# Supporting Information

# Automatic Conformational Search of Transition States for Catalytic Reactions Using Genetic Algorithm

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## Contents

# Genetic Simulation Setting

## Water Hexamer

The input water structure was optimized at gas phase HF/3-21G level and it was replicated six times by the program to generate water hexamers. A total of 50 GA simulations were carried out at HF/3-21G level. For each simulation, a population size of 100 was chosen and the simulation was continued for 100 generations. For each generation, every individual of the population was optimized for 2 cycles before they reproduced, by linking to the G16 suite of programs; every valid child structure generated by the program was optimized for a maximum of 10 cycles; the final outputted structures were optimized for a maximum of 100 cycles. When generating child structures, a minimal interatomic distance of 0.9 Å and a maximal inter-fragment distance of 2.5 Å were applied for pruning. If the structure generated did not pass these criteria, it was regenerated for a maximum of 1000 times. The system does not contain any rotatable bonds, and no restrains were used for the simulations.

## Water Heptamer

The input water structure was optimized at gas phase HF/3-21G level and it was replicated seven times by the program to generate water hepatmers. A total of 50 GA simulations were carried out at HF/3-21G level. For each simulation, a population size of 100 was chosen and the simulation was continued for 100 generations. For each generation, every individual of the population was optimized for 2 cycles before they reproduced, by linking to the G16 suite of programs; every valid child structure generated by the program was optimized for a maximum of 10 cycles; the final outputted structures were optimized for a maximum of 100 cycles. When generating child structures, a minimal interatomic distance of 0.9 Å and a maximal inter-fragment distance of 2.5 Å were applied for pruning. If the structure generated did not pass these criteria, it was regenerated for a maximum of 1000 times. The system does not contain any rotatable bonds, and no restrains were used for the simulations.

## Benzene Trimer

The input benzene structure was optimized at gas phase M06-2X/3-21G level and it was replicated three times by the program to generate benzene trimers. A total of 50 GA simulations were carried out at M06-2X/3-21G level. For each simulation, a small population size of 10 was chosen, due to the high cost of the DFT method, and the simulation was continued for 20 generations. For each generation, every individual of the population was optimized for 5 cycles before they reproduced, by linking to the G16 suite of programs; every valid child structure generated by the program was optimized for a maximum of 5 cycles; the final outputted structures were optimized for a maximum of 200 cycles. When generating child structures, a minimal interatomic distance of 1.5 Å and a maximal inter-fragment distance of 4.0 Å were applied for pruning. If the structure generated did not pass these criteria, it was regenerated for a maximum of 1000 times. The system does not contain any rotatable bonds, and no restrains were used for the simulations.

### Asymmetric Strecker Reaction

The input TS structures were taken from our early study, namely TS-R and TS-S of **Figure 8**, without optimization. A total of 100 GA simulations were carried out, 50 for each TS, at PM6 level. For each simulation, a population size of 20 was chosen and the simulation was continued for 500 generations. No optimizations were performed. When generating child structures, a minimal interatomic distance of 1.0 Å and a maximal inter-fragment distance of 1.8 Å were applied for pruning. If the structure generated did not pass these criteria, it was regenerated for a maximum of 1000 times. No restrains were used for this simulation.

### Asymmetric Methanolysis of Meso-cyclic Anhydride

The input TS structure, methanol and model amino alcohol were optimized at gas phase HF/3-21G level. The trimethyl amine catalyst was omitted from the TS structure, as shown in **Figure 9**. A total of 200 GA simulations were carried out, 50 for each of the four TSs of **Figure 10**, at HF/3-21G level. For each simulation, a population size of 20 was chosen and the simulation was continued for 30 generations. For each generation, every individual of the population was optimized for 5 cycles before they reproduced, by linking to the G16 suite of programs; every valid child structure generated by the program was optimized for a maximum of 10 cycles; the final outputted structures were optimized for a maximum of 100 cycles. When generating child structures, a minimal interatomic distance of 1.0 Å and a maximal inter-fragment distance of 2.0 Å were applied for pruning. If the structure generated did not pass these criteria, it was regenerated for a maximum of 100 times. All single bonds except the two C-N bonds between methyl carbon and nitrogen were considered free rotatable. A bias between the nitrogen atom of the amino alcohol catalyst and the hydroxyl proton of the *TS* was introduced, with an expected distance of 1.205 Å and a force constant of 2000 kcal/mol·Å$^2$.

## Method Selection for Asymmetric Methanolysis of meso-cyclic anhydride

We first considered the suitability of using the semi-empirical method PM6 for our GA simulations. However, after some preliminary tests, we found that the method describes poorly the interaction between two C-H bonds, as compared to the DFT method M06-2X, shown in **Figure S1**. Furthermore, the method seems to considerably underestimate the strength of hydrogen bond (**Table S1**). As a result, we chose to use the slightly more expensive HF/3-21G level of theory rather than PM6.

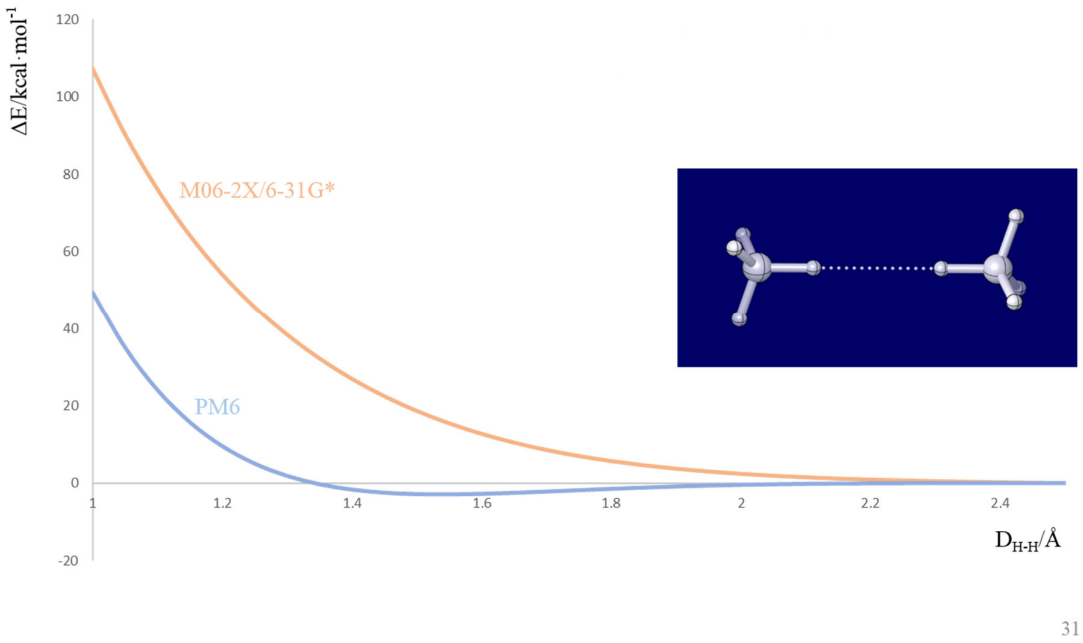
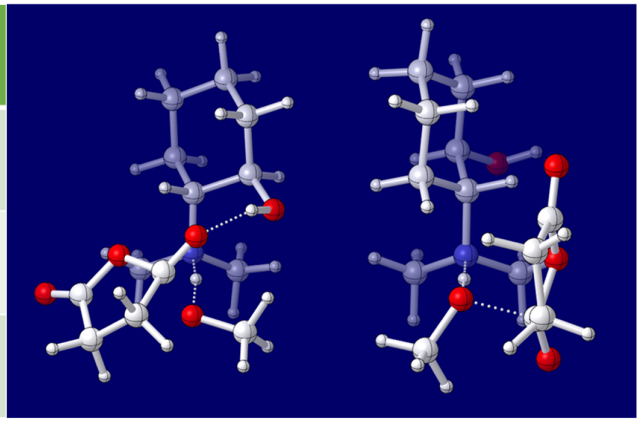



**Figure S1**. C-H···H-C interaction energy at PM6 and M06-2X levels of theory

**Table S1**. Relative energies of a hydrogen bonded TS and a non-hydrogen bonded TS, calculated at different levels of theory.

| | H-Bond | Non-H-Bond |
|---|---|---|
| PM6 | 0.0 | 6.6 |
| HF/3-21G | 0.0 | 35.4 |
| M06-2X | 0.0 | 35.2 |



## Cartesian Coordinates of Reported Structures

### Water Hexamer

The structures and thermodynamic data were calculated at HF/3-21G level.

water6-bag

| | | | |
|---|---|---|---|
| 0 | -1.12133700 | -0.76191300 | 1.36603600 |
| H | -1.70199500 | -0.30233800 | 0.72379800 |
| H | -0.52034700 | -0.07738700 | 1.73171500 |
| 0 | 0.54067300 | 1.48728400 | -0.91241500 |

H 0.85788700 2.21310400 -1.46125200
H 0.88719600 0.58626200 -1.24684500
0 0.35584900 -2.41251200 0.12901000
H -0.29341100 -1.90009000 0.70531200
H 0.77286200 -3.14204800 0.59687400
0 -2.08742900 0.97790500 -0.44083800
H -1.17495600 1.21652900 -0.71530500
H -2.52060700 1.75205300 -0.06049600
0 0.59178600 1.26884300 1.75380300
H 1.48026300 1.11222200 2.09577300
H 0.63441900 1.45618800 0.78775800
0 1.26207400 -0.82029300 -1.62113600
H 1.06105600 -1.15485100 -2.50278300
H 0.97601700 -1.49895800 -0.92900800
Zero-point correction= 0.159545 (Hartree/Particle)
Thermal correction to Energy= 0.172198
Thermal correction to Enthalpy= 0.173142
Thermal correction to Gibbs Free Energy= 0.121459
Sum of electronic and zero-point Energies= -453.515103
Sum of electronic and thermal Energies= -453.502450
Sum of electronic and thermal Enthalpies= -453.501506
Sum of electronic and thermal Free Energies= -453.553189

water6-book
0 2.02677700 -0.14026200 1.80996900
H 1.78741900 -0.52091700 0.90754400
H 2.98294700 -0.07453100 1.90808700
0 0.30073700 1.74304300 1.81500900
H 1.04443500 1.08045000 1.93671300
H -0.27414500 1.75035900 2.58782400
0 -0.68394700 -2.42682000 -1.19565000
H -1.40371000 -1.74988300 -1.20469900
H -0.64260900 -2.86171900 -2.05502000
0 1.24685700 -0.74017400 -0.54233600
H 0.74673800 0.06052000 -0.77727000
H 0.67205200 -1.51991500 -0.73015700
0 -2.23404600 -0.30750300 -1.28822100
H -3.01631800 -0.19037300 -0.73654400
H -1.58886200 0.42662000 -1.12973600
0 -0.46541700 1.51582200 -0.59315000
H -0.24999200 1.64745500 0.38690400
H -0.24404100 2.30380300 -1.10301800
Zero-point correction= 0.160109 (Hartree/Particle)
Thermal correction to Energy= 0.172614
Thermal correction to Enthalpy= 0.173558
Thermal correction to Gibbs Free Energy= 0.122091
Sum of electronic and zero-point Energies= -453.516804
Sum of electronic and thermal Energies= -453.504299

Sum of electronic and thermal Enthalpies= -453.503355
Sum of electronic and thermal Free Energies= -453.554821

water6-cage

| | | | |
|---|---|---|---|
| 0 | -1.91180800 | -1.10775000 | 1.83495400 |
| H | -2.02433900 | -1.33726100 | 2.76304400 |
| H | -1.62522400 | -0.16379000 | 1.72216400 |
| 0 | -0.78745900 | 1.17247500 | 1.10233800 |
| H | -0.99979000 | 1.17156300 | 0.14810300 |
| H | 0.16072300 | 0.96072200 | 1.16961100 |
| 0 | -0.82594100 | 0.64272100 | -1.60560200 |
| H | 0.12603400 | 0.89663500 | -1.78117800 |
| H | -1.41775400 | 0.95962700 | -2.29665600 |
| 0 | 1.74241000 | 1.09452700 | -1.70932000 |
| H | 2.32488000 | 0.65446000 | -2.33916100 |
| H | 1.90678400 | 0.75144300 | -0.79138500 |
| 0 | -0.21523000 | -1.60935500 | -0.14704300 |
| H | -0.58733900 | -1.03108900 | -0.84179000 |
| H | -0.87900300 | -1.67576100 | 0.58228200 |
| 0 | 1.67625300 | -0.10901300 | 0.61658800 |
| H | 0.99987300 | -0.82798900 | 0.33964200 |
| H | 2.33693100 | -0.44216800 | 1.23340800 |

Zero-point correction= 0.161692 (Hartree/Particle)
Thermal correction to Energy= 0.173681
Thermal correction to Enthalpy= 0.174625
Thermal correction to Gibbs Free Energy= 0.125423
Sum of electronic and zero-point Energies= -453.517022
Sum of electronic and thermal Energies= -453.505033
Sum of electronic and thermal Enthalpies= -453.504089
Sum of electronic and thermal Free Energies= -453.553292

water6-chair

| | | | |
|---|---|---|---|
| 0 | -0.77470600 | -1.08084400 | 1.17640200 |
| H | -0.09470700 | -1.72591300 | 0.86043700 |
| H | -1.29538800 | -0.77391000 | 0.41138700 |
| 0 | 0.21822800 | 1.91465100 | -0.38697000 |
| H | 0.52086800 | 2.79810700 | -0.62231200 |
| H | 0.33697200 | 1.70712100 | 0.60714200 |
| 0 | 0.86416600 | -0.44630200 | -1.74569500 |
| H | 0.96388700 | 0.42016100 | -1.31138000 |
| H | -0.08860900 | -0.53510600 | -1.91371300 |
| 0 | 1.15981400 | -2.41192200 | -0.02620700 |
| H | 1.20506700 | -1.74071900 | -0.75498200 |
| H | 2.03128700 | -2.54979100 | 0.36178800 |
| 0 | 0.37593600 | 1.04264400 | 2.00769200 |
| H | -0.04836100 | 0.13671000 | 1.82549500 |
| H | 0.04637200 | 1.42707300 | 2.82627200 |
| 0 | -1.69232300 | 0.24727500 | -1.08986000 |

H -2.58240100 0.50971700 -1.34938800
H -1.12444900 1.02803500 -0.87816900
Zero-point correction= 0.160734 (Hartree/Particle)
Thermal correction to Energy= 0.173027
Thermal correction to Enthalpy= 0.173971
Thermal correction to Gibbs Free Energy= 0.123799
Sum of electronic and zero-point Energies= -453.515454
Sum of electronic and thermal Energies= -453.503161
Sum of electronic and thermal Enthalpies= -453.502217
Sum of electronic and thermal Free Energies= -453.552389

water6-prism
0 -1.55907900 -0.41674200 -1.38229300
H -0.96335500 -1.12971100 -1.08280900
H -1.00616300 0.30511700 -1.73300000
0 1.91829500 0.12279900 -0.17990000
H 1.67156100 -0.76231500 -0.49918900
H 1.63571700 0.13654600 0.75369500
0 0.26102300 -2.05192700 -0.07262000
H 0.21478100 -3.00852100 0.03530400
H 0.17335600 -1.58514700 0.79199200
0 -1.40768200 1.15828400 0.76600100
H -0.89608000 1.76579200 0.19934500
H -1.83234100 0.54097900 0.13150200
0 0.27603800 -0.32135500 1.95860600
H -0.43290600 0.30937900 1.60664700
H 0.28028600 -0.35628300 2.92158800
0 0.19831200 1.71279300 -1.33072900
H 0.51650100 2.39745600 -1.92990600
H 0.95172900 1.18285700 -0.95422900
Zero-point correction= 0.162872 (Hartree/Particle)
Thermal correction to Energy= 0.174582
Thermal correction to Enthalpy= 0.175526
Thermal correction to Gibbs Free Energy= 0.127298
Sum of electronic and zero-point Energies= -453.517159
Sum of electronic and thermal Energies= -453.505450
Sum of electronic and thermal Enthalpies= -453.504505
Sum of electronic and thermal Free Energies= -453.552734

water6-ring
0 -1.39743500 -0.83965500 1.94680800
H -1.22053100 -1.52845600 2.59670400
H -1.50898200 -1.24896100 1.03841500
0 0.19189100 -1.40596000 -2.11886800
H 0.65586600 -0.51750500 -2.06856300
H 0.82057100 -2.08955300 -2.37482700
0 1.42069600 0.83597900 -1.94280800
H 1.49472300 1.26322400 -1.03516700

H 1.28035500 1.51393900 -2.61256300
0 -1.59931900 -1.93004600 -0.36100500
H -2.45255500 -1.98406700 -0.80508900
H -0.87779100 -1.74622200 -1.03744700
0 -0.19185800 1.40290800 2.12243100
H -0.82320400 2.07521400 2.40046100
H -0.64665400 0.50380800 2.07619500
0 1.57248700 1.95088900 0.35417200
H 0.85420600 1.75189100 1.02510900
H 2.42753600 1.99256900 0.79604100
Zero-point correction= 0.157741 (Hartree/Particle)
Thermal correction to Energy= 0.171123
Thermal correction to Enthalpy= 0.172067
Thermal correction to Gibbs Free Energy= 0.117653
Sum of electronic and zero-point Energies= -453.516399
Sum of electronic and thermal Energies= -453.503017
Sum of electronic and thermal Enthalpies= -453.502073
Sum of electronic and thermal Free Energies= -453.556487

Water Heptamer
The structures and thermodynamic data were calculated at MP2/6-311++G(d,p) level.

water7-1
0 -0.94052700 -1.38473800 1.18303100
H -0.71912000 -1.70387000 0.29587600
H -1.75635300 -0.86941300 1.04620900
0 0.18033200 -1.66591100 -1.47864800
H 0.30399400 -2.37014800 -2.11950900
H 1.08441000 -1.36510600 -1.24503600
0 -1.09748300 0.94908900 -1.49953800
H -0.35394400 1.42920000 -1.10415200
H -0.72147600 0.08085000 -1.70486400
0 1.11448000 2.07085400 -0.02279900
H 1.07517200 1.57719800 0.81658900
H 1.15588400 2.99587900 0.23122100
0 2.46070100 -0.51156200 -0.55562800
H 2.45447900 0.41863200 -0.81027600
H 2.28221300 -0.45740300 0.39623400
0 -2.91998300 0.41768300 0.46284900
H -2.38965300 0.71463000 -0.30464000
H -3.82128700 0.36076300 0.13975200
0 1.14376600 0.07507700 1.90293400
H 0.33361100 -0.47070800 1.72434200
H 1.28798800 0.01044100 2.84999200
Zero-point correction= 0.179734 (Hartree/Particle)
Thermal correction to Energy= 0.196660
Thermal correction to Enthalpy= 0.197605
Thermal correction to Gibbs Free Energy= 0.137055
Sum of electronic and zero-point Energies= -533.848039
Sum of electronic and thermal Energies= -533.831113

Sum of electronic and thermal Enthalpies= -533.830169
Sum of electronic and thermal Free Energies= -533.890718

water7-2

| | | | |
|---|---|---|---|
| 0 | -1.23659200 | -0.07687500 | -1.60508200 |
| H | -1.80905100 | 0.07946600 | -2.36022400 |
| H | -1.08795200 | 0.80352500 | -1.21569500 |
| 0 | 1.47165200 | -1.12625700 | -1.36705700 |
| H | 1.87319500 | -0.25329300 | -1.22797700 |
| H | 0.58465200 | -0.89688500 | -1.67657900 |
| 0 | -1.28605300 | 0.96774000 | 2.17222100 |
| H | -1.39952700 | 0.04069900 | 1.85120400 |
| H | -0.82022600 | 0.88751900 | 3.00730800 |
| 0 | 2.10751500 | 1.59709500 | -0.88819700 |
| H | 1.26527800 | 1.91894800 | -0.52734700 |
| H | 2.78055800 | 1.97967400 | -0.32160600 |
| 0 | -0.53132600 | 2.17755200 | -0.06384200 |
| H | -0.93005100 | 3.05169900 | -0.08205200 |
| H | -0.77074000 | 1.81262400 | 0.82407600 |
| 0 | -1.52789900 | -1.42290500 | 0.99546600 |
| H | -0.71690600 | -1.96416000 | 1.02066900 |
| H | -1.61652300 | -1.19733500 | 0.05989800 |
| 0 | 0.96957500 | -2.62007200 | 0.84973200 |
| H | 1.22924300 | -3.53042000 | 0.69444000 |
| H | 1.28314700 | -2.13225400 | 0.05926300 |

Zero-point correction= 0.178964 (Hartree/Particle)
Thermal correction to Energy= 0.196299
Thermal correction to Enthalpy= 0.197243
Thermal correction to Gibbs Free Energy= 0.134792
Sum of electronic and zero-point Energies= -533.845558
Sum of electronic and thermal Energies= -533.828223
Sum of electronic and thermal Enthalpies= -533.827279
Sum of electronic and thermal Free Energies= -533.889730

water7-3

| | | | |
|---|---|---|---|
| 0 | -0.56544100 | 0.17359700 | 2.74021300 |
| H | -0.56637800 | 0.43981800 | 3.66175400 |
| H | -0.60363400 | 1.00782400 | 2.23592100 |
| 0 | -0.08157600 | -2.84464300 | -0.48644600 |
| H | 0.45878100 | -2.30007400 | 0.13144900 |
| H | 0.51147300 | -3.52202300 | -0.81630000 |
| 0 | -0.62539600 | 1.28719500 | -1.68239700 |
| H | -1.06490900 | 0.40305300 | -1.70768400 |
| H | -0.92422900 | 1.72628600 | -2.48274200 |
| 0 | -0.32395600 | 2.32315300 | 1.01768800 |
| H | 0.62382200 | 2.32202400 | 0.83882900 |
| H | -0.68366400 | 2.11142900 | 0.14402400 |
| 0 | 1.28419100 | -1.18422200 | 1.11913500 |
| H | 1.61030800 | -0.41453400 | 0.63073700 |
| H | 0.70144700 | -0.80040200 | 1.79720200 |
| 0 | 1.89145900 | 1.13921200 | -0.51910600 |

H 1.13922600 1.16347500 -1.13758700
H 2.67366000 1.23695400 -1.06693000
0 -1.73838000 -1.14253700 -1.74504300
H -1.13774100 -1.81918100 -1.36155000
H -2.57906000 -1.30640700 -1.31116600
Zero-point correction= 0.178841 (Hartree/Particle)
Thermal correction to Energy= 0.196391
Thermal correction to Enthalpy= 0.197335
Thermal correction to Gibbs Free Energy= 0.133825
Sum of electronic and zero-point Energies= -533.845309
Sum of electronic and thermal Energies= -533.827759
Sum of electronic and thermal Enthalpies= -533.826815
Sum of electronic and thermal Free Energies= -533.890325

water7-4
0 0.96309300 0.61601100 1.00675200
H 0.42669000 1.43005800 1.01352900
H 0.47573200 -0.00066600 1.58063100
0 -1.41729000 -2.02000600 -0.50152600
H -0.61440700 -1.71980900 -0.97503400
H -1.66738500 -2.84665700 -0.92081200
0 -1.91514400 0.86566700 -1.32841900
H -2.21723200 0.01286100 -0.99305900
H -1.11252900 0.61605200 -1.80596300
0 0.62067100 -0.53087600 -1.47149500
H 1.52512900 -0.66718300 -1.77723900
H 0.77041200 -0.07842500 -0.61446200
0 -0.71456000 -1.30928800 2.13192200
H -0.52546900 -2.05282100 2.70816000
H -1.04847500 -1.70797000 1.31070700
0 3.30086600 -0.12744800 -0.39994600
H 4.12076400 0.36401600 -0.32456600
H 2.72217300 0.25850800 0.27499100
0 -0.83686500 2.64630700 0.51367500
H -1.36710400 2.11971200 -0.11298100
H -1.47261800 3.16127800 1.01405300
Zero-point correction= 0.178072 (Hartree/Particle)
Thermal correction to Energy= 0.196092
Thermal correction to Enthalpy= 0.197036
Thermal correction to Gibbs Free Energy= 0.133002
Sum of electronic and zero-point Energies= -533.842449
Sum of electronic and thermal Energies= -533.824429
Sum of electronic and thermal Enthalpies= -533.823485
Sum of electronic and thermal Free Energies= -533.887518

water7-5
0 -2.27588200 -1.77762900 -0.13570900
H -3.17282500 -1.55400200 0.12264600
H -1.97137600 -1.01270200 -0.66417300
0 2.88350500 0.83545000 -0.04646800
H 2.59203700 0.03999400 -0.53319500

H 3.80504500 0.68194800 0.16998800
0 -1.58461700 2.80536500 0.11206300
H -1.51011900 3.74018600 0.31261600
H -0.92189700 2.38363200 0.67840200
0 -0.96033400 0.32648800 -1.29713200
H -0.45044600 0.62055500 -0.51840100
H -1.41430200 1.14094200 -1.54296400
0 0.38289800 0.99027000 1.08418300
H 1.33104700 1.07385300 0.87235500
H 0.31034800 0.11632000 1.49420500
0 1.55716900 -1.30872500 -1.14367600
H 1.09762300 -1.67361700 -0.37242500
H 0.83704600 -0.96665300 -1.68689400
0 0.02528200 -1.87235700 1.28292500
H 0.13380200 -2.60945100 1.88879600
H -0.88077700 -1.96899600 0.92194800
Zero-point correction= 0.178174 (Hartree/Particle)
Thermal correction to Energy= 0.196069
Thermal correction to Enthalpy= 0.197013
Thermal correction to Gibbs Free Energy= 0.133398
Sum of electronic and zero-point Energies= -533.842081
Sum of electronic and thermal Energies= -533.824186
Sum of electronic and thermal Enthalpies= -533.823242
Sum of electronic and thermal Free Energies= -533.886857

water7-6
0 -1.12337700 2.44053000 -0.27675000
H -0.20466600 2.24768600 0.01406300
H -1.02215600 2.77655200 -1.17046000
0 1.24775000 1.49963800 0.56014600
H 2.18255700 1.66677400 0.39818200
H 1.17216000 0.55385900 0.33791900
0 -0.99303800 -1.50853900 1.83850500
H -0.91178500 -1.13740500 2.72014200
H -1.59535500 -0.90146900 1.37738300
0 -2.50890100 0.18840200 0.12905800
H -3.43120600 0.41525400 0.27337700
H -2.05885900 1.05508400 -0.02197900
0 -1.13368700 -1.30343400 -1.85230100
H -1.58674100 -2.06408600 -2.22242800
H -1.78668700 -0.88134800 -1.27092100
0 1.04051100 -1.22328000 -0.07676600
H 0.50118100 -1.51845700 0.67648700
H 0.43959400 -1.35006300 -0.83071100
0 3.59823700 -0.03467400 -0.32292300
H 4.40040700 -0.54260900 -0.19031900
H 2.88434500 -0.68757200 -0.27015100
Zero-point correction= 0.177813 (Hartree/Particle)
Thermal correction to Energy= 0.195942
Thermal correction to Enthalpy= 0.196886
Thermal correction to Gibbs Free Energy= 0.131559

Sum of electronic and zero-point Energies= -533.841803
Sum of electronic and thermal Energies= -533.823674
Sum of electronic and thermal Enthalpies= -533.822730
Sum of electronic and thermal Free Energies= -533.888057

water7-7

| | | | |
|---|---|---|---|
| 0 | -1.02554000 | 0.77643600 | -1.65507100 |
| H | -0.69129000 | -0.08222100 | -1.33210400 |
| H | -1.97308400 | 0.67915100 | -1.50417300 |
| 0 | -3.05729500 | -0.68321400 | -0.05985000 |
| H | -3.87346800 | -1.18802900 | -0.03893200 |
| H | -2.35622600 | -1.34764700 | -0.14878900 |
| 0 | -0.96498300 | 0.35652900 | 1.86682000 |
| H | -1.87527900 | 0.37081000 | 1.54820700 |
| H | -0.58037400 | 1.17487200 | 1.52387000 |
| 0 | 2.32038200 | -2.01248500 | -0.15521900 |
| H | 2.84916100 | -2.46096800 | 0.50802300 |
| H | 2.56273900 | -1.07229200 | -0.06713200 |
| 0 | -0.39626400 | -1.48087600 | -0.14355200 |
| H | 0.47952400 | -1.90281600 | -0.19109700 |
| H | -0.37416300 | -0.98132900 | 0.69263100 |
| 0 | 2.78291300 | 0.72697400 | 0.07261200 |
| H | 1.98523400 | 1.28260900 | 0.12372300 |
| H | 3.32593500 | 1.16129900 | -0.58910300 |
| 0 | 0.38165900 | 2.23408600 | 0.09278000 |
| H | 0.36489000 | 3.18289400 | -0.05521800 |
| H | -0.17077700 | 1.84688100 | -0.62669600 |

Zero-point correction= 0.178685 (Hartree/Particle)
Thermal correction to Energy= 0.196340
Thermal correction to Enthalpy= 0.197285
Thermal correction to Gibbs Free Energy= 0.134389
Sum of electronic and zero-point Energies= -533.841158
Sum of electronic and thermal Energies= -533.823502
Sum of electronic and thermal Enthalpies= -533.822558
Sum of electronic and thermal Free Energies= -533.885454

water7-8

| | | | |
|---|---|---|---|
| 0 | -1.81708600 | 2.21713900 | -0.50591800 |
| H | -2.03265100 | 2.91662700 | -1.12634300 |
| H | -0.95612300 | 2.49107300 | -0.12053500 |
| 0 | 0.40342400 | -1.56521800 | 0.14914800 |
| H | -0.15914700 | -2.11373300 | 0.71412600 |
| H | -0.26098900 | -1.14535700 | -0.42245200 |
| 0 | -2.17976200 | -2.38478400 | 1.03158900 |
| H | -2.39579900 | -1.68047000 | 0.40241500 |
| H | -2.78855000 | -2.25659000 | 1.76169100 |
| 0 | 2.98251600 | -1.37709400 | -0.96981600 |
| H | 2.13533800 | -1.74486800 | -0.67553100 |
| H | 3.55653100 | -2.13735300 | -1.07937700 |
| 0 | -1.91951400 | -0.43315900 | -1.02619000 |
| H | -1.92590600 | 0.54067900 | -0.88684600 |

H -2.21368900 -0.55685100 -1.93194900
0 0.60762500 2.89728300 0.49143700
H 0.72009800 3.39155900 1.30620600
H 1.19727100 2.11848800 0.59743200
0 2.04381500 0.64155000 0.87040300
H 1.42467600 -0.10593800 0.85890700
H 2.73643700 0.31628000 0.28037000
Zero-point correction= 0.177455 (Hartree/Particle)
Thermal correction to Energy= 0.195850
Thermal correction to Enthalpy= 0.196794
Thermal correction to Gibbs Free Energy= 0.130144
Sum of electronic and zero-point Energies= -533.841496
Sum of electronic and thermal Energies= -533.823101
Sum of electronic and thermal Enthalpies= -533.822157
Sum of electronic and thermal Free Energies= -533.888807

water7-9
0 0.24464700 -1.18065300 -0.84376200
H -0.48424800 -1.70035500 -1.20011000
H -0.10721100 -0.90899100 0.03255100
0 2.96154300 -1.06407900 -0.24904100
H 2.10249000 -1.39959400 -0.55042900
H 3.49094900 -1.84609900 -0.07962000
0 -0.74515500 -0.18498800 1.53005100
H -1.22822900 0.59449200 1.19995600
H 0.11806900 0.17989200 1.79652000
0 0.49896200 1.55251500 -1.37500100
H 0.52472900 0.58124800 -1.43888000
H 0.92145100 1.86698800 -2.17812100
0 -2.10942500 1.57411900 -0.14214400
H -2.56372400 0.84469900 -0.57758900
H -1.35913800 1.76684700 -0.72332500
0 -2.61163200 -1.53218400 -0.11777600
H -3.36508400 -2.09888200 0.06353200
H -2.20920800 -1.37753000 0.74801400
0 1.79233000 0.98165300 1.36494300
H 1.56861500 1.54064600 0.61110400
H 2.38625100 0.32565700 0.96827500
Zero-point correction= 0.177898 (Hartree/Particle)
Thermal correction to Energy= 0.195890
Thermal correction to Enthalpy= 0.196834
Thermal correction to Gibbs Free Energy= 0.133469
Sum of electronic and zero-point Energies= -533.838279
Sum of electronic and thermal Energies= -533.820287
Sum of electronic and thermal Enthalpies= -533.819343
Sum of electronic and thermal Free Energies= -533.882709
E(RHF/6-311+G**) = -532.431368550

water7-10
0 0.87197300 -0.83900000 1.45435300
H 0.43877000 -1.38798100 2.11205500

H 0.15334600 -0.55033300 0.85230000
0 3.04233100 0.93005700 1.63222900
H 2.21232300 0.44971100 1.78395800
H 2.85260100 1.83606800 1.88323000
0 -3.22040700 1.47221600 0.14453700
H -3.63631800 0.59826300 0.20914600
H -3.57003300 1.97219600 0.88471300
0 2.90447300 -0.61460600 -0.74067700
H 2.40777500 -1.17669800 -0.13356200
H 3.25149500 0.05391100 -0.12977300
0 0.92515700 0.34992500 -2.35099400
H 1.01841000 0.03300500 -3.25154200
H 1.72364000 0.03028300 -1.88105400
0 -0.94983500 -0.05953900 -0.42219000
H -1.49933800 0.72994100 -0.28788900
H -0.39639800 0.12209500 -1.20931800
0 -3.39732000 -1.31391400 0.04062500
H -3.77722100 -1.95806800 -0.56032400
H -2.48723300 -1.18188600 -0.27351400
Zero-point correction= 0.177232 (Hartree/Particle)
Thermal correction to Energy= 0.195740
Thermal correction to Enthalpy= 0.196685
Thermal correction to Gibbs Free Energy= 0.129334
Sum of electronic and zero-point Energies= -533.838627
Sum of electronic and thermal Energies= -533.820120
Sum of electronic and thermal Enthalpies= -533.819175
Sum of electronic and thermal Free Energies= -533.886526

water7-11
0 -1.35946500 0.44435900 1.08982900
H -2.20991100 0.00677200 0.94319000
H -1.39609600 1.27179600 0.57756300
0 -3.01531900 -1.57831400 -0.07095100
H -2.21415300 -1.81419000 -0.56069900
H -3.73296000 -1.71252200 -0.69316300
0 2.60203700 -1.59819600 -0.08078800
H 2.77304400 -0.82943700 -0.63969100
H 3.34986800 -2.18163600 -0.23209600
0 1.43115300 1.03029100 -1.14868300
H 1.48820600 0.95714500 -0.17756000
H 0.84874800 0.29424100 -1.38427800
0 -0.88759700 2.60083900 -0.61391600
H -0.78177000 3.54284500 -0.46527200
H -0.02793600 2.30085100 -0.95557200
0 1.41462800 0.56628900 1.61690100
H 1.79732900 -0.30870400 1.73600500
H 0.47749600 0.45817200 1.83457500
0 -0.24823400 -1.38119500 -0.73506000
H -0.48637100 -0.80116000 0.00970200
H 0.56156800 -1.82287500 -0.44961500
Zero-point correction= 0.177418 (Hartree/Particle)

Thermal correction to Energy= 0.195837
Thermal correction to Enthalpy= 0.196781
Thermal correction to Gibbs Free Energy= 0.132199
Sum of electronic and zero-point Energies= -533.833638
Sum of electronic and thermal Energies= -533.815219
Sum of electronic and thermal Enthalpies= -533.814275
Sum of electronic and thermal Free Energies= -533.878857

water7-12

| | | | |
|---|---|---|---|
| 0 | 2.83900000 | -1.57345000 | -1.10454600 |
| H | 3.11202900 | -0.94936600 | -0.41896000 |
| H | 3.63354500 | -2.06391000 | -1.32452000 |
| 0 | 2.34920900 | 0.29215600 | 1.05425900 |
| H | 1.56920200 | -0.30018700 | 0.96864100 |
| H | 2.53795600 | 0.32779300 | 1.99553600 |
| 0 | -2.24067700 | -0.42208300 | 1.64503200 |
| H | -2.91584200 | -0.64064800 | 0.98714300 |
| H | -1.60487100 | -1.14029300 | 1.55766100 |
| 0 | -3.59707200 | -0.34047500 | -0.90470900 |
| H | -2.83402700 | 0.18431900 | -1.18761300 |
| H | -3.85027600 | -0.84700400 | -1.67873500 |
| 0 | 0.32477400 | -1.30610800 | 0.21798900 |
| H | -0.18108700 | -0.65224400 | -0.29883300 |
| H | 0.89251500 | -1.75452300 | -0.42288400 |
| 0 | -1.11972000 | 0.93638000 | -0.55924700 |
| H | -0.45553100 | 1.64604500 | -0.57452600 |
| H | -1.44199200 | 0.90352500 | 0.35569300 |
| 0 | 1.18339000 | 2.51222200 | -0.26939700 |
| H | 1.72985200 | 1.84666800 | 0.18145600 |
| H | 1.76494800 | 2.90427000 | -0.92416500 |

Zero-point correction= 0.176616 (Hartree/Particle)
Thermal correction to Energy= 0.195372
Thermal correction to Enthalpy= 0.196316
Thermal correction to Gibbs Free Energy= 0.129450
Sum of electronic and zero-point Energies= -533.833406
Sum of electronic and thermal Energies= -533.814651
Sum of electronic and thermal Enthalpies= -533.813707
Sum of electronic and thermal Free Energies= -533.880573

Benzene Trimer
The structures were optimized at M06-2X/6-311++G(2d,p) level.

benzene3-1

| | | | |
|---|---|---|---|
| H | -0.89959000 | 1.17049600 | -1.67290600 |
| C | 0.12760400 | 1.32538900 | -1.36566600 |
| C | 2.76081300 | 1.69744300 | -0.56069800 |
| C | 0.49131800 | 2.48740700 | -0.69609600 |
| C | 1.07863600 | 0.34909300 | -1.63562200 |
| C | 2.39517000 | 0.53655500 | -1.23286600 |
| C | 1.80852400 | 2.67364200 | -0.29189800 |
| H | -0.25051600 | 3.24886300 | -0.48728600 |

| | | | |
|---|---|---|---|
| H | 0.78920700 | -0.55864500 | -2.15046200 |
| H | 3.13629600 | -0.22552500 | -1.44099900 |
| H | 2.09232400 | 3.57768100 | 0.23247400 |
| H | 3.78687400 | 1.84162800 | -0.24533400 |
| H | 1.28106500 | -3.97816900 | -2.37735300 |
| C | 0.41435600 | -3.35470000 | -2.19490600 |
| C | -1.81091200 | -1.75847900 | -1.72754700 |
| C | -0.31719800 | -2.85333900 | -3.26558200 |
| C | 0.03480800 | -3.05338100 | -0.89241800 |
| C | -1.07780300 | -2.25511600 | -0.65684100 |
| C | -1.43020900 | -2.05412900 | -3.03147000 |
| H | -0.02012300 | -3.08422800 | -4.28107500 |
| H | 0.60646400 | -3.43392400 | -0.05478100 |
| H | -1.36443500 | -2.01522000 | 0.35959700 |
| H | -1.99985800 | -1.66283400 | -3.86544200 |
| H | -2.67907600 | -1.13675400 | -1.54406800 |
| H | 1.05321100 | 0.50947100 | 1.28734500 |
| C | 0.36213900 | -0.14025900 | 1.80974700 |
| C | -1.42521800 | -1.81657000 | 3.12751000 |
| C | 0.77363900 | -1.39443800 | 2.24295200 |
| C | -0.94416400 | 0.27530800 | 2.03707500 |
| C | -1.83736100 | -0.56038800 | 2.69704000 |
| C | -0.11895500 | -2.23371500 | 2.89960700 |
| H | 1.79135800 | -1.71890300 | 2.06183700 |
| H | -1.26305700 | 1.25156000 | 1.69233700 |
| H | -2.85528100 | -0.23548200 | 2.87425600 |
| H | 0.20188300 | -3.21267500 | 3.23454600 |
| H | -2.12140800 | -2.46990300 | 3.63859800 |

benzene3-2

| | | | |
|---|---|---|---|
| C | -0.89257100 | 2.65922200 | 0.50167500 |
| C | 0.39599900 | 2.19215300 | 0.27753600 |
| C | 0.67516800 | 1.43284700 | -0.85323800 |
| C | -0.33677200 | 1.14695600 | -1.75994600 |
| C | -1.62829600 | 1.60820600 | -1.53383800 |
| C | -1.90607300 | 2.36357500 | -0.40303000 |
| H | -1.11021100 | 3.24907500 | 1.38393100 |
| H | 1.18713100 | 2.41281600 | 0.98441300 |
| H | 1.67841100 | 1.05863900 | -1.01836800 |
| H | -0.12187400 | 0.54959100 | -2.63796800 |
| H | -2.42042500 | 1.36748600 | -2.23201900 |
| H | -2.91429300 | 2.71489700 | -0.22135500 |
| C | -1.36011800 | -0.83038800 | 0.97076700 |
| C | -2.55499400 | -0.44121800 | 1.56178700 |
| C | -3.76638700 | -0.83831900 | 1.00970200 |
| C | -3.78265100 | -1.62763900 | -0.13381500 |
| C | -2.58735400 | -2.02099200 | -0.72289100 |
| C | -1.37698000 | -1.62104900 | -0.17029200 |
| H | -0.41528300 | -0.49076900 | 1.37776600 |
| H | -2.54139100 | 0.18599600 | 2.44482500 |
| H | -4.69807400 | -0.53039400 | 1.46819100 |

| | | | |
|---|---|---|---|
| H | -4.72678300 | -1.93609100 | -0.56568300 |
| H | -2.60012600 | -2.63310100 | -1.61638000 |
| H | -0.44304000 | -1.90202500 | -0.64303300 |
| C | 4.19229100 | 0.17928900 | -0.23703600 |
| C | 3.62472100 | 0.37228200 | 1.01681100 |
| C | 2.62065400 | -0.47812500 | 1.46317500 |
| C | 2.18423300 | -1.52206300 | 0.65706100 |
| C | 2.74832900 | -1.71226900 | -0.59850700 |
| C | 3.75288800 | -0.86230900 | -1.04556400 |
| H | 4.97515700 | 0.84163000 | -0.58494300 |
| H | 3.96640900 | 1.18502000 | 1.64603300 |
| H | 2.17734400 | -0.32767800 | 2.44024600 |
| H | 1.40458000 | -2.18724700 | 1.00857500 |
| H | 2.40803600 | -2.52607900 | -1.22730700 |
| H | 4.19389800 | -1.01151400 | -2.02326700 |

benzene3-3

| | | | |
|---|---|---|---|
| C | -0.47822500 | 0.96414800 | 1.29870400 |
| C | -0.21283200 | 2.12581800 | 0.58247500 |
| C | 0.26390100 | 2.04402600 | -0.71947000 |
| C | 0.48384300 | 0.80083600 | -1.30164400 |
| C | 0.22316100 | -0.35801400 | -0.58386000 |
| C | -0.26432300 | -0.27638300 | 0.71430200 |
| H | -0.86398800 | 1.02657000 | 2.30907500 |
| H | -0.38300300 | 3.09414000 | 1.03761600 |
| H | 0.47039100 | 2.94859900 | -1.27884500 |
| H | 0.87014500 | 0.73602900 | -2.31159700 |
| H | 0.40121900 | -1.32647900 | -1.03505900 |
| H | -0.48031900 | -1.18128600 | 1.26912000 |
| C | 4.01514500 | -0.30804300 | -1.11674500 |
| C | 3.80717500 | -1.57200100 | -0.57834600 |
| C | 3.33373500 | -1.70344300 | 0.72120600 |
| C | 3.06422900 | -0.57119900 | 1.47962400 |
| C | 3.26784200 | 0.69213300 | 0.94057900 |
| C | 3.74643200 | 0.82305700 | -0.35645200 |
| H | 4.38538900 | -0.20501100 | -2.12944800 |
| H | 4.01644700 | -2.45426300 | -1.17083700 |
| H | 3.17138300 | -2.68850200 | 1.14134700 |
| H | 2.68229500 | -0.67279700 | 2.48799600 |
| H | 3.03910600 | 1.57406400 | 1.52581300 |
| H | 3.89837200 | 1.80869300 | -0.77915500 |
| C | -3.80582400 | -1.59812300 | 0.54676900 |
| C | -4.02303000 | -0.35091400 | 1.11983000 |
| C | -3.75819000 | 0.80247700 | 0.39259100 |
| C | -3.27427600 | 0.71080400 | -0.90595900 |
| C | -3.06086800 | -0.53553500 | -1.47928100 |
| C | -3.32647200 | -1.69025400 | -0.75384800 |
| H | -4.01251800 | -2.49793300 | 1.11320400 |
| H | -4.39781300 | -0.27866700 | 2.13351000 |
| H | -3.91765600 | 1.77495100 | 0.84219000 |
| H | -3.04933500 | 1.61012000 | -1.46562300 |

| | | | |
|---|---|---|---|
| H | -2.67442300 | -0.60641800 | -2.48855100 |
| H | -3.15674300 | -2.66211800 | -1.20093200 |

benzene3-4

| | | | |
|---|---|---|---|
| C | 0.71536300 | 0.00777300 | -1.19141700 |
| C | 0.36061900 | -1.19951000 | -0.60337000 |
| C | -0.35315500 | -1.20964700 | 0.58839400 |
| C | -0.71561500 | -0.01254900 | 1.19237500 |
| C | -0.36090400 | 1.19471200 | 0.60432000 |
| C | 0.35292900 | 1.20484700 | -0.58743300 |
| H | 1.28841900 | 0.01575400 | -2.11053300 |
| H | 0.65088700 | -2.13318000 | -1.06998800 |
| H | -0.63738900 | -2.15125400 | 1.04262900 |
| H | -1.28866500 | -0.02052400 | 2.11149400 |
| H | -0.65120000 | 2.12838100 | 1.07091800 |
| H | 0.63719200 | 2.14645200 | -1.04165000 |
| C | 3.42526700 | -1.20396400 | 0.86275500 |
| C | 3.06512300 | -0.00539200 | 1.46446500 |
| C | 3.41902200 | 1.20026600 | 0.87333400 |
| C | 4.12660000 | 1.20834700 | -0.32209000 |
| C | 4.48193300 | 0.00878700 | -0.92653600 |
| C | 4.13285000 | -1.19787400 | -0.33267100 |
| H | 3.14234600 | -2.14402800 | 1.32033700 |
| H | 2.49596200 | -0.01095200 | 2.38566900 |
| H | 3.13118000 | 2.13478800 | 1.33912500 |
| H | 4.39960900 | 2.14917900 | -0.78418500 |
| H | 5.03306600 | 0.01434800 | -1.85899000 |
| H | 4.41077800 | -2.13317500 | -0.80298900 |
| C | -4.48246900 | -0.00684300 | 0.92566300 |
| C | -4.13330700 | 1.20005000 | 0.33228800 |
| C | -3.42510100 | 1.20657800 | -0.86275300 |
| C | -3.06434400 | 0.00821900 | -1.46455200 |
| C | -3.41830400 | -1.19764800 | -0.87391700 |
| C | -4.12657000 | -1.20616600 | 0.32110900 |
| H | -5.03410400 | -0.01275000 | 1.85781700 |
| H | -4.41169700 | 2.13517500 | 0.80268300 |
| H | -3.14216100 | 2.14681800 | -1.31996900 |
| H | -2.49463000 | 0.01412100 | -2.38541200 |
| H | -3.12996600 | -2.13199000 | -1.33975500 |
| H | -4.39962300 | -2.14717200 | 0.78282700 |

benzene3-5

| | | | |
|---|---|---|---|
| C | -0.50162300 | 3.64959600 | 0.55762600 |
| C | 0.46650100 | 3.66644200 | -0.43817100 |
| C | 0.95107100 | 2.47031700 | -0.95597900 |
| C | 0.46714500 | 1.25928000 | -0.47890000 |
| C | -0.50039800 | 1.24242800 | 0.51820700 |
| C | -0.98518500 | 2.43655200 | 1.03534300 |
| H | -0.87960400 | 4.58097400 | 0.96115900 |
| H | 0.84374900 | 4.61102400 | -0.81048900 |
| H | 1.70870900 | 2.48223700 | -1.73032400 |

| | | | |
|---|---|---|---|
| H | 0.84764600 | 0.32359100 | -0.87356700 |
| H | -0.87930800 | 0.29403300 | 0.88227500 |
| H | -1.74262500 | 2.42201700 | 1.80983000 |
| C | -1.59589000 | -1.72610900 | -1.11716200 |
| C | -2.39017200 | -0.67700600 | -1.56100300 |
| C | -3.40902500 | -0.18704400 | -0.75400900 |
| C | -3.63505700 | -0.74703000 | 0.49689100 |
| C | -2.84314100 | -1.79967400 | 0.94080800 |
| C | -1.82336300 | -2.28867200 | 0.13318100 |
| H | -0.79323300 | -2.09864300 | -1.74202400 |
| H | -2.20447900 | -0.22963800 | -2.52933400 |
| H | -4.01937300 | 0.63929500 | -1.09594600 |
| H | -4.42767500 | -0.36308500 | 1.12712400 |
| H | -3.02067400 | -2.23820100 | 1.91504800 |
| H | -1.20660300 | -3.10939300 | 0.47973700 |
| C | 2.48133200 | -0.60111500 | 1.50666700 |
| C | 1.66211500 | -1.66652900 | 1.15665500 |
| C | 1.81630500 | -2.28403300 | -0.07874700 |
| C | 2.78517200 | -1.83225300 | -0.96655300 |
| C | 3.60198200 | -0.76330100 | -0.61654800 |
| C | 3.45110900 | -0.14979800 | 0.62059000 |
| H | 2.35279000 | -0.11101900 | 2.46350200 |
| H | 0.89779500 | -2.01027500 | 1.84319300 |
| H | 1.18228300 | -3.11950600 | -0.35059100 |
| H | 2.90479500 | -2.31327400 | -1.92955500 |
| H | 4.35588400 | -0.40913300 | -1.30872000 |
| H | 4.08116200 | 0.68855100 | 0.88994100 |

benzene3-6

| | | | |
|---|---|---|---|
| C | -1.18462000 | 3.79017600 | -0.18724800 |
| C | -1.83129100 | 2.63234100 | -0.60255400 |
| C | -1.17109500 | 1.41069000 | -0.55866800 |
| C | 0.14009300 | 1.34577500 | -0.10147800 |
| C | 0.78648900 | 2.50400400 | 0.31273500 |
| C | 0.12490900 | 3.72569500 | 0.27167000 |
| H | -1.70100500 | 4.74170600 | -0.22005500 |
| H | -2.85315200 | 2.68101400 | -0.95869800 |
| H | -1.67890100 | 0.50720300 | -0.87434300 |
| H | 0.65712500 | 0.39260200 | -0.06698800 |
| H | 1.80764400 | 2.45055200 | 0.66969600 |
| H | 0.62967300 | 4.62713000 | 0.59699300 |
| C | -2.45623300 | -2.19053900 | -1.08608100 |
| C | -3.59826000 | -1.64103400 | -0.51615400 |
| C | -3.55304700 | -1.13100900 | 0.77596400 |
| C | -2.36710700 | -1.17094000 | 1.49796500 |
| C | -1.22503000 | -1.71936200 | 0.92812400 |
| C | -1.26909000 | -2.22794400 | -0.36371000 |
| H | -2.48976800 | -2.58432800 | -2.09433900 |
| H | -4.52239000 | -1.60781900 | -1.07977700 |
| H | -4.44126100 | -0.69714500 | 1.21807500 |
| H | -2.32892700 | -0.76158000 | 2.49954800 |

| | | | |
|---|---|---|---|
| H | -0.29427000 | -1.73122000 | 1.48227200 |
| H | -0.37459200 | -2.64168200 | -0.81268800 |
| C | 3.38397000 | -0.05740600 | 0.95732600 |
| C | 2.74383000 | -1.25145900 | 1.26591500 |
| C | 2.29787700 | -2.08358800 | 0.24608100 |
| C | 2.48600300 | -1.71819900 | -1.08138500 |
| C | 3.12328600 | -0.52273900 | -1.38946900 |
| C | 3.57467400 | 0.30596100 | -0.37006400 |
| H | 3.73245800 | 0.59004800 | 1.75270100 |
| H | 2.59524800 | -1.53453900 | 2.30080900 |
| H | 1.80362300 | -3.01751700 | 0.48738800 |
| H | 2.13661300 | -2.36486500 | -1.87711500 |
| H | 3.26439800 | -0.23491600 | -2.42353400 |
| H | 4.06863600 | 1.23902700 | -0.61155600 |

benzene3-7

| | | | |
|---|---|---|---|
| H | 3.65666700 | -0.21779600 | -0.67088000 |
| C | 2.73273900 | -0.46054200 | -1.18116100 |
| C | 0.35887000 | -1.08182200 | -2.48370700 |
| C | 2.32758800 | -1.78508200 | -1.29554100 |
| C | 1.95134700 | 0.55314500 | -1.72116100 |
| C | 0.76328200 | 0.24239700 | -2.37315500 |
| C | 1.14118500 | -2.09592000 | -1.94540700 |
| H | 2.93083000 | -2.57561000 | -0.86641700 |
| H | 2.26767500 | 1.58564300 | -1.63028300 |
| H | 0.14961600 | 1.03241900 | -2.78968800 |
| H | 0.81686900 | -3.12659700 | -2.01638600 |
| H | -0.57188100 | -1.32383700 | -2.98200700 |
| H | -0.90022900 | 5.38214400 | -0.48842700 |
| C | -0.98674800 | 4.48450400 | 0.11115400 |
| C | -1.21122600 | 2.18080900 | 1.65006800 |
| C | -0.34953300 | 3.31638700 | -0.28810600 |
| C | -1.73624800 | 4.50016500 | 1.28095900 |
| C | -1.84861000 | 3.34884600 | 2.05027600 |
| C | -0.46080400 | 2.16448800 | 0.48051000 |
| H | 0.23544500 | 3.30147600 | -1.20018400 |
| H | -2.23342900 | 5.41017100 | 1.59300700 |
| H | -2.43345200 | 3.36185300 | 2.96156500 |
| H | 0.03754300 | 1.25742500 | 0.15983200 |
| H | -1.30106800 | 1.28197900 | 2.24952800 |
| H | 0.48380600 | -0.39403400 | 1.69594600 |
| C | 0.07124100 | -1.34262000 | 1.37212700 |
| C | -0.96330300 | -3.77993400 | 0.52879300 |
| C | 0.73998900 | -2.52340400 | 1.67266200 |
| C | -1.11515700 | -1.38077500 | 0.65161000 |
| C | -1.63304900 | -2.60065300 | 0.23158500 |
| C | 0.22515900 | -3.74132000 | 1.24955300 |
| H | 1.66726100 | -2.49169700 | 2.23156700 |
| H | -1.63414800 | -0.46106000 | 0.40843600 |
| H | -2.55824400 | -2.62982900 | -0.33084100 |
| H | 0.74704000 | -4.66121700 | 1.48319500 |

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|---|---|---|---|
| H | -1.36701900 | -4.73010000 | 0.20096900 |

benzene3-8

| | | | |
|---|---|---|---|
| H | -0.75364900 | 4.64363400 | -1.97644600 |
| C | -0.80414100 | 4.34494200 | -0.93652200 |
| C | -0.93248000 | 3.58143600 | 1.73102500 |
| C | 0.35790200 | 4.01331200 | -0.25131800 |
| C | -2.03177500 | 4.29226400 | -0.28770200 |
| C | -2.09565100 | 3.91196800 | 1.04712800 |
| C | 0.29410500 | 3.62860100 | 1.08149400 |
| H | 1.31416700 | 4.04369800 | -0.75928500 |
| H | -2.93812200 | 4.55082900 | -0.82144700 |
| H | -3.05224800 | 3.87264100 | 1.55366300 |
| H | 1.19836600 | 3.35392300 | 1.61026400 |
| H | -0.98258900 | 3.27579800 | 2.76894700 |
| H | 0.29861100 | 1.03003600 | -2.09005600 |
| C | 0.22785600 | 0.71538100 | -1.05602000 |
| C | 0.04684800 | -0.07213000 | 1.60149500 |
| C | 1.37311900 | 0.34354200 | -0.36304100 |
| C | -1.00805900 | 0.69535400 | -0.42178200 |
| C | -1.09859800 | 0.29727000 | 0.90616800 |
| C | 1.28312800 | -0.04737300 | 0.96722300 |
| H | 2.33521400 | 0.35353000 | -0.85996500 |
| H | -1.89770000 | 1.00189500 | -0.95774100 |
| H | -2.06133600 | 0.28623700 | 1.40220900 |
| H | 2.17523000 | -0.34298100 | 1.50579700 |
| H | -0.02491200 | -0.37849800 | 2.63825300 |
| H | 0.74541800 | -5.43315300 | -2.85806400 |
| C | 0.73889000 | -4.92985500 | -1.89907200 |
| C | 0.72381000 | -3.63779800 | 0.55932200 |
| C | 0.14117400 | -3.68163300 | -1.77276500 |
| C | 1.32844000 | -5.53267300 | -0.79502700 |
| C | 1.32018800 | -4.88634900 | 0.43509400 |
| C | 0.13311000 | -3.03389900 | -0.54383300 |
| H | -0.31821700 | -3.21152700 | -2.63364400 |
| H | 1.79412000 | -6.50551200 | -0.89290800 |
| H | 1.77962900 | -5.35635100 | 1.29598700 |
| H | -0.32797400 | -2.05887700 | -0.44243400 |
| H | 0.71812100 | -3.12768100 | 1.51499900 |

benzene3-9

| | | | |
|---|---|---|---|
| C | -0.23181500 | 0.27884100 | 1.56217500 |
| C | -0.88395300 | 0.44583700 | 0.34628000 |
| C | -0.69512700 | 1.61219100 | -0.38477600 |
| C | 0.14720200 | 2.60792300 | 0.09551900 |
| C | 0.80121400 | 2.43828300 | 1.31013200 |
| C | 0.61006300 | 1.27441500 | 2.04423100 |
| H | -0.38140300 | -0.62971700 | 2.13321600 |
| H | -1.54237000 | -0.32746400 | -0.03029200 |
| H | -1.20871700 | 1.74060700 | -1.33007100 |
| H | 0.29600200 | 3.51529900 | -0.47674200 |

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|---|---|---|---|
| H | 1.46270500 | 3.21063500 | 1.68196800 |
| H | 1.12199500 | 1.14186400 | 2.98956000 |
| C | -3.87414800 | -0.21495800 | -1.68778400 |
| C | -4.24786500 | 0.65071600 | -0.66723800 |
| C | -4.38490100 | 0.17640500 | 0.63131700 |
| C | -4.15050500 | -1.16445600 | 0.90955900 |
| C | -3.77690900 | -2.03132900 | -0.11069700 |
| C | -3.63774700 | -1.55638200 | -1.40973500 |
| H | -3.76640600 | 0.15465000 | -2.70029200 |
| H | -4.42579300 | 1.69725800 | -0.88198500 |
| H | -4.66725700 | 0.85366800 | 1.42751900 |
| H | -4.25592300 | -1.53351900 | 1.92220500 |
| H | -3.59262700 | -3.07623800 | 0.10611800 |
| H | -3.34415700 | -2.23086200 | -2.20445500 |
| C | 2.81003500 | -0.13097200 | -0.42913900 |
| C | 3.19984800 | -0.92683000 | 0.64077800 |
| C | 4.44239600 | -1.54824700 | 0.63181600 |
| C | 5.29846100 | -1.37369000 | -0.44860500 |
| C | 4.91022300 | -0.57826100 | -1.51940600 |
| C | 3.66681400 | 0.04176700 | -1.50933200 |
| H | 1.84016300 | 0.35132600 | -0.41687400 |
| H | 2.52890400 | -1.05902500 | 1.48076200 |
| H | 4.74469600 | -2.16864700 | 1.46657300 |
| H | 6.26746000 | -1.85718000 | -0.45604300 |
| H | 5.57728600 | -0.44155700 | -2.36166600 |
| H | 3.36455100 | 0.66172500 | -2.34444500 |

benzene3-dta

| | | | |
|---|---|---|---|
| H | -0.57546700 | 2.52609800 | 0.42566100 |
| C | -0.58006100 | 1.44504200 | 0.35740600 |
| C | -0.59154200 | -1.32780800 | 0.18213900 |
| C | -0.04549800 | 0.68181800 | 1.38866500 |
| C | -1.12036300 | 0.82214400 | -0.76145200 |
| C | -1.12597700 | -0.56468200 | -0.84917600 |
| C | -0.05135500 | -0.70501900 | 1.30102700 |
| H | 0.38426500 | 1.16697300 | 2.25604900 |
| H | -1.54559200 | 1.41617700 | -1.56067100 |
| H | -1.55625600 | -1.04992000 | -1.71626200 |
| H | 0.37440900 | -1.29910000 | 2.09993300 |
| H | -0.59615600 | -2.40892900 | 0.11387200 |
| H | 5.19374600 | 2.05238900 | 0.31976500 |
| C | 4.64579500 | 1.14996200 | 0.07812600 |
| C | 3.23999400 | -1.16460600 | -0.53940200 |
| C | 3.34479900 | 1.23366400 | -0.40277800 |
| C | 5.24418100 | -0.09207400 | 0.25019900 |
| C | 4.54089000 | -1.24986100 | -0.05892400 |
| C | 2.64122600 | 0.07679800 | -0.71244500 |
| H | 2.87510500 | 2.20099200 | -0.53395500 |
| H | 6.25795200 | -0.15762900 | 0.62534600 |
| H | 5.00713800 | -2.21814300 | 0.07545200 |

| | | | |
|---|---|---|---|
| H | 1.62277300 | 0.14127800 | -1.07635500 |
| H | 2.68776400 | -2.06580300 | -0.77715900 |
| C | -5.70889300 | -1.28689100 | 0.45627000 |
| C | -4.41014400 | -1.25014900 | 0.94859900 |
| C | -3.81234900 | -0.03223700 | 1.24668100 |
| C | -4.51472400 | 1.14987100 | 1.05033000 |
| C | -5.81356300 | 1.11471600 | 0.55775900 |
| C | -6.41098400 | -0.10393000 | 0.26053800 |
| H | -6.17439000 | -2.23690800 | 0.22433600 |
| H | -3.85884000 | -2.17066400 | 1.09809000 |
| H | -2.79546300 | -0.00443700 | 1.61953700 |
| H | -4.04570900 | 2.09925000 | 1.27892200 |
| H | -6.36057800 | 2.03683400 | 0.40449400 |
| H | -7.42307000 | -0.13163100 | -0.12375300 |

benzene3-dtb

| | | | |
|---|---|---|---|
| H | 2.82893100 | -1.66094000 | 0.87926500 |
| C | 1.92082400 | -1.14117400 | 0.59877600 |
| C | -0.40702200 | 0.19076100 | -0.12019500 |
| C | 1.02930600 | -0.72165500 | 1.57859600 |
| C | 1.64718100 | -0.89385500 | -0.74093700 |
| C | 0.48253900 | -0.22782600 | -1.10259000 |
| C | -0.13587700 | -0.05462900 | 1.22063400 |
| H | 1.23803200 | -0.91219800 | 2.62428100 |
| H | 2.33931800 | -1.21845800 | -1.50823000 |
| H | 0.27186900 | -0.03694100 | -2.14825300 |
| H | -0.82857800 | 0.27134200 | 1.98743000 |
| H | -1.31522100 | 0.71036900 | -0.40067800 |
| H | 2.16835400 | -2.19457500 | -4.24503500 |
| C | 1.55355100 | -1.31773500 | -4.40716300 |
| C | -0.02685500 | 0.93059000 | -4.81721000 |
| C | 0.19357200 | -1.46057300 | -4.65278300 |
| C | 2.12301400 | -0.05104000 | -4.36371700 |
| C | 1.33270200 | 1.07323300 | -4.56786100 |
| C | -0.59651200 | -0.33630500 | -4.85915400 |
| H | -0.25108400 | -2.44742200 | -4.67928900 |
| H | 3.18198100 | 0.06098700 | -4.16603000 |
| H | 1.77558200 | 2.06047300 | -4.52850700 |
| H | -1.65670800 | -0.44732200 | -5.04946100 |
| H | -0.64291700 | 1.80701300 | -4.97519200 |
| H | -2.60680500 | 2.77696000 | 3.67659800 |
| C | -2.13106200 | 1.85372500 | 3.98301200 |
| C | -0.90802900 | -0.51651200 | 4.76228500 |
| C | -0.80381500 | 1.85964700 | 4.39393400 |
| C | -2.84654200 | 0.66259900 | 3.96051300 |
| C | -2.23455100 | -0.52303100 | 4.34881200 |
| C | -0.19294700 | 0.67465700 | 4.78504200 |
| H | -0.24414000 | 2.78641700 | 4.40522100 |
| H | -3.87982300 | 0.65746100 | 3.63662700 |
| H | -2.78979400 | -1.45227000 | 4.32549600 |
| H | 0.84243000 | 0.67953300 | 5.10300900 |

H -0.43090500 -1.44130300 5.06275200

Asymmetric Strecker Reaction

The structures and thermodynamic data were calculated at SMD(toluene)-M06-2X/6-31G* level.

TS-R

N -0.41733900 -0.61939000 0.55734500
C -1.56951200 -1.11988100 0.24406800
N -2.22262500 -1.82323700 1.24240000
N -2.26270000 -1.20123200 -0.91201100
C -0.20430700 -0.99326800 1.96714200
H 0.63561500 0.43521000 -0.25289000
C -3.53135600 -1.88473700 -0.66508600
C -1.18131700 -2.18070000 2.19532600
C -3.17545700 -2.71317800 0.60011800
H -4.04621500 -2.90693700 1.22934300
H -1.55315300 -2.23487800 3.22023900
H -2.70396000 -3.66738000 0.31950600
H -0.70645500 -3.13830400 1.92643900
H -3.76141600 -2.55379800 -1.49984700
H -0.51854800 -0.16117100 2.61660500
C 1.24895300 -1.29749300 2.24468200
C 1.97321600 -2.12623400 1.38073600
C 1.89823700 -0.73140000 3.34319300
C 3.31627200 -2.39486800 1.62549600
H 1.48512600 -2.53760800 0.49932100
C 3.24563000 -0.99575600 3.58747800
H 1.34430800 -0.07407600 4.01017200
C 3.95632700 -1.83098600 2.72932000
H 3.86845600 -3.03382400 0.94258200
H 3.73819400 -0.54631300 4.44488900
H 5.00681500 -2.03578200 2.91359700
C -4.70935100 -0.94375900 -0.44436700
C -5.96559800 -1.49338700 -0.16893000
C -4.58125300 0.44210500 -0.52603700
C -7.07024400 -0.67546400 0.03938500
H -6.07965600 -2.57484400 -0.12061900
C -5.68915500 1.26293200 -0.31695700
H -3.62228400 0.89044000 -0.76903100
C -6.93296800 0.71040400 -0.03040100
H -8.03848300 -1.11836600 0.25358900
H -5.57198500 2.34060900 -0.38280500
H -7.79353900 1.35260600 0.13122700
H -2.14888700 -0.51470100 -1.66969600
N 1.13771700 1.16099200 -0.85414400
C 0.54827100 2.30206200 -1.02799300
C 2.27557000 0.73965800 -1.68592700
C 3.57376000 1.19047100 -1.04335300
C 3.82082700 0.92565700 0.30758500
C 5.02308300 1.31525000 0.88713100
C 5.99018800 1.96991000 0.12375000

| | | | |
|---|---|---|---|
| C | 5.74906800 | 2.23251900 | -1.22118700 |
| C | 4.54250500 | 1.84355600 | -1.80228400 |
| C | 2.18870800 | -0.76288600 | -1.93394400 |
| C | 0.96344400 | -1.29696700 | -2.34625800 |
| C | 0.83471100 | -2.66104900 | -2.58237600 |
| C | 1.93348600 | -3.50602000 | -2.42435900 |
| C | 3.15973800 | -2.97489200 | -2.03584200 |
| C | 3.28756300 | -1.60811300 | -1.78636200 |
| C | -0.40775100 | 2.82090800 | -0.02991900 |
| C | -0.25937000 | 2.45665500 | 1.31226900 |
| C | -1.11622900 | 2.98101600 | 2.27537100 |
| C | -2.11666400 | 3.87468900 | 1.90424700 |
| C | -2.25281600 | 4.25590800 | 0.56870100 |
| C | -1.40014700 | 3.73623300 | -0.39592800 |
| H | 0.97395700 | 2.98766400 | -1.75388600 |
| H | 2.15986200 | 1.25377900 | -2.64971500 |
| H | 3.07238400 | 0.40688800 | 0.90465800 |
| H | 5.20442400 | 1.10346900 | 1.93680700 |
| H | 6.92800800 | 2.27457100 | 0.57832900 |
| H | 6.49661700 | 2.74324900 | -1.82052700 |
| H | 4.35304400 | 2.04782300 | -2.85331100 |
| H | 0.11001500 | -0.63634500 | -2.49027300 |
| H | -0.12722500 | -3.05984700 | -2.89056100 |
| H | 1.83513900 | -4.57119900 | -2.61190600 |
| H | 4.02343300 | -3.62366300 | -1.92115000 |
| H | 4.24545300 | -1.20742700 | -1.46919900 |
| H | 0.54316700 | 1.78345300 | 1.60200800 |
| H | -0.99586200 | 2.69606100 | 3.31612500 |
| H | -2.78801900 | 4.28025600 | 2.65500000 |
| H | -3.03064300 | 4.95513400 | 0.27861300 |
| H | -1.51762200 | 3.99608800 | -1.44287100 |
| C | -1.03499800 | 1.76269600 | -2.74249600 |
| N | -1.80740200 | 0.89138700 | -2.88169200 |

Zero-point correction= 0.650444 (Hartree/Particle)
Thermal correction to Energy= 0.673469
Thermal correction to Enthalpy= 0.674207
Thermal correction to Gibbs Free Energy= 0.600705
Sum of electronic and zero-point Energies= -1741.493138
Sum of electronic and thermal Energies= -1741.470112
Sum of electronic and thermal Enthalpies= -1741.469375
Sum of electronic and thermal Free Energies= -1741.542877

TS-R-new

| | | | |
|---|---|---|---|
| N | -0.33690700 | -1.30515900 | -0.17176200 |
| C | -1.45813700 | -1.25877500 | -0.82363200 |
| N | -2.31919000 | -2.32884600 | -0.65053700 |
| N | -1.97148100 | -0.40461900 | -1.73007000 |
| C | -0.37914200 | -2.58077800 | 0.57061900 |
| H | 0.60690700 | 0.08865000 | 0.26711400 |
| C | -3.29302500 | -0.86037700 | -2.15384300 |
| C | -1.48928800 | -3.40756400 | -0.14247100 |

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|---|---|---|---|
| C | -3.20883100 | -2.37100100 | -1.79870400 |
| H | -4.18367300 | -2.79287700 | -1.54734600 |
| H | -2.02953100 | -4.06738000 | 0.53945100 |
| H | -2.76338900 | -2.94270500 | -2.62720500 |
| H | -1.06367500 | -4.00446500 | -0.96522600 |
| H | -3.39878400 | -0.73429400 | -3.23567200 |
| H | -0.70187000 | -2.38792400 | 1.60515600 |
| C | 0.94935000 | -3.29908300 | 0.60384600 |
| C | 1.41055900 | -3.88289400 | 1.78374600 |
| C | 1.70840600 | -3.43616400 | -0.56225500 |
| C | 2.59983800 | -4.61067500 | 1.79954800 |
| H | 0.82968400 | -3.77244700 | 2.69714200 |
| C | 2.89056800 | -4.16772200 | -0.55139700 |
| H | 1.37241300 | -2.95062300 | -1.47460800 |
| C | 3.33837900 | -4.76074600 | 0.62933400 |
| H | 2.94545300 | -5.06208400 | 2.72497100 |
| H | 3.47266200 | -4.26321800 | -1.46330700 |
| H | 4.26305100 | -5.33046500 | 0.63700400 |
| C | -4.45098600 | -0.15536300 | -1.45912200 |
| C | -5.75705500 | -0.54255700 | -1.77651200 |
| C | -4.25532300 | 0.86924900 | -0.53507300 |
| C | -6.84782200 | 0.06910700 | -1.16937300 |
| H | -5.92035500 | -1.33011300 | -2.51015600 |
| C | -5.34927000 | 1.48367500 | 0.07380700 |
| H | -3.25098700 | 1.20816000 | -0.29944100 |
| C | -6.64526500 | 1.08521500 | -0.23601300 |
| H | -7.85567000 | -0.24400900 | -1.42577500 |
| H | -5.17940000 | 2.28075400 | 0.79172100 |
| H | -7.49485500 | 1.56623500 | 0.23938800 |
| H | -1.64976700 | 0.56160000 | -1.83927900 |
| N | 1.04232100 | 1.05312100 | 0.36271900 |
| C | 0.37981200 | 1.94930200 | 1.02662400 |
| C | 1.98794200 | 1.36701500 | -0.71574700 |
| C | 2.58688100 | 2.75765900 | -0.57203700 |
| C | 3.58307200 | 3.01158800 | 0.37586700 |
| C | 4.10959200 | 4.29109800 | 0.51610100 |
| C | 3.65111600 | 5.32813100 | -0.29576800 |
| C | 2.66105700 | 5.08034300 | -1.24157500 |
| C | 2.12636700 | 3.80013600 | -1.37791900 |
| C | 3.05247000 | 0.28825900 | -0.79084000 |
| C | 3.67549800 | 0.03633900 | -2.01438500 |
| C | 4.71292000 | -0.88669200 | -2.09937400 |
| C | 5.13859300 | -1.56724600 | -0.95972300 |
| C | 4.51425400 | -1.32792700 | 0.26098400 |
| C | 3.47281900 | -0.40686700 | 0.34457900 |
| C | -0.59246800 | 1.54967100 | 2.06085900 |
| C | -0.46604000 | 0.31765900 | 2.71034100 |
| C | -1.36765000 | -0.03623600 | 3.71001800 |
| C | -2.39189100 | 0.83677300 | 4.06569000 |
| C | -2.51126900 | 2.07183200 | 3.42737600 |
| C | -1.61374900 | 2.43084200 | 2.43068600 |

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|---|---|---|---|
| H | 0.73460300 | 2.97340400 | 1.00378300 |
| H | 1.38150300 | 1.35170800 | -1.63424600 |
| H | 3.95517700 | 2.20125500 | 0.99761900 |
| H | 4.88391100 | 4.47780500 | 1.25404500 |
| H | 4.06622600 | 6.32588800 | -0.18952200 |
| H | 2.29715100 | 5.88370900 | -1.87468900 |
| H | 1.33140400 | 3.61005400 | -2.09287700 |
| H | 3.34901200 | 0.57527300 | -2.90060000 |
| H | 5.19023000 | -1.07384800 | -3.05664600 |
| H | 5.94745000 | -2.28904900 | -1.02557600 |
| H | 4.82531800 | -1.86952200 | 1.14919100 |
| H | 2.98480400 | -0.22865800 | 1.29969800 |
| H | 0.34885200 | -0.35323000 | 2.45039600 |
| H | -1.26379700 | -0.99172300 | 4.21495900 |
| H | -3.09647500 | 0.55785300 | 4.84310800 |
| H | -3.31029600 | 2.75240200 | 3.70392800 |
| H | -1.71445300 | 3.37131700 | 1.89831800 |
| C | -1.01445700 | 2.73312600 | -0.73732700 |
| N | -1.07985600 | 2.43013800 | -1.86984000 |

Zero-point correction= 0.650606 (Hartree/Particle)
Thermal correction to Energy= 0.673835
Thermal correction to Enthalpy= 0.674573
Thermal correction to Gibbs Free Energy= 0.600073
Sum of electronic and zero-point Energies= -1741.490712
Sum of electronic and thermal Energies= -1741.467483
Sum of electronic and thermal Enthalpies= -1741.466745
Sum of electronic and thermal Free Energies= -1741.541245

TS-S

| | | | |
|---|---|---|---|
| C | 1.25821900 | -0.94879100 | 2.84301400 |
| C | 0.09533300 | -1.01291900 | 1.81251000 |
| C | 1.71638700 | 0.21099500 | 0.96005700 |
| C | 3.92882200 | 0.83616500 | 0.96399400 |
| C | 3.54487200 | 0.20228600 | 2.33131500 |
| H | 1.46674100 | -1.91405800 | 3.30811500 |
| H | 1.05133900 | -0.20220000 | 3.62749800 |
| H | 4.41008300 | 1.80554500 | 1.12793700 |
| H | 3.33969900 | 0.98335400 | 3.07947200 |
| N | 0.44299900 | 0.02520500 | 0.82151400 |
| H | -0.69106800 | 0.44569700 | -0.35295100 |
| N | 2.60646000 | 1.03739900 | 0.36671600 |
| H | 0.11426500 | -1.99708600 | 1.31919800 |
| H | 4.31820600 | -0.46858700 | 2.70934000 |
| N | 2.33308400 | -0.51050200 | 1.96679700 |
| H | 2.47556700 | 1.32730900 | -0.60858700 |
| C | 4.87006300 | -0.04534400 | 0.15261000 |
| C | 6.12501400 | -0.35033500 | 0.69085700 |
| C | 4.54098600 | -0.53146500 | -1.11185500 |
| C | 7.02623400 | -1.14529800 | -0.00777500 |
| H | 6.40119700 | 0.04260600 | 1.66770000 |
| C | 5.44670100 | -1.32804200 | -1.81344000 |

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|---|---|---|---|
| H | 3.59141400 | -0.26946500 | -1.56993200 |
| C | 6.68556200 | -1.64249000 | -1.26500500 |
| H | 7.99482300 | -1.37466400 | 0.42671700 |
| H | 5.17799200 | -1.69606300 | -2.79932100 |
| H | 7.38682400 | -2.26281000 | -1.81506900 |
| C | -1.27890100 | -0.79623600 | 2.39976900 |
| C | -1.65015300 | 0.46382400 | 2.88078400 |
| C | -2.20749500 | -1.83620400 | 2.44765100 |
| C | -2.92879100 | 0.68225600 | 3.38586000 |
| H | -0.92827000 | 1.27640400 | 2.84391700 |
| C | -3.48726900 | -1.62393400 | 2.95899100 |
| H | -1.92766800 | -2.81453300 | 2.06511700 |
| C | -3.85188400 | -0.36355400 | 3.42535000 |
| H | -3.20643300 | 1.66722300 | 3.75018400 |
| H | -4.20192900 | -2.44135200 | 2.98274300 |
| H | -4.84987000 | -0.19491500 | 3.81939100 |
| N | -1.28766100 | 0.64925500 | -1.21673100 |
| C | -1.15834300 | 1.80258500 | -1.79310600 |
| C | -0.76306800 | 2.99944700 | -1.02715400 |
| C | -0.19107200 | 4.10309600 | -1.66935900 |
| C | 0.10291600 | 5.24907900 | -0.94456400 |
| C | -0.17563600 | 5.30542800 | 0.42230300 |
| C | -0.75766400 | 4.21476800 | 1.06074800 |
| C | -1.05709500 | 3.06370200 | 0.33755100 |
| C | 0.91455600 | 1.52996700 | -2.95252900 |
| N | 1.98599800 | 1.30410200 | -2.53269800 |
| C | -1.92593900 | -0.48561600 | -1.89906300 |
| C | -3.41721800 | -0.49417800 | -1.62008900 |
| C | -4.30907200 | -0.83087600 | -2.63774000 |
| C | -5.67805600 | -0.88897100 | -2.38541400 |
| C | -6.16344200 | -0.61100100 | -1.11043400 |
| C | -5.27528700 | -0.27706800 | -0.08907200 |
| C | -3.90782300 | -0.21892700 | -0.34057100 |
| C | -1.20979200 | -1.77491100 | -1.50745500 |
| C | -1.86644200 | -2.84928200 | -0.91043600 |
| C | -1.15982800 | -4.00822400 | -0.58153200 |
| C | 0.20442200 | -4.09370600 | -0.83773600 |
| C | 0.86547600 | -3.01786200 | -1.43350000 |
| C | 0.16162300 | -1.86807400 | -1.77144700 |
| H | -1.61746900 | 1.93486700 | -2.76824100 |
| H | 0.05299400 | 4.03311900 | -2.72450700 |
| H | 0.55789200 | 6.09917700 | -1.44270500 |
| H | 0.05771500 | 6.20376500 | 0.98584600 |
| H | -0.99046900 | 4.26113800 | 2.12037100 |
| H | -1.54291500 | 2.22244000 | 0.82249100 |
| H | -1.76862100 | -0.32734300 | -2.97455800 |
| H | -3.92893300 | -1.04948800 | -3.63280700 |
| H | -6.36379300 | -1.14701100 | -3.18667500 |
| H | -7.23029900 | -0.65243700 | -0.91283800 |
| H | -5.64408200 | -0.06179300 | 0.90947300 |
| H | -3.21985400 | 0.03615700 | 0.46395800 |

| | | | |
|---|---|---|---|
| H | -2.93010800 | -2.79031100 | -0.70055500 |
| H | -1.68276400 | -4.84265700 | -0.12289800 |
| H | 0.75334400 | -4.99419900 | -0.57853600 |
| H | 1.93146500 | -3.07354300 | -1.63283500 |
| H | 0.67532700 | -1.02424200 | -2.23017600 |

Zero-point correction= 0.650683 (Hartree/Particle)
Thermal correction to Energy= 0.673742
Thermal correction to Enthalpy= 0.674480
Thermal correction to Gibbs Free Energy= 0.601452
Sum of electronic and zero-point Energies= -1741.490631
Sum of electronic and thermal Energies= -1741.467572
Sum of electronic and thermal Enthalpies= -1741.466834
Sum of electronic and thermal Free Energies= -1741.539863

TS-S-new

| | | | |
|---|---|---|---|
| C | -1.04367400 | -3.37672100 | 0.66519500 |
| C | 0.08045200 | -2.34102900 | 0.96048500 |
| C | -1.25582300 | -1.50858800 | -0.58068800 |
| C | -3.27212700 | -1.56947500 | -1.69628100 |
| C | -3.02112400 | -2.91519000 | -0.96102500 |
| H | -1.44631000 | -3.83463900 | 1.57091800 |
| H | -0.67958400 | -4.16622800 | -0.01229400 |
| H | -3.50556400 | -1.75882100 | -2.74883300 |
| H | -2.63281200 | -3.67319800 | -1.65840200 |
| N | -0.05560900 | -1.34190100 | -0.11888100 |
| H | 0.91551100 | 0.09601400 | -0.25839300 |
| N | -1.95093700 | -0.94824400 | -1.59218000 |
| H | -0.12727000 | -1.85802600 | 1.92743200 |
| H | -3.91841900 | -3.29827400 | -0.47234900 |
| N | -2.00673500 | -2.51643300 | -0.00043100 |
| H | -1.73398000 | -0.01806200 | -1.95900400 |
| C | -4.40582500 | -0.75526100 | -1.08263400 |
| C | -5.67393200 | -1.33590900 | -0.97543800 |
| C | -4.23141800 | 0.56450700 | -0.66735300 |
| C | -6.74095200 | -0.62371100 | -0.43903400 |
| H | -5.83147700 | -2.35595200 | -1.31993300 |
| C | -5.30229700 | 1.27917800 | -0.13091900 |
| H | -3.26864800 | 1.05195700 | -0.79013800 |
| C | -6.55565700 | 0.68884700 | -0.00783200 |
| H | -7.71740400 | -1.09242000 | -0.35937000 |
| H | -5.15148100 | 2.30731500 | 0.18496400 |
| H | -7.38649700 | 1.24843900 | 0.41129400 |
| C | 1.44898600 | -2.97698900 | 1.02395500 |
| C | 2.12754800 | -3.33331000 | -0.14576500 |
| C | 2.02864700 | -3.27499600 | 2.25802900 |
| C | 3.36309100 | -3.97201400 | -0.07782900 |
| H | 1.68227000 | -3.09593700 | -1.10899600 |
| C | 3.26496700 | -3.91436600 | 2.32854400 |
| H | 1.50298800 | -3.00011000 | 3.16959500 |
| C | 3.93619100 | -4.26294400 | 1.15969200 |
| H | 3.87797100 | -4.25292500 | -0.99248800 |

| | | | |
|---|---|---|---|
| H | 3.70375200 | -4.13862600 | 3.29642000 |
| H | 4.90000300 | -4.76037700 | 1.21104300 |
| N | 1.18229500 | 1.12242100 | -0.26443800 |
| C | 1.71108000 | 1.63094200 | -1.33294000 |
| C | 2.46058300 | 0.79003800 | -2.27983400 |
| C | 2.69487800 | 1.25727200 | -3.57702300 |
| C | 3.43990600 | 0.49313400 | -4.46423500 |
| C | 3.95892700 | -0.73819600 | -4.06110300 |
| C | 3.73274600 | -1.20167100 | -2.76796900 |
| C | 2.98669600 | -0.43953600 | -1.87430500 |
| C | -0.31928100 | 2.07103200 | -2.51907400 |
| N | -1.42755400 | 1.95567600 | -2.14728300 |
| C | 0.36580000 | 1.88143700 | 0.69173800 |
| C | 0.79869700 | 3.33508600 | 0.79560700 |
| C | 0.08056000 | 4.31356000 | 0.10420000 |
| C | 0.47464900 | 5.64904700 | 0.16630200 |
| C | 1.58976700 | 6.01468900 | 0.91445200 |
| C | 2.31327500 | 5.04060900 | 1.60108700 |
| C | 1.91902200 | 3.70776400 | 1.54353200 |
| C | 0.35892700 | 1.14248500 | 2.01671100 |
| C | 1.50494600 | 0.50786400 | 2.50166700 |
| C | 1.48397800 | -0.13692100 | 3.73675100 |
| C | 0.31244200 | -0.16826500 | 4.48960000 |
| C | -0.83932500 | 0.44605400 | 3.99996300 |
| C | -0.81483300 | 1.09836500 | 2.77059600 |
| H | 1.81493400 | 2.70917400 | -1.39123600 |
| H | 2.25298000 | 2.19987500 | -3.88467100 |
| H | 3.61175600 | 0.85259400 | -5.47374000 |
| H | 4.54261300 | -1.33369500 | -4.75655200 |
| H | 4.14523700 | -2.15264000 | -2.44488900 |
| H | 2.83569600 | -0.79332100 | -0.85810300 |
| H | -0.64927400 | 1.86715900 | 0.26633100 |
| H | -0.77321900 | 4.01937100 | -0.50031200 |
| H | -0.09179100 | 6.40167700 | -0.37355100 |
| H | 1.89607200 | 7.05526800 | 0.96397400 |
| H | 3.18308100 | 5.32027500 | 2.18780200 |
| H | 2.47720900 | 2.95552900 | 2.09383000 |
| H | 2.41605300 | 0.50801500 | 1.90749900 |
| H | 2.38374100 | -0.62202200 | 4.10365900 |
| H | 0.29425000 | -0.67380500 | 5.45044900 |
| H | -1.76027600 | 0.41424700 | 4.57408300 |
| H | -1.71529100 | 1.57060800 | 2.38548100 |

Zero-point correction= 0.650770 (Hartree/Particle)
Thermal correction to Energy= 0.673361
Thermal correction to Enthalpy= 0.674098
Thermal correction to Gibbs Free Energy= 0.601969
Sum of electronic and zero-point Energies= -1741.492224
Sum of electronic and thermal Energies= -1741.469633
Sum of electronic and thermal Enthalpies= -1741.468895
Sum of electronic and thermal Free Energies= -1741.541025

Asymmetric Methanolysis Reaction
The model TS was optimized at HF/3-21G level.

amma-model-ts

| | | | |
|---|---|---|---|
| N | -2.04333100 | 0.31921600 | -0.02698700 |
| C | -2.18974400 | 0.16345700 | 1.43156800 |
| H | -1.32421200 | 0.60805600 | 1.92124100 |
| H | -2.21699100 | -0.89927400 | 1.67623600 |
| H | -3.11377500 | 0.65272300 | 1.76206400 |
| C | -1.88847400 | 1.73522000 | -0.40466100 |
| H | -1.02326000 | 2.15193200 | 0.11296900 |
| H | -2.79390200 | 2.29416000 | -0.14044700 |
| H | -1.72249000 | 1.79836700 | -1.48268600 |
| C | -3.16670700 | -0.30344400 | -0.74511000 |
| H | -2.99190900 | -0.22822500 | -1.82086700 |
| H | -4.10597300 | 0.20296400 | -0.49364700 |
| H | -3.23609600 | -1.35573200 | -0.46067600 |
| H | -0.96164200 | -0.29176700 | -0.40998600 |
| 0 | 0.13736600 | -0.90967900 | -0.83341400 |
| C | -0.18764600 | -2.25469500 | -1.09311700 |
| H | -0.47204500 | -2.77600000 | -0.16894700 |
| H | 0.67075800 | -2.77520500 | -1.53751000 |
| H | -1.01677900 | -2.30980800 | -1.80964400 |
| C | 1.05082100 | -0.77528400 | 0.68843700 |
| 0 | 0.53247500 | -1.45884700 | 1.55112400 |
| 0 | 0.83253800 | 0.68043100 | 0.76377300 |
| C | 1.65135900 | 1.32251600 | -0.08736400 |
| 0 | 1.54411600 | 2.50102100 | -0.31679700 |
| C | 2.46594100 | -0.91690400 | 0.13374400 |
| H | 2.56748700 | -1.83966300 | -0.43925800 |
| H | 3.14222800 | -0.96602200 | 0.99304400 |
| C | 2.67041600 | 0.35853700 | -0.67290300 |
| H | 3.66856000 | 0.79593300 | -0.60423300 |
| H | 2.42560500 | 0.22321700 | -1.72980100 |

Zero-point correction= 0.273090 (Hartree/Particle)
Thermal correction to Energy= 0.287252
Thermal correction to Enthalpy= 0.288196
Thermal correction to Gibbs Free Energy= 0.232815
Sum of electronic and zero-point Energies= -662.753331
Sum of electronic and thermal Energies= -662.739169
Sum of electronic and thermal Enthalpies= -662.738225
Sum of electronic and thermal Free Energies= -662.793606

TS-major-no-meoh-docked

| | | | |
|---|---|---|---|
| C | -3.6919093 | 1.5252560 | 1.3563807 |
| H | -4.7728168 | 1.4477222 | 1.3710405 |
| C | -3.1196042 | 0.7025202 | 2.5195227 |
| H | -2.0730165 | 0.9345730 | 2.5947188 |
| C | -3.3141487 | 3.0009065 | 1.5722575 |
| H | -2.2374913 | 3.1044006 | 1.5952795 |
| H | -3.6958651 | 3.6208271 | 0.7712559 |

| | | | |
|---|---|---|---|
| C | -3.9440845 | 3.4823935 | 2.9010407 |
| H | -3.6575411 | 4.5134326 | 3.0758336 |
| H | -5.0263743 | 3.4562216 | 2.8065140 |
| C | -3.8125207 | 1.1195289 | 3.8154022 |
| H | -3.4392325 | 0.4957056 | 4.6184352 |
| H | -4.8806669 | 0.9460958 | 3.7307100 |
| C | -3.5204874 | 2.6053476 | 4.0953516 |
| H | -2.4553625 | 2.7286123 | 4.2657876 |
| H | -4.0356576 | 2.9307718 | 4.9924635 |
| N | -3.2632017 | 0.9313896 | 0.0148331 |
| C | -3.0538318 | 1.9350523 | -1.0751711 |
| H | -3.9677018 | 2.4793566 | -1.2712739 |
| H | -2.7571832 | 1.3940007 | -1.9621112 |
| H | -2.2636301 | 2.6126254 | -0.7996313 |
| C | -4.3091465 | -0.0635805 | -0.4025616 |
| H | -5.2574717 | 0.4440605 | -0.5286614 |
| H | -4.3697794 | -0.7978010 | 0.3808147 |
| H | -4.0212503 | -0.5133627 | -1.3403804 |
| O | -3.2745995 | -0.7058997 | 2.2824025 |
| H | -2.3732807 | -1.0804302 | 2.2258685 |
| H | -2.2120374 | 0.3374865 | -0.0122798 |
| O | -1.1094634 | -0.2269555 | -0.3769348 |
| C | -1.2732384 | -1.5679045 | -0.8629838 |
| H | -1.2876704 | -2.2610915 | -0.0300888 |
| H | -0.4610594 | -1.8295505 | -1.5312408 |
| H | -2.2016464 | -1.6615385 | -1.4170648 |
| C | -0.1235164 | -0.1673555 | 1.1144022 |
| O | -0.5956464 | -0.9329615 | 1.9361222 |
| O | -0.3722944 | 1.2686315 | 1.2517852 |
| C | 0.3048456 | 1.9692415 | 0.3088022 |
| O | 0.0508546 | 3.1160505 | 0.0592532 |
| C | 1.2580826 | -0.2214015 | 0.4674422 |
| H | 1.3832736 | -1.1198125 | -0.1117828 |
| H | 1.9813116 | -0.2168785 | 1.2734392 |
| C | 1.3363776 | 1.0671945 | -0.3510888 |
| H | 2.3059846 | 1.5425525 | -0.3482748 |
| H | 1.0158416 | 0.9042935 | -1.3695068 |

TS-minor-no-meoh-docked

| | | | |
|---|---|---|---|
| C | -3.43833000 | 1.02233500 | -1.69065400 |
| H | -2.45436000 | 1.25764900 | -2.06221700 |
| C | -3.89510300 | -0.33141800 | -2.26469000 |
| H | -4.93226700 | -0.48885400 | -1.99934000 |
| C | -4.42369800 | 2.10887100 | -2.15015000 |
| H | -5.43086700 | 1.87156400 | -1.82091000 |
| H | -4.15463300 | 3.07472400 | -1.74383700 |
| C | -4.38773700 | 2.19150800 | -3.69418600 |
| H | -5.08841100 | 2.94684900 | -4.03212500 |
| H | -3.39470400 | 2.50430800 | -4.00164200 |
| C | -3.79756800 | -0.27379700 | -3.79369700 |
| H | -4.08062700 | -1.24244100 | -4.18720500 |

| | | | |
|---|---|---|---|
| H | -2.76551500 | -0.08812100 | -4.07421900 |
| C | -4.71628100 | 0.83284100 | -4.34271700 |
| H | -5.74990700 | 0.57555900 | -4.12854000 |
| H | -4.61558100 | 0.90371000 | -5.41986100 |
| N | -3.24453800 | 0.92943300 | -0.18844300 |
| C | -4.33097600 | 0.18741200 | 0.52231400 |
| H | -5.28701200 | 0.66477400 | 0.35220500 |
| H | -4.11350000 | 0.20190600 | 1.58145900 |
| H | -4.33386600 | -0.82583200 | 0.16265500 |
| C | -3.02070600 | 2.26003700 | 0.45772800 |
| H | -3.94549900 | 2.81678400 | 0.50834400 |
| H | -2.27297500 | 2.81262600 | -0.08456900 |
| H | -2.65487000 | 2.07953700 | 1.45903100 |
| O | -3.17884900 | -1.43239300 | -1.70939700 |
| H | -2.21903000 | -1.36309200 | -1.91141100 |
| H | -2.21203740 | 0.33748650 | 0.01227980 |
| O | -1.10946340 | -0.22695550 | 0.37693480 |
| C | -1.27323840 | -1.56790450 | 0.86298380 |
| H | -1.28767040 | -2.26109150 | 0.03008880 |
| H | -0.46105940 | -1.82955050 | 1.53124080 |
| H | -2.20164640 | -1.66153850 | 1.41706480 |
| C | -0.12351640 | -0.16735550 | -1.11440220 |
| O | -0.59564640 | -0.93296150 | -1.93612220 |
| O | -0.37229440 | 1.26863150 | -1.25178520 |
| C | 0.30484560 | 1.96924150 | -0.30880220 |
| O | 0.05085460 | 3.11605050 | -0.05925320 |
| C | 1.25808260 | -0.22140150 | -0.46744220 |
| H | 1.38327360 | -1.11981250 | 0.11178280 |
| H | 1.98131160 | -0.21687850 | -1.27343920 |
| C | 1.33637760 | 1.06719450 | 0.35108880 |
| H | 2.30598460 | 1.54255250 | 0.34827480 |
| H | 1.01584160 | 0.90429350 | 1.36950680 |

TS-mjaor-2-meoh-docked

| | | | |
|---|---|---|---|
| C | -3.35638500 | 1.62110600 | 1.40822500 |
| H | -2.43947400 | 2.17037200 | 1.52516900 |
| C | -4.53322700 | 2.59279200 | 1.57070800 |
| H | -5.47226000 | 2.07765900 | 1.43691800 |
| C | -3.40928300 | 0.54610900 | 2.51208600 |
| H | -4.34573400 | 0.00097000 | 2.45789000 |
| H | -2.58716500 | -0.14230400 | 2.38468100 |
| C | -3.31738500 | 1.20966200 | 3.89866700 |
| H | -3.33944400 | 0.44279900 | 4.66470200 |
| H | -2.36827400 | 1.72922100 | 3.98260000 |
| C | -4.47108700 | 3.24034900 | 2.96316200 |
| H | -5.31072900 | 3.91998600 | 3.05008400 |
| H | -3.56105300 | 3.82999100 | 3.00666600 |
| C | -4.47608100 | 2.20133000 | 4.09379900 |
| H | -5.41740500 | 1.65851000 | 4.08566500 |
| H | -4.39564100 | 2.70021300 | 5.05362200 |
| N | -3.23666100 | 0.96658100 | 0.04249100 |

| | | | |
|---|---|---|---|
| C | -3.01670500 | 1.92172400 | -1.10590500 |
| H | -3.95430200 | 2.32800600 | -1.43355600 |
| H | -2.55290600 | 1.34984000 | -1.89661800 |
| H | -2.34926600 | 2.70609000 | -0.79963600 |
| C | -4.39374900 | 0.07854700 | -0.31269200 |
| H | -5.27996400 | 0.68025300 | -0.44562900 |
| H | -4.53045900 | -0.67227400 | 0.44734700 |
| H | -4.16348300 | -0.40837000 | -1.24962700 |
| O | -4.52365800 | 3.64908700 | 0.58197400 |
| H | -3.65976200 | 4.12308600 | 0.60376400 |
| O | -6.24959400 | 2.61145000 | -1.09366600 |
| H | -5.67347000 | 3.17434300 | -0.53184100 |
| C | -7.38504600 | 3.31988700 | -1.60676000 |
| H | -7.09650000 | 4.15933800 | -2.23239600 |
| H | -8.02854400 | 3.69145900 | -0.81494400 |
| H | -7.95355300 | 2.62670100 | -2.20972200 |
| O | -2.07044700 | 4.66470900 | 0.82925200 |
| H | -1.27963000 | 4.12477600 | 0.63107500 |
| C | -1.76623800 | 6.07490900 | 0.86109700 |
| H | -1.41076100 | 6.42546200 | -0.10018000 |
| H | -1.02325600 | 6.29792900 | 1.61665900 |
| H | -2.68185600 | 6.58985900 | 1.10737800 |
| H | -2.21203740 | 0.33748650 | -0.01227980 |
| O | -1.10946340 | -0.22695550 | -0.37693480 |
| C | -1.27323840 | -1.56790450 | -0.86298380 |
| H | -1.28767040 | -2.26109150 | -0.03008880 |
| H | -0.46105940 | -1.82955050 | -1.53124080 |
| H | -2.20164640 | -1.66153850 | -1.41706480 |
| C | -0.12351640 | -0.16735550 | 1.11440220 |
| O | -0.59564640 | -0.93296150 | 1.93612220 |
| O | -0.37229440 | 1.26863150 | 1.25178520 |
| C | 0.30484560 | 1.96924150 | 0.30880220 |
| O | 0.05085460 | 3.11605050 | 0.05925320 |
| C | 1.25808260 | -0.22140150 | 0.46744220 |
| H | 1.38327360 | -1.11981250 | -0.11178280 |
| H | 1.98131160 | -0.21687850 | 1.27343920 |
| C | 1.33637760 | 1.06719450 | -0.35108880 |
| H | 2.30598460 | 1.54255250 | -0.34827480 |
| H | 1.01584160 | 0.90429350 | -1.36950680 |

TS-minor-2-meoh-docked

| | | | |
|---|---|---|---|
| C | -3.18300000 | 2.11900000 | 0.63300000 |
| H | -2.28500000 | 2.62600000 | 0.32800000 |
| C | -4.34900000 | 3.10400000 | 0.48600000 |
| H | -5.28300000 | 2.62400000 | 0.73500000 |
| C | -3.00200000 | 1.71100000 | 2.10900000 |
| H | -3.89800000 | 1.23000000 | 2.48200000 |
| H | -2.18100000 | 1.01000000 | 2.16700000 |
| C | -2.71900000 | 2.95400000 | 2.97200000 |
| H | -2.57300000 | 2.65500000 | 4.00400000 |
| H | -1.80400000 | 3.42900000 | 2.63100000 |

| | | | |
|---|---|---|---|
| C | -4.11200000 | 4.32700000 | 1.38800000 |
| H | -4.96200000 | 4.98900000 | 1.28000000 |
| H | -3.24000000 | 4.84800000 | 1.00500000 |
| C | -3.89000000 | 3.94500000 | 2.85800000 |
| H | -4.78900000 | 3.48400000 | 3.25700000 |
| H | -3.69200000 | 4.83600000 | 3.44500000 |
| N | -3.23600000 | 0.88900000 | -0.24700000 |
| C | -3.20300000 | 1.15500000 | -1.73900000 |
| H | -4.20700000 | 1.30800000 | -2.08900000 |
| H | -2.74500000 | 0.29200000 | -2.19700000 |
| H | -2.59300000 | 2.01400000 | -1.93300000 |
| C | -4.38700000 | -0.03400000 | 0.02800000 |
| H | -5.30400000 | 0.42700000 | -0.30700000 |
| H | -4.43100000 | -0.27800000 | 1.07700000 |
| H | -4.21800000 | -0.94100000 | -0.53700000 |
| O | -4.49200000 | 3.56800000 | -0.87300000 |
| H | -3.63800000 | 3.95500000 | -1.18100000 |
| O | -2.01200000 | 4.44300000 | -1.39800000 |
| H | -1.25500000 | 4.01800000 | -0.94800000 |
| C | -1.58000000 | 5.39900000 | -2.39000000 |
| H | -0.99600000 | 4.92200000 | -3.16800000 |
| H | -0.99600000 | 6.19300000 | -1.94100000 |
| H | -2.47000000 | 5.82300000 | -2.82900000 |
| O | -6.40300000 | 1.90700000 | -1.57500000 |
| H | -5.76600000 | 2.64600000 | -1.47100000 |
| C | -7.54000000 | 2.26500000 | -2.37000000 |
| H | -7.26000000 | 2.56900000 | -3.37400000 |
| H | -8.11900000 | 3.06600000 | -1.92000000 |
| H | -8.17000000 | 1.39000000 | -2.44400000 |
| H | -2.21200000 | 0.33700000 | 0.01200000 |
| O | -1.10900000 | -0.22700000 | 0.37700000 |
| C | -1.27300000 | -1.56800000 | 0.86300000 |
| H | -1.28800000 | -2.26100000 | 0.03000000 |
| H | -0.46100000 | -1.83000000 | 1.53100000 |
| H | -2.20200000 | -1.66200000 | 1.41700000 |
| C | -0.12400000 | -0.16700000 | -1.11400000 |
| O | -0.59600000 | -0.93300000 | -1.93600000 |
| O | -0.37200000 | 1.26900000 | -1.25200000 |
| C | 0.30500000 | 1.96900000 | -0.30900000 |
| O | 0.05100000 | 3.11600000 | -0.05900000 |
| C | 1.25800000 | -0.22100000 | -0.46700000 |
| H | 1.38300000 | -1.12000000 | 0.11200000 |
| H | 1.98100000 | -0.21700000 | -1.27300000 |
| C | 1.33600000 | 1.06700000 | 0.35100000 |
| H | 2.30600000 | 1.54300000 | 0.34800000 |
| H | 1.01600000 | 0.90400000 | 1.37000000 |

The structures and thermodynamic data were calculated at SMD(toluene)-M06-2X/6-31G* level of theory and 258 K.

TS-major

| | | | |
|---|---|---|---|
| H | -2.34389800 | -2.11126700 | -3.22994700 |
| C | -2.36610500 | -1.89274900 | -2.15693500 |
| C | -2.13595700 | -0.07812300 | -0.42760700 |
| C | -3.73897300 | -1.95978200 | -0.05780700 |
| C | -3.49645400 | -0.46302300 | 0.17837900 |
| C | -3.68984900 | -2.33825200 | -1.53744300 |
| C | -2.12914600 | -0.40010400 | -1.92766400 |
| H | -1.36185300 | -0.68989300 | 0.05132200 |
| H | -2.96416900 | -2.51697600 | 0.48955100 |
| H | -4.28253000 | 0.10590000 | -0.33995300 |
| H | -4.52083800 | -1.85173700 | -2.06716000 |
| H | -2.91879500 | 0.16564500 | -2.44009500 |
| H | -1.53768200 | -2.44423900 | -1.69704500 |
| H | -4.70272100 | -2.22089900 | 0.39139200 |
| H | -3.82889200 | -3.41852000 | -1.65652300 |
| H | -1.16752700 | -0.11445800 | -2.35786500 |
| N | -1.69107100 | 1.33098400 | -0.18629300 |
| C | -1.97216200 | 3.74609700 | -0.63523500 |
| C | -0.61800900 | 2.97381100 | 1.31868800 |
| C | -1.51836000 | 4.08753900 | 0.78400400 |
| C | -1.33152700 | 1.62867700 | 1.23545800 |
| C | -2.62666100 | 2.36724700 | -0.68731000 |
| H | -1.10508100 | 3.75558900 | -1.30866900 |
| H | 0.30755600 | 2.93346000 | 0.73264100 |
| H | -2.39951900 | 4.18794100 | 1.43212100 |
| H | -2.24865500 | 1.63903800 | 1.82911000 |
| H | -3.53096400 | 2.35042400 | -0.06386300 |
| H | -0.59298600 | 1.39815100 | -0.78160500 |
| H | -2.68524700 | 4.48685600 | -1.01150600 |
| H | -0.33776500 | 3.15444200 | 2.36102200 |
| H | -0.99677500 | 5.05000100 | 0.79600800 |
| H | -0.69689400 | 0.81454200 | 1.59031600 |
| H | -2.91078700 | 2.11673100 | -1.71186200 |
| 0 | -3.62047300 | -0.14646700 | 1.54448400 |
| H | -2.90999100 | -0.64502100 | 2.00563500 |
| 0 | 0.55568100 | 1.44025800 | -1.28570900 |
| C | 0.50918300 | 1.72406600 | -2.65674000 |
| H | -0.48912900 | 2.07554900 | -2.96148600 |
| H | 0.73117000 | 0.82632500 | -3.25606700 |
| H | 1.23061100 | 2.50892000 | -2.92434200 |
| C | 1.46338500 | -0.21963200 | -0.90877900 |
| 0 | 0.92221400 | -1.12942500 | -1.52364800 |
| 0 | 1.17954000 | -0.10226500 | 0.47473000 |
| C | 2.05501100 | 0.74765400 | 1.07685700 |
| 0 | 1.90033800 | 1.10657000 | 2.21338400 |
| C | 2.85816300 | 0.32756500 | -1.15634400 |
| H | 2.86844300 | 0.96401500 | -2.04131200 |
| C | 3.20655100 | 1.06474700 | 0.14694900 |
| H | 3.31965000 | 2.14599200 | 0.04608600 |
| C | 3.98080900 | -0.75759900 | -1.26494100 |
| H | 4.05048100 | -1.21488500 | -2.25167500 |

| | | | |
|---|---|---|---|
| C | 4.54581600 | 0.37245800 | 0.60456100 |
| H | 5.11970100 | 0.95876400 | 1.32137800 |
| C | 5.17233700 | 0.09554800 | -0.77743700 |
| H | 5.32990800 | 1.00125400 | -1.37319400 |
| H | 6.10195800 | -0.47494300 | -0.70820800 |
| C | 3.82796100 | -1.70628100 | -0.08867300 |
| H | 3.40280100 | -2.70189000 | -0.14993800 |
| C | 4.17494600 | -1.04233900 | 1.01875500 |
| H | 4.08684500 | -1.38131200 | 2.04516900 |
| H | -0.97077800 | -2.06076500 | 1.73387200 |
| 0 | -1.44869300 | -1.60378000 | 2.46078700 |
| C | -0.50201300 | -1.23431800 | 3.44731900 |
| H | -0.11185700 | -2.11610900 | 3.97251200 |
| H | -1.01274800 | -0.59946500 | 4.17661500 |
| H | 0.33860900 | -0.67127800 | 3.02518900 |
| H | 0.25182300 | -2.26950500 | -0.29461300 |
| 0 | -0.08125000 | -2.82222600 | 0.44611400 |
| C | -0.20424900 | -4.17136000 | 0.04348600 |
| H | 0.75641800 | -4.57722100 | -0.29661700 |
| H | -0.94402000 | -4.30462800 | -0.75671100 |
| H | -0.53342300 | -4.74382000 | 0.91398200 |

Zero-point correction= 0.640403 (Hartree/Particle)
Thermal correction to Energy= 0.665774
Thermal correction to Enthalpy= 0.666591
Thermal correction to Gibbs Free Energy= 0.589805
Sum of electronic and zero-point Energies= -1481.166924
Sum of electronic and thermal Energies= -1481.141553
Sum of electronic and thermal Enthalpies= -1481.140736
Sum of electronic and thermal Free Energies= -1481.217522

TS-minor-1

| | | | |
|---|---|---|---|
| N | -2.06467900 | 1.04127200 | 0.24479000 |
| C | -1.30220000 | 3.37536400 | -0.08308200 |
| C | -2.60868400 | 2.74465400 | 1.95229000 |
| C | -2.29867400 | 3.86915500 | 0.96508700 |
| C | -3.06727500 | 1.47196800 | 1.23899500 |
| C | -1.83517800 | 2.11187300 | -0.74984500 |
| H | -0.33677400 | 3.15983100 | 0.39092900 |
| H | -1.70783300 | 2.51977800 | 2.53830800 |
| H | -3.22566600 | 4.18013700 | 0.46407600 |
| H | -4.03888700 | 1.64767900 | 0.74897500 |
| H | -2.77912700 | 2.35486100 | -1.26088000 |
| H | -1.12690200 | 4.13408800 | -0.85225100 |
| H | -3.38533400 | 3.04799400 | 2.66233900 |
| H | -1.90953900 | 4.74552500 | 1.49341200 |
| H | -3.19045700 | 0.66993700 | 1.96967800 |
| H | -1.13086800 | 1.73589900 | -1.49771500 |
| C | -2.35527900 | -0.26273600 | -0.41329400 |
| C | -2.70289600 | -2.72733800 | -0.08785600 |
| C | -3.56635000 | -1.60944900 | -2.16103400 |
| C | -3.79615900 | -2.73846700 | -1.15668800 |

| | | | |
|---|---|---|---|
| C | -3.47583200 | -0.24633500 | -1.46437700 |
| C | -2.63463100 | -1.37143600 | 0.61375200 |
| H | -1.73109900 | -2.92885700 | -0.55884400 |
| H | -2.62260900 | -1.79889000 | -2.68953200 |
| H | -4.77748000 | -2.61060500 | -0.67818700 |
| H | -4.43632700 | -0.00795800 | -0.98544100 |
| H | -3.60860900 | -1.18409200 | 1.08604600 |
| H | -1.42353000 | -0.53216100 | -0.93061400 |
| H | -2.87598100 | -3.49891700 | 0.66967800 |
| H | -4.36439800 | -1.58981300 | -2.91117300 |
| H | -3.81464100 | -3.70611800 | -1.66870900 |
| H | -3.28691300 | 0.52781500 | -2.21408000 |
| 0 | -1.69163300 | -1.36684300 | 1.66618000 |
| H | -0.81301600 | -1.51373000 | 1.26360100 |
| H | -0.73311300 | 0.89560800 | 0.97037600 |
| 0 | 0.25642600 | 0.90474400 | 1.39334000 |
| C | 0.26199200 | 0.52918100 | 2.76888600 |
| H | 0.72546900 | 1.32882000 | 3.35476400 |
| H | 0.84201800 | -0.39305200 | 2.89695400 |
| H | -0.75671300 | 0.34994300 | 3.11750800 |
| C | 1.66517400 | 1.57055600 | -1.10397500 |
| 0 | 1.39641200 | 2.36411300 | -1.95948200 |
| 0 | 0.85436100 | 0.48920900 | -0.86618500 |
| C | 1.24598600 | -0.19129300 | 0.29496800 |
| 0 | 0.82934900 | -1.35641500 | 0.41760800 |
| C | 2.87529600 | 1.51338500 | -0.19826300 |
| H | 2.98382900 | 2.45685700 | 0.34035200 |
| C | 2.63290900 | 0.28062700 | 0.69224700 |
| H | 2.68652200 | 0.47987000 | 1.76349100 |
| H | 1.81125400 | -2.15064900 | 1.75993700 |
| 0 | 2.15330500 | -2.33780800 | 2.65424800 |
| C | 1.16684700 | -3.11849000 | 3.29890100 |
| H | 1.12531100 | -4.14109800 | 2.89884900 |
| H | 0.16326900 | -2.67687500 | 3.21358000 |
| H | 1.42563600 | -3.17704600 | 4.35964400 |
| 0 | 0.00516400 | -2.12370500 | -2.28850400 |
| H | 0.31792200 | -1.77800100 | -1.43368700 |
| C | 0.09436300 | -1.10392100 | -3.25758400 |
| H | 1.11636400 | -0.71513500 | -3.36394900 |
| H | -0.56862200 | -0.25231600 | -3.04222200 |
| H | -0.20937600 | -1.53947300 | -4.21375500 |
| C | 4.18838200 | 1.13157900 | -0.98401400 |
| H | 4.69708700 | 1.98902800 | -1.42289400 |
| C | 3.78023100 | -0.69932000 | 0.27219800 |
| H | 3.92623500 | -1.51645300 | 0.97867800 |
| C | 4.91654400 | 0.33409100 | 0.11674900 |
| H | 5.84710600 | -0.11406000 | -0.23954800 |
| H | 5.10184800 | 0.91447500 | 1.02698900 |
| C | 3.81054300 | 0.00218400 | -1.92824100 |
| H | 3.66550100 | 0.11609300 | -2.99728900 |
| C | 3.55395300 | -1.07859400 | -1.18246700 |

H 3.14974500 -2.02761900 -1.51867900
Zero-point correction= 0.642834 (Hartree/Particle)
Thermal correction to Energy= 0.667814
Thermal correction to Enthalpy= 0.668631
Thermal correction to Gibbs Free Energy= 0.592813
Sum of electronic and zero-point Energies= -1481.164796
Sum of electronic and thermal Energies= -1481.139817
Sum of electronic and thermal Enthalpies= -1481.138999
Sum of electronic and thermal Free Energies= -1481.214818

TS-minor-2

| | | | |
|---|---|---|---|
| N | -1.88789200 | 0.76014300 | -0.68741300 |
| C | -2.96911900 | 2.80333200 | -1.65459900 |
| C | -1.45573800 | 2.97984200 | 0.32089800 |
| C | -2.67423300 | 3.58292700 | -0.37485900 |
| C | -1.67282300 | 1.49625300 | 0.59473600 |
| C | -3.08507400 | 1.30792400 | -1.37750500 |
| H | -2.17657900 | 2.98443600 | -2.38865800 |
| H | -0.55638600 | 3.10798300 | -0.29160100 |
| H | -3.54265100 | 3.52406200 | 0.29473800 |
| H | -2.54196500 | 1.34095700 | 1.23890800 |
| H | -3.95121600 | 1.12938200 | -0.72779700 |
| H | -3.90706900 | 3.13630100 | -2.11134900 |
| H | -1.25889300 | 3.48275000 | 1.27395400 |
| H | -2.51118400 | 4.64145400 | -0.60131700 |
| H | -0.79602500 | 1.05507300 | 1.06866900 |
| H | -3.23351500 | 0.75625100 | -2.30828900 |
| C | -1.94608900 | -0.73874800 | -0.52765600 |
| C | -3.17465000 | -2.79121000 | 0.22746900 |
| C | -1.64555900 | -2.94530700 | -1.74692500 |
| C | -2.93675900 | -3.46885800 | -1.12025800 |
| C | -1.67464500 | -1.41993500 | -1.87758000 |
| C | -3.24830500 | -1.26761200 | 0.09693000 |
| H | -2.35354400 | -3.04047600 | 0.91477800 |
| H | -0.79459400 | -3.23385900 | -1.12028000 |
| H | -3.78445500 | -3.25887300 | -1.78774200 |
| H | -2.46210500 | -1.14841400 | -2.59371500 |
| H | -4.08716800 | -1.03043900 | -0.57228200 |
| H | -1.12585800 | -0.98301700 | 0.15900400 |
| H | -4.10419500 | -3.13338300 | 0.69416000 |
| H | -1.48648000 | -3.39047900 | -2.73527600 |
| H | -2.89090700 | -4.55614700 | -0.99720700 |
| H | -0.72743200 | -1.04564500 | -2.27998300 |
| 0 | -3.55104900 | -0.66460600 | 1.33429600 |
| H | -2.76647500 | -0.79026500 | 1.91371800 |
| H | -0.77927000 | 0.93646400 | -1.26240900 |
| 0 | 0.41148700 | 0.99170000 | -1.67363200 |
| C | 0.63710800 | 2.09862000 | -2.50274800 |
| H | -0.30079700 | 2.46508500 | -2.94023000 |
| H | 1.29706300 | 1.83725100 | -3.34188800 |
| H | 1.09510400 | 2.93161700 | -1.94581100 |

| | | | |
|---|---|---|---|
| C | 1.63868100 | -1.34371100 | -0.38000800 |
| 0 | 1.21056700 | -2.45284500 | -0.19861400 |
| 0 | 1.13313200 | -0.26966500 | 0.27933500 |
| C | 1.68116500 | 0.94099500 | -0.22679900 |
| 0 | 1.54783300 | 1.94968400 | 0.45279800 |
| C | 2.80339300 | -0.93289200 | -1.25262400 |
| H | 2.63911000 | -1.26765900 | -2.27882900 |
| C | 2.89183200 | 0.59076500 | -1.07485400 |
| H | 2.88588700 | 1.14611800 | -2.01187800 |
| H | 1.02685000 | 1.38538500 | 2.08095300 |
| 0 | 0.74545900 | 1.00836900 | 2.94330500 |
| C | 0.04372100 | 2.00173400 | 3.66849000 |
| H | 0.59623900 | 2.94826100 | 3.69213600 |
| H | -0.07394100 | 1.64134000 | 4.69335700 |
| H | -0.95793900 | 2.18734700 | 3.25586700 |
| 0 | -1.15900900 | -0.94113500 | 2.75697600 |
| H | -0.45920800 | -0.25086500 | 2.70721600 |
| C | -0.50028900 | -2.19080400 | 2.87031600 |
| H | 0.25141000 | -2.16829100 | 3.66951000 |
| H | -0.00788200 | -2.48252300 | 1.93398200 |
| H | -1.24959200 | -2.94376500 | 3.13066200 |
| C | 4.18073600 | -1.44237000 | -0.68049300 |
| H | 4.44599000 | -2.44743600 | -1.00653700 |
| C | 4.26596800 | 0.78782300 | -0.35158700 |
| H | 4.62234600 | 1.81743200 | -0.36828300 |
| C | 5.08391500 | -0.27221200 | -1.12044100 |
| H | 6.10657500 | -0.36956400 | -0.74776500 |
| H | 5.09125700 | -0.11244200 | -2.20421100 |
| C | 4.13692200 | -1.19815500 | 0.81913600 |
| H | 3.96848800 | -1.96732300 | 1.56490900 |
| C | 4.17399000 | 0.12458500 | 1.01171800 |
| H | 4.04398100 | 0.65497400 | 1.94845200 |

Zero-point correction= 0.640517 (Hartree/Particle)
Thermal correction to Energy= 0.665916
Thermal correction to Enthalpy= 0.666733
Thermal correction to Gibbs Free Energy= 0.589430
Sum of electronic and zero-point Energies= -1481.162657
Sum of electronic and thermal Energies= -1481.137258
Sum of electronic and thermal Enthalpies= -1481.136441
Sum of electronic and thermal Free Energies= -1481.213744