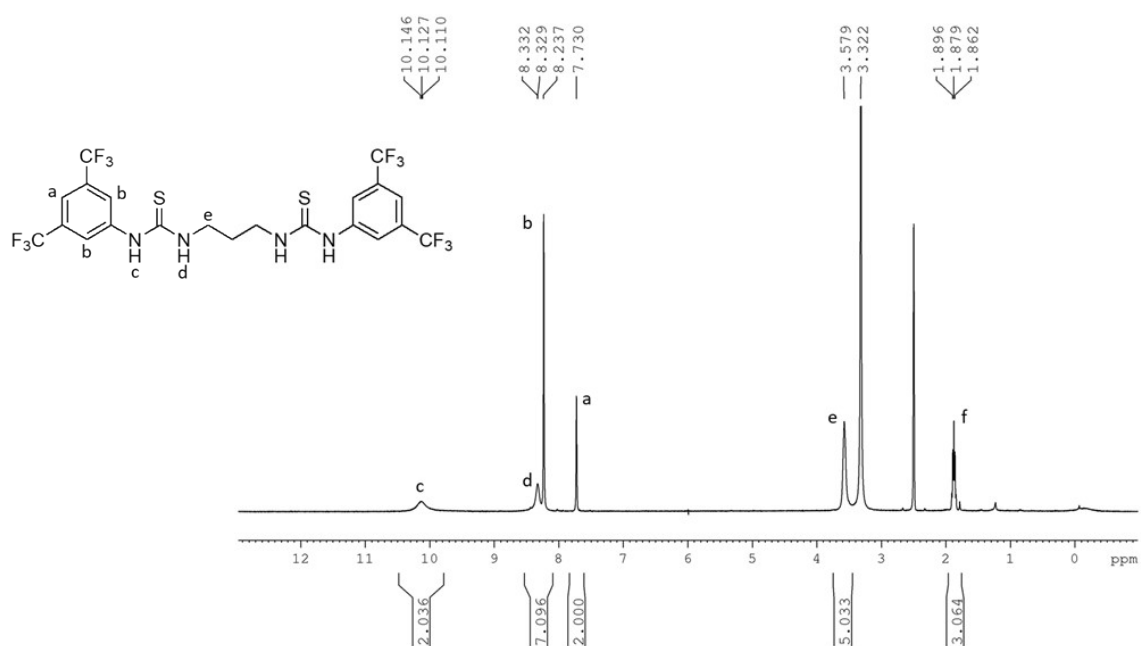
### Bis-(thio)ureas and peraza-macrocycles as binary organocatalysts for the ROP of lactide.

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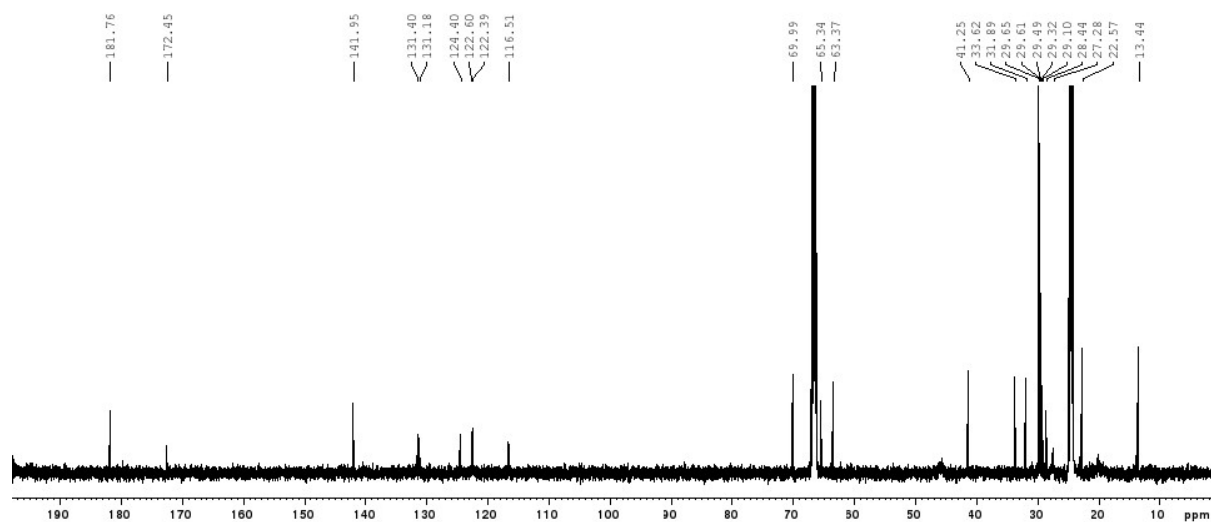


**Figure S1.** <sup>1</sup>H NMR spectrum (300 MHz, DMSO-d<sub>6</sub>, 298 K) of bis(thio)urea TU. <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>, 298 K): δ 10.1 (s, 2H, NH, c), 8.33 (s, 2H, NH, d), 8.24 (s, 4H, CH, b), 7.73 (s, 2H, CH, a), 3.58 (s, 4H, CH<sub>2</sub>, e), 1.88 (t, 2H, CH<sub>2</sub>, f).

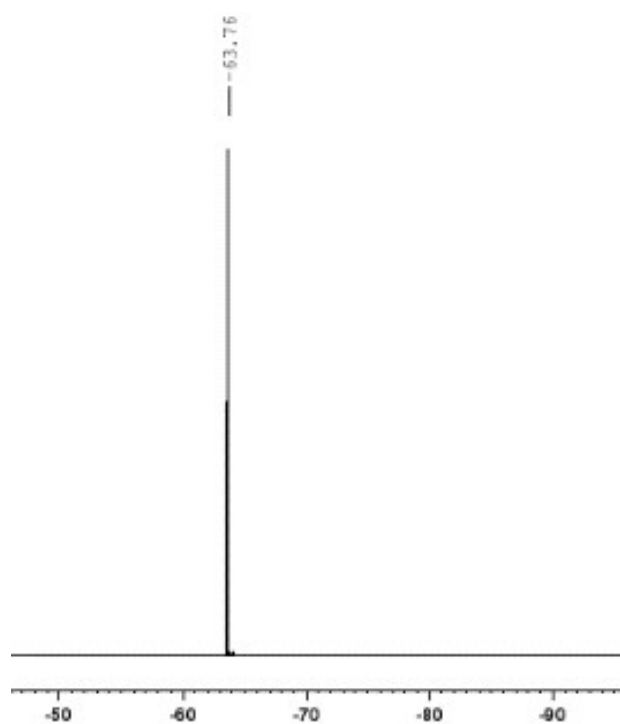


**Figure S2.** <sup>1</sup>H NMR spectrum (400 MHz, THF d<sub>8</sub>, 298 K) of the bis(thio)urea TU

$^1\text{H}$  NMR (400 MHz, THF  $d_8$ , 298 K):  $\delta$  9.29 (s, 2H, NH), 8.14 (s, 4H, CH), 7.67 (s, 2H, NH), 7.67 (s, 2H, CH), 3.72 (s, 4H,  $\text{CH}_2$ ), 1.92 (t, 2H,  $\text{CH}_2$ ).



**Figure S3.**  $^{13}\text{C}$  NMR spectrum (100 MHz, THF  $d_8$ , 298 K) of the bis(thio)urea TU



**Figure S4.**  $^{19}\text{F}$  NMR spectrum (376 MHz, THF  $d_8$ , 298 K) of the bis(thio)urea TU. This chemical shift is reported relative to an external  $\text{CFCl}_3$  reference.

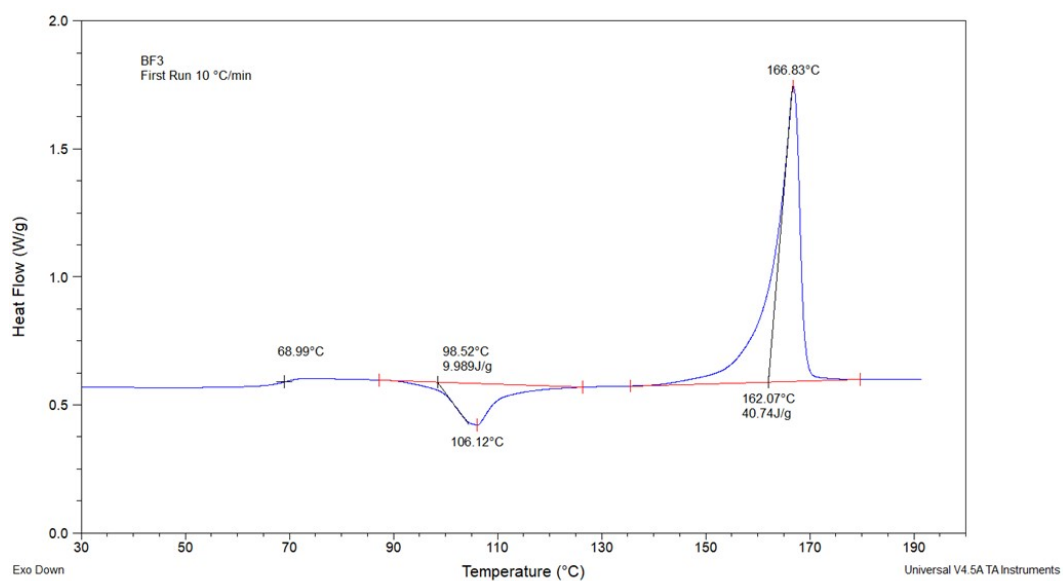


Figure S5. DSC thermograms of the sample obtained by run 3 table 1

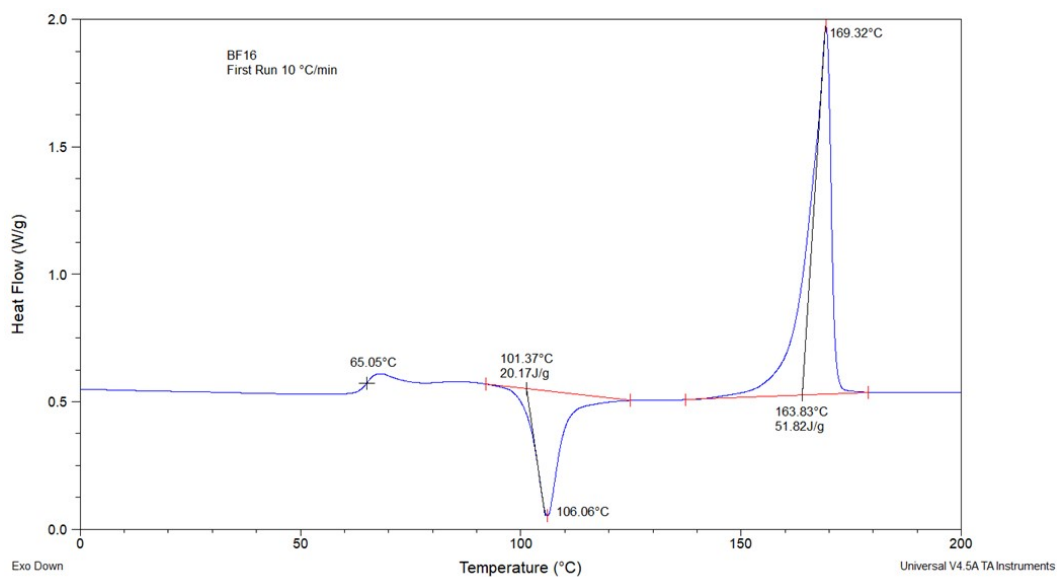


Figure S6. DSC thermograms of the sample obtained by run 4 table 1

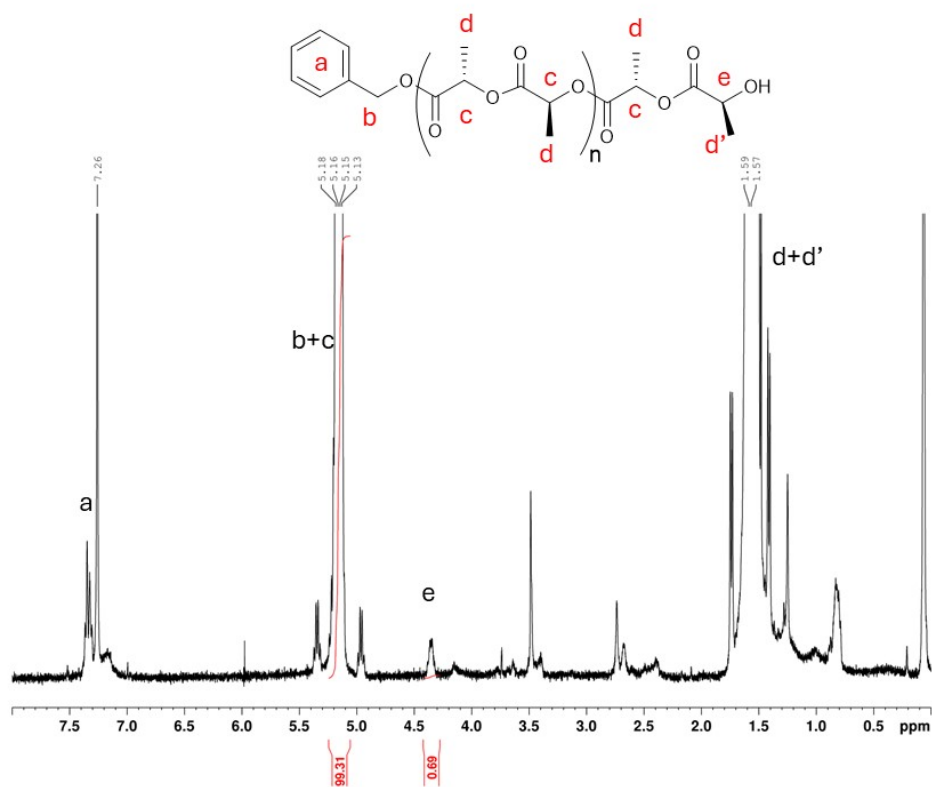


Figure S7. <sup>1</sup>H NMR of the sample obtained in run 2 of Table 1.

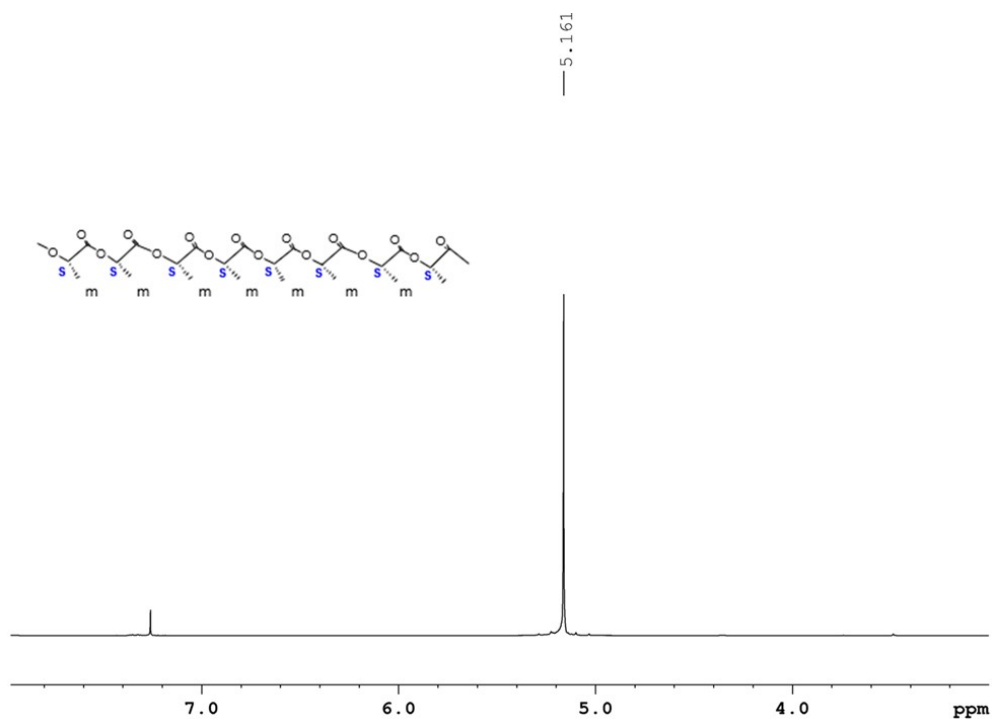
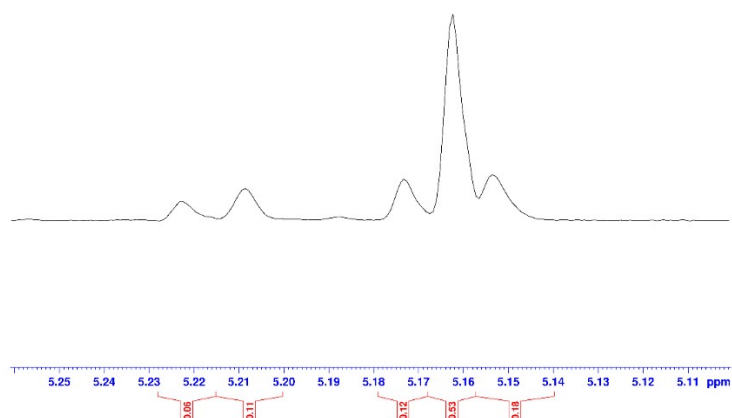


Figure S8. Methine region of the homonuclear decoupled <sup>1</sup>H NMR spectrum (600 MHz, CDCl<sub>3</sub>, 298 K)



**Figure S9.** Methine region of the homonuclear decoupled  $^1\text{H}$  NMR spectrum (600 MHz,  $\text{CDCl}_3$ , 298 K) of Poly(rac-LA) obtained in run 7 Table 1.

**Table S1** Correlation between  $M_n$  and conversions

Conversion (%)	Molecular Mass KDa	$\bar{D}$
<b>23</b>	<b>5.4</b>	<b>1.07</b>
<b>40</b>	<b>9.9</b>	<b>1.07</b>
<b>78</b>	<b>21.2</b>	<b>1.08</b>
<b>100</b>	<b>28.8</b>	<b>1.11</b>

Chromatogram Plot

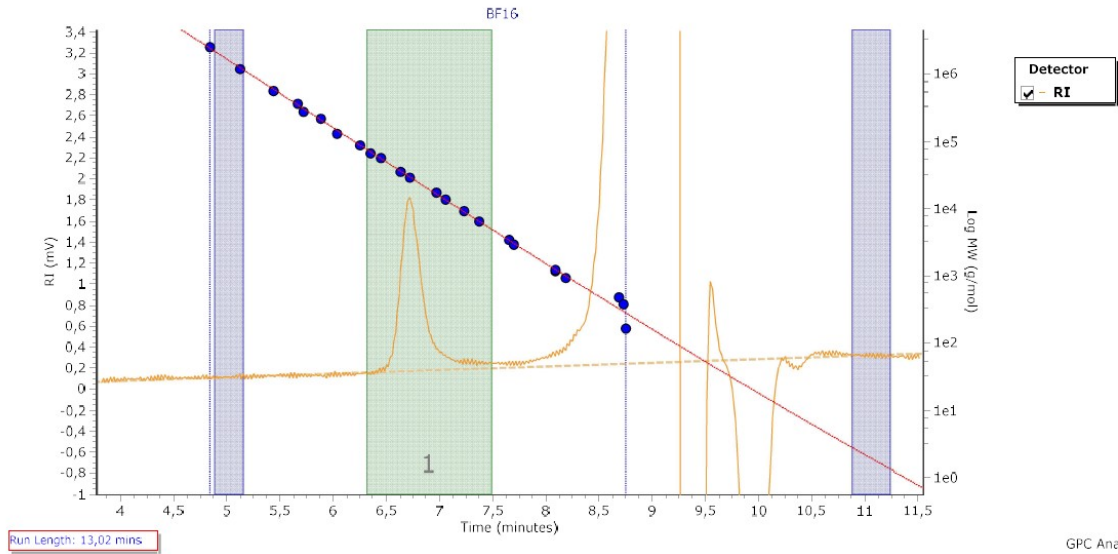


Figure S10. GPC analysis of PLA obtained in run 6.

Chromatogram Plot

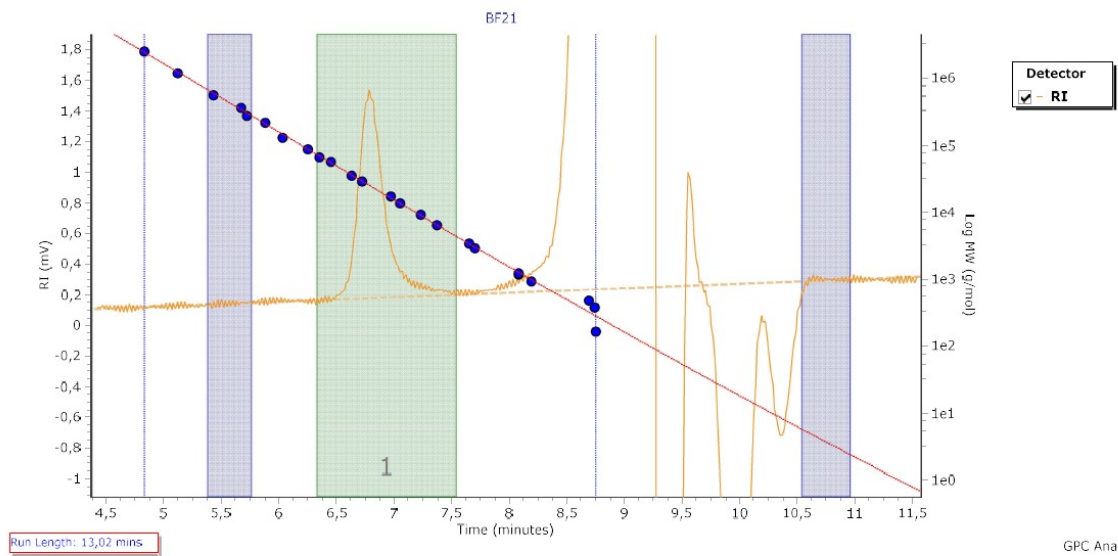


Figure S11. GPC analysis of PLA obtained in run 2

## Cartesian Coordinates

### Me<sub>3</sub>TACN/Alcohol

49

symmetry c1

C	-1.348573000	1.147333000	2.096068000
H	-1.931910000	1.851148000	2.741110000
H	-1.138345000	0.278990000	2.755721000
C	-2.275869000	0.701604000	0.948467000
H	-3.225240000	0.307622000	1.408886000
H	-2.572182000	1.596667000	0.357922000
C	-0.103135000	3.198150000	1.670244000
H	-0.981253000	3.583918000	1.110742000
H	0.805135000	3.596070000	1.170711000
H	-0.142720000	3.639655000	2.704868000
C	-1.185308000	-1.504435000	0.596344000
H	-1.807411000	-2.374886000	0.276799000
H	-1.295588000	-1.469994000	1.701066000
C	0.285350000	-1.802174000	0.234782000
H	0.568389000	-2.784822000	0.710357000
H	0.353956000	-1.962204000	-0.863257000
C	-2.514112000	-0.460207000	-1.171632000
H	-1.991791000	-1.121401000	-1.891791000
H	-2.685748000	0.505228000	-1.689353000
C	1.299005000	-0.341137000	1.965923000
H	2.279924000	-0.649387000	2.410962000
H	0.539575000	-0.899215000	2.553875000
C	1.127418000	1.173360000	2.220179000
H	1.219675000	1.347137000	3.330982000
H	1.985342000	1.712053000	1.759789000



C	2.451072000	-0.739750000	-0.160335000
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H	3.096010000	-1.629284000	0.080320000
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C	2.540421000	4.179442000	-4.539090000
C	1.597810000	2.183254000	-5.553240000
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C	1.097281000	1.781535000	-4.301154000
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H	2.711174000	3.696692000	-6.659114000
C	0.762806000	2.157682000	-1.803817000
H	1.600055000	2.186839000	-1.058519000
H	0.041731000	2.949226000	-1.467737000
O	0.160514000	0.892197000	-1.873118000
H	-0.172995000	0.633163000	-0.968338000
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**Bn<sub>3</sub>TACN/Alcohol**

79

symmetry c1

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H	-0.271640000	-2.647828000	0.412091000
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O	0.423861000	0.562865000	0.082839000
H	0.455425000	0.135013000	-0.815823000

#### Me<sub>4</sub>cyclen/Alcohol

60

symmetry c1

C	1.559073000	2.095602000	1.591066000
H	1.873550000	3.022661000	2.147498000
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H	-0.493909000	2.001049000	2.287463000
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H	-1.146820000	0.522551000	-2.311892000
O	-0.601987000	-1.230990000	-1.348175000
H	0.129977000	-1.270270000	-0.670402000

#### **Bn4cyclen/Alcohol**

100

symmetry c1

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H	2.069505000	-1.944938000	-2.304153000
H	2.620078000	-1.549644000	-0.664638000
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H	3.188183000	1.724357000	0.917279000
H	3.477710000	0.051284000	0.388050000
C	4.546866000	1.539868000	-0.760181000
C	5.332254000	0.614660000	-1.484935000
H	5.084344000	-0.459069000	-1.439321000
C	6.438767000	1.037346000	-2.242426000
H	7.038936000	0.297486000	-2.796211000
C	6.785002000	2.398903000	-2.284771000
H	7.653964000	2.732140000	-2.874328000
C	6.022791000	3.331303000	-1.558636000
H	6.296954000	4.398536000	-1.572642000
C	4.916583000	2.903204000	-0.805321000
H	4.337354000	3.640741000	-0.225180000
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H	-0.457672000	-2.763410000	-2.382111000
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H	1.391649000	-2.543051000	0.911510000
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C	2.304270000	-4.583029000	-0.624646000
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H	3.675035000	-6.112486000	-1.339766000
C	1.593876000	-6.682845000	-1.634997000
H	1.839150000	-7.653101000	-2.095688000
C	0.252677000	-6.306297000	-1.448736000

H	-0.559184000	-6.983554000	-1.759667000
C	-0.056344000	-5.069309000	-0.855846000
H	-1.112609000	-4.796642000	-0.693486000
C	-2.406964000	0.650476000	-1.413435000
H	-3.383856000	0.680209000	-1.960347000
H	-1.633821000	0.536886000	-2.199950000
C	-2.197648000	2.001326000	-0.708130000
H	-2.562388000	2.809392000	-1.396739000
H	-2.863970000	2.051487000	0.177803000
C	-3.505711000	-0.683648000	0.360263000
H	-3.594539000	0.232498000	0.979356000
H	-3.259819000	-1.500670000	1.069549000
C	-4.834295000	-0.970669000	-0.330409000
C	-5.219977000	-2.292394000	-0.650813000
H	-4.571209000	-3.132680000	-0.353239000
C	-6.425969000	-2.554954000	-1.322443000
H	-6.708366000	-3.594192000	-1.555945000
C	-7.276196000	-1.495627000	-1.686203000
H	-8.223168000	-1.699685000	-2.210892000
C	-6.916329000	-0.175977000	-1.362891000
H	-7.583385000	0.659604000	-1.629455000
C	-5.708950000	0.080259000	-0.689724000
H	-5.447836000	1.117450000	-0.420593000
C	0.074433000	2.617785000	-1.333725000
H	-0.081962000	3.682192000	-1.661504000
H	-0.188400000	2.008013000	-2.223943000
C	1.579556000	2.461667000	-1.048848000
H	2.118413000	2.893405000	-1.935032000
H	1.854546000	3.117772000	-0.194576000
C	-0.728072000	3.026795000	0.980441000



H	0.329910000	3.008793000	1.315928000
H	-1.307140000	2.480244000	1.754486000
C	-1.204329000	4.474950000	0.886191000
C	-0.334807000	5.506224000	0.462260000
H	0.723156000	5.273734000	0.255092000
C	-0.787227000	6.830277000	0.325916000
H	-0.089004000	7.617229000	-0.002184000
C	-2.123889000	7.152305000	0.618436000
H	-2.479843000	8.189935000	0.516559000
C	-2.999240000	6.142729000	1.056357000
H	-4.044099000	6.388464000	1.306184000
C	-2.541177000	4.820729000	1.188444000
H	-3.231345000	4.041271000	1.553063000
N	2.031042000	1.110283000	-0.714856000
N	0.540602000	-1.692620000	-0.802742000
N	-2.322221000	-0.516057000	-0.523033000
N	-0.826289000	2.229434000	-0.254308000
C	0.874090000	-1.015163000	3.290314000
C	0.030721000	-1.986430000	3.865013000
C	2.242319000	-1.014753000	3.642934000
H	-1.034461000	-1.974649000	3.588467000
H	2.914742000	-0.253461000	3.210453000
C	0.542488000	-2.941204000	4.762347000
C	2.756451000	-1.967868000	4.537692000
H	-0.131388000	-3.694851000	5.202132000
H	3.827772000	-1.955078000	4.797028000
C	1.906494000	-2.938063000	5.101205000
H	2.307893000	-3.687322000	5.802337000
C	0.324458000	0.038718000	2.337954000
H	0.958127000	0.106485000	1.423269000

H	0.427202000	1.029073000	2.853128000
O	-1.026673000	-0.181141000	1.989633000
H	-1.115749000	-0.205489000	0.996537000

### **Bn<sub>6</sub>hexacyclen/Alcohol**

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symmetry c1

N	4.151112000	0.074194000	-0.339353000
N	2.302331000	3.393274000	-0.211651000
N	-3.433246000	0.270647000	-0.438008000
N	-1.440550000	3.481180000	-0.849361000
N	-1.608133000	-3.077424000	-0.267350000
N	2.211212000	-3.193707000	-0.479557000
C	6.552751000	-0.416423000	0.169542000
C	-2.987864000	1.643027000	-0.171754000
H	-2.634066000	1.777691000	0.883601000
H	-3.867101000	2.311025000	-0.289245000
C	-5.853244000	0.761180000	-0.850807000
C	-1.881068000	2.112260000	-1.132807000
H	-1.004268000	1.438360000	-1.033158000
H	-2.237710000	1.988655000	-2.188475000
C	-2.197800000	5.865652000	-0.809242000
C	3.761761000	-1.255020000	-0.822353000
H	4.671429000	-1.890994000	-0.824146000
H	3.394689000	-1.231694000	-1.881724000
C	5.549296000	0.394058000	-0.638095000
H	5.708476000	1.470809000	-0.408398000
H	5.782617000	0.286940000	-1.732312000
C	-6.994429000	1.337233000	-0.254340000
H	-7.106266000	1.302527000	0.842547000
C	0.879801000	3.121914000	0.012034000

H	0.525842000	3.499823000	1.006555000
H	0.735082000	2.021425000	0.042617000
C	2.944431000	-5.478602000	-1.192073000
C	3.195746000	2.320542000	0.232376000
H	2.937565000	1.940259000	1.255989000
H	4.217068000	2.749004000	0.311112000
C	3.997980000	5.228591000	-0.347076000
C	2.707861000	4.713855000	0.274278000
H	2.800651000	4.741610000	1.394158000
H	1.891897000	5.429392000	0.027622000
C	3.228345000	1.136263000	-0.750190000
H	2.209984000	0.698347000	-0.819407000
H	3.461048000	1.527597000	-1.775704000
C	6.330678000	-0.678940000	1.539247000
H	5.391207000	-0.329762000	1.996256000
C	7.746612000	-0.880092000	-0.421584000
H	7.928243000	-0.690780000	-1.493192000
C	2.688188000	-1.917005000	0.061447000
H	3.087946000	-2.017895000	1.105109000
H	1.821040000	-1.227557000	0.136250000
C	-0.235944000	-2.779572000	-0.739704000
H	-0.060388000	-1.694494000	-0.589684000
H	-0.147007000	-2.959718000	-1.841891000
C	-5.719683000	0.827346000	-2.255161000
H	-4.821190000	0.390917000	-2.719542000
C	-0.015748000	3.715262000	-1.091147000
H	0.143790000	4.813890000	-1.125110000
H	0.323729000	3.320981000	-2.085639000
C	-2.562338000	-2.049360000	-0.735669000
H	-3.580227000	-2.481117000	-0.649778000
H	-2.406267000	-1.815615000	-1.819549000

C	-4.815082000	0.041029000	-0.002458000
H	-4.965004000	0.310009000	1.076747000
H	-5.015467000	-1.051565000	-0.064738000
C	-2.300441000	4.494454000	-1.462255000
H	-3.352820000	4.143495000	-1.372494000
H	-2.113631000	4.597014000	-2.565986000
C	3.172625000	-4.283206000	-0.278377000
H	3.192809000	-4.632434000	0.789190000
H	4.190377000	-3.882772000	-0.478806000
C	-3.356994000	-4.919131000	-0.197320000
C	-2.504755000	-0.743590000	0.073768000
H	-2.687442000	-0.967815000	1.156197000
H	-1.479062000	-0.323945000	0.016100000
C	-2.019574000	-4.431566000	-0.727272000
H	-1.231834000	-5.143623000	-0.407294000
H	-2.036269000	-4.460546000	-1.846997000
C	0.869369000	-3.567439000	-0.015657000
H	0.746179000	-3.457445000	1.091565000
H	0.744616000	-4.648810000	-0.229310000
C	-7.984764000	1.954705000	-1.038941000
H	-8.868457000	2.400187000	-0.554243000
C	8.473443000	-1.831055000	1.700008000
H	9.219038000	-2.382206000	2.295182000
C	-7.842776000	2.012468000	-2.435946000
H	-8.614798000	2.500422000	-3.052245000
C	7.281942000	-1.380427000	2.297837000
H	7.093379000	-1.577003000	3.365823000
C	-6.704464000	1.448309000	-3.040898000
H	-6.584160000	1.491702000	-4.135675000
C	-4.448815000	-5.104064000	-1.072925000
H	-4.328291000	-4.868578000	-2.143813000

C	8.702987000	-1.578735000	0.336684000
H	9.629321000	-1.933716000	-0.143053000
C	4.236969000	5.083512000	-1.731550000
H	3.492695000	4.547164000	-2.341488000
C	-2.219941000	7.040186000	-1.589616000
H	-2.267299000	6.958113000	-2.688805000
C	-5.839165000	-5.895881000	0.761184000
H	-6.802764000	-6.277352000	1.135292000
C	-5.681793000	-5.588535000	-0.600577000
H	-6.521251000	-5.726229000	-1.300761000
C	-3.525014000	-5.236100000	1.170380000
H	-2.686115000	-5.091034000	1.870160000
C	-2.122858000	5.989139000	0.595574000
H	-2.089386000	5.070805000	1.203242000
C	2.657864000	-5.291644000	-2.562413000
H	2.553529000	-4.263363000	-2.943823000
C	4.960231000	5.898091000	0.437046000
H	4.791005000	6.009542000	1.521490000
C	6.355046000	6.273229000	-1.524446000
H	7.271917000	6.677529000	-1.982494000
C	6.129019000	6.420535000	-0.145377000
H	6.870016000	6.939103000	0.484094000
C	-2.108829000	8.420591000	0.414352000
H	-2.072513000	9.413525000	0.890469000
C	2.898071000	-7.901197000	-1.554439000
H	2.987591000	-8.922549000	-1.150637000
C	-4.757139000	-5.718092000	1.643121000
H	-4.870998000	-5.964847000	2.711120000
C	2.617233000	-7.703543000	-2.916998000
H	2.488396000	-8.568046000	-3.587765000
C	5.404856000	5.600649000	-2.315288000

H	5.575748000	5.479592000	-3.397386000
C	3.056518000	-6.795454000	-0.699767000
H	3.269781000	-6.956035000	0.370615000
C	2.495853000	-6.393750000	-3.417537000
H	2.273160000	-6.230678000	-4.484607000
C	-2.078495000	7.255004000	1.202347000
H	-2.020834000	7.334080000	2.300189000
C	-2.179751000	8.309229000	-0.984688000
H	-2.196354000	9.215435000	-1.611426000
C	-4.359327000	-0.064907000	4.933362000
C	-3.062969000	0.480547000	4.988154000
C	-4.553358000	-1.331198000	4.354467000
H	-2.900915000	1.474493000	5.435947000
H	-5.565030000	-1.766026000	4.306224000
C	-1.973911000	-0.238118000	4.468182000
C	-3.460393000	-2.050323000	3.837159000
H	-0.960934000	0.198374000	4.511912000
H	-3.602765000	-3.040721000	3.378280000
C	-2.159160000	-1.512666000	3.889157000
H	-5.214888000	0.497850000	5.339928000
O	-1.265706000	-3.413951000	2.564088000
C	-0.958548000	-2.306989000	3.380355000
H	-0.245381000	-1.600252000	2.884264000
H	-1.471878000	-3.126691000	1.623660000
H	-0.410913000	-2.705373000	4.266750000

**Bn<sub>3</sub>TACN/TU**

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symmetry c1

C	-1.915937000	1.840908000	0.818751000
H	-2.218195000	2.842863000	1.207755000

H	-1.644957000	1.267736000	1.729204000
C	-3.162055000	1.197422000	0.172354000
H	-3.939343000	1.110667000	0.976779000
H	-3.593222000	1.888691000	-0.583456000
C	-0.595402000	3.202217000	-0.774267000
H	-1.527565000	3.376851000	-1.353768000
H	0.214647000	3.068189000	-1.522980000
C	-0.311567000	4.435544000	0.079162000
C	0.992757000	4.713752000	0.549864000
H	1.832822000	4.065014000	0.251375000
C	1.240722000	5.821522000	1.378305000
H	2.264016000	6.019205000	1.734195000
C	0.186639000	6.677418000	1.746461000
H	0.380902000	7.547323000	2.393974000
C	-1.112138000	6.425012000	1.272965000
H	-1.940144000	7.100413000	1.542152000
C	-1.355922000	5.314350000	0.445513000
H	-2.373387000	5.138590000	0.056326000
C	-2.313086000	-1.109460000	0.365536000
H	-3.050103000	-1.924009000	0.550979000
H	-2.135389000	-0.687041000	1.375172000
C	-1.033401000	-1.800185000	-0.129240000
H	-0.872074000	-2.656256000	0.575442000
H	-1.225820000	-2.255817000	-1.127752000
C	-4.030871000	-0.577549000	-1.320905000
H	-3.654662000	-1.428066000	-1.929404000
H	-4.305059000	0.225185000	-2.036182000
C	-5.282583000	-1.010469000	-0.563576000
C	-6.254766000	-0.059713000	-0.175182000
H	-6.134488000	0.993042000	-0.477510000
C	-7.390404000	-0.444914000	0.556910000

H	-8.138862000	0.311325000	0.843087000
C	-7.580499000	-1.793035000	0.909836000
H	-8.472570000	-2.096015000	1.480843000
C	-6.635515000	-2.754218000	0.512471000
H	-6.787137000	-3.815949000	0.765175000
C	-5.500417000	-2.364370000	-0.220472000
H	-4.781314000	-3.131505000	-0.554574000
C	0.486099000	-0.087765000	0.882014000
H	1.482674000	-0.322980000	1.312585000
H	-0.215892000	-0.276826000	1.722174000
C	0.498590000	1.412848000	0.530430000
H	0.805114000	1.962652000	1.460602000
H	1.312632000	1.593647000	-0.205279000
C	1.350770000	-1.809675000	-0.674121000
H	1.088000000	-2.267257000	-1.653533000
H	2.198163000	-1.116289000	-0.856027000
C	1.818007000	-2.904902000	0.280987000
C	1.246211000	-4.197873000	0.246791000
H	0.482389000	-4.433945000	-0.512544000
C	1.656199000	-5.195967000	1.147243000
H	1.199075000	-6.197394000	1.100087000
C	2.655704000	-4.922041000	2.097328000
H	2.979998000	-5.704454000	2.801706000
C	3.252196000	-3.649678000	2.129616000
H	4.053061000	-3.432487000	2.854352000
C	2.838875000	-2.654676000	1.226850000
H	3.338561000	-1.671342000	1.241775000
N	-0.741540000	1.923582000	-0.053243000
N	-2.895115000	-0.076863000	-0.507071000
N	0.188993000	-0.982675000	-0.254383000
S	-0.148519000	1.265286000	-5.548451000



N	-1.744753000	0.943295000	-3.377416000
N	0.467385000	0.364129000	-3.090090000
C	-3.295554000	0.951252000	-5.303198000
C	-4.468615000	1.440449000	-5.897551000
C	-5.271308000	2.400777000	-5.247902000
C	-4.870310000	2.878904000	-3.993142000
C	-3.680422000	2.413319000	-3.400716000
C	-2.891427000	1.436188000	-4.035902000
C	-0.484645000	0.832103000	-3.948928000
H	-1.821399000	0.803790000	-2.347498000
H	0.206117000	0.114537000	-2.110175000
S	4.919638000	2.480033000	-0.638553000
N	5.724672000	4.643101000	-2.111429000
N	4.744759000	2.933559000	-3.276164000
C	5.906340000	5.434401000	0.250095000
C	6.354381000	6.439181000	1.128192000
C	7.041071000	7.570500000	0.665143000
C	7.281492000	7.691721000	-0.717494000
C	6.843340000	6.703484000	-1.605252000
C	6.147214000	5.560773000	-1.134564000
C	5.124184000	3.391043000	-2.039712000
H	5.942334000	4.957469000	-3.062232000
H	4.695071000	3.610515000	-4.043737000
H	5.382844000	4.543392000	0.622030000
C	4.078107000	1.654527000	-3.507032000
H	4.289862000	1.352910000	-4.555266000
H	4.558631000	0.913068000	-2.834157000
C	2.565780000	1.704949000	-3.243643000
H	2.412642000	2.043289000	-2.196915000
H	2.080728000	2.442980000	-3.918497000
C	1.879380000	0.343699000	-3.449341000

H	1.949400000	0.046197000	-4.518179000
H	2.378846000	-0.435953000	-2.839130000
H	7.044582000	6.823503000	-2.681448000
H	7.382743000	8.342519000	1.368131000
C	8.008965000	8.918454000	-1.232420000
F	8.242904000	8.853100000	-2.567439000
F	7.294563000	10.048641000	-1.002213000
F	9.206932000	9.076632000	-0.617023000
C	6.106664000	6.250069000	2.613247000
F	4.816286000	5.896967000	2.861625000
F	6.886080000	5.265418000	3.124427000
F	6.361221000	7.376334000	3.321397000
C	-4.876290000	0.956875000	-7.275190000
F	-6.223400000	0.803427000	-7.369966000
F	-4.514377000	1.842093000	-8.239373000
F	-4.308401000	-0.232135000	-7.589250000
C	-5.710496000	3.876932000	-3.228632000
F	-6.714764000	4.390582000	-3.972397000
F	-6.280546000	3.304366000	-2.125279000
F	-4.963109000	4.916030000	-2.770773000
H	-3.348343000	2.837348000	-2.442177000
H	-6.198157000	2.763166000	-5.713399000
H	-2.693057000	0.186956000	-5.808615000

### **Bn4cyclen/TU**

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symmetry c1

C	1.607357000	0.065986000	2.294519000
H	2.650811000	-0.187525000	2.620043000
H	0.960538000	-0.349919000	3.093816000
C	1.509297000	1.600818000	2.326433000

H	1.817111000	1.899154000	3.361421000
H	2.275176000	2.045558000	1.652532000
C	2.223061000	-0.363424000	-0.052203000
H	1.788026000	-0.795435000	-0.976705000
H	2.276041000	0.732649000	-0.220392000
C	-0.921750000	1.670847000	2.729410000
H	-0.989003000	2.178229000	3.722157000
H	-0.717572000	0.609642000	2.954875000
C	-2.281806000	1.754320000	2.007206000
H	-3.077158000	2.003170000	2.757821000
H	-2.263027000	2.603647000	1.292253000
C	0.263939000	3.685103000	1.973350000
H	-0.686651000	4.057885000	1.536306000
H	1.070601000	4.001362000	1.282868000
C	-2.942238000	-0.581362000	2.136206000
H	-3.980941000	-0.491747000	2.550864000
H	-2.284178000	-0.516886000	3.026635000
C	-2.826345000	-1.992851000	1.539646000
H	-3.150321000	-2.695528000	2.352770000
H	-3.580842000	-2.115016000	0.730479000
C	-3.594905000	0.764315000	0.169787000
H	-3.665889000	-0.169944000	-0.425690000
H	-3.167592000	1.533220000	-0.507673000
C	-0.402043000	-2.327923000	1.906010000
H	-0.322445000	-3.286394000	2.478235000
H	-0.606489000	-1.554805000	2.672049000
C	0.965928000	-2.034679000	1.254473000
H	1.761995000	-2.520638000	1.876142000
H	1.007195000	-2.545147000	0.269780000
C	-1.601725000	-3.625527000	0.194982000
H	-0.650686000	-3.752869000	-0.365458000

H	-2.402130000	-3.499902000	-0.567286000
N	1.250243000	-0.604265000	1.039415000
N	0.212484000	2.193625000	1.945960000
N	-2.608530000	0.537585000	1.249217000
N	-1.528012000	-2.358037000	0.961684000
S	-0.721491000	1.595142000	-3.754813000
N	-0.115653000	2.226850000	-1.189525000
N	-0.892294000	0.079241000	-1.544030000
C	-0.346816000	4.410031000	-2.326634000
C	0.191754000	5.668440000	-2.633548000
C	1.476648000	6.039187000	-2.184512000
C	2.221666000	5.124230000	-1.429381000
C	1.697344000	3.849281000	-1.136519000
C	0.405769000	3.488765000	-1.560638000
C	-0.578534000	1.283428000	-2.096758000
H	0.021131000	1.952681000	-0.188839000
H	-0.815162000	-0.064373000	-0.520107000
S	1.211746000	-5.090450000	-2.353734000
N	2.451074000	-4.921856000	-4.786966000
N	0.572904000	-3.640205000	-4.520439000
C	4.097616000	-6.146750000	-3.361838000
C	5.321426000	-6.836237000	-3.299057000
C	6.100626000	-7.061854000	-4.444457000
C	5.629525000	-6.584693000	-5.681572000
C	4.415083000	-5.892229000	-5.762599000
C	3.633258000	-5.659705000	-4.603444000
C	1.434766000	-4.525011000	-3.925418000
H	2.326402000	-4.622134000	-5.759083000
H	0.883397000	-3.180692000	-5.382371000
H	3.491452000	-5.980905000	-2.461535000
C	-0.556884000	-3.005928000	-3.842966000

H	-1.297407000	-2.728689000	-4.623799000
H	-1.019395000	-3.774991000	-3.189922000
C	-0.138573000	-1.777004000	-3.023512000
H	0.589410000	-2.107523000	-2.253159000
H	0.369684000	-1.040202000	-3.682581000
C	-1.318603000	-1.059439000	-2.344189000
H	-2.026669000	-0.693880000	-3.120143000
H	-1.853711000	-1.749029000	-1.662843000
H	4.077103000	-5.515945000	-6.741307000
H	7.060890000	-7.591205000	-4.375042000
C	6.430150000	-6.861264000	-6.939338000
F	6.082115000	-6.031881000	-7.955964000
F	7.759554000	-6.711751000	-6.725228000
F	6.239439000	-8.131971000	-7.378037000
C	5.773305000	-7.390006000	-1.960322000
F	5.431627000	-6.568301000	-0.932588000
F	5.203365000	-8.594556000	-1.705931000
F	7.116290000	-7.564441000	-1.912099000
C	-0.623021000	6.682271000	-3.411455000
F	-1.028551000	7.706719000	-2.611563000
F	0.102929000	7.238217000	-4.415283000
F	-1.734491000	6.140553000	-3.960768000
C	3.581101000	5.487502000	-0.876315000
F	4.080629000	6.619589000	-1.420171000
F	3.523858000	5.683352000	0.475583000
F	4.488170000	4.496558000	-1.078804000
H	2.314169000	3.117108000	-0.594539000
H	1.891625000	7.028172000	-2.424748000
H	-1.350233000	4.134353000	-2.672977000
C	-1.878298000	-4.899004000	0.990896000
C	3.635491000	-0.907080000	0.149341000

C	0.488840000	4.354216000	3.325294000
C	-4.994955000	1.190076000	0.606435000
C	3.961990000	-2.235453000	-0.208719000
C	5.251824000	-2.749126000	0.009994000
C	6.245083000	-1.939343000	0.589316000
C	5.942529000	-0.611450000	0.936704000
C	4.650365000	-0.103120000	0.715983000
H	3.201990000	-2.876546000	-0.686102000
H	5.482079000	-3.785957000	-0.281691000
H	7.257249000	-2.339916000	0.758958000
H	6.718847000	0.036505000	1.374496000
H	4.433398000	0.948702000	0.968173000
C	-3.198344000	-5.292444000	1.309680000
C	-3.447789000	-6.445337000	2.073534000
C	-2.376857000	-7.232991000	2.531646000
C	-1.058777000	-6.866267000	2.209658000
C	-0.814784000	-5.712214000	1.444769000
H	-4.047796000	-4.697373000	0.935257000
H	-4.485260000	-6.736222000	2.304505000
H	-2.570405000	-8.138927000	3.127880000
H	-0.214111000	-7.487808000	2.547655000
H	0.221132000	-5.449893000	1.172972000
C	-5.309418000	2.552679000	0.812079000
C	-6.582928000	2.945135000	1.257525000
C	-7.573149000	1.977829000	1.504688000
C	-7.283193000	0.619165000	1.291846000
C	-6.007231000	0.233001000	0.845099000
H	-4.548606000	3.322094000	0.600439000
H	-6.807291000	4.014119000	1.402785000
H	-8.573165000	2.283898000	1.850938000
H	-8.057624000	-0.144910000	1.466871000

H	-5.799087000	-0.833816000	0.657435000
C	1.797184000	4.623479000	3.788125000
C	2.013458000	5.226115000	5.039028000
C	0.921080000	5.577077000	5.851694000
C	-0.387270000	5.333719000	5.398946000
C	-0.598447000	4.731379000	4.146454000
H	2.658720000	4.385034000	3.143350000
H	3.041649000	5.434035000	5.375944000
H	1.089160000	6.053191000	6.830796000
H	-1.249922000	5.623743000	6.020003000
H	-1.629663000	4.570999000	3.789510000

### **Bn<sub>6</sub>hexacyclen/TU**

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N	20.252433000	-13.677512000	-1.298463000
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N	15.744986000	-9.052652000	-0.370064000
N	13.925479000	-14.820840000	-2.716517000
N	17.598281000	-15.871690000	-2.961619000
C	22.043450000	-15.120601000	-0.320114000
C	13.830085000	-10.654722000	-0.159241000
H	14.349455000	-11.097876000	0.731597000
H	13.157693000	-9.864635000	0.236044000
C	10.785884000	-10.517015000	-0.524430000
C	14.881595000	-10.003052000	-1.076574000
H	15.524527000	-10.801793000	-1.504278000
H	14.357210000	-9.535714000	-1.950194000
C	15.778191000	-6.931306000	0.939982000
C	19.719527000	-14.681316000	-2.226487000

H	20.329305000	-15.598456000	-2.097772000
H	19.844557000	-14.367883000	-3.297278000
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H	22.050999000	-12.980826000	-0.478557000
H	22.275942000	-13.812590000	-2.036475000
C	9.944802000	-10.050395000	0.507033000
H	9.946888000	-10.566702000	1.482041000
C	18.010010000	-10.072394000	-0.405412000
H	17.950077000	-10.082623000	0.713300000
H	17.603010000	-11.048552000	-0.743814000
C	17.855659000	-18.134011000	-4.086844000
C	20.112593000	-11.266894000	-0.579818000
H	19.788260000	-11.696958000	0.401856000
H	21.194892000	-11.044116000	-0.489544000
C	21.518304000	-8.581673000	-0.659793000
C	20.108427000	-8.877376000	-0.170779000
H	20.139681000	-9.052760000	0.936489000
H	19.491740000	-7.961000000	-0.299441000
C	19.888467000	-12.312799000	-1.682522000
H	18.810300000	-12.314499000	-1.947511000
H	20.434847000	-11.984577000	-2.607804000
C	21.305781000	-15.498893000	0.823617000
H	20.446771000	-14.880768000	1.129801000
C	23.132735000	-15.923018000	-0.718347000
H	23.713212000	-15.642735000	-1.613635000
C	18.240974000	-15.003236000	-1.950763000
H	18.160288000	-15.453447000	-0.927532000
H	17.670758000	-14.053219000	-1.914663000
C	15.343330000	-14.700053000	-3.067351000
H	15.755725000	-13.838092000	-2.504403000
H	15.486974000	-14.458336000	-4.151450000



C	10.778873000	-9.836576000	-1.762210000
H	11.445141000	-10.190689000	-2.564878000
C	17.096412000	-8.947908000	-0.920334000
H	17.507721000	-7.969775000	-0.594331000
H	17.097517000	-8.935893000	-2.042169000
C	13.292806000	-13.519564000	-2.469238000
H	12.193792000	-13.668783000	-2.514453000
H	13.538006000	-12.770198000	-3.266996000
C	11.648574000	-11.754620000	-0.325198000
H	11.657076000	-12.026765000	0.765354000
H	11.157523000	-12.609902000	-0.840628000
C	15.112532000	-7.743124000	-0.160551000
H	14.052281000	-7.922684000	0.120311000
H	15.078204000	-7.135297000	-1.103550000
C	18.202852000	-17.228280000	-2.918104000
H	17.928748000	-17.741649000	-1.960587000
H	19.303996000	-17.106607000	-2.900175000
C	11.817776000	-16.093664000	-3.170127000
C	13.650720000	-12.920867000	-1.097535000
H	13.404085000	-13.666856000	-0.298305000
H	14.749847000	-12.771873000	-1.036543000
C	13.167011000	-15.620298000	-3.688237000
H	13.772290000	-16.517062000	-3.947513000
H	13.019303000	-15.071384000	-4.655850000
C	16.141802000	-15.965590000	-2.709921000
H	15.939333000	-16.223683000	-1.638307000
H	15.758124000	-16.816014000	-3.310831000
C	9.107002000	-8.938411000	0.307185000
H	8.457380000	-8.587995000	1.125342000
C	22.747252000	-17.437332000	1.150497000
H	23.020397000	-18.338293000	1.722575000

C	9.105389000	-8.271401000	-0.929624000
H	8.453537000	-7.397402000	-1.087615000
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H	21.069572000	-16.928783000	2.443287000
C	9.946505000	-8.723642000	-1.963345000
H	9.952529000	-8.204744000	-2.935528000
C	10.676536000	-16.050298000	-3.998161000
H	10.758819000	-15.629424000	-5.013973000
C	23.486171000	-17.071755000	0.012638000
H	24.340392000	-17.686556000	-0.313266000
C	21.868037000	-8.637536000	-2.026986000
H	21.123418000	-8.965766000	-2.768489000
C	16.222251000	-5.613635000	0.707898000
H	16.100253000	-5.163792000	-0.290828000
C	9.323759000	-17.065704000	-2.243842000
H	8.353554000	-17.442898000	-1.882847000
C	9.438392000	-16.535637000	-3.540110000
H	8.557202000	-16.492310000	-4.200076000
C	11.691261000	-16.624040000	-1.867304000
H	12.578608000	-16.642653000	-1.214390000
C	15.953585000	-7.487583000	2.227326000
H	15.622239000	-8.522428000	2.410403000
C	18.441929000	-17.923262000	-5.357706000
H	19.131012000	-17.075173000	-5.504516000
C	22.505266000	-8.181313000	0.267378000
H	22.253776000	-8.140950000	1.340473000
C	24.131787000	-7.886723000	-1.521956000
H	25.145338000	-7.615691000	-1.857320000
C	23.798352000	-7.831897000	-0.157654000
H	24.551307000	-7.520090000	0.583639000
C	16.984264000	-5.423199000	3.013532000

H	17.452245000	-4.837031000	3.820657000
C	16.720993000	-20.111924000	-4.989870000
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C	10.454821000	-17.105691000	-1.407410000
H	10.371745000	-17.516558000	-0.388032000
C	17.312614000	-19.892577000	-6.246135000
H	17.095188000	-20.571699000	-7.084832000
C	23.162227000	-8.294204000	-2.454757000
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C	16.993230000	-19.239349000	-3.920576000
H	16.537155000	-19.425257000	-2.934120000
C	18.174365000	-18.794932000	-6.428172000
H	18.644740000	-18.618815000	-7.408469000
C	16.547668000	-6.739756000	3.256229000
H	16.670704000	-7.185239000	4.256841000
C	16.822389000	-4.862466000	1.735967000
H	17.167733000	-3.838286000	1.526312000
S	16.596437000	-13.465932000	-8.063829000
N	16.089354000	-15.656755000	-6.517546000
N	17.820276000	-14.328902000	-5.827487000
C	13.914929000	-15.245490000	-7.655925000
C	12.692221000	-15.775713000	-8.095188000
C	12.387694000	-17.144231000	-7.961493000
C	13.337276000	-17.983960000	-7.360553000
C	14.565337000	-17.471004000	-6.911262000
C	14.871454000	-16.098525000	-7.052319000
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H	17.774722000	-14.876709000	-4.942368000
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N	19.149873000	-9.703329000	-4.403357000
C	17.242121000	-5.756655000	-5.172426000
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C	17.160472000	-3.518743000	-4.172871000
C	17.993784000	-3.969316000	-3.133837000
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C	18.337491000	-11.947569000	-5.197560000
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H	17.461895000	-11.531638000	-5.738647000
C	18.791113000	-13.245615000	-5.891851000
H	18.991485000	-13.041482000	-6.965095000
H	19.735910000	-13.613944000	-5.431464000
H	19.133670000	-5.614455000	-2.304296000
H	16.812177000	-2.477090000	-4.203231000
C	18.352197000	-3.020108000	-2.010226000
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C	15.827100000	-3.978136000	-6.263492000
F	16.014202000	-4.650273000	-7.421844000
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F	15.957073000	-2.653586000	-6.529965000
C	11.630274000	-14.844012000	-8.644326000

F	10.927867000	-15.418920000	-9.652086000
F	10.723465000	-14.515764000	-7.675719000
F	12.146518000	-13.685631000	-9.109458000
C	13.075195000	-19.466285000	-7.196503000
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F	13.951267000	-20.212226000	-7.924414000
F	13.223552000	-19.856200000	-5.900436000
H	15.299928000	-18.147148000	-6.446981000
H	11.430239000	-17.546605000	-8.318323000
H	14.141905000	-14.179584000	-7.784252000