Supporting Information

Perylene bisimide cyclophanes as receptors for planar transition structures – Catalysis of stereoinversions by shape-complementarity and noncovalent π–π interactions
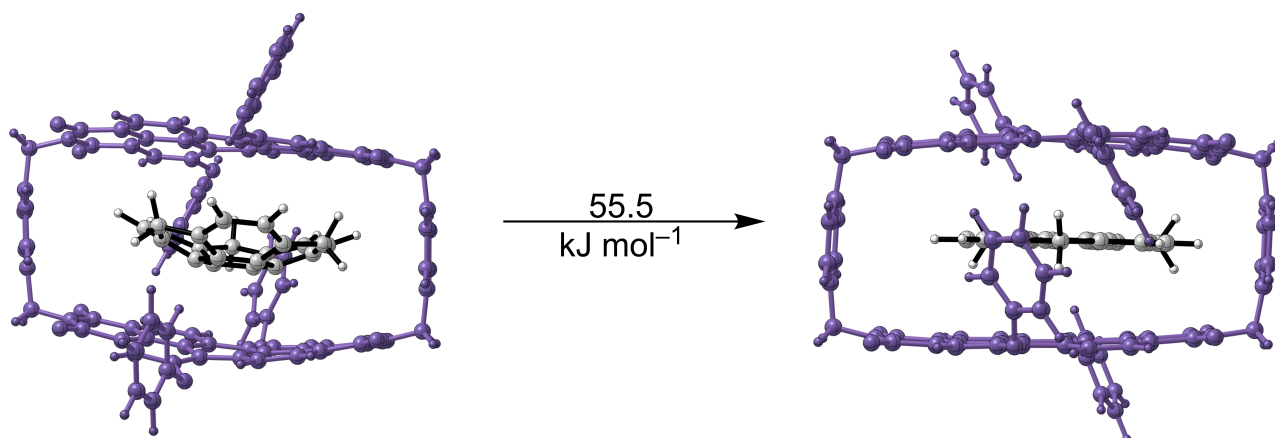
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1. Catalysis of the sumanene bowl inversion with a di-core-substituted PBI cyclophane

Compound	$\Delta G^{\ddagger}_{uncat}$	$\Delta G^{\ddagger}_{cat}$	$\Delta\Delta G^{\ddagger}_{cat}$	$\Delta G_{complex}$	% reduction
4	82.8	55.5	27.3	-38.9	33.0

Figure S1. 3D representations of lowest energy equilibrium and transition structure host–guest complexes between sumanene and the di-core-substituted PBI cyclophane along with reaction barrier heights at 298 K for the uncatalyzed ($\Delta G^{\ddagger}_{uncat}$) and catalyzed ($\Delta G^{\ddagger}_{cat}$) inversion, catalytic enhancement ($\Delta\Delta G^{\ddagger}_{cat}$) from complexation and complexation energy between reactant and cyclophane ($\Delta G_{complex}$) in kJ mol^{-1}, as well as resulting percentage barrier reduction (% reduction) obtained at the SMD(chloroform)-PW6B95-D3(BJ)/Def2-QZVP' level of theory.

2. Stereoinversion paths obtained from intrinsic reaction coordinate calculations
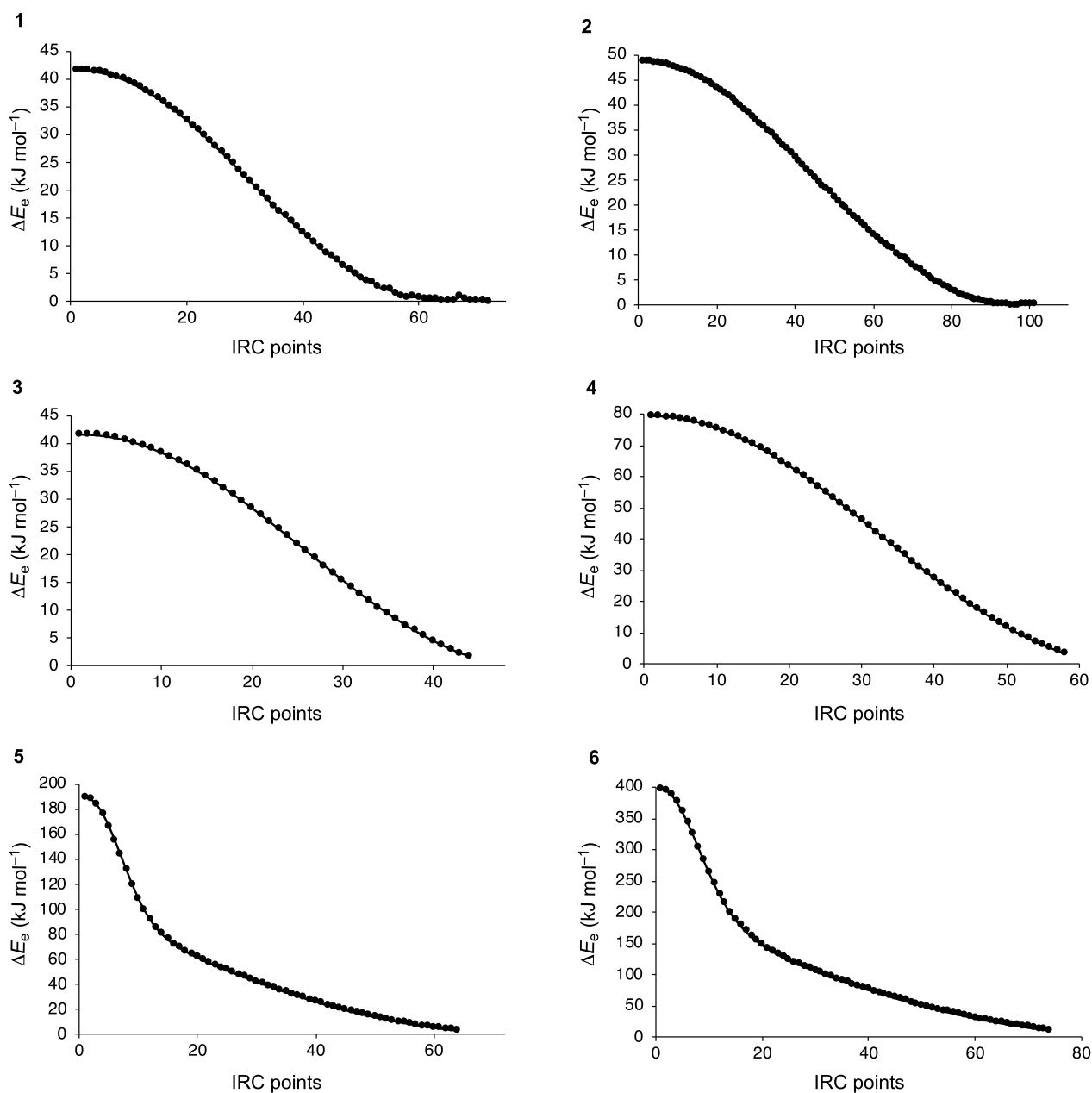
Figure S2. Intrinsic reaction coordinates (IRCs) for the free stereoinversions of **1–6**, obtained at the PBE-D3(BJ)/6-31G(d) level of theory. Electronic energies (ΔE_e) are given relative to the energies of the most stable optimized reactant complex obtained at the same level of theory.
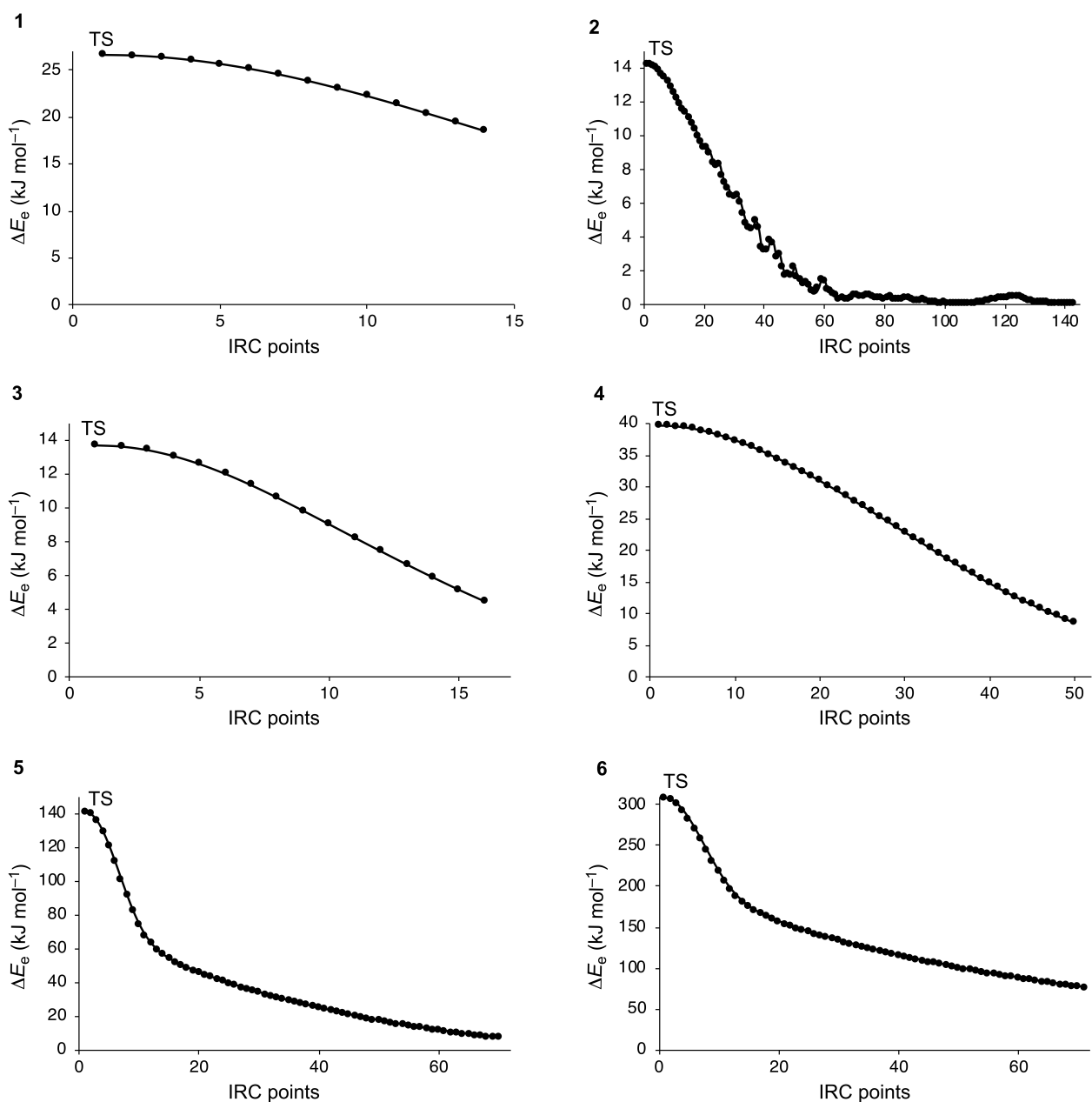
Figure S3. Intrinsic reaction coordinates (IRCs) for the PBI cyclophane catalyzed stereoinversions of **1–6**, obtained at the PBE-D3(BJ)/6-31G(d) level of theory. Electronic energies (ΔE_e) are given relative to the energies of the most stable optimized reactant complex obtained at the same level of theory.

3. Reaction barrier heights and reductions, as well as supramolecular interaction energies given in kcal mol^{-1}

Table S1. Reaction barrier heights at 298 K for the uncatalyzed ($\Delta G^{\ddagger}_{uncat}$) and catalyzed ($\Delta G^{\ddagger}_{cat}$) inversions of compounds **1–6**, catalytic enhancements ($\Delta\Delta G^{\ddagger}_{cat}$), as well as supramolecular interaction energies ($\Delta G_{complex}$) in kcal mol^{-1}.

Compound	$\Delta G^{\ddagger}_{uncat}$	$\Delta G^{\ddagger}_{cat}$	$\Delta\Delta G^{\ddagger}_{cat}$	$\Delta G_{complex}$
1	12.9	9.0	3.9	0.0
2	10.7	1.9	8.9	–3.1
3	11.3	4.1	7.2	–13.1
4	19.8	13.0	6.7	–11.3
5	44.4	33.4	11.0	–16.3
6	93.1	77.8	15.3	–9.9

4. Comparison of reaction barrier heights and reductions, as well as supramolecular interaction energies resulting from calculations including solvation corrections for chloroform and toluene

Table S2. Reaction barrier heights at 298 K for the uncatalyzed ($\Delta G^{\ddagger}_{uncat}$) and catalyzed ($\Delta G^{\ddagger}_{cat}$) inversions of compounds **1–6**, catalytic enhancements ($\Delta\Delta G^{\ddagger}_{cat}$), as well as supramolecular interaction energies ($\Delta G_{complex}$) in kJ mol^{-1} obtained from calculations using solvation corrections for chloroform and toluene (in brackets).

Compound	$\Delta G^{\ddagger}_{uncat}$	$\Delta G^{\ddagger}_{cat}$	$\Delta\Delta G^{\ddagger}_{cat}$	$\Delta G_{complex}$
1	53.9 (54.2)	37.6 (37.3)	16.3 (15.9)	0.0 (–0.3)
2	45.0 (45.2)	7.9 (N/A*)	37.1 (N/A*)	–12.8 (–14.5)
3	47.4 (47.0)	17.1 (15.9)	30.2 (31.1)	–54.7 (–56.2)
4	82.8 (83.0)	54.6 (55.0)	28.2 (28.0)	–47.1 (–47.0)
5	185.7 (186.1)	139.7 (139.1)	46.0 (47.0)	–68.3 (–70.4)
6	389.3 (389.5)	325.3 (329.2)	64.0 (60.2)	–41.3 (–42.2)

* The solvation free energy of the transition structure complex with compound **2** for toluene could not be obtained due to numerical issues.

5. Comparison of reaction barrier heights and reductions, as well as supramolecular interaction energies obtained from calculations using the def2-QZVP' and the def2-TZVPP basis set

Table S3. Reaction barrier heights at 298 K for the uncatalyzed ($\Delta G^{\ddagger}_{uncat}$) and catalyzed ($\Delta G^{\ddagger}_{cat}$) inversions of compounds **1–6**, catalytic enhancements ($\Delta\Delta G^{\ddagger}_{cat}$), as well as supramolecular interaction energies ($\Delta G_{complex}$) in kJ mol^{-1} obtained from calculations at the SMD(chloroform)-PW6B95-D3(BJ)/def2-QZVP' and SMD(chloroform)-PW6B95-D3(BJ)/def2-TZVPP (in brackets) levels of theory.

Compound	$\Delta G^{\ddagger}_{uncat}$	$\Delta G^{\ddagger}_{cat}$	$\Delta\Delta G^{\ddagger}_{cat}$	$\Delta G_{complex}$
1	53.9 (53.7)	37.6 (37.8)	16.3 (16.0)	0.0 (0.0)
2	45.0 (45.0)	7.9 (9.7)	37.1 (35.3)	−12.8 (−13.0)
3	47.4 (46.8)	17.1 (18.8)	30.2 (28.0)	−54.7 (−54.2)
4	82.8 (82.3)	54.6 (57.5)	28.2 (24.7)	−47.1 (−47.1)
5	185.7 (186.0)	139.7 (142.1)	46.0 (43.8)	−68.3 (−69.3)
6	389.3 (390.2)	325.3 (325.9)	64.0 (64.3)	−41.3 (−42.0)

6. 3D representations of overlaid host and guest geometries from free and complex optimizations, as well as energy differences in kJ mol^{-1} between respective pairs for both equilibrium and transition structures

(Substrate geometries before complexation are represented in red, while substrate geometries after complexation are represented in blue. The PBI cyclophane catalyst geometry before complexation is represented in green, whereas catalyst geometries from host–guest complexes are represented in blue.)

Equilibrium structures

Substrates

1
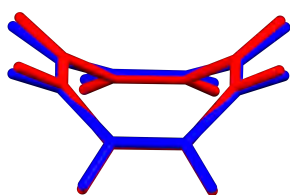
$\Delta E_e = 5.1$

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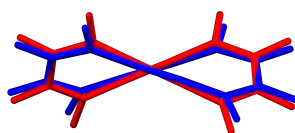
$\Delta E_e = 10.6$

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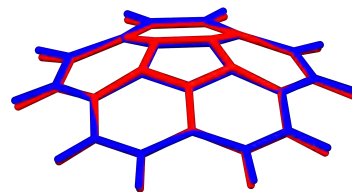
$\Delta E_e = 6.7$

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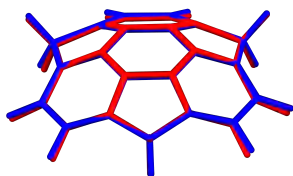
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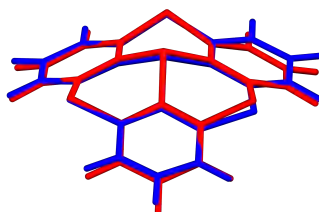
$\Delta E_e = 12.1$

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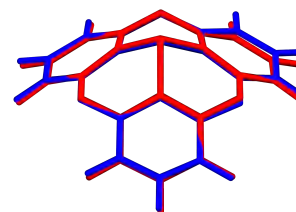
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Cyclophanes

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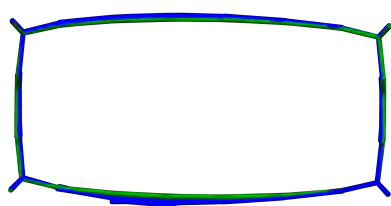
$\Delta E_e = 1.6$

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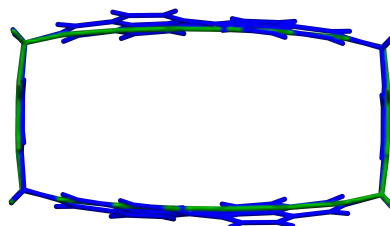
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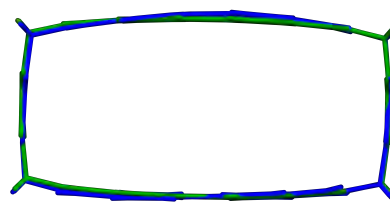
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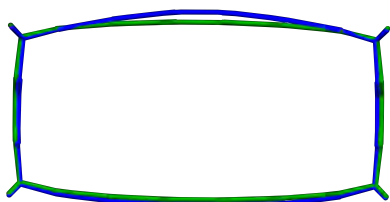
$\Delta E_e = 2.5$

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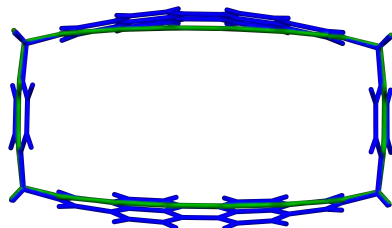
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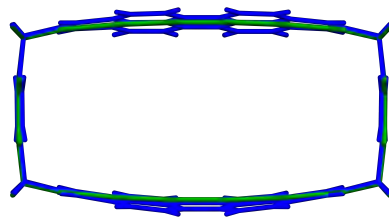
$\Delta E_e = 1.1$

Transition structures

Substrates

1
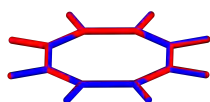
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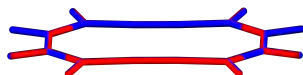
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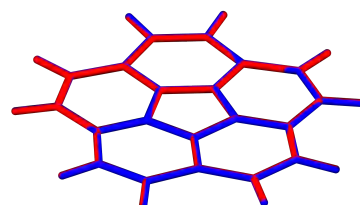
$\Delta E_e = 2.6$

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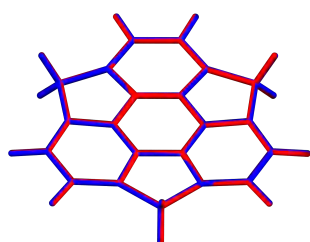
$\Delta E_e = 1.9$

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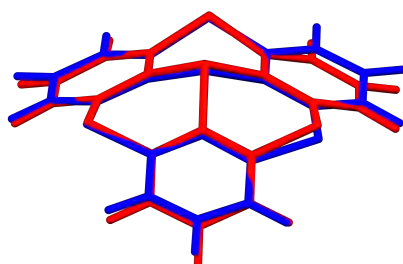
$\Delta E_e = -1.1$

6
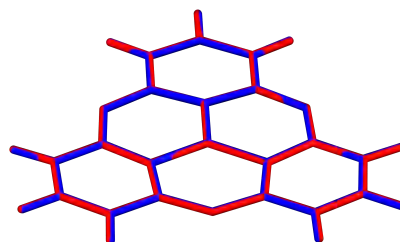
$\Delta E_e = -2.8$

Cyclophanes

1

$\Delta E_e = -0.2$

2

$\Delta E_e = -1.9$

3

$\Delta E_e = -1.9$

4   **5**   **6**
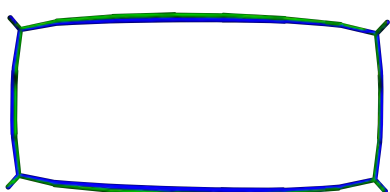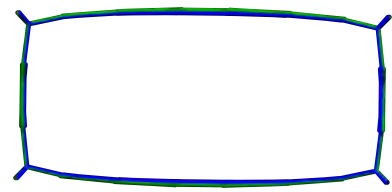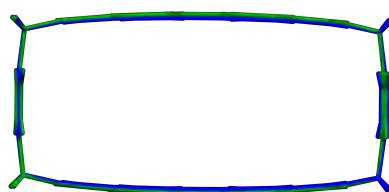
$\Delta E_e = -1.1$ $\Delta E_e = 4.5$ $\Delta E_e = 10.9$
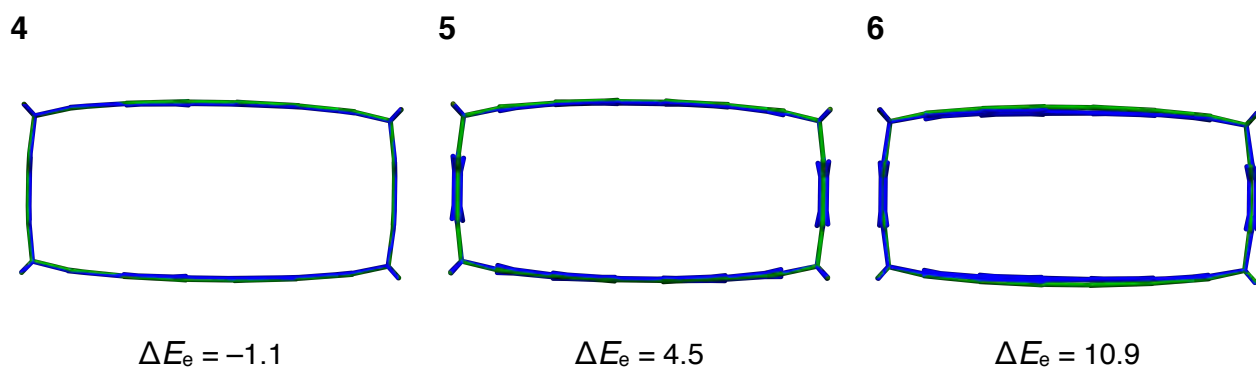
Figure S4. Overlays of 3D host and guest geometries from free optimizations and from complex optimizations. Differences in electronic energies (ΔE_e, PW6B95-D3(BJ)/Def2-TZVPP) between substrates from free and host–guest complex optimizations, calculated as $\Delta E_e = E_{e,complex} - E_{e,free}$, are given in kJ mol^{-1}.

7. Optimized structures (PBE-D3(BJ)/6-31G(d), Cartesian coordinates (in Å), computed absolute energies (SMD-(chloroform)-PW6B95-D3(BJ)/Def2-QZVP'// PBE-D3(BJ)/6-31G(d), in Hartree) and imaginary frequencies for transition structures

Free equilibrium structures

1

C	-0.675821	1.568634	0.378891
H	-1.181996	2.368535	0.938987
C	0.675821	1.568634	0.378891
H	1.181996	2.368535	0.938987
C	1.568634	0.675821	-0.378891
H	2.368535	1.181996	-0.938987
C	1.568634	-0.675821	-0.378891
H	2.368535	-1.181996	-0.938987
C	-1.568634	0.675821	-0.378891
H	-2.368535	1.181996	-0.938987
C	-1.568634	-0.675821	-0.378891
H	-2.368535	-1.181996	-0.938987
C	-0.675821	-1.568634	0.378891
C	0.675821	-1.568634	0.378891
H	-1.181996	-2.368535	0.938987
H	1.181996	-2.368535	0.938987

Number of imaginary frequencies = 0
Computed total Gibbs free energy = -310.03868 a.u.

2

C	0.568926	1.378691	0.244833
C	-0.568926	1.378691	-0.244833
C	0.568926	-1.378691	-0.244833
C	-0.568926	-1.378691	0.244833
C	-1.847142	1.377409	-0.819835
H	-2.044955	2.141475	-1.584502
C	-2.891780	0.554909	-0.459355
H	-3.865830	0.799191	-0.901821
C	-2.891780	-0.554909	0.459355
H	-3.865830	-0.799191	0.901821
C	-1.847142	-1.377409	0.819835
H	-2.044955	-2.141475	1.584502
C	1.847142	-1.377409	-0.819835
H	2.044955	-2.141475	-1.584502
C	2.891780	-0.554909	-0.459355
H	3.865830	-0.799191	-0.901821
C	2.891780	0.554909	0.459355
H	3.865830	0.799191	0.901821
C	1.847142	1.377409	0.819835
H	2.044955	2.141475	1.584502

Number of imaginary frequencies = 0
Computed total Gibbs free energy = -462.61718 a.u.

3

C	1.312055	2.994372	-0.262767
C	2.442370	2.173150	-0.262767
C	-1.312055	2.994372	-0.262767
C	-0.000000	2.495473	0.097602
C	-0.000000	1.210560	0.641712
C	2.373336	0.771144	0.097602
C	-2.442370	2.173150	-0.262767
C	3.253264	-0.322527	-0.262767
C	0.698573	-3.193704	-0.262767
C	-0.698573	-3.193704	-0.262767
C	1.466802	-2.018880	0.097602
C	0.711549	-0.979364	0.641712
C	-0.711549	-0.979364	0.641712
C	-1.466802	-2.018880	0.097602
C	-2.821522	-1.651291	-0.262767
C	-3.253264	-0.322527	-0.262767
C	-2.373336	0.771144	0.097602
C	-1.151311	0.374084	0.641712
C	2.821522	-1.651291	-0.262767
C	1.151311	0.374084	0.641712
H	-4.257598	-0.100804	-0.641340
H	-3.503720	-2.421001	-0.641340
H	-1.219800	-4.080367	-0.641340
H	1.219800	-4.080367	-0.641340
H	3.503720	-2.421001	-0.641340
H	4.257598	-0.100804	-0.641340
H	3.385218	2.584106	-0.641340
H	1.411541	4.018066	-0.641340
H	-1.411541	4.018066	-0.641340
H	-3.385218	2.584106	-0.641340

Number of imaginary frequencies = 0
Computed total Gibbs free energy = -769.34369 a.u.

4

C	-3.232425	1.037756	0.454098
C	-2.514936	2.280484	0.454098
C	-1.213935	2.371146	-0.069751
C	-2.660440	-0.134274	-0.069751
C	-2.859167	-1.650741	0.194143
C	3.232425	1.037756	0.454098
C	2.660440	-0.134274	-0.069751
C	2.859167	-1.650741	0.194143
C	2.514936	2.280484	0.454098
C	1.213935	2.371146	-0.069751
C	0.718597	1.220576	-0.710672
C	1.416348	0.012035	-0.710672
C	0.697751	-1.232611	-0.710672

```
C     1.446505   -2.236872   -0.069751
C     0.717489   -3.318240    0.454098
C    -0.717489   -3.318240    0.454098
C    -1.446505   -2.236872   -0.069751
C    -0.697751   -1.232611   -0.710672
C    -1.416348    0.012035   -0.710672
C    -0.718597    1.220576   -0.710672
C     0.000000    3.301482    0.194143
H     2.960253    3.122008    0.996864
H     4.183865    1.002650    0.996864
H     0.000000    3.685476    1.228925
H    -2.960253    3.122008    0.996864
H    -4.183865    1.002650    0.996864
H    -3.625784   -2.093347   -0.471608
H    -1.223612   -4.124658    0.996864
H     1.223612   -4.124658    0.996864
H     3.191716   -1.842738    1.228925
H    -3.191716   -1.842738    1.228925
H     0.000000    4.186695   -0.471608
H     3.625784   -2.093347   -0.471608
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Number of imaginary frequencies = 0
Computed total Gibbs free energy = -808.67271 a.u.

5
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P    -0.000030    0.000041    1.140919
S    -1.672934    2.754952    0.444935
S    -1.549325   -2.826345    0.444857
S     3.222361    0.071357    0.445380
C    -1.636700   -0.036242    0.284387
C     0.786949    1.435425    0.284265
C     0.161728   -2.596548   -0.003688
C     0.849700   -1.399190    0.284290
C     2.167947    1.438319   -0.003279
C    -2.276118   -1.260286   -0.003313
C    -3.620520    1.132226   -0.560156
H    -4.129264    2.074880   -0.781300
C     0.664987    3.734386   -0.560705
H     0.063137    4.620425   -0.782098
C     2.901829   -2.443080   -0.560173
H     3.970190   -2.364946   -0.781130
C    -2.329717    1.158266   -0.003359
C     0.046640    2.601188   -0.003614
C     0.829679   -3.701265   -0.560750
H     0.267658   -4.613103   -0.782124
C     2.790779    2.569145   -0.560294
H     3.861560    2.538420   -0.781235
C     2.229494   -1.340959   -0.003218
C    -4.239666   -0.093898   -0.824286
H    -5.245334   -0.116197   -1.254811
C    -3.566831   -1.291383   -0.560083
H    -4.033371   -2.255643   -0.781160
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C     2.201145   -3.624391   -0.824771
H     2.723267   -4.484092   -1.255491
C     2.038495    3.718280   -0.824848
H     2.522038    4.600242   -1.255605
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Number of imaginary frequencies = 0
Computed total Gibbs free energy = -2229.743 a.u.

6
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P    -0.000086    0.000001    1.546851
C    -1.519656   -0.060210    0.547578
C     0.707697    1.346132    0.547732
C     0.079264   -2.401499    0.119318
C     0.811985   -1.285964    0.547783
C     2.040211    1.269343    0.119572
C    -2.023233   -1.296275    0.119340
C    -3.338866    1.096815   -0.567104
H    -3.813547    2.029566   -0.881701
C     0.445205    3.485805   -0.567482
H    -0.192883    4.315299   -0.882283
C     2.796431   -2.128375   -0.567191
H     3.833917   -1.990477   -0.881718
C    -2.119453    1.132170    0.119402
C    -0.110961    2.400223    0.119287
C     0.719571   -3.439669   -0.567478
H     0.149101   -4.317045   -0.882263
C     2.619279    2.342899   -0.567228
H     3.664426    2.287522   -0.881750
C     2.134236   -1.103978    0.119572
C    -3.903785   -0.154628   -0.865853
H    -4.858582   -0.192440   -1.398806
C    -3.241609   -1.357461   -0.567205
H    -3.641014   -2.324836   -0.881818
C     2.085823   -3.303153   -0.866193
H     2.595956   -4.111014   -1.399329
C     1.817973    3.457779   -0.866226
H     2.262595    4.303450   -1.399389
O    -1.494286    2.366710    0.339070
O     2.796805    0.110803    0.339484
O    -1.302438   -2.477485    0.339014
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Number of imaginary frequencies = 0
Computed total Gibbs free energy = -1260.0827 a.u.

PBI cyclophane catalyst
```
C    -5.054488   -3.328914    1.249444
C    -3.577653   -3.456762    1.226549
C    -2.862475   -3.489893    0.000011
C    -3.577622   -3.456211   -1.226527
C    -5.054442   -3.328225   -1.249379
C    -2.881430   -3.501491    2.432441
C    -1.428459   -3.543275    0.000006
```

C	-0.729685	-3.562643	1.253519
C	-1.481457	-3.556105	2.441528
C	0.737652	-3.561873	1.253530
C	1.436419	-3.542204	0.000023
C	0.737666	-3.562064	-1.253490
C	-0.729672	-3.562427	-1.253502
C	-1.481424	-3.555324	-2.441522
C	-2.881389	-3.500486	-2.432429
H	-3.453793	-3.475376	-3.363702
H	-0.975715	-3.577818	-3.409264
H	-3.453843	-3.476880	3.363721
H	-0.975757	-3.578916	3.409267
C	1.489405	-3.554152	2.441546
C	2.870398	-3.487728	0.000030
C	1.489439	-3.554917	-2.441495
C	3.585533	-3.453511	1.226552
C	2.889333	-3.498295	2.432453
H	3.461704	-3.472678	3.363730
C	3.585555	-3.454113	-1.226494
C	2.889378	-3.499336	-2.432394
H	3.461781	-3.474258	-3.363666
C	5.062245	-3.324084	1.249414
C	5.062279	-3.324957	-1.249380
H	0.983761	-3.577998	-3.409238
H	0.983718	-3.576883	3.409293
O	-5.697395	-3.269009	2.303262
O	-5.697340	-3.267681	-2.303164
O	5.705023	-3.263180	2.303240
O	5.705116	-3.264905	-2.303229
N	-5.698779	-3.251337	0.000046
N	5.706500	-3.246048	0.000005
C	-5.062299	3.324970	1.249307
C	-3.585574	3.454125	1.226442
C	-2.870398	3.487730	-0.000070
C	-3.585514	3.453497	-1.226603
C	-5.062226	3.324071	-1.249486
C	-2.889416	3.499354	2.432353
C	-1.436419	3.542207	-0.000042
C	-0.737684	3.562078	1.253481
C	-1.489477	3.554934	2.441475
C	0.729655	3.562444	1.253514
C	1.428459	3.543275	0.000015
C	0.729702	3.562632	-1.253506
C	-0.737634	3.561859	-1.253539
C	-1.489368	3.554119	-2.441566
C	-2.889296	3.498263	-2.432494
H	-3.461652	3.472633	-3.363780
H	-0.983664	3.576831	-3.409305
H	-3.461832	3.474280	3.363617
H	-0.983815	3.578016	3.409226
C	1.481392	3.555365	2.441544
C	2.862475	3.489893	0.000030

```
C      1.481489    3.556089   -2.441506
C      3.577606    3.456225    1.226578
C      2.881357    3.500523    2.432470
H      3.453749    3.475427    3.363751
C      3.577670    3.456753   -1.226498
C      2.881463    3.501474   -2.432400
H      3.453888    3.476859   -3.363672
C      5.054425    3.328231    1.249451
C      5.054505    3.328904   -1.249372
H      0.975802    3.578899   -3.409252
H      0.975672    3.577882    3.409280
O     -5.705151    3.264919    2.303147
O     -5.704988    3.263169   -2.303322
O      5.697308    3.267692    2.303246
O      5.697425    3.268982   -2.303181
N     -5.706500    3.246046   -0.000086
N      5.698779    3.251339    0.000036
C     -7.145810   -2.923000    0.000075
H     -7.572112   -3.382820   -0.901862
H     -7.572066   -3.382982    0.901956
C      7.152819   -2.914704   -0.000087
H      7.580026   -3.373638   -0.902041
H      7.580197   -3.373649    0.901786
C      7.145810    2.922999    0.000024
H      7.572100    3.382791    0.901982
H      7.572080    3.383009   -0.901836
C     -7.152819    2.914703   -0.000013
H     -7.580039    3.373661    0.901922
H     -7.580185    3.373622   -0.901904
C     -7.323493   -1.417375    0.000173
C     -7.347956   -0.704041    1.212838
C     -7.349500   -0.704146   -1.212515
C     -7.349712    0.695393    1.212775
H     -7.326072   -1.255077    2.157908
C     -7.351251    0.695296   -1.212582
H     -7.328828   -1.255229   -2.157588
C     -7.327059    1.408681    0.000046
H     -7.329334    1.246535    2.157824
H     -7.332018    1.246337   -2.157713
C      7.327060   -1.408683   -0.000098
C      7.349723   -0.695352   -1.212802
C      7.351241   -0.695340    1.212556
C      7.347966    0.704082   -1.212814
H      7.329353   -1.246460   -2.157870
C      7.349491    0.704102    1.212538
H      7.332001   -1.246415    2.157667
C      7.323493    1.417374   -0.000125
H      7.326088    1.255151   -2.157866
H      7.328812    1.255152    2.157631
```

Number of imaginary frequencies = 0
Computed total Gibbs free energy = -3284.2371 a.u.

Free transition structures

1

C	-0.000079	0.737744	1.696220
H	-0.000181	1.136817	2.718055
C	0.000079	-0.737744	1.696220
H	0.000181	-1.136817	2.718055
C	0.000079	-1.696218	0.737744
H	0.000194	-2.718054	1.136816
C	0.000079	-1.696218	-0.737744
H	0.000194	-2.718054	-1.136816
C	-0.000079	1.696218	0.737744
H	-0.000194	2.718054	1.136816
C	-0.000079	1.696218	-0.737744
H	-0.000194	2.718054	-1.136816
C	-0.000079	0.737744	-1.696220
C	0.000079	-0.737744	-1.696220
H	-0.000181	1.136817	-2.718055
H	0.000181	-1.136817	-2.718055

Number of imaginary frequencies = 1 (-151.3 cm^{-1})
Computed total Gibbs free energy = -310.01815 a.u.

2

C	0.000000	1.567435	0.614921
C	0.000000	1.567435	-0.614921
C	-0.000000	-1.567435	0.614921
C	-0.000000	-1.567435	-0.614921
C	0.000000	1.685244	-2.023284
H	0.000000	2.724270	-2.383030
C	0.000000	0.730522	-3.002740
H	0.000000	1.144775	-4.018503
C	-0.000000	-0.730522	-3.002740
H	-0.000000	-1.144775	-4.018503
C	-0.000000	-1.685244	-2.023284
H	-0.000000	-2.724270	-2.383030
C	-0.000000	-1.685244	2.023284
H	-0.000000	-2.724270	2.383030
C	-0.000000	-0.730522	3.002740
H	-0.000000	-1.144775	4.018503
C	-0.000000	0.730522	3.002740
H	-0.000000	1.144775	4.018503
C	-0.000000	1.685244	2.023284
H	-0.000000	2.724270	2.383030

Number of imaginary frequencies = 1 (-97.3 cm^{-1})
Computed total Gibbs free energy = -462.60005 a.u.

3

C	1.369389	3.086768	0.000000
C	2.512526	2.256230	-0.000000

```
C     -1.369389    3.086768    -0.000000
C      0.000000    2.569965    -0.000000
C      0.000000    1.193053    -0.000000
C      2.444182    0.794163    -0.000000
C     -2.512526    2.256230     0.000000
C      3.358855   -0.348503     0.000000
C      0.706498   -3.302154     0.000000
C     -0.706498   -3.302154    -0.000000
C      1.510587   -2.079145    -0.000000
C      0.701259   -0.965200    -0.000000
C     -0.701259   -0.965200    -0.000000
C     -1.510587   -2.079145    -0.000000
C     -2.922216   -1.692341     0.000000
C     -3.358855   -0.348503     0.000000
C     -2.444182    0.794163    -0.000000
C     -1.134661    0.368674    -0.000000
C      2.922216   -1.692341     0.000000
C      1.134661    0.368674    -0.000000
H     -3.698377   -2.465942     0.000000
H     -4.441494   -0.178862    -0.000000
H     -3.488112    2.755348     0.000000
H     -1.542606    4.168840     0.000000
H      1.542606    4.168840     0.000000
H      3.488112    2.755348    -0.000000
H      4.441494   -0.178862     0.000000
H      3.698377   -2.465942     0.000000
H      1.202389   -4.279384     0.000000
H     -1.202389   -4.279384    -0.000000
```

Number of imaginary frequencies = 1 (-110.8 cm⁻¹)
Computed total Gibbs free energy = -769.32565 a.u.

4
```
C      2.684763   -2.392675     0.000000
C      3.414499   -1.128735    -0.000000
C      2.763718    0.137593     0.000000
C      1.262700   -2.462247     0.000000
C      0.000000   -3.437831     0.000000
C     -0.729736    3.521410     0.000000
C     -1.501018    2.324653     0.000000
C     -2.977249    1.718915     0.000000
C      0.729736    3.521410     0.000000
C      1.501018    2.324653     0.000000
C      0.686608    1.206106     0.000000
C     -0.686608    1.206106    -0.000000
C     -1.387822   -0.008433     0.000000
C     -2.763718    0.137593    -0.000000
C     -3.414499   -1.128735     0.000000
C     -2.684763   -2.392675    -0.000000
C     -1.262700   -2.462247     0.000000
C     -0.701214   -1.197673     0.000000
C      0.701214   -1.197673     0.000000
```

```
C      1.387822   -0.008433   -0.000000
C      2.977249    1.718915    0.000000
H      1.205096    4.508867    0.000000
H     -1.205096    4.508867   -0.000000
H      4.507341   -1.210790   -0.000000
H      3.302245   -3.298077    0.000000
H     -3.302245   -3.298077    0.000000
H     -4.507341   -1.210790    0.000000
H     -3.549987    2.049586    0.884770
H     -3.549987    2.049586   -0.884770
H      3.549987    2.049586   -0.884770
H      3.549987    2.049586    0.884770
H     -0.000000   -4.099172   -0.884770
H     -0.000000   -4.099172    0.884770
```

Number of imaginary frequencies = 1 (-121.3 cm^{-1})
Computed total Gibbs free energy = -808.64118 a.u.

5
```
P     -0.000002   -0.001799   -0.001559
C     -1.505147   -0.866450   -0.036819
C     -2.718718   -0.146770   -0.114191
C     -1.484984   -2.277858    0.043162
C     -3.926332   -0.860832   -0.117660
C     -2.699580   -2.975707   -0.028208
C     -3.908643   -2.264758   -0.098472
H     -4.877957   -0.321716   -0.152181
H     -2.702271   -4.069510   -0.000318
H     -4.853736   -2.813988   -0.129675
C      0.000315    1.732947    0.023998
C     -1.233986    2.419449    0.076280
C      1.234835    2.418989    0.076676
C     -1.223271    3.808799    0.268208
C      1.224595    3.808350    0.268567
C      0.000776    4.489882    0.373931
H     -2.167310    4.359827    0.317627
H      2.168831    4.359017    0.318272
H      0.000949    5.572918    0.524971
C      1.504825   -0.867000   -0.036961
C      2.718683   -0.147764   -0.114226
C      1.484067   -2.278407    0.042855
C      3.925974   -0.862372   -0.118213
C      2.698356   -2.976763   -0.028856
C      3.907681   -2.266310   -0.099334
H      4.877841   -0.323684   -0.152802
H      2.700609   -4.070570   -0.001132
H      4.852533   -2.815931   -0.130921
S     -2.830509    1.649950   -0.287473
S      2.831335    1.648936   -0.286286
S     -0.000585   -3.247256    0.395329
```

Number of imaginary frequencies = 1 (-347.3 cm^{-1})
Computed total Gibbs free energy = -2229.6723 a.u.

6

P	-0.000001	-0.000028	-0.000355
C	1.344716	-0.962899	-0.000301
C	1.070607	-2.337765	-0.000123
C	2.558033	-0.260549	-0.000065
C	2.214769	-3.141893	0.000210
C	3.687852	-1.084701	0.000275
C	3.482264	-2.493487	0.000371
H	2.152485	-4.233033	0.000353
H	4.700754	-0.674211	0.000459
H	4.371191	-3.130009	0.000600
C	-1.506236	-0.683061	-0.000684
C	-1.504674	-2.085002	-0.000226
C	-2.559887	0.241716	-0.000264
C	-2.783304	-2.651401	0.000379
C	-3.828346	-0.347094	0.000345
C	-3.900578	-1.768984	0.000570
H	-2.934251	-3.733847	0.000725
H	-4.742146	0.252441	0.000671
H	-4.896280	-2.220566	0.000962
C	0.161533	1.645915	-0.000447
C	-1.053356	2.345585	-0.000196
C	1.489249	2.096041	-0.000097
C	-0.904512	3.736096	0.000245
C	1.613590	3.488974	0.000351
C	0.418317	4.262462	0.000456
H	-1.766445	4.408064	0.000436
H	2.589711	3.980556	0.000610
H	0.525064	5.350561	0.000744
O	2.605441	1.181606	-0.000139
O	-0.279435	-2.847109	-0.000194
O	-2.326043	1.665597	-0.000296

Number of imaginary frequencies = 1 (-437.5 cm^{-1})
Computed total Gibbs free energy = -1259.9344 a.u.

Lowest energy equilibrium structure host-guest complexes between guests 1-6 and the PBI cyclophane catalyst

1

C	5.215092	-3.398000	-1.233484
C	3.740860	-3.545666	-1.209195
C	3.027662	-3.596100	0.018006
C	3.743231	-3.552166	1.244022
C	5.217614	-3.398373	1.265692
C	3.043865	-3.596652	-2.414572
C	1.594863	-3.674887	0.019110
C	0.894592	-3.695395	-1.233654

```
C      1.645078   -3.672819   -2.422626
C     -0.571803   -3.702883   -1.231750
C     -1.269638   -3.706004    0.021566
C     -0.570556   -3.728726    1.273313
C      0.896710   -3.712601    1.272710
C      1.649680   -3.694903    2.460308
C      3.048460   -3.612417    2.450202
H      3.620909   -3.578784    3.381205
H      1.145257   -3.730960    3.428315
H      3.615011   -3.560163   -3.346261
H      1.138513   -3.699258   -3.389713
C     -1.321211   -3.667511   -2.419708
C     -2.701105   -3.641889    0.022774
C     -1.319754   -3.716866    2.462802
C     -3.414060   -3.574147   -1.202768
C     -2.719705   -3.601428   -2.409597
H     -3.290892   -3.540757   -3.339812
C     -3.414459   -3.600658    1.249301
C     -2.718511   -3.650274    2.455294
H     -3.289245   -3.613228    3.387065
C     -4.883154   -3.392249   -1.223881
C     -4.886583   -3.437656    1.274347
H     -0.812703   -3.736439    3.429894
H     -0.815010   -3.663725   -3.387239
O      5.856646   -3.329565   -2.287791
O      5.860460   -3.326359    2.318890
O     -5.521310   -3.266885   -2.276231
O     -5.530424   -3.367064    2.327191
N      5.859534   -3.313497    0.015523
N     -5.529055   -3.327815    0.024900
C      5.264016    3.332740   -1.231803
C      3.793979    3.519926   -1.196528
C      3.089688    3.569323    0.036005
C      3.811052    3.490238    1.256819
C      5.282556    3.314843    1.267406
C      3.090571    3.602111   -2.396527
C      1.659556    3.681725    0.047691
C      0.953364    3.755691   -1.199421
C      1.694307    3.719698   -2.393963
C     -0.511340    3.815104   -1.187764
C     -1.200935    3.741234    0.066917
C     -0.495728    3.733587    1.315502
C      0.970030    3.698513    1.306042
C      1.727776    3.636580    2.488623
C      3.124855    3.536283    2.468568
H      3.702452    3.472985    3.394810
H      1.228089    3.646815    3.459767
H      3.653977    3.556231   -3.332520
H      1.180717    3.763100   -3.357048
C     -1.271641    3.900852   -2.366966
C     -2.631851    3.665114    0.073592
C     -1.240640    3.736976    2.508814
```

```
C    -3.353524    3.655551   -1.148120
C    -2.669517    3.810577   -2.352351
H    -3.248141    3.829978   -3.280122
C    -3.336837    3.587360    1.302758
C    -2.638350    3.660487    2.506641
H    -3.205908    3.621338    3.440486
C    -4.816893    3.429157   -1.168258
C    -4.800860    3.366312    1.329171
H    -0.729224    3.774101    3.473299
H    -0.773311    4.008471   -3.333106
O     5.896581    3.252036   -2.290696
O     5.931756    3.226887    2.315592
O    -5.461427    3.343050   -2.219654
O    -5.429622    3.222135    2.384738
N     5.914777    3.227607    0.012495
N    -5.448411    3.286504    0.083128
C     7.304108   -2.976213    0.013151
H     7.733741   -3.431076    0.916047
H     7.731995   -3.436908   -0.887670
C    -6.962106   -2.945662    0.028745
H    -7.404933   -3.398089    0.926362
H    -7.406367   -3.379367   -0.877447
C    -6.879652    2.902892    0.086196
H    -7.324777    3.356258   -0.810086
H    -7.319250    3.340605    0.993017
C     7.352966    2.864500    0.000861
H     7.781596    3.312599   -0.905893
H     7.797947    3.316613    0.897761
C     7.478039   -1.470227    0.008427
C     7.495502   -0.759348   -1.205869
C     7.515424   -0.754888    1.219423
C     7.506241    0.640036   -1.208478
H     7.463561   -1.312332   -2.149492
C     7.527526    0.644510    1.216779
H     7.498311   -1.304284    2.165614
C     7.501060    1.355747    0.002953
H     7.482379    1.189900   -2.154274
H     7.520096    1.197828    2.160672
C    -7.087677   -1.434255    0.044212
C    -7.095755   -0.731682    1.264437
C    -7.087133   -0.706444   -1.161006
C    -7.066052    0.668283    1.278327
H    -7.090527   -1.292814    2.203896
C    -7.055831    0.692777   -1.145937
H    -7.078103   -1.248521   -2.111347
C    -7.028565    1.393955    0.073299
H    -7.040666    1.210017    2.228605
H    -7.020986    1.253904   -2.084790
C    -2.235689    0.483038   -1.997503
H    -2.584301    1.040510   -2.878328
C    -0.899976    0.449464   -1.793108
H    -0.274542    0.983259   -2.523743
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C    -0.135769   -0.284935   -0.771836
H     0.760714   -0.794231   -1.153419
C    -0.335520   -0.328481    0.564582
H     0.416783   -0.869120    1.156513
C    -3.315711   -0.177720   -1.249994
H    -4.111137   -0.601130   -1.878722
C    -3.523511   -0.218827    0.087305
H    -4.473476   -0.657687    0.418909
C    -2.719892    0.356922    1.172733
C    -1.379890    0.323610    1.369232
H    -3.321146    0.808207    1.973906
H    -1.014242    0.762090    2.308320
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Number of imaginary frequencies = 0
Computed total Gibbs free energy = -3594.2758 a.u.

2
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C     4.897608   -3.336937   -1.398855
C     3.433009   -3.533008   -1.314606
C     2.790751   -3.698053   -0.058987
C     3.565714   -3.751058    1.129766
C     5.037305   -3.591628    1.087500
C     2.671609   -3.476509   -2.480330
C     1.362540   -3.769965    0.011394
C     0.601404   -3.761229   -1.202534
C     1.277211   -3.602881   -2.423516
C    -0.855614   -3.875679   -1.125673
C    -1.490372   -3.740820    0.151823
C    -0.730410   -3.674946    1.364980
C     0.727054   -3.806099    1.295868
C     1.531963   -3.914346    2.443443
C     2.931636   -3.895395    2.363730
H     3.552020   -3.954828    3.262297
H     1.067793   -4.000903    3.428826
H     3.188587   -3.318881   -3.430612
H     0.709529   -3.534859   -3.354354
C    -1.659207   -4.074623   -2.261535
C    -2.917239   -3.645971    0.212754
C    -1.409811   -3.456724    2.575172
C    -3.690122   -3.767754   -0.972591
C    -3.058028   -4.026325   -2.188149
H    -3.677987   -4.146847   -3.080918
C    -3.560934   -3.406943    1.455174
C    -2.802700   -3.310363    2.620572
H    -3.321377   -3.108913    3.561726
C    -5.155746   -3.559617   -0.949010
C    -5.023719   -3.192023    1.523123
H    -0.847019   -3.361843    3.506694
H    -1.192316   -4.253509   -3.233330
O     5.482608   -3.134887   -2.468753
O     5.739184   -3.619186    2.104986
O    -5.849549   -3.604643   -1.972090
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O	-5.612422	-2.938571	2.579677
N	5.605827	-3.362622	-0.180737
N	-5.725699	-3.258427	0.302678
C	5.155749	3.559576	-0.948819
C	3.690135	3.767706	-0.972356
C	2.917288	3.645900	0.212997
C	3.560978	3.406636	1.455371
C	5.023817	3.192090	1.523338
C	3.058103	4.026519	-2.187876
C	1.490422	3.740819	0.152056
C	0.855697	3.876092	-1.125414
C	1.659303	4.075160	-2.261252
C	-0.601312	3.761704	-1.202306
C	-1.362471	3.769962	0.011597
C	-0.727031	3.805787	1.296087
C	0.730423	3.674515	1.365163
C	1.409772	3.455654	2.575277
C	2.802672	3.309425	2.620678
H	3.321333	3.107632	3.561770
H	0.846873	3.360089	3.506668
H	3.678109	4.146944	-3.080624
H	1.192399	4.254255	-3.233012
C	-1.277105	3.603793	-2.423356
C	-2.790685	3.698044	-0.058861
C	-1.531924	3.913944	2.443686
C	-3.432925	3.533278	-1.314529
C	-2.671486	3.477290	-2.480259
H	-3.188428	3.319934	-3.430610
C	-3.565632	3.750806	1.129913
C	-2.931594	3.894921	2.363918
H	-3.552049	3.954353	3.262438
C	-4.897502	3.336974	-1.398838
C	-5.037224	3.591470	1.087557
H	-1.067700	4.000521	3.429043
H	-0.709372	3.536129	-3.354179
O	5.849479	3.604455	-1.971959
O	5.612548	2.938716	2.579894
O	-5.482457	3.134724	-2.468726
O	-5.739166	3.618665	2.105016
N	5.725820	3.258775	0.302912
N	-5.605738	3.362889	-0.180771
C	7.038109	-2.987008	-0.224259
H	7.526526	-3.514491	0.606362
H	7.429116	-3.344312	-1.186587
C	-7.145731	-2.836782	0.320583
H	-7.567087	-3.174880	1.277040
H	-7.634663	-3.353670	-0.516371
C	-7.038068	2.987491	-0.224243
H	-7.429097	3.344828	-1.186551
H	-7.526357	3.515069	0.606391
C	7.145882	2.837182	0.320700
H	7.634686	3.354161	-0.516268

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H     7.567328    3.175217    1.277143
C     7.180966   -1.483755   -0.089473
C     7.157125   -0.658693   -1.229688
C     7.251696   -0.887982    1.183591
C     7.186425    0.734645   -1.098045
H     7.092933   -1.118787   -2.220338
C     7.276028    0.505593    1.315117
H     7.262143   -1.526617    2.072164
C     7.234926    1.330656    0.176737
H     7.152894    1.374063   -1.985825
H     7.300228    0.965671    2.307369
C    -7.234807   -1.330243    0.176770
C    -7.275479   -0.505207    1.315160
C    -7.186830   -0.734173   -1.098014
C    -7.251237    0.888397    1.183663
H    -7.299238   -0.965279    2.307427
C    -7.157706    0.659157   -1.229643
H    -7.153640   -1.373557   -1.985835
C    -7.181073    1.484237   -0.089387
H    -7.261184    1.526973    2.072281
H    -7.093902    1.119232   -2.220330
C     0.599847   -0.155097    1.007434
C    -0.599041    0.154167    1.007721
C     0.587086    0.193441   -1.861234
C    -0.588684   -0.193960   -1.861126
C    -1.940981    0.564685    1.071781
H    -2.206916    1.175705    1.945228
C    -2.964329    0.264186    0.203650
H    -3.963410    0.583860    0.527677
C    -2.944511   -0.433392   -1.059241
H    -3.926028   -0.794554   -1.390794
C    -1.904797   -0.680204   -1.925416
H    -2.140348   -1.296592   -2.803422
C     1.903157    0.679666   -1.926602
H     2.138001    1.296039   -2.804829
C     2.943552    0.433026   -1.061210
H     3.924733    0.794393   -1.393550
C     2.964600   -0.264266    0.201868
H     3.964055   -0.583520    0.525173
C     1.941974   -0.565073    1.070776
H     2.208747   -1.175872    1.944140
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Number of imaginary frequencies = 0
Computed total Gibbs free energy = -3746.8592 a.u.

3
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C     4.778601   -3.511839   -1.337950
C     3.300407   -3.573570   -1.332000
C     2.572225   -3.566902   -0.114171
C     3.271916   -3.539944    1.120511
C     4.746353   -3.433012    1.159445
C     2.617642   -3.587073   -2.546585
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C     1.139437    -3.565719    -0.130687
C     0.455359    -3.549269    -1.390462
C     1.218085    -3.571114    -2.571450
C    -1.008180    -3.499337    -1.406047
C    -1.721509    -3.529546    -0.162352
C    -1.037947    -3.587069     1.097086
C     0.426424    -3.574406     1.114502
C     1.161195    -3.568525     2.311459
C     2.560770    -3.544112     2.318091
H     3.121301    -3.510636     3.255645
H     0.642632    -3.553154     3.271885
H     3.201798    -3.593143    -3.470901
H     0.720940    -3.574355    -3.543535
C    -1.742957    -3.412768    -2.601840
C    -3.154159    -3.483166    -0.177238
C    -1.800718    -3.644460     2.275999
C    -3.852916    -3.382226    -1.408642
C    -3.141778    -3.351311    -2.606873
H    -3.703086    -3.263691    -3.541269
C    -3.881905    -3.509592     1.041467
C    -3.199668    -3.605920     2.252629
H    -3.783563    -3.627163     3.176924
C    -5.324649    -3.227043    -1.440768
C    -5.354642    -3.363790     1.055673
H    -1.304073    -3.701962     3.246232
H    -1.222731    -3.376487    -3.561123
O     5.438279    -3.488997    -2.384098
O     5.377315    -3.314818     2.217503
O    -5.955392    -3.088217    -2.495053
O    -6.010054    -3.343554     2.104165
N     5.412067    -3.446700    -0.081317
N    -5.981197    -3.201827    -0.195071
C     5.102392     3.151110    -1.435594
C     3.646975     3.418408    -1.391376
C     2.961064     3.536029    -0.153600
C     3.688722     3.450199     1.061963
C     5.144796     3.187974     1.064026
C     2.935926     3.501459    -2.586377
C     1.536053     3.696327    -0.131864
C     0.818238     3.736832    -1.373372
C     1.544919     3.663155    -2.573775
C    -0.647077     3.771442    -1.348502
C    -1.323651     3.740206    -0.083788
C    -0.604435     3.761629     1.157310
C     0.860842     3.752722     1.132340
C     1.628945     3.712414     2.309445
C     3.019288     3.559639     2.279395
H     3.601924     3.488576     3.201512
H     1.139134     3.759512     3.283940
H     3.487221     3.408200    -3.525944
H     1.022938     3.691633    -3.532300
C    -1.416457     3.759396    -2.524212
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C    -2.753524    3.637840   -0.059619
C    -1.332140    3.712324    2.359146
C    -3.486889    3.591928   -1.274887
C    -2.813686    3.670463   -2.491975
H    -3.401546    3.638761   -3.413353
C    -3.442865    3.554278    1.178690
C    -2.727233    3.603400    2.373604
H    -3.280424    3.532775    3.313888
C    -4.958015    3.428437   -1.274365
C    -4.911738    3.375617    1.225034
H    -0.808139    3.716838    3.316816
H    -0.926218    3.792715   -3.499296
O     5.719764    3.001510   -2.496742
O     5.799729    3.072456    2.106581
O    -5.621518    3.367978   -2.316139
O    -5.535101    3.261631    2.287012
N     5.761057    3.052555   -0.195088
N    -5.578635    3.329283   -0.014383
C     6.872993   -3.193466   -0.070318
H     7.265412   -3.649076    0.848933
H     7.284795   -3.698904   -0.954531
C    -7.404806   -2.787522   -0.190974
H    -7.865661   -3.250691    0.691867
H    -7.855188   -3.183349   -1.111127
C    -7.030765    3.038303    0.004825
H    -7.462788    3.540618   -0.871634
H    -7.425094    3.479082    0.930715
C     7.181733    2.634169   -0.210315
H     7.619637    3.043111   -1.131119
H     7.653233    3.087284    0.672412
C     7.130536   -1.700542   -0.107922
C     7.151024   -1.015742   -1.338152
C     7.229517   -0.962340    1.086408
C     7.219167    0.381471   -1.370882
H     7.075031   -1.587168   -2.267915
C     7.299550    0.435928    1.052736
H     7.209051   -1.491084    2.044054
C     7.271735    1.121880   -0.175344
H     7.194768    0.913345   -2.326681
H     7.334021    1.009647    1.983615
C    -7.470824   -1.274147   -0.136461
C    -7.399206   -0.605060    1.100323
C    -7.474522   -0.518586   -1.323279
C    -7.297661    0.789949    1.146785
H    -7.393782   -1.190225    2.024961
C    -7.375130    0.876635   -1.276174
H    -7.521450   -1.035976   -2.286155
C    -7.268355    1.542648   -0.041834
H    -7.210750    1.306352    2.107582
H    -7.345087    1.459913   -2.201289
C    -2.956332   -0.106517    0.290470
C    -2.581987   -0.070590   -1.060858
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C     -2.008251   -0.242447    2.775979
C     -2.001000    0.108943    1.366137
C     -0.760888    0.552011    0.921527
C     -1.212564    0.181579   -1.482873
C     -0.835055   -0.294849    3.545199
C     -0.488384   -0.092314   -2.713210
C      3.148571   -0.161929   -1.315038
C      3.645147   -0.193257   -0.003521
C      1.754839    0.130530   -1.614595
C      1.034549    0.562887   -0.507381
C      1.532664    0.522653    0.817830
C      2.797461    0.055333    1.151693
C      2.930745   -0.282799    2.558371
C      1.830672   -0.308761    3.429433
C      0.478287    0.006892    2.995174
C      0.423080    0.509108    1.700821
C      0.914959   -0.118446   -2.774628
C     -0.382755    0.585742   -0.444041
H      3.901280   -0.621936    2.937616
H      1.999691   -0.658339    4.454659
H     -0.918474   -0.643389    4.581432
H     -2.946974   -0.555406    3.246078
H     -3.993512   -0.369367    0.529127
H     -3.345297   -0.314412   -1.807443
H     -1.047201   -0.364468   -3.615783
H      1.381333   -0.410438   -3.722319
H      3.836494   -0.434878   -2.122918
H      4.691703   -0.478937    0.141816
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Number of imaginary frequencies = 0
Computed total Gibbs free energy = -4053.6017 a.u.

4
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C      5.010187   -3.352817   -1.261364
C      3.554775   -3.622423   -1.237887
C      2.849127   -3.733277   -0.011146
C      3.556792   -3.630639    1.215139
C      5.011972   -3.359782    1.238057
C      2.864387   -3.724478   -2.443764
C      1.425020   -3.902781   -0.010525
C      0.726994   -3.949184   -1.262737
C      1.473978   -3.890372   -2.452007
C     -0.739175   -3.953035   -1.261624
C     -1.435449   -3.916377   -0.008237
C     -0.737150   -3.960077    1.243768
C      0.729053   -3.957717    1.242467
C      1.478105   -3.907879    2.430846
C      2.868498   -3.741767    2.421424
H      3.437464   -3.668188    3.352333
H      0.973740   -3.960699    3.397888
H      3.431830   -3.644432   -3.375066
H      0.968015   -3.936037   -3.418608
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C    -1.486960   -3.892304   -2.450269
C    -2.860893   -3.757843   -0.006724
C    -1.483007   -3.904600    2.433939
C    -3.568637   -3.652241   -1.233444
C    -2.877992   -3.739560   -2.440610
H    -3.444972   -3.652463   -3.371172
C    -3.566446   -3.656129    1.221574
C    -2.873787   -3.749342    2.427204
H    -3.438980   -3.664719    3.359080
C    -5.025164   -3.391275   -1.255899
C    -5.022463   -3.391853    1.247302
H    -0.975767   -3.934562    3.400183
H    -0.981192   -3.917091   -3.417419
O     5.645287   -3.220090   -2.314102
O     5.648438   -3.232170    2.290589
O    -5.665720   -3.269680   -2.306425
O    -5.660486   -3.268580    2.299131
N     5.648194   -3.238745   -0.011777
N    -5.657277   -3.256197   -0.003632
C     5.079952    3.478064   -1.244186
C     3.609102    3.644864   -1.221357
C     2.894534    3.677995    0.004530
C     3.606982    3.629573    1.231127
C     5.077845    3.463809    1.254526
C     2.915981    3.708413   -2.428106
C     1.462883    3.740032    0.003672
C     0.765802    3.776156   -1.249594
C     1.517022    3.777646   -2.437867
C    -0.699004    3.797125   -1.250823
C    -1.397657    3.770720    0.001544
C    -0.700965    3.778645    1.255344
C     0.763741    3.758467    1.256173
C     1.512853    3.744971    2.445606
C     2.911833    3.677408    2.437394
H     3.484407    3.642022    3.368419
H     1.004882    3.770555    3.412031
H     3.490093    3.684139   -3.358534
H     1.010866    3.816442   -3.404851
C    -1.447494    3.825546   -2.439316
C    -2.830055    3.730789    0.000171
C    -1.451127    3.789630    2.442955
C    -3.542874    3.707001   -1.227813
C    -2.846476    3.776302   -2.432267
H    -3.418017    3.764073   -3.364320
C    -3.544913    3.693869    1.226757
C    -2.850248    3.744529    2.433063
H    -3.423375    3.721671    3.363922
C    -5.012414    3.531526   -1.253496
C    -5.015285    3.525126    1.248231
H    -0.945539    3.805587    3.410330
H    -0.940441    3.858463   -3.405527
O     5.721644    3.393048   -2.297711
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O	5.717872	3.367640	2.308094
O	-5.652082	3.440922	-2.307790
O	-5.658283	3.433499	2.300315
N	5.721156	3.380378	0.005229
N	-5.653531	3.422723	-0.003713
C	7.076762	-2.849729	-0.011691
H	7.521853	-3.295333	0.888592
H	7.520578	-3.290458	-0.915005
C	-7.076022	-2.833504	-0.002199
H	-7.530889	-3.263680	0.900543
H	-7.532931	-3.265035	-0.903303
C	-7.079683	3.019258	-0.005864
H	-7.528590	3.455000	-0.908735
H	-7.532011	3.456296	0.894675
C	7.153169	2.996108	0.004552
H	7.597964	3.440695	-0.896014
H	7.597789	3.435464	0.907790
C	7.218116	-1.340953	-0.007673
C	7.243232	-0.624949	-1.218331
C	7.249112	-0.631886	1.206874
C	7.269659	0.774515	-1.214898
H	7.211705	-1.174840	-2.163716
C	7.275652	0.767619	1.211321
H	7.222106	-1.187068	2.149322
C	7.270341	1.484946	0.000290
H	7.262004	1.329174	-2.158164
H	7.272282	1.316947	2.157672
C	-7.174663	-1.320690	-0.003265
C	-7.188281	-0.606160	1.209292
C	-7.178057	-0.607531	-1.216778
C	-7.193084	0.793634	1.208340
H	-7.172533	-1.158205	2.153968
C	-7.182704	0.792151	-1.217527
H	-7.154486	-1.160932	-2.160429
C	-7.184025	1.506673	-0.004976
H	-7.182094	1.346163	2.152782
H	-7.164094	1.343561	-2.162545
C	-2.377962	0.390886	-2.522538
C	-1.129484	0.389204	-3.241422
C	0.060782	-0.099304	-2.662005
C	-2.466600	-0.086261	-1.199591
C	-3.405322	0.134056	0.025009
C	3.338148	0.202923	0.722348
C	2.200070	-0.189101	1.459599
C	1.617351	0.070477	2.883147
C	3.333100	0.209449	-0.717530
C	2.190120	-0.176153	-1.450605
C	1.147355	-0.720431	-0.689699
C	1.152124	-0.726394	0.700915
C	-0.084527	-0.701213	1.419201
C	0.079248	-0.123286	2.686263
C	-1.107106	0.359405	3.278467

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C    -2.360516    0.367324    2.568103
C    -2.458261   -0.097178    1.241250
C    -1.292877   -0.687189    0.729649
C    -1.297835   -0.681176   -0.701400
C    -0.094208   -0.689008   -1.399323
C     1.597548    0.096539   -2.867659
H     4.218680    0.616922   -1.216901
H     4.227102    0.605897    1.219357
H     1.839204    1.115483   -3.213952
H    -1.117073    0.885236   -4.219145
H    -3.232641    0.886510   -2.995655
H    -4.260114   -0.569945    0.024576
H    -3.212174    0.857665    3.052021
H    -1.088249    0.845621    4.261034
H     1.861537    1.086111    3.237456
H    -3.850973    1.140330    0.031049
H     2.005139   -0.602080   -3.623940
H     2.030024   -0.635220    3.630037
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Number of imaginary frequencies = 0
Computed total Gibbs free energy = -4092.9278 a.u.

5
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C     5.002063    3.434104    1.460383
C     3.550434    3.718464    1.428531
C     2.845054    3.797832    0.198419
C     3.551039    3.656081   -1.025790
C     5.000533    3.356366   -1.040548
C     2.861238    3.860905    2.631326
C     1.422562    3.979276    0.193920
C     0.724100    4.054857    1.445199
C     1.471538    4.029688    2.635509
C    -0.742094    4.057198    1.443227
C    -1.437073    3.977465    0.190282
C    -0.738587    4.016627   -1.062326
C     0.727289    4.020145   -1.060475
C     1.477641    3.948971   -2.247601
C     2.865234    3.757778   -2.234176
H     3.431583    3.652547   -3.163162
H     0.974218    3.991705   -3.214974
H     3.427717    3.802260    3.564505
H     0.966011    4.099002    3.600927
C    -1.493225    4.040768    2.631427
C    -2.859337    3.794514    0.191658
C    -1.485331    3.937979   -2.251225
C    -3.568369    3.721766    1.420047
C    -2.883012    3.872644    2.624051
H    -3.452502    3.820917    3.555812
C    -3.561404    3.645320   -1.033900
C    -2.872356    3.742450   -2.240781
H    -3.435735    3.630479   -3.170772
C    -5.020008    3.436993    1.449145
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C    -5.009910    3.341012   -1.051164
H    -0.979080    3.977169   -3.217204
H    -0.990750    4.117601    3.597907
O     5.637402    3.326521    2.516261
O     5.636631    3.179548   -2.085945
O    -5.658733    3.336229    2.503650
O    -5.641963    3.153380   -2.097152
N     5.635668    3.263926    0.213162
N    -5.649001    3.256361    0.200989
C     5.046971   -3.698209    1.015839
C     3.582487   -3.903944    0.948181
C     2.868295   -3.686564   -0.259740
C     3.578358   -3.375641   -1.448568
C     5.046448   -3.206601   -1.437058
C     2.890650   -4.265735    2.102775
C     1.436906   -3.765540   -0.275095
C     0.741186   -4.100320    0.933203
C     1.494761   -4.375859    2.087759
C    -0.724459   -4.102066    0.934477
C    -1.422993   -3.768116   -0.272364
C    -0.726158   -3.495473   -1.496615
C     0.737250   -3.494951   -1.498194
C     1.484318   -3.215239   -2.655235
C     2.882084   -3.163897   -2.636226
H     3.452477   -2.926133   -3.537437
H     0.975831   -3.007530   -3.598740
H     3.463151   -4.438588    3.018298
H     0.990312   -4.647922    3.016695
C    -1.475438   -4.380272    2.090080
C    -2.854516   -3.691622   -0.254207
C    -1.475867   -3.214853   -2.651717
C    -3.566089   -3.910470    0.955043
C    -2.871512   -4.272426    2.107877
H    -3.441889   -4.446851    3.024430
C    -3.567327   -3.381534   -1.441541
C    -2.873703   -3.166598   -2.630137
H    -3.446395   -2.928148   -3.529676
C    -5.030680   -3.706012    1.025773
C    -5.035983   -3.217670   -1.427771
H    -0.969519   -3.003755   -3.595605
H    -0.968900   -4.652569    3.017802
O     5.685163   -3.794908    2.070735
O     5.694016   -2.913550   -2.449631
O    -5.666477   -3.802303    2.082137
O    -5.686646   -2.929939   -2.439838
N     5.687290   -3.352731   -0.191747
N    -5.673890   -3.362613   -0.180814
C     7.060113    2.863265    0.219998
H     7.531654    3.343141   -0.648802
H     7.484761    3.260899    1.152319
C    -7.071969    2.850348    0.205752
H    -7.542989    3.323687   -0.666906
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H	-7.500791	3.251285	1.134758
C	-7.105352	-2.988637	-0.115755
H	-7.514309	-3.495911	0.768826
H	-7.582954	-3.368955	-1.029329
C	7.117696	-2.973920	-0.128422
H	7.530585	-3.483389	0.753068
H	7.594454	-3.348701	-1.044704
C	7.195763	1.355520	0.149512
C	6.995570	0.568800	1.300927
C	7.449825	0.717629	-1.076648
C	7.017714	-0.828217	1.218047
H	6.799412	1.062951	2.257643
C	7.476031	-0.680580	-1.159349
H	7.588834	1.325926	-1.975389
C	7.243050	-1.467308	-0.017397
H	6.834542	-1.437160	2.109148
H	7.636130	-1.173083	-2.122861
C	-7.201257	1.341677	0.142614
C	-7.456278	0.696932	-1.079686
C	-6.993709	0.561212	1.297013
C	-7.476408	-0.701761	-1.155770
H	-7.600853	1.300231	-1.980920
C	-7.009729	-0.836258	1.220765
H	-6.796778	1.060785	2.250747
C	-7.236355	-1.482102	-0.010968
H	-7.637283	-1.199468	-2.116450
H	-6.821008	-1.440015	2.114288
P	-0.000986	0.913889	0.244868
S	-2.796499	-0.031427	1.681697
S	2.796026	-0.029458	1.684168
S	0.000740	0.856102	-3.118366
C	-0.000266	-0.265582	1.638202
C	-1.432912	0.342220	-0.744554
C	2.650453	0.043083	-0.092074
C	1.433121	0.345021	-0.743046
C	-1.429130	0.406117	-2.153416
C	1.215933	-0.642967	2.244547
C	-1.217132	-1.403989	3.426796
H	-2.168504	-1.695208	3.880988
C	-3.845286	-0.112349	-0.819768
H	-4.780557	-0.324469	-0.295094
C	2.624060	0.243767	-2.881578
H	2.601473	0.302954	-3.974317
C	-1.216649	-0.644537	2.243373
C	-2.650307	0.038673	-0.094531
C	3.846375	-0.104777	-0.816431
H	4.781903	-0.314368	-0.291211
C	-2.621939	0.238980	-2.883881
H	-2.598738	0.298688	-3.976589
C	1.430532	0.408979	-2.151976
C	-0.000690	-1.768567	4.017150
H	-0.000792	-2.347530	4.946219

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C      1.215867   -1.401942    3.428398
H      2.167038   -1.691442    3.884015
C      3.830769    0.026308   -2.208683
H      4.763989   -0.084754   -2.766362
C     -3.828767    0.018814   -2.212021
H     -4.761314   -0.093155   -2.770682
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Number of imaginary frequencies = 0
Computed total Gibbs free energy = -5514.0061 a.u.

6
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C      5.055636   -2.983486   -2.173272
C      3.577777   -3.052626   -2.168029
C      2.863993   -3.379363   -0.985823
C      3.577741   -3.664145    0.208076
C      5.049805   -3.517468    0.268285
C      2.882606   -2.742792   -3.335156
C      1.430816   -3.390559   -0.990278
C      0.732682   -3.055653   -2.197838
C      1.482660   -2.740999   -3.344736
C     -0.733533   -3.054465   -2.197763
C     -1.431991   -3.390431   -0.990711
C     -0.733331   -3.728032    0.215563
C      0.731838   -3.727207    0.216061
C      1.480178   -4.038664    1.364058
C      2.879586   -3.994998    1.367291
H      3.448761   -4.191864    2.279725
H      0.973546   -4.287479    2.297617
H      3.457180   -2.492140   -4.231037
H      0.975891   -2.484416   -4.277453
C     -1.483145   -2.736567   -3.344012
C     -2.865162   -3.379065   -0.986667
C     -1.482015   -4.041703    1.362725
C     -3.578613   -3.049650   -2.168360
C     -2.883092   -2.737383   -3.334621
H     -3.457369   -2.484184   -4.229977
C     -3.579229   -3.666274    0.206422
C     -2.881436   -3.998875    1.365364
H     -3.450941   -4.197666    2.277174
C     -5.056426   -2.979975   -2.173785
C     -5.051314   -3.519833    0.266502
H     -0.975638   -4.291734    2.296076
H     -0.976060   -2.477710   -4.275932
O      5.706547   -2.725958   -3.191928
O      5.687569   -3.642592    1.321236
O     -5.706986   -2.719815   -3.191987
O     -5.689293   -3.647391    1.319021
N      5.698424   -3.183331   -0.935715
N     -5.699629   -3.183090   -0.937001
C      5.036459    3.503615   -1.386534
C      3.571151    3.716167   -1.359945
C      2.857757    3.750854   -0.133633
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C    3.563298    3.610475    1.091050
C    5.021469    3.352124    1.108660
C    2.880363    3.840042   -2.564318
C    1.430206    3.889697   -0.132436
C    0.732267    3.958625   -1.384128
C    1.484336    3.955837   -2.572211
C   -0.733981    3.959156   -1.383650
C   -1.431194    3.889424   -0.131577
C   -0.732490    3.908193    1.120177
C    0.732192    3.908853    1.119721
C    1.479410    3.829696    2.309440
C    2.871047    3.668736    2.298010
H    3.436034    3.561126    3.227790
H    0.973525    3.855218    3.275849
H    3.452805    3.818267   -3.495747
H    0.980130    4.020884   -3.538910
C   -1.486890    3.958400   -2.571239
C   -2.858755    3.750408   -0.132118
C   -1.478977    3.827867    2.310274
C   -3.572928    3.716862   -1.357990
C   -2.882925    3.842508   -2.562628
H   -3.455945    3.822080   -3.493733
C   -3.563464    3.608789    1.092873
C   -2.870534    3.666264    2.299457
H   -3.434958    3.557740    3.229470
C   -5.038249    3.504192   -1.383909
C   -5.021644    3.350576    1.111152
H   -0.972699    3.852942    3.276489
H   -0.983335    4.025337   -3.538157
O    5.684069    3.466731   -2.439103
O    5.650581    3.162764    2.155735
O   -5.686499    3.467918   -2.436091
O   -5.650103    3.160080    2.158439
N    5.668130    3.319041   -0.142007
N   -5.669219    3.319159   -0.138996
C    7.141345   -2.848330   -0.868475
H    7.553942   -3.417039   -0.024341
H    7.592681   -3.182349   -1.812745
C   -7.142499   -2.847792   -0.869346
H   -7.555132   -3.417357   -0.025808
H   -7.593993   -3.180699   -1.813941
C   -7.103790    2.950700   -0.154433
H   -7.562565    3.498330   -0.989271
H   -7.521348    3.293129    0.802270
C    7.102771    2.950719   -0.158147
H    7.560854    3.497820   -0.993714
H    7.520954    3.293908    0.798014
C    7.296682   -1.353037   -0.672901
C    7.392993   -0.495865   -1.784710
C    7.226510   -0.792384    0.616986
C    7.374944    0.893223   -1.613648
H    7.443975   -0.926913   -2.788529
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C      7.205330    0.597145    0.787466
H      7.160299   -1.456339    1.485137
C      7.259840    1.453051   -0.328603
H      7.412762    1.556173   -2.482953
H      7.114930    1.029789    1.788664
C     -7.297643   -1.352666   -0.672255
C     -7.224623   -0.793001    0.617970
C     -7.396586   -0.494680   -1.783132
C     -7.203515    0.596352    0.789481
H     -7.156552   -1.457633    1.485476
C     -7.378301    0.894307   -1.611044
H     -7.449544   -0.924855   -2.787206
C     -7.260695    1.453121   -0.325858
H     -7.111156    1.028270    1.790788
H     -7.417697    1.557894   -2.479794
P      0.000895    0.805019    2.447672
C     -1.313265    0.298382    1.314341
C      1.316665    0.299615    1.315769
C     -1.222035   -1.387906    3.626109
C      0.000990   -0.778682    3.315468
C      2.440712   -0.358717    1.832699
C     -2.437437   -0.360830    1.829824
C     -2.323261    0.380620   -0.884349
H     -2.259458    0.614018   -1.949874
C      2.328645    0.381292   -0.881931
H      2.265889    0.614005   -1.947670
C      1.234631   -2.527873    4.441238
H      2.183659   -2.992599    4.721377
C     -1.202521    0.551973   -0.059956
C      1.207018    0.552646   -0.058695
C     -1.232099   -2.529465    4.439294
H     -2.180983   -2.995421    4.717903
C      3.583702   -0.507922    1.039475
H      4.488798   -0.959330    1.451213
C      1.224309   -1.386470    3.627889
C     -3.516725   -0.088610   -0.305884
H     -4.412269   -0.183486   -0.927947
C     -3.579746   -0.509742    1.035523
H     -4.485168   -0.961281    1.446319
C      0.001256   -3.059766    4.862997
H      0.001309   -3.942447    5.509886
C      3.521709   -0.087352   -0.302222
H      4.417696   -0.182538   -0.923632
O      0.002399    0.985630   -0.626428
O      2.431005   -0.872268    3.140222
O     -2.428761   -0.875399    3.136844
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Number of imaginary frequencies = 0
Computed total Gibbs free energy = -4544.3356 a.u.

Lowest energy transition structure complexes between the inversion TSs of 1-6 and the PBI cyclophane catalyst

1

C	-4.949902	-3.294822	1.251059
C	-3.473146	-3.386715	1.227759
C	-2.757785	-3.397022	0.000786
C	-3.473322	-3.388395	-1.226100
C	-4.950074	-3.296254	-1.249324
C	-2.776209	-3.393472	2.432972
C	-1.323790	-3.405424	0.000698
C	-0.625100	-3.401774	1.253235
C	-1.375467	-3.401229	2.441584
C	0.840952	-3.382942	1.253729
C	1.539395	-3.365514	0.000499
C	0.840803	-3.384452	-1.252630
C	-0.625256	-3.403534	-1.251930
C	-1.375786	-3.404797	-2.440179
C	-2.776538	-3.396951	-2.431392
H	-3.349429	-3.381163	-3.362612
H	-0.868753	-3.402266	-3.407456
H	-3.348986	-3.376379	3.364238
H	-0.868301	-3.397200	3.408782
C	1.592092	-3.374546	2.442112
C	2.973839	-3.325515	0.000394
C	1.591806	-3.377152	-2.441105
C	3.689438	-3.304050	1.226968
C	2.991764	-3.332851	2.433302
H	3.565026	-3.316706	3.364302
C	3.689304	-3.305009	-1.226285
C	2.991480	-3.335063	-2.432500
H	3.564615	-3.319595	-3.363592
C	5.168768	-3.226231	1.249936
C	5.168622	-3.226750	-1.249481
H	1.085106	-3.396127	-3.408365
H	1.085497	-3.392450	3.409445
O	-5.596145	-3.239429	2.303984
O	-5.596428	-3.241894	-2.302235
O	5.813686	-3.185183	2.303833
O	5.813387	-3.185873	-2.303476
N	-5.595687	-3.237653	0.000879
N	5.816296	-3.182713	0.000180
C	-4.949117	3.296506	1.249379
C	-3.472361	3.388465	1.226166
C	-2.756838	3.397252	-0.000727
C	-3.472196	3.387184	-1.227703
C	-4.948958	3.295484	-1.251010
C	-2.775564	3.396655	2.431457
C	-1.322841	3.405466	-0.000637
C	-0.624295	3.403365	1.251982
C	-1.374813	3.404368	2.440239
C	0.841765	3.384343	1.252672
C	1.540349	3.365378	-0.000459
C	0.841893	3.382820	-1.253683

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C    -0.624160    3.401883   -1.253181
C    -1.374525    3.401608   -2.441533
C    -2.775265    3.394015   -2.432919
H    -3.348051    3.377116   -3.364183
H    -0.867355    3.397670   -3.408730
H    -3.348453    3.380679    3.362675
H    -0.867764    3.401498    3.407506
C     1.592786    3.377218    2.441135
C     2.974792    3.325349   -0.000365
C     1.593028    3.374298   -2.442066
C     3.690276    3.304944    1.226304
C     2.992466    3.335147    2.432521
H     3.565606    3.319792    3.363610
C     3.690388    3.303797   -1.226940
C     2.992705    3.332541   -2.433266
H     3.565952    3.316299   -3.364273
C     5.169596    3.226525    1.249494
C     5.169721    3.225831   -1.249912
H     1.086434    3.392156   -3.409400
H     1.086107    3.396382    3.408403
O    -5.595478    3.241937    2.302275
O    -5.595215    3.240227   -2.303936
O     5.814348    3.185729    2.303497
O     5.814615    3.184745   -2.303818
N    -5.594744    3.238355   -0.000833
N     5.817262    3.182176   -0.000164
C    -7.043159   -2.918307    0.000850
H    -7.468634   -3.378469   -0.901176
H    -7.468571   -3.377905    0.903193
C     7.275390   -2.911229    0.000079
H     7.683901   -3.386147   -0.902221
H     7.684029   -3.386116    0.902338
C     7.276275    2.910197   -0.000066
H     7.684934    3.384976    0.902239
H     7.685070    3.384961   -0.902318
C    -7.042314    2.919443   -0.000829
H    -7.467669    3.379702    0.901205
H    -7.467574    3.379196   -0.903165
C    -7.217936   -1.412695    0.000399
C    -7.238953   -0.698954    1.213151
C    -7.238623   -0.699654   -1.212773
C    -7.238746    0.700840    1.212748
H    -7.220204   -1.250365    2.157976
C    -7.238426    0.700138   -1.213178
H    -7.219630   -1.251617   -2.157274
C    -7.217516    1.413875   -0.000416
H    -7.219800    1.252797    2.157251
H    -7.219263    1.251547   -2.157995
C     7.498239   -1.412419    0.000042
C     7.531846   -0.700139   -1.212905
C     7.531720   -0.700076    1.212960
C     7.532066    0.698976   -1.212940
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H	7.508372	-1.251283	-2.157727
C	7.531901	0.699037	1.212924
H	7.508167	-1.251175	2.157801
C	7.498644	1.411325	-0.000027
H	7.508796	1.250081	-2.157786
H	7.508506	1.250187	2.157744
C	-2.741534	0.000774	0.735756
H	-3.764019	0.001149	1.135514
C	-2.741634	-0.000322	-0.735839
H	-3.764170	-0.000270	-1.135472
C	-1.778661	-0.001382	-1.693300
H	-2.177663	-0.002014	-2.714952
C	-0.305801	-0.002032	-1.691039
H	0.094436	-0.003446	-2.713340
C	-1.778439	0.001553	1.693093
H	-2.177311	0.002425	2.714795
C	-0.305574	0.001578	1.690653
H	0.094790	0.002774	2.712905
C	0.659313	0.000393	0.735725
C	0.659209	-0.001311	-0.736232
H	1.680150	0.000774	1.137784
H	1.679991	-0.002228	-1.138427

Number of imaginary frequencies = 1 (-113.7 cm^{-1})
Computed total Gibbs free energy = -3594.2615 a.u.

2

C	5.054804	-3.300283	-1.250168
C	3.579037	-3.406192	-1.226922
C	2.864621	-3.424581	0.000032
C	3.579006	-3.406206	1.227001
C	5.054772	-3.300333	1.250285
C	2.882405	-3.426532	-2.432850
C	1.431179	-3.447420	0.000014
C	0.732586	-3.454496	-1.252495
C	1.482557	-3.451501	-2.441435
C	-0.732633	-3.454430	-1.252516
C	-1.431260	-3.447405	-0.000028
C	-0.732669	-3.454617	1.252480
C	0.732551	-3.454553	1.252502
C	1.482490	-3.451477	2.441461
C	2.882340	-3.426490	2.432912
H	3.455134	-3.406166	3.364082
H	0.974948	-3.455857	3.408234
H	3.455223	-3.406244	-3.364006
H	0.975039	-3.455939	-3.408219
C	-1.482571	-3.451292	-2.441477
C	-2.864701	-3.424552	-0.000045
C	-1.482644	-3.451772	2.441417
C	-3.579083	-3.406083	-1.227013
C	-2.882419	-3.426304	-2.432925
H	-3.455213	-3.405931	-3.364094

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C   -3.579123   -3.406279    1.226906
C   -2.882493   -3.426775    2.432833
H   -3.455311   -3.406594    3.363992
C   -5.054850   -3.300218   -1.250292
C   -5.054889   -3.300332    1.250159
H   -0.975130   -3.456361    3.408203
H   -0.975030   -3.455636   -3.408250
O    5.700891   -3.237956   -2.302820
O    5.700839   -3.238066    2.302952
O   -5.700914   -3.237924   -2.302959
O   -5.700975   -3.238086    2.302815
N    5.700260   -3.240360    0.000065
N   -5.700339   -3.240275   -0.000073
C    5.054860    3.300341   -1.250095
C    3.579095    3.406294   -1.226826
C    2.864687    3.424555    0.000133
C    3.579083    3.406088    1.227093
C    5.054851    3.300254    1.250356
C    2.882454    3.426799   -2.432746
C    1.431246    3.447399    0.000130
C    0.732643    3.454640   -1.252371
C    1.482606    3.451806   -2.441316
C   -0.732576    3.454603   -1.252379
C   -1.431194    3.447421    0.000114
C   -0.732590    3.454439    1.252617
C    0.732630    3.454393    1.252626
C    1.482580    3.451243    2.441577
C    2.882431    3.426281    2.433012
H    3.455234    3.405913    3.364175
H    0.975050    3.455570    3.408357
H    3.455262    3.406620   -3.363910
H    0.975081    3.456403   -3.408096
C   -1.482525    3.451610   -2.441333
C   -2.864636    3.424589    0.000107
C   -1.482551    3.451375    2.441562
C   -3.579030    3.406293   -1.226859
C   -2.882375    3.426646   -2.432774
H   -3.455177    3.406383   -3.363940
C   -3.579042    3.406135    1.227064
C   -2.882400    3.426401    2.432987
H   -3.455210    3.406062    3.364147
C   -5.054796    3.300418   -1.250138
C   -5.054809    3.300241    1.250316
H   -0.975026    3.455765    3.408342
H   -0.974990    3.456040   -3.408110
O    5.700932    3.238079   -2.302759
O    5.700931    3.237988    2.303015
O   -5.700868    3.238195   -2.302805
O   -5.700892    3.237868    2.302967
N    5.700325    3.240304    0.000128
N   -5.700274    3.240388    0.000083
C    7.146882   -2.918717    0.000090
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H     7.573079  -3.377885   0.902303
H     7.573117  -3.377891  -0.902103
C    -7.146960  -2.918625  -0.000092
H    -7.573200  -3.377818   0.902089
H    -7.573161  -3.377766  -0.902317
C    -7.146897   2.918751   0.000053
H    -7.573093   3.377944  -0.902148
H    -7.573132   3.377904   0.902257
C     7.146946   2.918660   0.000132
H     7.573174   3.377841  -0.902061
H     7.573159   3.377812   0.902346
C     7.320222  -1.413168   0.000094
C     7.341252  -0.699930  -1.212958
C     7.341187  -0.699947   1.213158
C     7.341274   0.699891  -1.212949
H     7.322607  -1.251866  -2.157469
C     7.341210   0.699873   1.213168
H     7.322488  -1.251895   2.157661
C     7.320266   1.413110   0.000113
H     7.322652   1.251839  -2.157454
H     7.322539   1.251807   2.157679
C    -7.320285  -1.413076  -0.000055
C    -7.341339  -0.699878   1.213019
C    -7.341184  -0.699818  -1.213099
C    -7.341316   0.699943   1.213052
H    -7.322751  -1.251845   2.157513
C    -7.341160   0.700004  -1.213063
H    -7.322479  -1.251736  -2.157618
C    -7.320239   1.413203   0.000014
H    -7.322704   1.251862   2.157573
H    -7.322427   1.251969  -2.157555
C     0.614863   0.000041  -1.561632
C    -0.616107   0.000099  -1.561218
C     0.616203  -0.000146   1.560549
C    -0.614767  -0.000187   1.560959
C    -2.025076   0.000185  -1.679675
H    -2.384793   0.000366  -2.718127
C    -3.009787   0.000067  -0.729072
H    -4.025784   0.000148  -1.143781
C    -3.009151  -0.000153   0.730740
H    -4.024786  -0.000228   1.146324
C    -2.023641  -0.000260   1.680518
H    -2.382508  -0.000436   2.719265
C     2.025170  -0.000100   1.679018
H     2.384882  -0.000093   2.717471
C     3.009880  -0.000069   0.728414
H     4.025880  -0.000054   1.143117
C     3.009246  -0.000054  -0.731397
H     4.024884  -0.000071  -1.146971
C     2.023740  -0.000023  -1.681180
H     2.382615  -0.000032  -2.719925
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Number of imaginary frequencies = 1 (-65.3 cm^{-1})
Computed total Gibbs free energy = -3746.8562 a.u.

3

C	4.981880	-3.285596	-1.379868
C	3.506221	-3.394456	-1.353572
C	2.794376	-3.405157	-0.125380
C	3.509224	-3.357627	1.099687
C	4.983062	-3.236243	1.119471
C	2.808294	-3.431648	-2.558519
C	1.361429	-3.436867	-0.123247
C	0.660976	-3.458051	-1.374779
C	1.408453	-3.462556	-2.565144
C	-0.804106	-3.457367	-1.372616
C	-1.500364	-3.442436	-0.119013
C	-0.799664	-3.435300	1.133240
C	0.665436	-3.429476	1.131194
C	1.415985	-3.402686	2.318901
C	2.814518	-3.363147	2.307437
H	3.387112	-3.313264	3.237032
H	0.910180	-3.382489	3.285857
H	3.379979	-3.417884	-3.490461
H	0.899334	-3.477766	-3.530662
C	-1.555316	-3.454261	-2.560920
C	-2.933477	-3.415404	-0.116737
C	-1.546179	-3.422543	2.323571
C	-3.649649	-3.398957	-1.342321
C	-2.955035	-3.423860	-2.549822
H	-3.529846	-3.404360	-3.479795
C	-3.644572	-3.380458	1.111554
C	-2.945410	-3.391900	2.316590
H	-3.515927	-3.357407	3.248515
C	-5.125347	-3.291696	-1.363253
C	-5.120171	-3.273065	1.137161
H	-1.037286	-3.410055	3.288945
H	-1.048725	-3.461943	-3.528047
O	5.626057	-3.235707	-2.434768
O	5.629768	-3.139445	2.169290
O	-5.773373	-3.235836	-2.415139
O	-5.763991	-3.202753	2.190724
N	5.629627	-3.213024	-0.131821
N	-5.768627	-3.225306	-0.112085
C	4.987287	3.283569	-1.380987
C	3.511723	3.393565	-1.353627
C	2.800574	3.402830	-0.125044
C	3.516114	3.354549	1.099606
C	4.990062	3.234272	1.118375
C	2.813186	3.433134	-2.558152
C	1.367635	3.434737	-0.122077
C	0.666558	3.458834	-1.373197
C	1.413367	3.465244	-2.563976
C	-0.798529	3.459702	-1.370255

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C   -1.494190    3.442520   -0.116353
C   -0.792847    3.431381    1.135525
C    0.672247    3.425371    1.132699
C    1.423456    3.398028    2.319976
C    2.822016    3.358978    2.307699
H    3.395093    3.309008    3.237005
H    0.918240    3.377773    3.287229
H    3.384384    3.420463   -3.490403
H    0.903744    3.482910   -3.529194
C   -1.550311    3.460218   -2.558189
C   -2.927329    3.417085   -0.113465
C   -1.538788    3.415585    2.326159
C   -3.644125    3.404241   -1.338730
C   -2.950056    3.431229   -2.546515
H   -3.525331    3.414344   -3.476248
C   -3.637871    3.379998    1.115110
C   -2.938053    3.386789    2.319774
H   -3.508137    3.350285    3.251887
C   -5.119928    3.298086   -1.359261
C   -5.113598    3.275039    1.141127
H   -1.029496    3.399129    3.291257
H   -1.044196    3.469826   -3.525544
O    5.630609    3.233106   -2.436374
O    5.637596    3.137904    2.167732
O   -5.768388    3.244330   -2.410989
O   -5.757154    3.203646    2.194793
N    5.635839    3.210990   -0.133377
N   -5.762727    3.230679   -0.107938
C    7.081797   -2.916739   -0.136151
H    7.502938   -3.380353    0.766199
H    7.495551   -3.387110   -1.038538
C   -7.217454   -2.912764   -0.111009
H   -7.640394   -3.374610    0.791422
H   -7.640656   -3.374922   -1.013111
C   -7.212053    2.920589   -0.106464
H   -7.635073    3.385078   -1.007468
H   -7.633607    3.381583    0.797041
C    7.087670    2.912637   -0.138372
H    7.501519    3.381607   -1.041439
H    7.510085    3.376343    0.763323
C    7.284324   -1.415214   -0.141652
C    7.252439   -0.702172   -1.355131
C    7.375070   -0.702164    1.067792
C    7.253874    0.696820   -1.355643
H    7.185902   -1.254903   -2.296926
C    7.376594    0.698420    1.067260
H    7.396364   -1.253564    2.012438
C    7.287409    1.410713   -0.142737
H    7.188340    1.249101   -2.297763
H    7.398919    1.250558    2.011427
C   -7.399649   -1.408515   -0.110936
C   -7.430846   -0.696603    1.102519
```

42

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C     -7.412518    -0.694645    -1.323695
C     -7.429437     0.702961     1.103582
H     -7.417435    -1.249446     2.046512
C     -7.411303     0.704667    -1.322642
H     -7.385411    -1.246092    -2.268269
C     -7.397011     1.416672    -0.108800
H     -7.414888     1.254300     2.048442
H     -7.383100     1.257510    -2.266364
C     -3.106375     0.000138     0.057092
C     -2.640089     0.000103    -1.277535
C     -2.312449    -0.001023     2.674601
C     -2.212624    -0.000711     1.215981
C     -0.892534    -0.001061     0.819654
C     -1.218919    -0.000426    -1.633638
C     -1.185529    -0.001068     3.530556
C     -0.386161    -0.000331    -2.837555
C      3.217639    -0.001840    -1.153909
C      3.627337    -0.001886     0.199513
C      1.812162    -0.001276    -1.569419
C      0.976269    -0.001202    -0.474760
C      1.381742    -0.001564     0.867938
C      2.683340    -0.001658     1.318535
C      2.721109    -0.001501     2.781025
C      1.559061    -0.001118     3.588381
C      0.197733    -0.001261     3.045412
C      0.227034    -0.001361     1.668203
C      1.029619    -0.000757    -2.807224
C     -0.430041    -0.000826    -0.504449
H      3.688403    -0.001259     3.295557
H      1.712042    -0.000890     4.673823
H     -1.384166    -0.001126     4.608602
H     -3.300133    -0.000952     3.148946
H     -4.193312     0.000763     0.203971
H     -3.402156     0.000544    -2.064308
H     -0.861088     0.000119    -3.825326
H      1.546105    -0.000631    -3.773764
H      4.014240    -0.002597    -1.906132
H      4.705740    -0.002545     0.391750
```

Number of imaginary frequencies = 1 (-73.2 cm^{-1})
Computed total Gibbs free energy = -4053.5951 a.u.

4
```
C      5.052548     3.339065     1.250844
C      3.577334     3.452964     1.227135
C      2.863757     3.480604    -0.000825
C      3.577060     3.451423    -1.228942
C      5.052300     3.337693    -1.252880
C      2.879650     3.454589     2.432926
C      1.430765     3.504191    -0.000646
C      0.732378     3.501014     1.252372
C      1.480142     3.478571     2.441507
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C	-0.733317	3.502546	1.252249
C	-1.432148	3.483091	-0.000364
C	-0.733566	3.502135	-1.253124
C	0.732100	3.499847	-1.253502
C	1.479542	3.475583	-2.442775
C	2.879048	3.451338	-2.434542
H	3.450275	3.408439	-3.365549
H	0.971832	3.444160	-3.408369
H	3.451133	3.413025	3.363835
H	0.972753	3.448733	3.407345
C	-1.483358	3.521239	2.440628
C	-2.864947	3.445406	-0.000208
C	-1.483810	3.521270	-2.441381
C	-3.578847	3.421150	1.226301
C	-2.883253	3.475628	2.431935
H	-3.457071	3.466881	3.362896
C	-3.579068	3.421679	-1.226606
C	-2.883711	3.476255	-2.432374
H	-3.457802	3.468052	-3.363172
C	-5.053035	3.292986	1.249699
C	-5.053285	3.294128	-1.249758
H	-0.975918	3.561255	-3.407306
H	-0.975278	3.561058	3.406431
O	5.700114	3.277259	2.302353
O	5.699679	3.275033	-2.304441
O	-5.697567	3.221235	2.302721
O	-5.698116	3.223666	-2.302698
N	5.696178	3.261974	-0.001042
N	-5.698903	3.231843	0.000021
C	5.041340	-3.343075	1.252409
C	3.565958	-3.454464	1.228484
C	2.852656	-3.482566	0.000400
C	3.566212	-3.455282	-1.227579
C	5.041613	-3.343787	-1.251314
C	2.868054	-3.454233	2.434144
C	1.419640	-3.504933	0.000309
C	0.721016	-3.500496	1.253187
C	1.468541	-3.477284	2.442469
C	-0.744670	-3.501648	1.252808
C	-1.443251	-3.482234	0.000071
C	-0.744484	-3.502449	-1.252556
C	0.721210	-3.501424	-1.252672
C	1.468936	-3.479104	-2.441837
C	2.868461	-3.455983	-2.433336
H	3.439935	-3.414762	-3.364267
H	0.961474	-3.448701	-3.407602
H	3.439425	-3.412290	3.365100
H	0.960952	-3.446181	3.408155
C	-1.494957	-3.520207	2.441035
C	-2.876022	-3.443169	-0.000032
C	-1.494602	-3.521716	-2.440893
C	-3.590130	-3.418105	1.226330

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C   -2.894814   -3.473451    2.432087
H   -3.468772   -3.464331    3.362957
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C   -2.894472   -3.475038   -2.432153
H   -3.468338   -3.466475   -3.363087
C   -5.064163   -3.287702    1.249459
C   -5.063967   -3.288585   -1.249961
H   -0.986609   -3.562779   -3.406715
H   -0.987085   -3.560668    3.406923
O    5.688804   -3.281154    2.303982
O    5.689261   -3.282471   -2.302804
O   -5.708770   -3.215730    2.302404
O   -5.708415   -3.217286   -2.303063
N    5.685460   -3.268919    0.000590
N   -5.709647   -3.224053   -0.000313
C    7.137232    2.916400   -0.000959
H    7.570915    3.368496   -0.903173
H    7.570847    3.368883    0.901088
C   -7.148462    2.922567    0.000000
H   -7.569587    3.386592   -0.902226
H   -7.569654    3.386425    0.902289
C   -7.158241   -2.910142   -0.000538
H   -7.581117   -3.372849    0.901548
H   -7.580673   -3.372565   -0.902972
C    7.127520   -2.927329    0.000712
H    7.559708   -3.380637    0.903034
H    7.559981   -3.381169   -0.901219
C    7.289495    1.407913   -0.000572
C    7.304055    0.694458    1.212584
C    7.304207    0.693734   -1.213300
C    7.301562   -0.705201    1.213003
H    7.285581    1.246635    2.157041
C    7.301676   -0.705916   -1.212872
H    7.285895    1.245350   -2.158090
C    7.284430   -1.419334    0.000270
H    7.281202   -1.256754    2.157781
H    7.281399   -1.258094   -2.157283
C   -7.341632    1.419620   -0.000141
C   -7.370643    0.706631   -1.213097
C   -7.371782    0.706416    1.212646
C   -7.373021   -0.693292   -1.213221
H   -7.348554    1.258609   -2.157523
C   -7.374177   -0.693503    1.212526
H   -7.350577    1.258234    2.157184
C   -7.346471   -1.406580   -0.000396
H   -7.353003   -1.245172   -2.157761
H   -7.355093   -1.245521    2.157009
C    1.169420   -0.001930   -3.412854
C    2.434568   -0.002342   -2.683676
C    2.504859   -0.001940   -1.260940
C   -0.101622   -0.000942   -2.763320
C   -1.686783   -0.000078   -2.973473
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C    1.174454   -0.000132    3.412514
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C    2.438512   -0.000787    2.681500
C    2.506679   -0.001092    1.258673
C    1.239275   -0.000618    0.701479
C    0.048855    0.000201    1.388757
C   -1.168255    0.000775    0.688288
C   -2.286912    0.001183    1.502179
C   -3.487908    0.001123    0.732912
C   -3.488912    0.000933   -0.726445
C   -2.289052    0.000691   -1.497457
C   -1.169220    0.000560   -0.685193
C    0.046882   -0.000439   -1.387466
C    1.238293   -0.001041   -0.701913
C    3.481336   -0.001452   -0.001837
H    3.347263   -0.001114    3.293635
H    1.259241   -0.000100    4.505570
H    3.342400   -0.003126   -3.297170
H    1.252624   -0.002472   -4.506035
H   -4.478092    0.000622   -1.197870
H   -4.476433    0.000934    1.205743
H   -2.016338   -0.884740    3.545288
H   -2.015734    0.886653    3.545428
H    4.150219    0.874961   -0.002658
H    4.151718   -0.876710   -0.001991
H   -2.020639    0.885652   -3.541199
H   -2.021660   -0.885623   -3.540854
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Number of imaginary frequencies = 1 (-94.3 cm^{-1})
Computed total Gibbs free energy = -4092.907 a.u.

5
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C   -5.046471    3.252322   -1.302329
C   -3.577463    3.423002   -1.283146
C   -2.865617    3.482274   -0.056883
C   -3.578825    3.469731    1.172023
C   -5.051190    3.349913    1.197977
C   -2.882160    3.452715   -2.490995
C   -1.432359    3.528647   -0.058347
C   -0.734043    3.544086   -1.312438
C   -1.484484    3.524718   -2.501727
C    0.730437    3.544547   -1.312234
C    1.428418    3.528811   -0.057964
C    0.729337    3.537195    1.194247
C   -0.733622    3.537627    1.194047
C   -1.482403    3.545855    2.387093
C   -2.880044    3.518425    2.378067
H   -3.453080    3.504116    3.309056
H   -0.973789    3.552923    3.352791
H   -3.454714    3.398280   -3.420540
H   -0.976864    3.533982   -3.468250
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C    1.481215    3.526229   -2.501322
C    2.861679    3.482686   -0.056148
C    1.477768    3.543876    2.387529
C    3.573901    3.424492   -1.282253
C    2.878925    3.454847   -2.490277
H    3.451739    3.401409   -3.419719
C    3.574541    3.469303    1.172955
C    2.875411    3.516502    2.378852
H    3.448195    3.501150    3.309978
C    5.043011    3.254597   -1.301179
C    5.046945    3.350155    1.199203
H    0.968902    3.549535    3.353112
H    0.973849    3.535999   -3.467966
O   -5.687040    3.105681   -2.351108
O   -5.702233    3.321660    2.249616
O    5.683933    3.109203   -2.349910
O    5.697711    3.321389    2.250998
N   -5.694229    3.234368   -0.053009
N    5.690422    3.236101   -0.051696
C   -5.043812   -3.254054   -1.302262
C   -3.574688   -3.423823   -1.283491
C   -2.862467   -3.482872   -0.057434
C   -3.575331   -3.470420    1.171678
C   -5.047744   -3.351162    1.198057
C   -2.879725   -3.453078   -2.491545
C   -1.429194   -3.528893   -0.059314
C   -0.731221   -3.543486   -1.313610
C   -1.482009   -3.524280   -2.502681
C    0.733262   -3.542887   -1.313809
C    1.431589   -3.528490   -0.059710
C    0.732865   -3.538614    1.192681
C   -0.730103   -3.538262    1.192882
C   -1.478528   -3.545932    2.386148
C   -2.876179   -3.518555    2.377525
H   -3.448930   -3.503918    3.308683
H   -0.969626   -3.552212    3.351701
H   -3.452579   -3.398896   -3.420918
H   -0.974668   -3.533200   -3.469357
C    1.483707   -3.522556   -2.503071
C    2.864839   -3.482048   -0.058220
C    1.481645   -3.547757    2.385723
C    3.576702   -3.421921   -1.284440
C    2.881398   -3.450699   -2.492310
H    3.453936   -3.395672   -3.421829
C    3.578040   -3.470310    1.170701
C    2.879279   -3.520077    2.376712
H    3.452323   -3.506370    3.307705
C    5.045740   -3.251452   -1.303522
C    5.050382   -3.350220    1.196741
H    0.973050   -3.555824    3.351434
H    0.976082   -3.530986   -3.469593
O   -5.684786   -3.107992   -2.350874
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O	-5.698469	-3.322913	2.249889
O	5.686346	-3.104500	-2.352227
O	5.701375	-3.322307	2.248419
N	-5.691229	-3.236328	-0.052762
N	5.693457	-3.234075	-0.054172
C	-7.141162	2.916357	-0.045584
H	-7.558251	3.385919	0.855825
H	-7.572474	3.368832	-0.948846
C	7.137671	2.919579	-0.044087
H	7.554039	3.389073	0.857690
H	7.568734	3.373014	-0.946990
C	7.140429	-2.916263	-0.046567
H	7.571751	-3.368535	-0.949930
H	7.557371	-3.386158	0.854735
C	-7.138433	-2.919535	-0.045040
H	-7.569559	-3.372573	-0.948111
H	-7.554908	-3.389278	0.856559
C	-7.329979	1.412525	-0.032251
C	-7.480144	0.698706	-1.234972
C	-7.234835	0.698262	1.178090
C	-7.479483	-0.702432	-1.234843
H	-7.549780	1.250600	-2.177166
C	-7.234132	-0.701304	1.178216
H	-7.121128	1.250720	2.115581
C	-7.328616	-1.415876	-0.031988
H	-7.548588	-1.254577	-2.176927
H	-7.119815	-1.253500	2.115786
C	7.328130	1.415958	-0.031533
C	7.233517	0.700963	1.178414
C	7.479331	0.702906	-1.234585
C	7.234183	-0.698593	1.177796
H	7.119061	1.252781	2.116188
C	7.480021	-0.698236	-1.235198
H	7.548701	1.255382	-2.176460
C	7.329497	-1.412469	-0.032764
H	7.120246	-1.251347	2.115086
H	7.549898	-1.249773	-2.177584
P	0.000959	-0.000183	0.149772
C	1.501978	0.000681	-0.723496
C	2.720415	0.000141	-0.002358
C	1.486388	0.001538	-2.135119
C	3.931446	0.000660	-0.711558
C	2.707806	0.002100	-2.827087
C	3.915187	0.001671	-2.114735
H	4.885395	-0.000038	-0.176648
H	2.715585	0.002786	-3.921346
H	4.865884	0.002058	-2.652131
C	0.001515	-0.000705	1.876392
C	1.240496	-0.001126	2.565668
C	-1.237052	-0.000856	2.566397
C	1.225996	-0.001507	3.969600
C	-1.221728	-0.001389	3.970318

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C      0.002340   -0.001654    4.658595
H      2.170403   -0.001750    4.522764
H     -2.165811   -0.001564    4.524034
H      0.002663   -0.002002    5.752150
C     -1.500507    0.000021   -0.722699
C     -2.718504   -0.000507   -0.000858
C     -1.485642    0.000438   -2.134323
C     -3.929928   -0.000770   -0.709368
C     -2.707455    0.000124   -2.825608
C     -3.914422   -0.000527   -2.112568
H     -4.883593   -0.001130   -0.173953
H     -2.715886    0.000440   -3.919860
H     -4.865393   -0.000762   -2.649474
S      2.865423   -0.001570    1.787955
S     -2.862425   -0.000264    1.789595
S      0.000098    0.002086   -3.157027
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Number of imaginary frequencies = 1 (-328.9 cm⁻¹)
Computed total Gibbs free energy = -5513.9529 a.u.

6
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C      5.038850   -3.271483   -1.483500
C      3.563426   -3.349455   -1.457975
C      2.850913   -3.323725   -0.229843
C      3.565112   -3.269209    0.996381
C      5.035637   -3.164629    1.016085
C      2.864000   -3.411627   -2.664797
C      1.415998   -3.337732   -0.229251
C      0.716434   -3.369982   -1.481579
C      1.466644   -3.422514   -2.674103
C     -0.747556   -3.347456   -1.479958
C     -1.446727   -3.342288   -0.226235
C     -0.745212   -3.333142    1.027477
C      0.716827   -3.311361    1.026387
C      1.469836   -3.286707    2.219387
C      2.866094   -3.257231    2.205318
H      3.440569   -3.209828    3.133971
H      0.963450   -3.271798    3.186496
H      3.438791   -3.438688   -3.594630
H      0.956887   -3.472660   -3.638217
C     -1.499660   -3.317967   -2.671173
C     -2.882859   -3.327824   -0.223740
C     -1.497717   -3.344281    2.219597
C     -3.595350   -3.300525   -1.450770
C     -2.896676   -3.291997   -2.659760
H     -3.472185   -3.260678   -3.588936
C     -3.598837   -3.311004    1.004405
C     -2.895476   -3.329461    2.209317
H     -3.467503   -3.310127    3.140921
C     -5.071680   -3.236138   -1.474955
C     -5.071195   -3.201154    1.028967
H     -0.989931   -3.347071    3.186337
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H	-0.990538	-3.302689	-3.637089
O	5.686524	-3.252928	-2.538791
O	5.682833	-3.040286	2.065235
O	-5.720176	-3.211164	-2.529338
O	-5.723592	-3.118936	2.078124
N	5.685192	-3.189721	-0.234270
N	-5.718595	-3.172062	-0.224963
C	5.038770	3.271766	-1.483236
C	3.563347	3.349760	-1.457679
C	2.850845	3.323749	-0.229546
C	3.565052	3.268987	0.996661
C	5.035576	3.164469	1.016333
C	2.863910	3.412231	-2.664478
C	1.415931	3.337733	-0.228934
C	0.716356	3.370310	-1.481246
C	1.466553	3.423145	-2.673765
C	-0.747633	3.347774	-1.479617
C	-1.446793	3.342324	-0.225891
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C	0.716772	3.311054	1.026705
C	1.469790	3.286134	2.219695
C	2.866047	3.256717	2.205604
H	3.440536	3.209143	3.134238
H	0.963417	3.270989	3.186806
H	3.438690	3.439512	-3.594312
H	0.956786	3.473561	-3.637860
C	-1.499745	3.318550	-2.670833
C	-2.882924	3.327876	-0.223390
C	-1.497760	3.343787	2.219941
C	-3.595427	3.300840	-1.450420
C	-2.896762	3.292575	-2.659417
H	-3.472276	3.261441	-3.588597
C	-3.598888	3.310819	1.004760
C	-2.895518	3.329013	2.209669
H	-3.467538	3.309512	3.141274
C	-5.071756	3.236393	-1.474606
C	-5.071245	3.200988	1.029311
H	-0.989968	3.346379	3.186678
H	-0.990630	3.303455	-3.636756
O	5.686434	3.253380	-2.538537
O	5.682790	3.039954	2.065453
O	-5.720260	3.211552	-2.528987
O	-5.723639	3.118600	2.078456
N	5.685118	3.189799	-0.234024
N	-5.718652	3.172079	-0.224618
C	7.141004	-2.911413	-0.241063
H	7.558891	-3.376702	0.662051
H	7.546571	-3.389528	-1.143055
C	-7.178020	-2.911339	-0.230023
H	-7.587143	-3.377751	0.676284
H	-7.579901	-3.398396	-1.129204
C	-7.178064	2.911295	-0.229689

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H    -7.579968    3.398427   -1.128819
H    -7.587201    3.377601    0.676666
C     7.140936    2.911533   -0.240849
H     7.546494    3.389760   -1.142785
H     7.558800    3.376736    0.662321
C     7.355491   -1.412023   -0.250748
C     7.311662   -0.699357   -1.463676
C     7.463642   -0.699863    0.957318
C     7.311646    0.699563   -1.463634
H     7.236732   -1.252480   -2.404783
C     7.463641    0.699912    0.957355
H     7.502328   -1.252648    1.900455
C     7.355474    1.412148   -0.250663
H     7.236698    1.252748   -2.404703
H     7.502317    1.252646    1.900520
C    -7.417712   -1.414487   -0.246796
C    -7.600237   -0.701320    0.951551
C    -7.323826   -0.699265   -1.456887
C    -7.600233    0.701128    0.951639
H    -7.681020   -1.252848    1.893636
C    -7.323820    0.699363   -1.456798
H    -7.201766   -1.251020   -2.393468
C    -7.417703    1.414436   -0.246618
H    -7.681024    1.252542    1.893791
H    -7.201750    1.251237   -2.393308
P     0.056131   -0.000095    0.755460
C     0.619622    0.000007   -0.788432
C    -0.391469    0.000135   -1.767269
C     2.024775    0.000080   -0.894124
C     0.104015    0.000294   -3.073256
C     2.492322    0.000241   -2.209324
C     1.518663    0.000331   -3.246492
H    -0.561095    0.000402   -3.939928
H     3.559742    0.000306   -2.442551
H     1.892839    0.000457   -4.273927
C    -1.563622   -0.000165    1.043542
C    -2.359623   -0.000014   -0.116503
C    -1.903488   -0.000256    2.408290
C    -3.731301    0.000009    0.144221
C    -3.280981   -0.000231    2.641807
C    -4.137703   -0.000117    1.508879
H    -4.484842    0.000114   -0.647569
H    -3.703317   -0.000315    3.648922
H    -5.212501   -0.000143    1.696242
C     1.125008   -0.000234    2.009359
C     0.518866   -0.000331    3.276036
C     2.475939   -0.000130    1.625524
C     1.438615   -0.000368    4.334006
C     3.374841   -0.000178    2.696772
C     2.823215   -0.000298    4.007085
H     1.117138   -0.000445    5.378354
H     4.456866   -0.000061    2.542406
```

```
H      3.530589   -0.000325    4.840909
O      2.872211    0.000053    0.256042
O     -1.779040    0.000108   -1.429204
O     -0.902366   -0.000372    3.439860
```

Number of imaginary frequencies = 1 (-356.7 cm^{-1})
Computed total Gibbs free energy = -4544.2117 a.u.

Catalysis of the sumanene bowl inversion with a di-core-substituted PBI cyclophane

di-core-substituted PBI cyclophane

```
C     -5.008913   -1.441554   -2.827290
C     -3.532367   -1.350572   -2.723469
C     -2.858651   -0.107523   -2.850048
C     -3.612991    1.072137   -3.071496
C     -5.091163    1.032797   -3.161218
C     -2.812941   -2.503222   -2.450536
C     -1.428072   -0.060231   -2.762135
C     -0.676422   -1.278884   -2.627123
C     -1.408048   -2.467368   -2.366109
C      0.775336   -1.221219   -2.795900
C      1.427289    0.061318   -2.762017
C      0.675646    1.279976   -2.626745
C     -0.776146    1.222349   -2.795490
C     -1.563977    2.369504   -3.034075
C     -2.953780    2.293835   -3.187431
H     -3.550944    3.188352   -3.386073
H     -1.081116    3.341722   -3.104922
H     -3.354633   -3.442060   -2.311464
C      1.562997   -2.368332   -3.035198
C      2.857878    0.108473   -2.849891
C      1.407422    2.468388   -2.365770
C      3.612087   -1.071150   -3.071958
C      2.952792   -2.292736   -3.188581
H      3.549849   -3.187176   -3.387876
C      3.531726    1.351404   -2.722913
C      2.812336    2.504074   -2.450039
H      3.354101    3.442867   -2.310951
C      5.090229   -1.031889   -3.161885
C      5.008309    1.442269   -2.826470
H      1.079975   -3.340427   -3.106697
O     -5.614163   -2.513753   -2.722416
O     -5.771596    2.050821   -3.330841
O      5.770550   -2.049886   -3.332197
O      5.613679    2.514320   -2.720904
N     -5.699245   -0.232064   -3.027130
N      5.698470    0.232835   -3.027193
C     -5.090309   -1.031717    3.162367
C     -3.612190   -1.071321    3.072282
C     -2.857758    0.108160    2.850222
```

```
C   -3.531316    1.351257    2.723261
C   -5.007858    1.442452    2.826896
C   -2.953164   -2.293063    3.188723
C   -1.427195    0.060658    2.762233
C   -0.775499   -1.222025    2.795988
C   -1.563397   -2.368985    3.035228
C    0.676230   -1.280004    2.627077
C    1.428158   -0.061506    2.762106
C    0.776484    1.221199    2.795571
C   -0.675304    1.279147    2.626937
C   -1.406781    2.467754    2.365987
C   -2.811680    2.503774    2.450335
H   -3.353258    3.442680    2.311276
H   -3.550434   -3.187379    3.387945
H   -1.080630   -3.341224    3.106532
C    1.407576   -2.468614    2.365987
C    2.858721   -0.109102    2.849943
C    1.564534    2.368203    3.034175
C    3.532199   -1.352275    2.723099
C    2.812485   -2.504744    2.450169
H    3.353954   -3.443686    2.310925
C    3.613261    1.070403    3.071528
C    2.954316    2.292237    3.187524
H    3.551694    3.186604    3.386206
C    5.008731   -1.443547    2.826708
C    5.091394    1.030715    3.161494
H    1.081870    3.340520    3.105077
O   -5.770889   -2.049571    3.332519
O   -5.613076    2.514566    2.721123
O    5.613862   -2.515745    2.721165
O    5.772060    2.048529    3.331454
N   -5.698240    0.233177    3.027900
N    5.699214   -0.234270    3.027302
C   -7.177611   -0.266252   -2.878895
H   -7.572197    0.570859   -3.470217
H   -7.518301   -1.225116   -3.292213
C    7.176883    0.266781   -2.879473
H    7.517588    1.225830   -3.292352
H    7.571111   -0.570048   -3.471436
C    7.177598   -0.268650    2.879313
H    7.518069   -1.227752    3.292260
H    7.572216    0.568139    3.471066
C   -7.176639    0.267440    2.880120
H   -7.571062   -0.569425    3.471901
H   -7.517190    1.226473    3.293156
C   -7.498383   -0.131355   -1.404066
C   -7.549793   -1.272626   -0.582541
C   -7.552301    1.142561   -0.808845
C   -7.549531   -1.141998    0.810224
H   -7.519169   -2.264960   -1.041397
C   -7.552202    1.273190    0.583954
H   -7.524906    2.032668   -1.444501
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C    -7.497969    0.132052    1.405440
H    -7.519908   -2.032006    1.445900
H    -7.523429    2.265614    1.042746
C     7.498283    0.131040   -1.404843
C     7.552103    1.271960   -0.583018
C     7.550314   -1.143157   -0.810012
C     7.552170    1.140929    0.809735
H     7.522991    2.264498   -1.041542
C     7.550566   -1.274192    0.582723
H     7.521100   -2.033000   -1.445941
C     7.498626   -0.133191    1.404583
H     7.524380    2.030829    1.445657
H     7.520308   -2.266679    1.041267
O     0.717979    3.626413   -2.079713
O    -0.718371   -3.625170   -2.079744
O    -0.716982    3.625544    2.079932
O     0.717695   -3.626422    2.079979
C     1.300299   -4.564547    1.223612
C     1.144151   -5.911862    1.566511
C     1.940495   -4.180885    0.036120
C     1.651873   -6.894885    0.708137
H     0.625263   -6.171091    2.492886
C     2.455654   -5.176301   -0.802563
H     2.027960   -3.124669   -0.231078
C     2.316093   -6.532054   -0.472129
H     1.530290   -7.950368    0.970012
H     2.967855   -4.882555   -1.723564
H     2.722269   -7.302954   -1.133601
C     1.301452    4.564702   -1.224082
C     1.146468    5.911914   -1.567847
C     1.941550    4.181214   -0.036470
C     1.655141    6.895045   -0.710122
H     0.627747    6.171038   -2.494341
C     2.457606    5.176695    0.801558
H     2.028327    3.125074    0.231284
C     2.319095    6.532374    0.470328
H     1.534463    7.950466   -0.972661
H     2.969692    4.883115    1.722682
H     2.725972    7.303326    1.131311
C    -1.300113    4.564184    1.224451
C    -1.144032    5.911302    1.568118
C    -1.940842    4.181113    0.037068
C    -1.652319    6.894770    0.710566
H    -0.624730    6.170064    2.494388
C    -2.456499    5.176951   -0.800804
H    -2.028370    3.125043   -0.230695
C    -2.316979    6.532528   -0.469627
H    -1.530784    7.950115    0.973015
H    -2.969100    4.883693   -1.721740
H    -2.723545    7.303753   -1.130481
C    -1.302001   -4.563673   -1.224480
C    -1.147352   -5.910792   -1.568766
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C	-1.941719	-4.180507	-0.036555
C	-1.655898	-6.894130	-0.711231
H	-0.628945	-6.169674	-2.495508
C	-2.457715	-5.176197	0.801270
H	-2.028232	-3.124435	0.231555
C	-2.319463	-6.531777	0.469544
H	-1.535452	-7.949482	-0.974155
H	-2.969508	-4.882834	1.722623
H	-2.726215	-7.302920	1.130382

Number of imaginary frequencies = 0
Computed total Gibbs free energy = -4511.029 a.u.

Equilibrium structure complex with compound **4**

C	-4.918090	-1.198572	3.261324
C	-3.497350	-1.606806	3.382443
C	-2.891915	-2.481248	2.442101
C	-3.692384	-3.035672	1.412877
C	-5.132830	-2.717412	1.294799
C	-2.764142	-1.138853	4.460219
C	-1.491776	-2.788707	2.538860
C	-0.707170	-2.203045	3.593123
C	-1.404851	-1.470726	4.590485
C	0.752551	-2.306391	3.517663
C	1.346472	-3.128556	2.493841
C	0.543632	-3.896068	1.572947
C	-0.908316	-3.673070	1.560979
C	-1.761670	-4.238578	0.587453
C	-3.120326	-3.922195	0.507598
H	-3.758035	-4.369277	-0.260000
H	-1.363634	-4.945380	-0.131507
H	-3.258035	-0.513808	5.208222
C	1.606179	-1.534307	4.335173
C	2.776659	-3.123138	2.355740
C	1.236917	-4.746656	0.671677
C	3.583214	-2.269571	3.152106
C	2.988657	-1.492623	4.140344
H	3.620123	-0.833866	4.742209
C	3.405508	-3.949396	1.389085
C	2.636065	-4.787542	0.597693
H	3.126762	-5.446745	-0.123053
C	5.035094	-2.133905	2.906624
C	4.870586	-3.919926	1.174437
H	1.178701	-0.913481	5.116416
O	-5.438672	-0.374373	4.022150
O	-5.855932	-3.215147	0.424278
O	5.736606	-1.303747	3.499717
O	5.435528	-4.642519	0.345136
N	-5.657426	-1.808186	2.231718
N	5.595922	-2.992223	1.942918
C	-5.081330	3.682703	-1.908799

C	-3.610140	3.592645	-2.040325
C	-2.991245	2.525263	-2.739215
C	-3.811388	1.566755	-3.389310
C	-5.291319	1.645100	-3.332356
C	-2.818240	4.525755	-1.380000
C	-1.561824	2.386380	-2.768508
C	-0.763018	3.330126	-2.025112
C	-1.427579	4.387630	-1.365661
C	0.690678	3.143974	-1.960952
C	1.289301	2.098946	-2.755868
C	0.493431	1.222679	-3.576498
C	-0.965576	1.290446	-3.485131
C	-1.843216	0.313463	-4.034522
C	-3.238800	0.471793	-4.015848
H	-3.892357	-0.274163	-4.474726
H	-3.308288	5.343600	-0.844783
H	-0.845799	5.109849	-0.802389
C	1.573654	3.949189	-1.192179
C	2.716143	1.940442	-2.780632
C	1.158590	0.342958	-4.460554
C	3.533384	2.736955	-1.938273
C	2.958487	3.718730	-1.151790
H	3.595525	4.328450	-0.506882
C	3.336686	0.994169	-3.634604
C	2.551474	0.228870	-4.491749
H	3.045782	-0.467774	-5.174541
C	4.997455	2.535312	-1.859404
C	4.802212	0.791215	-3.628040
H	0.574670	-0.267027	-5.143707
O	-5.634685	4.563907	-1.240066
O	-6.021504	0.823793	-3.896207
O	5.709257	3.161614	-1.061887
O	5.362475	-0.040917	-4.350505
N	-5.832767	2.677276	-2.546449
N	5.547853	1.583123	-2.729129
C	-7.078831	-1.426344	2.076600
H	-7.629563	-2.342797	1.820468
H	-7.398988	-1.053729	3.059751
C	7.025839	-2.803125	1.608581
H	7.402514	-3.782660	1.283277
H	7.526702	-2.488579	2.534389
C	6.989238	1.270045	-2.574354
H	7.488746	2.209480	-2.300611
H	7.338748	0.922119	-3.555946
C	-7.265990	2.560890	-2.185051
H	-7.593748	3.567751	-1.892974
H	-7.806468	2.226523	-3.080883
C	-7.252612	-0.373375	1.002146
C	-6.953087	0.975147	1.275062
C	-7.651826	-0.736262	-0.294527
C	-7.021810	1.934492	0.259415
H	-6.647532	1.260200	2.287272

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C    -7.716669    0.222457   -1.312587
H    -7.868089   -1.786011   -0.512282
C    -7.386171    1.562362   -1.050447
H    -6.769695    2.979112    0.469077
H    -7.980434   -0.074671   -2.331768
C     7.172643   -1.761340    0.517909
C     7.073299   -2.130808   -0.836264
C     7.313943   -0.401008    0.846751
C     7.071360   -1.154974   -1.839540
H     6.960036   -3.188018   -1.093913
C     7.313801    0.575511   -0.155915
H     7.387278   -0.111945    1.899375
C     7.169133    0.209553   -1.507220
H     6.955992   -1.442504   -2.888992
H     7.386028    1.635205    0.105528
O    -1.305410   -0.810674   -4.624625
O     1.084177    4.968051   -0.400675
O     0.545736   -5.616422   -0.157665
O    -0.747060   -1.125069    5.750565
C    -2.033694   -2.005079   -4.653196
C    -2.607984   -2.548479   -3.494516
C    -2.080413   -2.681779   -5.876949
C    -3.244649   -3.792129   -3.577255
H    -2.555815   -2.012796   -2.544232
C    -2.716194   -3.929227   -5.941168
H    -1.624321   -2.223561   -6.758904
C    -3.300548   -4.485857   -4.794881
H    -3.699155   -4.217880   -2.677736
H    -2.759442   -4.461901   -6.896243
H    -3.800781   -5.457142   -4.849544
C     1.766681    6.184637   -0.382228
C     2.349288    6.727493   -1.537943
C     1.766758    6.887970    0.828491
C     2.955530    7.987542   -1.462965
H     2.324607    6.169647   -2.477865
C     2.370045    8.150598    0.884258
H     1.297939    6.435112    1.704519
C     2.970134    8.702760   -0.256513
H     3.412826    8.414459   -2.360888
H     2.374524    8.701430    1.829905
H     3.445367    9.686662   -0.206758
C     0.584724   -5.423281   -1.538575
C    -0.167375   -6.340238   -2.289652
C     1.250952   -4.357894   -2.160378
C    -0.264500   -6.172388   -3.675240
H    -0.672130   -7.162150   -1.773787
C     1.139728   -4.205279   -3.550057
H     1.828577   -3.644291   -1.569754
C     0.383189   -5.103245   -4.312894
H    -0.862077   -6.878848   -4.259553
H     1.644812   -3.360461   -4.030679
H     0.284797   -4.965109   -5.392770
```

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C    -1.076037    0.079535    6.381006
C    -1.363799    0.042856    7.749139
C    -1.017521    1.287079    5.673582
C    -1.606243    1.250501    8.419240
H    -1.393442   -0.919667    8.266782
C    -1.263065    2.483617    6.356137
H    -0.762461    1.283642    4.611214
C    -1.560433    2.469918    7.727528
H    -1.835878    1.234116    9.489111
H    -1.201929    3.429790    5.808646
H    -1.750956    3.407651    8.257860
C     0.894503    3.804035    2.817105
C     2.284339    3.461675    2.658991
C     2.684806    2.164727    2.283078
C    -0.130675    2.865231    2.594667
C    -1.640013    2.915297    2.206247
C     2.606912   -1.158595   -1.023534
C     1.269345   -1.187905   -0.577711
C    -0.131238   -1.432993   -1.210754
C     3.626901   -0.432909   -0.312609
C     3.323601    0.301864    0.849824
C     2.021026    0.133488    1.346431
C     1.041419   -0.584222    0.668656
C    -0.340767   -0.253779    0.836286
C    -1.092039   -0.625002   -0.289388
C    -2.340907    0.016554   -0.416410
C    -2.722867    1.101253    0.447260
C    -1.861246    1.566776    1.459684
C    -0.708572    0.795022    1.675115
C     0.303733    1.550847    2.351118
C     1.648401    1.218149    2.201016
C     3.932403    1.515857    1.609911
H     4.619853   -0.379958   -0.769286
H     2.889264   -1.579871   -1.994961
H     3.012183    4.278547    2.725370
H     0.653447    4.855136    3.011846
H    -3.655509    1.624941    0.211666
H    -3.010777   -0.199624   -1.255122
H    -0.162378   -1.089234   -2.256434
H    -0.392007   -2.507274   -1.235811
H     4.666583    1.172046    2.365573
H     4.468552    2.208754    0.940346
H    -2.299125    3.016900    3.090636
H    -1.857896    3.772638    1.546038
```

Number of imaginary frequencies = 1 (-356.7 cm^{-1})
Computed total Gibbs free energy = -5319.711 a.u.

Transition structure complex with compound **4**

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C    -5.091962   -0.122976   -4.143460
C    -3.611894   -0.073741   -4.096423
```

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C    -2.914025    1.051228   -3.586971
C    -3.667341    2.177096   -3.164049
C    -5.146457    2.171107   -3.172136
C    -2.904089   -1.196572   -4.494791
C    -1.478110    1.037807   -3.496590
C    -0.746342   -0.139811   -3.897685
C    -1.510676   -1.243804   -4.367345
C     0.717701   -0.130426   -3.779744
C     1.378110    1.020549   -3.216068
C     0.646709    2.201194   -2.827924
C    -0.813995    2.200128   -2.956336
C    -1.611769    3.292928   -2.549712
C    -3.004256    3.288008   -2.658081
H    -3.597358    4.144763   -2.326022
H    -1.137569    4.162030   -2.107888
H    -3.445346   -2.064435   -4.880339
C     1.519648   -1.209683   -4.214246
C     2.808537    0.982543   -3.076060
C     1.411040    3.305669   -2.357092
C     3.558036   -0.158585   -3.454666
C     2.905188   -1.237299   -4.041309
H     3.494727   -2.102278   -4.356573
C     3.501685    2.098730   -2.541120
C     2.806268    3.244647   -2.205047
H     3.352501    4.099813   -1.801240
C     5.020431   -0.236942   -3.231651
C     4.965868    2.075499   -2.316222
H     1.045030   -2.051524   -4.707027
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O    -5.817286    3.124242   -2.758103
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O     5.571219    3.030278   -1.809865
N    -5.770819    1.000987   -3.645022
N     5.644386    0.909280   -2.698639
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C    -3.733613   -2.677088    2.146857
C    -3.097206   -1.576404    2.773175
C    -3.893624   -0.483177    3.196449
C    -5.354804   -0.440605    2.954227
C    -2.968183   -3.761675    1.734449
C    -1.671616   -1.542812    2.956990
C    -0.899492   -2.688086    2.537305
C    -1.586938   -3.769981    1.941887
C     0.556935   -2.680139    2.723317
C     1.182923   -1.477619    3.215133
C     0.410590   -0.320508    3.598850
C    -1.051887   -0.382962    3.542319
C    -1.916680    0.646428    4.018062
C    -3.306375    0.600590    3.825885
H    -3.945472    1.425448    4.148622
H    -3.471350   -4.606045    1.254774
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C    3.413429   -2.518791    2.946818
C    2.808627   -3.699452    2.552234
H    3.435554   -4.561790    2.313057
C    3.266536   -0.200099    3.684122
C    2.501873    0.908155    4.027476
H    3.008913    1.833285    4.312407
C    4.893719   -2.459176    2.953698
C    4.739860   -0.078636    3.667384
H    0.554515    1.750109    4.213731
O   -5.757212   -3.621924    1.309154
O   -6.054473    0.523114    3.289571
O    5.598378   -3.424096    2.634518
O    5.322719    0.983364    3.927710
N   -5.914144   -1.553835    2.305346
N    5.469565   -1.227214    3.310529
C   -7.229474    0.866907   -3.417066
H   -7.655879    1.876132   -3.494086
H   -7.619279    0.222356   -4.216381
C    7.090525    0.821215   -2.378851
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H    7.526563    0.126871   -3.109996
C    6.933169   -1.079195    3.121813
H    7.372910   -2.068604    3.307026
H    7.279193   -0.357779    3.874545
C   -7.343746   -1.478997    1.924453
H   -7.732369   -2.506160    1.954887
H   -7.836612   -0.860355    2.687064
C   -7.447094    0.261708   -2.044370
C   -7.475880   -1.135186   -1.879743
C   -7.478506    1.085988   -0.903591
C   -7.490710   -1.698008   -0.598329
H   -7.443153   -1.778528   -2.764071
C   -7.495634    0.523183    0.377370
H   -7.451869    2.172596   -1.028847
C   -7.480152   -0.874787    0.541860
H   -7.470723   -2.784647   -0.472588
H   -7.487514    1.165126    1.263574
C    7.280665    0.330072   -0.958080
C    7.278580    1.243041    0.112683
C    7.326681   -1.048938   -0.678918
C    7.240747    0.785973    1.434590
H    7.249220    2.315136   -0.100680
C    7.292672   -1.506505    0.644683
H    7.330710   -1.761977   -1.509043
C    7.208957   -0.592780    1.712813
H    7.179987    1.498528    2.262079
H    7.272447   -2.579789    0.856694
O   -1.360467    1.739070    4.640122
O    0.875042   -4.983354    2.023923
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O	0.778394	4.463866	-1.969242
O	-0.908027	-2.431899	-4.764866
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C	-2.149808	3.979631	4.864390
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C	-2.877144	4.945731	5.573410
H	-1.561906	4.228909	3.976193
C	-3.610337	3.252762	7.153224
H	-2.865307	1.235279	6.792818
C	-3.610476	4.585204	6.712740
H	-2.870938	5.984629	5.229328
H	-4.176246	2.968749	8.045664
H	-4.180388	5.341832	7.259975
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C	1.147982	-7.082141	0.973561
C	2.181718	-5.123751	-0.057335
C	1.616340	-7.876432	-0.080387
H	0.565923	-7.505089	1.797026
C	2.647701	-5.934255	-1.099806
H	2.392627	-4.052514	-0.046611
C	2.372379	-7.308969	-1.117597
H	1.395372	-8.948369	-0.082637
H	3.224739	-5.476262	-1.909149
H	2.745592	-7.935309	-1.933317
C	1.416305	5.692077	-2.144491
C	2.033483	6.030123	-3.357834
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C	2.583004	7.310067	-3.501278
H	2.077433	5.300220	-4.170949
C	1.873210	7.885368	-1.252929
H	0.841602	6.293232	-0.160879
C	2.505110	8.240026	-2.453645
H	3.068138	7.582431	-4.443647
H	1.809843	8.606073	-0.431656
H	2.935358	9.238556	-2.574089
C	-0.988997	-3.540271	-3.918652
C	-0.085911	-4.577889	-4.200332
C	-1.874395	-3.637387	-2.836055
C	-0.045678	-5.698363	-3.363352
H	0.581078	-4.486349	-5.062712
C	-1.820603	-4.768387	-2.008285
H	-2.575490	-2.830267	-2.621063
C	-0.901924	-5.795931	-2.255693
H	0.674435	-6.496032	-3.567490
H	-2.502679	-4.827773	-1.154013
H	-0.840251	-6.661302	-1.589945
C	3.047010	-1.361931	-0.365793
C	3.859269	-0.251561	0.118927
C	3.294183	0.973941	0.572209
C	1.622113	-1.322135	-0.413500
C	0.302303	-2.113560	-0.825264
C	0.042277	4.401869	1.709355

C	-0.811726	3.353764	1.254742
C	-2.324333	2.912303	0.991255
C	1.499531	4.281009	1.747136
C	2.189870	3.106967	1.329700
C	1.296200	2.131740	0.914520
C	-0.073950	2.243392	0.881171
C	-0.854730	1.172660	0.419609
C	-2.215243	1.431070	0.417203
C	-2.950349	0.319065	-0.081361
C	-2.306519	-0.913964	-0.523163
C	-0.893649	-1.107385	-0.500580
C	-0.250560	0.011782	0.002146
C	1.147076	-0.106662	0.049909
C	1.911375	0.943926	0.496303
C	3.620715	2.424915	1.139089
H	2.039859	5.160958	2.114649
H	-0.362891	5.363727	2.047994
H	4.939122	-0.413825	0.107798
H	3.614248	-2.233765	-0.712719
H	-2.990597	-1.699692	-0.858828
H	-4.044450	0.339587	-0.153735
H	-2.921335	2.939709	1.920967
H	-2.826959	3.584727	0.274329
H	4.256145	2.990994	0.434511
H	4.181586	2.363556	2.088865
H	0.323770	-2.392007	-1.890548
H	0.186004	-3.061111	-0.273283

Number of imaginary frequencies = 1 (-84.4 cm^{-1})
Computed total Gibbs free energy = -5319.695 a.u.