

Supporting Information to:

**A Computational Study on the Stereoselective
Organocatalytic Epoxidation of α,β -Unsaturated
Aldehydes with Hydrogen Peroxide**

Filipe J. S. Duarte and A. Gil Santos*

REQUIMTE, CQFB, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade
Nova de Lisboa, 2829-516 Caparica (Portugal)

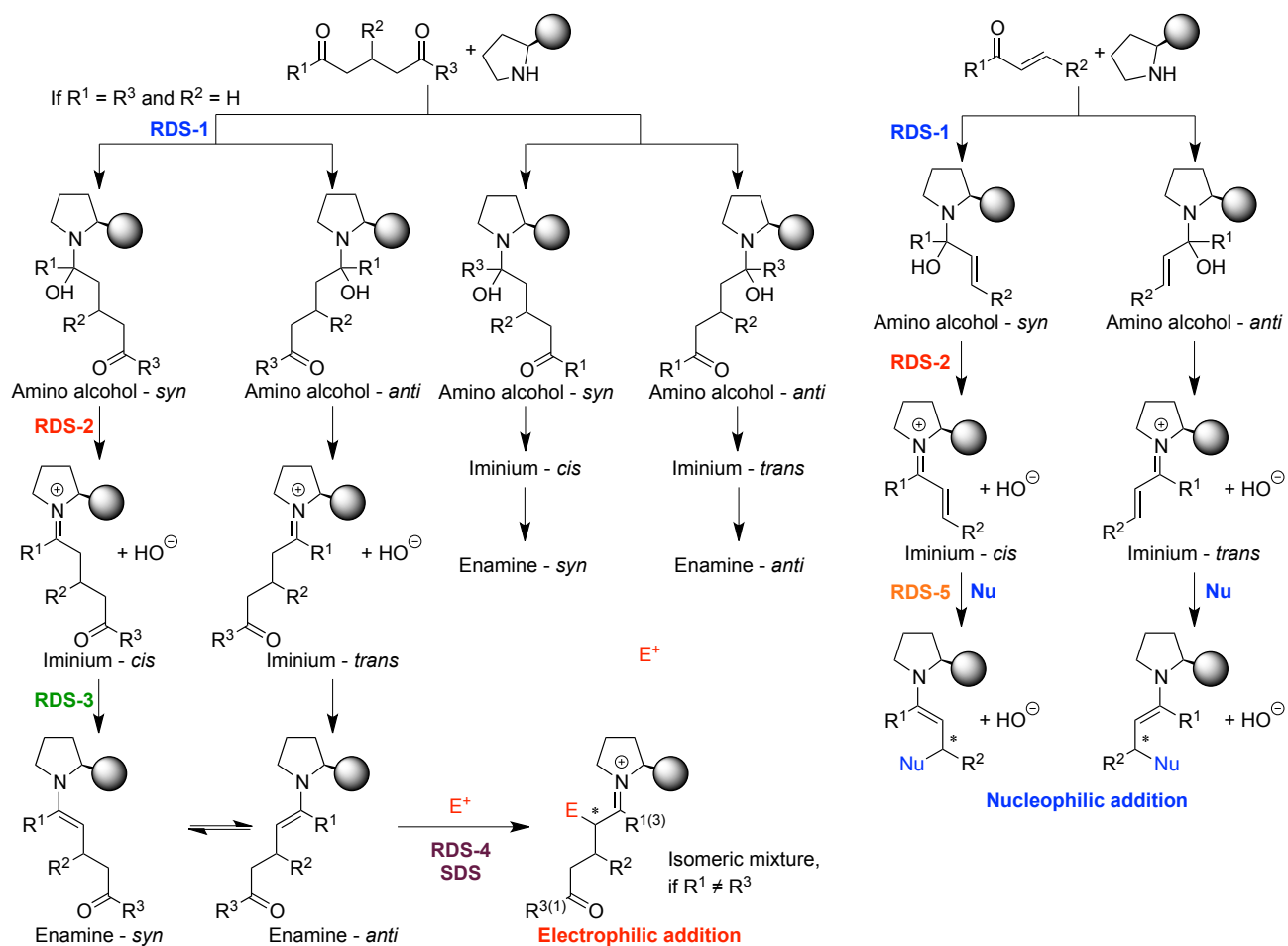
*E-mail address: ags@fct.unl.pt

Contents:

Selectivity control in mechanisms via enamine and iminium intermediates	S3
Alternative reaction mechanisms via the intermediate aminoalcohol	S5
Non-covalent reaction mechanism with co-catalysis by hydrogen peroxide during the second step of the reaction	S7
Cartesian coordinates and computed total energies for the:	
reactants	S8
structures presented in Scheme 5	S9
structures presented in Scheme 6	S12
structures presented in Scheme 7	S22
structures presented in Scheme 8	S25
structures presented in Scheme 9 and Scheme S4	S44
structures presented in Scheme S3	S50

Selectivity control in mechanisms via enamine and iminium intermediates

When aldehydes or ketones react via the covalent mechanism, they can follow two possible reaction pathways, with the carbonyl compound being initially converted either to the iminium or to the enamine intermediates, which then react according to their own chemistries (Scheme S1).^{42,46-48} There are known systems in which the RDS occurs after the enamine formation (RDS-4).^{35,36,49-51} There is also a case in which the enamine formation is the RDS (RDS-3).³⁹ However, in most known cases, theoretical and experimental studies indicate that the RDS is one of the iminium formation steps (RDS-1 or RDS-2).^{34,38,40,41,43,44} In these cases, and when the reaction proceeds via the enamine (Scheme S1, left), the RDS is important to the definition of the final stereochemistry only when the initial aldehyde or ketone has two different carbonyl groups of similar reactivity, as, for instance, in *meso* compounds (Scheme S1).^{40,43} With simple ketones or aldehydes, the previous steps are not important to the definition of the final selectivity, because the enamine intermediate can freely rotate through the enamine bond. In such cases, the RDS is the electrophilic addition (Scheme S1, left). On the other hand, if the reaction proceeds via the iminium intermediate (Scheme S1, right), the above scenario can change considerably. Therefore, if the RDS is one of the iminium formation steps (RDS-1 or RDS-2), and because the iminium intermediate has two different non-equilibrating configurations, the selectivity induced in the RDS (that leads to the two possible iminium configurations) directly influences the final reaction selectivity (Scheme S1). However, if the RDS occurs after the iminium formation steps (RDS-5), then the iminium formation does not influence the final reaction selectivity, as all the steps before the RDS are in equilibrium through the free reagents.

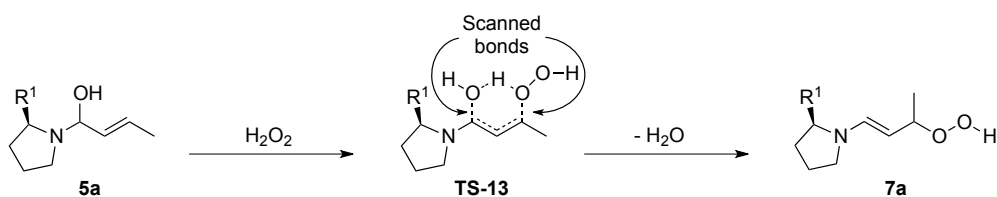


Scheme S1 – Possible rate-determining steps in catalytic asymmetric reactions through enamine (left) and iminium (right) intermediates.

Alternative reaction mechanisms via the intermediate aminoalcohol

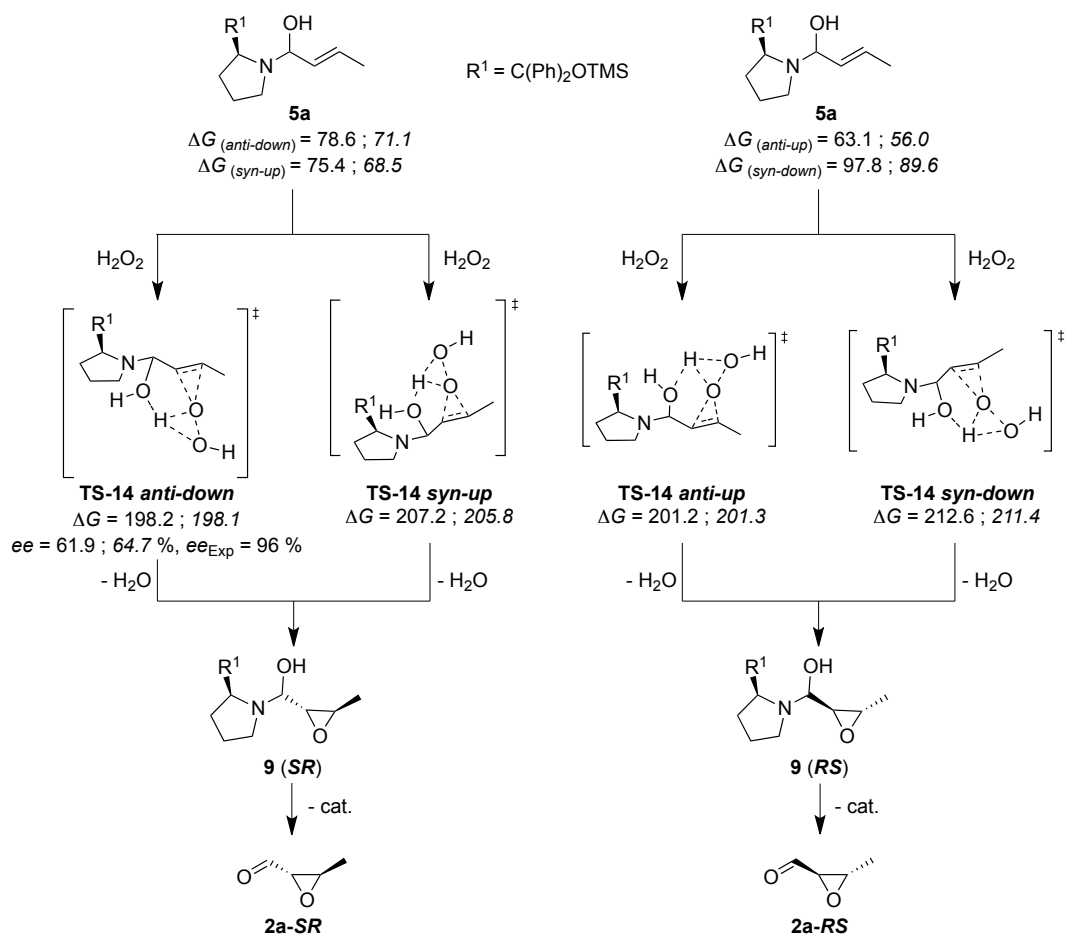
A different mechanism for the epoxidation with hydrogen peroxide can be envisaged, in which the reacting species is the aminoalcohol intermediate **5a** (Scheme S2) and not the iminium ion that can result from it.

Intermediate **5a** does not have its double bond activated by the iminium group. However, as the protonated hydroxyl group can be a very good leaving group, an interesting possibility would be the addition of hydrogen peroxide with the concerted elimination of water, as shown in Scheme S2. To find such a TS, we double scanned the bonds marked in Scheme S2, but no concerted TS was found. The hydrogen transfer from the peroxide to the hydroxide is clearly shown as a ridge along the potential energy surface (PES), with the energy diminishing with the increasing of the C-O bond lengths, reaching a stable value when the C-O bond lengths are over 2.3 Å. All attempts to optimize structures obtained from the ridge as TSs, when the C-O bond lengths are over 2 Å, converged to **TS-7**, **TS-9** or to the iminium ion.



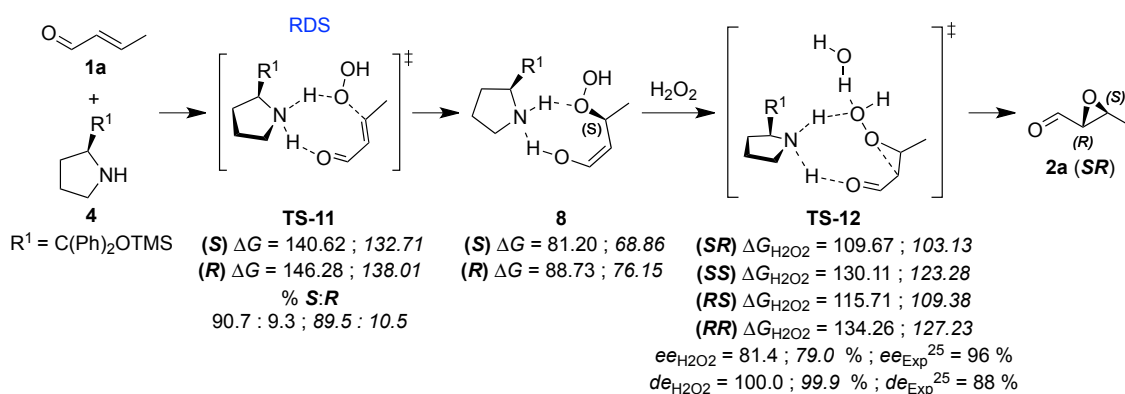
Scheme S2 – Proposed concerted pathway for the epoxidation of the aminoalcohol intermediates with hydrogen peroxide, with concerted elimination of water.

All attempts to optimize structures obtained from the ridge as TSs, when the C-O bond lengths are shorter than 2 Å, converged to **TS-14**, Scheme S3. In this TS the hydroxyl group is not eliminated and the epoxide ring is formed in a concerted process, which implies that the final products should be formed as a single enantiomeric pair, in disagreement with the experimental results. On the other hand, the energy values calculated for **TS-14** are too high when compared with the values found for the two-step pathway (Scheme 8), which also renders this possibility of very low probability.



Scheme S3 – Concerted ring formation obtained for the epoxidation of the aminoalcohol intermediate with hydrogen peroxide. *Syn/anti* refers to the relative orientation between the carbon chain and the catalyst substituent. *Up/down* refers to the orientation between the catalyst substituent and the hydrogen peroxide. The energies, in kJ mol^{-1} , were calculated in DCM with B2PLY/6-311+G**//M062X/6-31+G** (roman) and mPW2PLYP/6-311+G**//M062X/6-31+G** (*italic*).

Non-covalent reaction mechanism with co-catalysis by hydrogen peroxide during the second step of the reaction



Scheme S4 – Calculated non-covalent pathway for the epoxidation reaction. The second reaction step (ring closure) was calculated with the explicit inclusion of a hydrogen peroxide molecule. The energies, in kJ mol⁻¹, were calculated in DCM with B2PLY/6-311+G**//M062X/6-31+G** (roman) and mPW2PLYP/6-311+G**//M062X/6-31+G** (*italic*).

Cartesian coordinates and computed total energies for the reactants.

H₂O

M06-2X/6-31+G**, $E = -76.4021309209$ a.u.
Thermal correction to Gibbs Free Energy = 0.003883 a.u.
SP at B2PLYP/6-311+G**, $E = -76.399599502028$ a.u.
SP at mPW2PLYP/6-311+G**, $E = -76.398738558598$ a.u.

0,1

O,0,0.591146511,0.0000000002,-0.758711804
H,0,0.591146511,0.766395627,-0.1748439521
H,0,0.591146511,-0.766395627,-0.1748439529

H₂O₂

M06-2X/6-31+G**, $E = -151.496317109$ a.u.
Thermal correction to Gibbs Free Energy = 0.003883 a.u.
SP at B2PLYP/6-311+G**, $E = -151.48478385045$ a.u.
SP at mPW2PLYP/6-311+G**, $E = -151.48308028770$ a.u.

0,1

O,0,-0.2259186733,1.0515218743,-0.6736414358
O,0,-0.1673654103,1.5047818212,0.6757604181
H,0,0.5924070334,1.0128324751,1.0221496375
H,0,-0.9856900378,0.4501790245,-0.6521982988

1a (R² = Me, R³ = H)

M06-2X/6-31+G**, $E = -231.142247608$ a.u.
Thermal correction to Gibbs Free Energy = 0.061598 a.u.
SP at B2PLYP/6-311+G**, $E = -231.07615604980$ a.u.
SP at mPW2PLYP/6-311+G**, $E = -231.07683215687$ a.u.

0,1

O,0,-1.2571739057,-1.2327960081,-2.7889196285
C,0,-2.1443723573,-0.4139870248,-2.9533212649
H,0,-2.9098626848,-0.5718337345,-3.7384514964
C,0,-2.2938858098,0.8141679119,-2.1686933178
H,0,-1.5617018532,1.0072568709,-1.3876122608
C,0,-3.3083562675,1.652546934,-2.4261666909
H,0,-4.0018895246,1.3882842863,-3.2266448276
C,0,-3.5758086649,2.9311834732,-1.7047539595
H,0,-4.5711560001,2.9064047264,-1.2488426737
H,0,-2.833172985,3.1168544005,-0.9264427673
H,0,-3.572097382,3.7700651601,-2.4083989766

1b (R² = R³ = Me)

M06-2X/6-31+G**, $E = -270.441131611$ a.u.
Thermal correction to Gibbs Free Energy = 0.087401 a.u.
SP at B2PLYP/6-311+G**, $E = -270.35657387838$ a.u.
SP at mPW2PLYP/6-311+G**, $E = -270.35820928183$ a.u.

0,1

O,0,-0.9561015472,-1.0643315343,-2.7722417361
C,0,-1.9462684266,-0.3916549774,-3.0186680092
H,0,-2.6168011669,-0.7006374389,-3.838753438
C,0,-2.2897671304,0.8155954247,-2.2704428288
H,0,-1.593562928,1.0748890864,-1.47548347
C,0,-3.3702529764,1.5929164106,-2.4931259602
C,0,-3.6116108572,2.8113308973,-1.6484708087
H,0,-4.5851667043,2.7359070481,-1.1512728583
H,0,-2.8375119316,2.9460591682,-0.8912700281
H,0,-3.6481039393,3.7049526084,-2.2815005211
C,0,-4.4128386945,1.3573153562,-3.5502586593
H,0,-4.2327318547,0.4820642899,-4.1717826559
H,0,-5.3928827871,1.2482583481,-3.0735833874
H,0,-4.4739286407,2.2370248589,-4.199806105

1c (R² = Et, R³ = H)

M06-2X/6-31+G**, $E = -270.437196416$ a.u.
Thermal correction to Gibbs Free Energy = a.u.
SP at B2PLYP/6-311+G**, $E = -270.35352994894$ a.u.
SP at mPW2PLYP/6-311+G**, $E = -270.35508179312$ a.u.

0,1

O,0,-1.2556912733,-1.24423209,-2.7684045593
C,0,-2.1381624325,-0.4228611308,-2.9444240513
H,0,-2.8934154735,-0.5777572675,-3.7399521187
C,0,-2.2947665432,0.8055433843,-2.1607688376
H,0,-1.5715702516,0.9964261337,-1.3706964259
C,0,-3.304774369,1.6462156381,-2.4283065851
H,0,-3.9890213158,1.3887391366,-3.2408721514
C,0,-3.5760257934,2.9340695902,-1.7194753896
H,0,-4.559999176,2.8640823445,-1.2387055096
H,0,-2.8353674944,3.0852088467,-0.9282827706
C,0,-3.5783085666,4.1216235355,-2.6904834147
H,0,-4.3255891723,3.980767012,-3.4770766147
H,0,-3.8129269978,5.0483852622,-2.1614323782
H,0,-2.6004869706,4.2359189045,-3.1663018234

4

M06-2X/6-31+G**, $E = -1197.55070311$ a.u.
Thermal correction to Gibbs Free Energy = 0.375934 a.u.
SP at B2PLYP/6-311+G**, $E = -1197.0933450939$ a.u.
SP at mPW2PLYP/6-311+G**, $E = -1197.1196084427$ a.u.

0,1

N,0,-1.9986770505,-0.8973491456,-1.1680179142
C,0,-0.7517569156,-1.6495443673,-0.995282494
C,0,0.1724587153,-1.1703498043,-2.1337208602
C,0,-0.4630344935,0.1388904309,-2.61421387
C,0,-1.953184492,-0.1414384984,-2.4269323345
C,0,-0.1471068176,-1.439446993,0.4286744263
C,0,0.3056066908,0.0123860751,0.5742974929
C,0,-1.1412547335,-1.8579241046,1.5245978123
O,0,0.9758639564,-2.3149617264,0.4538310843
C,0,1.6474439057,0.363195239,0.412788905
C,0,2.0480580983,1.7005813222,0.4471532402
C,0,1.1078940652,2.7095106399,0.6434453856
C,0,-0.2363324589,2.3697988956,0.8079618193
C,0,-0.6327734407,1.0355031038,0.7721800201
C,0,-1.1199820715,-1.2572884001,2.7885725782
C,0,-1.9286923744,-1.7233038509,3.8250273472
C,0,-2.786610656,-2.800849182,3.6149955416
C,0,-2.8241063049,-3.4059931384,2.3596012929
C,0,-2.0071393556,-2.9412924761,1.3307320633
Si,0,1.8137267789,-3.036673664,1.7216624471
C,0,3.2630662895,-3.8399287972,0.8476849477
C,0,2.4542174113,-1.794596527,2.9779988477
C,0,0.7925039025,-4.3458738899,2.5963400144
H,0,-0.9005135046,-2.7308102541,-1.0947475882
H,0,0.1516408878,-1.9075510551,-2.9432103075
H,0,1.2096826555,-1.0640848904,-1.8084173635
H,0,-0.1531934596,0.9738748582,-1.9771854955
H,0,-0.2112747332,0.379745757,-3.6500231336
H,0,-2.3328009836,-0.7255090985,-3.2800464293
H,0,-2.5511007998,0.7724334467,-2.3475630689
H,0,2.3849808185,-0.4157496154,0.2477116362
H,0,1.4176960738,3.7498298232,0.6703889084
H,0,-1.6801962194,0.778159417,0.8863720662
H,0,-0.4646688726,-0.4117681638,2.9721986395
H,0,-3.4193607365,-3.1642069901,4.418785321
H,0,-2.0433634857,-3.4525571664,0.3742861852
H,0,3.8572450718,-3.0907149987,0.3141762884
H,0,3.9163280696,-4.3432261834,1.5682658725
H,0,2.9191046563,-4.5831225563,0.1215487868
H,0,2.9623150136,-2.3410001047,3.7813120644
H,0,1.65282997,-1.2044019975,3.4305941424

H,0,3.1752139129,-1.1046974392,2.5291328999
H,0,0.0209388062,-3.9089642656,3.238634565
H,0,0.3006960101,-5.0055729727,1.8739579642
H,0,1.4540522972,-4.9568633758,3.221313144
H,0,3.0972298347,1.9496972145,0.3181216146
H,0,-0.9795278969,3.146336767,0.9626652704
H,0,-1.8855931666,-1.2399754168,4.7964775133
H,0,-3.4858090245,-4.2478596431,2.1792367042
H,0,-2.8193209938,-1.4877610872,-1.0971894828

Cartesian coordinates and computed total energies for the structures presents in Scheme 5. The structures with H₂O₂ are in the Scheme 6, see page S9.

TS-6 *syn-up*

M06-2X/6-31+G**, $E = -1428.65865370$ a.u.

Thermal correction to Gibbs Free Energy = 0.461227 a.u.

1 imaginary frequency = -1460.60 cm⁻¹

SP at B2PLYP/6-311+G**, $E = -1428.1228351706$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1428.1512426956$ a.u.

O,1
C,0,-0.7145630005,0.7294408406,0.6677836949
N,0,-1.3954393188,2.0792815357,1.021136535
C,0,-2.1787035648,2.2472919442,2.277635528
C,0,-1.4641289288,3.3524382278,3.0824585895
C,0,-0.1038273324,3.5036487031,2.3897319829
C,0,-0.4685078158,3.23682748,0.9356140843
O,0,-1.1340724967,0.7181704224,-0.6439731506
H,0,0.3735356287,0.8440183602,0.8139632127
H,0,-1.7992732378,1.7470705777,-0.0790087447
C,0,-3.6844867597,2.468672046,1.9453995909
C,0,-4.5015310663,2.6789669156,3.2291495858
C,0,-5.6922330087,3.4146945345,3.217669108
C,0,-4.1531801481,2.0093137977,4.4089214285
C,0,-6.5081984452,3.481530846,4.3465878054
H,0,-5.9942797871,3.9409538894,2.3181820143
C,0,-4.9611300518,2.0793361846,5.5416141252
H,0,-3.2536884165,1.4043158878,4.4555187998
C,0,-6.1454152763,2.8144610577,5.5148203257
H,0,-7.4285858571,4.0559254354,4.3088271122
H,0,-4.6676965355,1.5490838357,6.4422699564
H,0,-6.7788468783,2.8643473498,6.3948477787
C,0,-3.8241487538,3.6127556723,0.9337871473
C,0,-3.8527448302,3.321989046,-0.4341520675
C,0,-3.8194300397,4.9585312309,1.3244314245
C,0,-3.8642391781,4.3412030664,-1.3855462881
H,0,-3.8608996458,2.2857066356,-0.7578165475
C,0,-3.8303058726,5.9800826503,0.3758617815
H,0,-3.8255738053,5.2204503454,2.3783894096
C,0,-3.8480569138,5.6756518194,-0.9848246648
H,0,-3.8822139819,4.0876296911,-2.4410349877
H,0,-3.8294667146,7.0148289937,0.7043548165
H,0,-3.855939445,6.4710612138,-1.7235744541
O,0,-4.062971376,1.2417562471,1.337917373
Si,0,-5.5626722429,0.4986742807,1.1294198071
C,0,-6.2554840899,-0.1229802876,2.7585137886
H,0,-7.0922296188,-0.8021442702,2.5583699932
H,0,-5.4911046704,-0.679719327,3.3114844002
H,0,-6.6169246606,0.6886866602,3.3980814176
C,0,-6.8034855674,1.62078534,0.2787909485
H,0,-6.4360497052,1.9585847522,-0.6948819138
H,0,-7.7301748734,1.0582851612,0.1153032343
H,0,-7.0512857918,2.5029349982,0.8755974643
C,0,-5.1439509645,-0.9489286799,0.0201207358
H,0,-4.6518498311,-0.607479947,-0.8961685775
H,0,-4.4717862331,-1.6505991872,0.5246190416
H,0,-6.0526214563,-1.4926429267,-0.259212146
C,0,-1.2302841676,-0.4104984543,1.4909275627

H,0,-2.2930365973,-0.6253470316,1.3718286345
C,0,-0.4525400238,-1.1636955101,2.2710868341
H,0,0.6075813429,-0.9141604639,2.3475504182
C,0,-0.9209971087,-2.3530292347,3.0551277719
H,0,-1.9923256127,-2.5206662005,2.9151331088
H,0,-0.7269311365,-2.2161306072,4.1242674223
H,0,-0.3854012263,-3.2574692724,2.7480013085
H,0,-2.1195456573,1.2947745816,2.8066806728
H,0,-1.3804947293,3.0835364919,4.1374482698
H,0,-2.0137028916,4.2950628253,3.0245327842
H,0,0.3476259315,4.4861011685,2.5415883177
H,0,0.5983039976,2.7398422578,2.7433732011
H,0,0.3646774161,2.9933464163,0.2739719974
H,0,-1.024166715,4.0825025035,0.5134868564

TS-6 *syn-up* with H₂O

M06-2X/6-31+G**, $E = -1505.10596355$ a.u.

Thermal correction to Gibbs Free Energy = 0.486862 a.u.

1 imaginary frequency = -377.04 cm⁻¹

SP at B2PLYP/6-311+G**, $E = -1504.5561433608$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1504.5859477880$ a.u.

O,1
C,0,-6.5188486642,-2.1071046355,-6.2159675376
C,0,-5.397307548,-1.144902081,-6.4612454288
H,0,-7.4487520129,-1.7310550512,-6.6565583492
H,0,-5.5187203672,-0.1387500338,-6.0557725139
H,0,-6.3019059134,-3.0875474498,-6.6474168418
C,0,-4.2842124488,-1.4324395243,-7.1373228003
C,0,-3.1898154735,-0.4380548846,-7.3782063591
H,0,-4.1172124344,-2.4359423078,-7.5316729402
N,0,-3.2558770807,0.1557873245,-8.8264740379
C,0,-4.3905516748,1.1069589983,-9.0146525138
C,0,-3.3621726277,-0.9051761637,-9.8819000642
C,0,-5.5178517168,0.3074385615,-9.6810084052
H,0,-4.6672349696,1.5172041532,-8.0412573984
H,0,-2.9736956526,-1.8218821886,-9.430705145
C,0,-2.4250077768,-0.5983623523,-11.0907056434
H,0,-2.2868378025,0.6655723711,-8.8129480977
O,0,-0.9582541034,1.0584327295,-8.0483991464
O,0,-1.9461799001,-0.9698456687,-7.2244003177
H,0,-3.3536900256,0.4618144536,-6.7639424443
H,0,-1.2954231521,-0.1017396486,-7.5216705647
H,0,-5.9524245511,0.8835306463,-10.5008556255
H,0,-6.3116695486,0.0881112508,-8.963776351
H,0,-4.0433663302,1.9264155427,-9.6460545128
C,0,-4.8699789937,-0.9980872952,-10.1863011481
H,0,-5.0488457995,-1.158486986,-11.2499862246
H,0,-5.2909193785,-1.8591510627,-9.6601591153
C,0,-2.5798692901,-1.6407585482,-12.208247496
C,0,-2.0502410379,-1.3464784537,-13.4706670867
C,0,-3.1164500283,-2.9132193071,-11.992156316
C,0,-2.0552992886,-2.294364862,-14.4889692783
H,0,-1.6180902922,-0.3662150636,-13.652013848
C,0,-3.1190156801,-3.8690743321,-13.0094766471
H,0,-3.5413588847,-3.1824939297,-11.0298758476
C,0,-2.5890637228,-3.563405358,-14.2604851579
H,0,-1.63573998,-2.0452790616,-15.458792438
H,0,-3.5400808372,-4.851524185,-12.8199516129
H,0,-2.5924816612,-4.3065109535,-15.0518393747
C,0,-2.6882192481,0.8158379352,-11.619057527
C,0,-1.8530114497,1.8727549266,-11.2510795214
C,0,-3.8027760442,1.0869674652,-12.4225559331
C,0,-2.1426053567,3.1788411346,-11.6488288049
H,0,-0.9810438382,1.6689306052,-10.6416371334
C,0,-4.0972145863,2.390706754,-12.8140655111
H,0,-4.4417007143,0.2765530092,-12.7620746542
C,0,-3.2712498098,3.4448502124,-12.4208665199
H,0,-1.484216138,3.9882571341,-11.3488212125
H,0,-4.9681297255,2.5818938855,-13.4335510956

H,0,-3.4998034513,4.461200011,-12.7260621391
O,0,-1.0969575566,-0.6321446759,-10.594340674
Si,0,-0.0441300721,-1.9296103006,-10.33115291
C,0,-0.8015948281,-3.3179766497,-9.3233966601
H,0,-1.2108570668,-2.9351565491,-8.3833461023
H,0,-1.58215919,-3.8561398484,-9.8697476096
H,0,-0.0081680202,-4.0385141645,-9.090969158
C,0,0.5971275041,-2.628917447,-11.9514569685
H,0,1.4663795905,-3.2637391566,-11.7436731095
H,0,-0.1579056374,-3.239477727,-12.4582467816
H,0,0.910279002,-1.8341047888,-12.6360041124
C,0,1.3608488192,-1.1463414497,-9.3733867727
H,0,2.2032403816,-1.8434353379,-9.3118044985
H,0,1.714846082,-0.2334795973,-9.8647440231
H,0,1.0538510106,-0.8977888319,-8.3525083316
H,0,-6.7010341929,-2.2290797545,-5.1435226999
H,0,-0.2297491747,0.9317451927,-8.6661055056

TS-6 anti-up

M06-2X/6-31+G**, $E = -1428.65727883$ a.u.

Thermal correction to Gibbs Free Energy = 0.459945 a.u.

1 imaginary frequency = -1468.98 cm^{-1}

SP at B2PLYP/6-311+G**, $E = -1428.1218381298$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1428.1501367096$ a.u.

0,1
C,0,-0.9297000297,0.570358188,0.4254621436
N,0,-1.38780201,1.9950662489,0.8353281935
C,0,-2.0833864825,2.1599224799,2.1432824101
C,0,-1.2954734692,3.232447109,2.9182364991
C,0,0.044522062,3.3179564764,2.1771977932
C,0,-0.3865489518,3.0861093116,0.734624796
O,0,-1.4094526714,0.6382972236,-0.860061339
H,0,-1.503065809,-0.0961114439,2.5925945401
H,0,-1.9032619445,1.7269893071,-0.2401354382
C,0,-3.5996346556,2.4092544355,1.8981664207
C,0,-4.3624312306,2.5759911176,3.2200183598
C,0,-5.5675228145,3.2867815064,3.2615315262
C,0,-3.9546913512,1.902574892,4.3774990324
C,0,-6.3421328866,3.325242827,4.4198480617
H,0,-5.9110001959,3.8179039094,2.3798044741
C,0,-4.7219619034,1.9443124788,5.5406991942
H,0,-3.0387053443,1.3213617843,4.3867711142
C,0,-5.9213992896,2.6536579594,5.5661901489
H,0,-7.2742456594,3.8816306577,4.4228016049
H,0,-4.3831977957,1.4135068451,6.425039568
H,0,-6.5215916727,2.6820662399,6.4701100358
C,0,-3.7771752183,3.5990454319,0.9461170851
C,0,-3.893120606,3.376079005,-0.4295190159
C,0,-3.740809414,4.9233791158,1.4027919613
C,0,-3.9584203975,4.4425561132,-1.3261885362
H,0,-3.931355495,2.3570378185,-0.8022043017
C,0,-3.8041461849,5.991291935,0.5094441351
H,0,-3.6861491012,5.1307979516,2.4673971627
C,0,-3.90883767,5.7550266881,-0.8609713191
H,0,-4.0465960673,4.2428070363,-2.3896909038
H,0,-3.7780769017,7.0083302679,0.8882863538
H,0,-3.9592298057,6.586288747,-1.5572465983
O,0,-4.0102793243,1.2134845122,1.2537789589
Si,0,-5.4999219071,0.4440511562,1.0883395467
C,0,-6.0996996314,-0.2496194002,2.7255840634
H,0,-6.9395759256,-0.9302353617,2.5443474699
H,0,-5.3033071802,-0.8175459903,3.2180627462
H,0,-6.4355995623,0.5337498118,3.4128971516
C,0,-6.8071933896,1.5664129804,0.3427276894
H,0,-6.4798802528,1.9763904808,-0.6175433051
H,0,-7.7168661332,0.9797664469,0.1688965995
H,0,-7.0695321497,2.3999670438,1.0002303073
C,0,-5.0837057571,-0.9417838064,-0.0963845825
H,0,-4.6786018514,-0.539103973,-1.030305084

H,0,-4.3287530316,-1.6048444691,0.3381024231
H,0,-5.970934489,-1.5383638163,-0.3322483617
C,0,0.5346730988,0.286841682,0.5709424481
H,0,1.1971368484,0.7397616921,-0.1671268811
C,0,1.025868927,-0.523154521,1.511960677
H,0,0.3296460926,-0.9856115114,2.2145335595
C,0,2.4757859479,-0.862695722,1.6825936949
H,0,3.0898965257,-0.3668604004,0.9265677093
H,0,2.633977155,-1.9434384103,1.605364545
H,0,2.8318595257,-0.5588547568,2.6728517567
H,0,-2.0087462721,1.194995256,2.6521782442
H,0,-1.1881627237,2.9643541834,3.9713249779
H,0,-1.8029867476,4.1987797423,2.8711417168
H,0,0.5494863645,4.2756844618,2.3187033131
H,0,0.7171953081,2.514704909,2.4965356502
H,0,0.4093861273,2.8083512061,0.0432461258
H,0,-0.9028185845,3.9692637462,0.3401152254

TS-6 anti-up with H₂O

M06-2X/6-31+G**, $E = -1505.10595253$ a.u.

Thermal correction to Gibbs Free Energy = 0.486414 a.u.

1 imaginary frequency = -310.85 cm^{-1}

SP at B2PLYP/6-311+G**, $E = -1504.5579848785$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1504.5876388156$ a.u.

0,1
C,0,-5.5012822051,-3.7890114858,-7.5854155449
C,0,-4.2973560859,-2.9281755902,-7.8174550123
H,0,-5.2752137687,-4.5923678756,-6.8770808792
H,0,-3.4054179098,-3.4299982494,-8.1992712814
H,0,-6.3377529955,-3.2039544967,-7.1949573747
C,0,-4.246889097,-1.6138555448,-7.5950259361
C,0,-3.0279189701,-0.7807022181,-7.848502442
H,0,-5.1092138196,-1.0835405,-7.1887614255
N,0,-3.1896228684,0.0730724987,-9.140073168
C,0,-4.3523513307,1.01084282,-9.0657271798
C,0,-3.3434571196,-0.7605820997,-10.3705917733
C,0,-5.5011846706,0.3301148921,-9.8189959143
H,0,-4.5570152002,1.2105690137,-8.0126945863
H,0,-2.9719514802,-1.7575534217,-11.105955708
C,0,-2.4217290554,-0.230169077,-11.5056667968
H,0,-2.2648967359,0.673401548,-9.0564966787
O,0,-1.2313433794,1.376295924,-8.1470080209
O,0,-2.7629995395,0.0748654789,-6.8190097324
H,0,-2.1707397882,-1.4224750256,-8.1112852344
H,0,-1.9977096615,0.7558327916,-7.2378979481
H,0,-6.0216190408,1.0549319902,-10.4493606706
H,0,-6.230379023,-0.0865304451,-9.1202873847
H,0,-4.0500369777,1.9457522603,-9.5427453814
C,0,-4.8567795761,-0.7933787622,-10.657966568
H,0,-5.0569606239,-0.6750440428,-11.7232551246
H,0,-5.2569501512,-1.7667461223,-10.3629580618
C,0,-2.5588540277,-1.0605027143,-12.7878365702
C,0,-2.0242872156,-0.546365473,-13.9757665482
C,0,-3.0843016559,-2.3552459793,-12.7991802201
C,0,-2.0112347051,-1.3051962041,-15.1420394606
H,0,-1.6045730755,0.4560291778,-13.9802430728
C,0,-3.0699341829,-3.1213828511,-13.9665277607
H,0,-3.5158694179,-2.7906478704,-11.9027837585
C,0,-2.5323213039,-2.5998805576,-15.1405011521
H,0,-1.5886758217,-0.888450996,-16.0510184367
H,0,-3.4823745224,-4.1253872204,-13.9528660516
H,0,-2.5217423932,-3.1952467935,-16.0479676448
C,0,-2.7113388767,1.2527409081,-11.7649868012
C,0,-1.894470966,2.2340741211,-11.1981165709
C,0,-3.8305163145,1.6504929372,-12.5072268913
C,0,-2.2086884992,3.5861662101,-11.3438261229
H,0,-1.0287701994,1.9304850117,-10.6201623613
C,0,-4.1473377561,2.9998531609,-12.6470706889
H,0,-4.4531676061,0.9083640887,-12.9985657764

C,0,-3.340618555,3.9741953593,-12.0578982331
H,0,-1.5655840537,4.3361973337,-10.8929379725
H,0,-5.0200635184,3.2888382263,-13.2244797133
H,0,-3.5863498654,5.0259748125,-12.166963379
O,0,-1.0970833353,-0.3239564684,-11.0126194414
Si,0,0.0194883786,-1.5871182431,-10.9679806811
C,0,-0.6738559759,-3.1492750462,-10.1808376555
H,0,-0.9625719735,-2.995540826,-9.1362646774
H,0,-1.5292100685,-3.5579233977,-10.728659182
H,0,0.1146675821,-3.9111855664,-10.1922736666
C,0,0.6557770063,-2.0166311828,-12.6780990218
H,0,1.5551675652,-2.6355047928,-12.5799335073
H,0,-0.0835400194,-2.5766577036,-13.2608357277
H,0,0.9206971559,-1.1153021545,-13.2397427105
C,0,1.3769567693,-0.8859444911,-9.895716266
H,0,2.1761620332,-1.6200342485,-9.7504319912
H,0,1.810712192,0.0100363943,-10.3506182228
H,0,0.9739688413,-0.6069756988,-8.9169049127
H,0,-5.8169928801,-4.2666832981,-8.519359525
H,0,-1.3347195349,2.3344892657,-8.1307384161

TS-7 anti-down with H₂O

M06-2X/6-31+G**, $E = -1505.08713897$ a.u.

Thermal correction to Gibbs Free Energy = 0.481213 a.u.

1 imaginary frequency = -169.62 cm⁻¹

SP at B2PLYP/6-311+G**, $E = -1504.5516268719$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1504.5804908154$ a.u.

0,1
C,0,-1.5291187084,-0.6081127219,-3.4585850865
C,0,-0.5812713116,0.3441866996,-3.4313507956
H,0,-0.7760040163,1.34611215,-3.8052635296
C,0,0.7175520955,0.0232079664,-2.8764077587
H,0,0.8496683894,-0.9476882145,-2.4147859167
N,0,1.6541850387,0.9086135981,-2.6874154767
C,0,1.6822792417,2.2146497487,-3.3718736428
C,0,2.9667779873,0.5006711418,-2.1620062136
C,0,3.0881929724,2.7518081254,-3.1049117197
C,0,3.929231488,1.4942156947,-2.8300196757
H,0,0.8947766815,2.8634918878,-2.9796723894
H,0,3.0816051601,3.4131543734,-2.2355374933
H,0,1.5087892738,2.0375463398,-4.4390286969
H,0,3.4645371559,3.3162181265,-3.9597520786
H,0,4.8026753615,1.7094406916,-2.2106166371
H,0,4.2780073701,1.0604607597,-3.7722563165
H,0,3.1233548666,-0.524184379,-2.5131202005
C,0,2.9700613239,0.4801710932,-0.6003802104
H,0,-1.2605577088,-1.6018656831,-3.0961348214
O,0,0.6677940891,-3.0377364125,-3.365267342
H,0,1.1438095403,-2.291607677,-3.9583969523
C,0,-2.9119927211,-0.4156358395,-3.9809952262
H,0,-3.073685627,0.6023465499,-4.3416165141
H,0,-3.1039024409,-1.1187714767,-4.7983955406
H,0,-3.6455403651,-0.6381189118,-3.1988522144
O,0,1.8350398183,-0.2736650096,-0.2156799956
Si,0,1.5674970009,-1.8014796282,0.4520917418
C,0,1.5900250408,-1.7187187117,2.329974699
H,0,1.1083049739,-0.8007757099,2.6837577622
H,0,1.0316513751,-2.5698196583,2.7356034782
H,0,2.6038310878,-1.7561342037,-2.737272712
C,0,2.7945990137,-3.0766491977,-0.1690559661
H,0,3.7737506512,-2.9779621929,0.3107852472
H,0,2.4029475352,-4.0785327296,0.0420772617
H,0,2.9269790024,-2.991119311,-1.2536678349
C,0,-0.1613649985,-2.2162720434,-0.1339508569
H,0,-0.1398511002,-2.5372286278,-1.1819266086
H,0,-0.5809329629,-3.031854462,0.4651896963
H,0,-0.8232269976,-1.3480660048,-0.0394325753
O,0,1.7206747596,-1.1661742595,-4.5946585432
H,0,1.2114907144,-0.9501888213,-5.384930688

C,0,2.785630484,1.9042335932,-0.0678717853
C,0,3.877949801,2.7260132066,0.2278434937
C,0,1.494912045,2.4348112638,0.0290942098
C,0,3.6864355794,4.0586015668,0.5903361192
H,0,4.8873310089,2.3280615876,0.1746611057
C,0,1.3024427401,3.7678234371,0.3896910024
H,0,0.6442352492,1.793910851,-0.181023297
C,0,2.3978688668,4.5866437607,0.6641312442
H,0,4.5456155919,4.6825695371,0.8163152491
H,0,0.2947725722,4.1667033707,0.4578529084
H,0,2.2476841141,5.624753296,0.9439302658
C,0,4.2531673368,-0.1601707619,-0.061611798
C,0,4.4219451571,-0.1994315933,1.3282120441
C,0,5.221623676,-0.7620537787,-0.8672250359
C,0,5.5108772964,-0.8479087646,1.9012115641
H,0,3.6839887955,0.281833428,1.9657245082
C,0,6.3231438657,-1.4039589107,-0.2966428329
H,0,5.1370130108,-0.753769275,-1.9485964502
C,0,6.4675801939,-1.4571148773,1.0866569987
H,0,5.6154029076,-0.8753972292,2.9815953488
H,0,7.062845757,-1.8679675431,-0.9414814031
H,0,7.3199975029,-1.9625565429,1.5294634374
H,0,1.2713444049,-3.7848926179,-3.3029134361

TS-7 syn-down with H₂O

M06-2X/6-31+G**, $E = -1505.08382589$ a.u.

Thermal correction to Gibbs Free Energy = 0.483080 a.u.

1 imaginary frequency = -131.43 cm⁻¹

SP at B2PLYP/6-311+G**, $E = -1504.5496804379$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1504.5783437836$ a.u.

0,1
C,0,-0.9088232933,0.9990873825,-1.4440722086
C,0,0.276208945,0.4995096187,-1.8278272428
H,0,1.0656654798,0.3017683016,-1.111041022
C,0,0.5058675814,0.2568798699,-3.2381218737
H,0,-0.3149382639,0.4549115125,-3.9222604858
N,0,1.6538083239,0.0096718799,-3.7963725976
C,0,1.7318140746,-0.3427032355,-5.2261951234
C,0,2.8732684153,-0.4410788396,-3.0941261893
C,0,2.4500626801,-1.6869594927,-5.1699213645
C,0,3.4859076979,-1.4891460231,-4.0493788009
H,0,2.5515333119,-0.897294705,-2.1560537207
C,0,3.801172572,0.7661628279,-2.7315732645
H,0,-1.6591759641,1.203337411,-2.2088902621
O,0,-1.5043216484,-0.9319798961,-5.2886534573
H,0,-1.0557731293,-1.4444462927,-4.4617498411
C,0,-1.2887149938,1.3003450385,-0.0328530253
H,0,-0.5192722174,0.9741885375,0.6700319883
H,0,-1.4500659106,2.376642991,0.096183493
H,0,-2.2321772711,0.8055577179,0.2190854061
O,0,3.0854222729,1.4485537404,-1.7147485527
Si,0,3.5902551821,2.610223496,-0.5954268449
C,0,4.4952892804,4.0364163007,-1.4123395181
H,0,3.836467585,4.5890921157,-2.0891167172
H,0,4.8456778289,4.725903342,-0.6358313598
H,0,5.3660007911,3.7041389774,-1.9846691412
C,0,4.6413479278,1.8434075947,0.7541019773
H,0,5.6317926389,1.5418208424,0.398904187
H,0,4.7732484163,2.5700421377,1.563927204
H,0,4.1443923403,0.9599375818,1.1686904603
C,0,1.9628564582,3.1939240193,0.1208351181
H,0,1.4690295478,2.3812478203,0.6629791101
H,0,2.1184217216,4.0221589816,0.8200750969
H,0,1.2867565585,3.5325085669,-0.6715993914
O,0,-0.3330912721,-1.9413786649,-3.3657619082
H,0,-0.9183325742,-2.0511071317,-2.6071734504
C,0,3.9434467795,1.6674556063,-3.964012285
C,0,4.8747120298,1.4175461263,-4.9796109316
C,0,3.0209447396,2.702691892,-4.1498971026

C,0,4.8814230208,2.1806292364,-6.1474830057
H,0,5.6131415912,0.6301334019,-4.8648485481
C,0,3.0245972825,3.466290381,-5.3154096144
H,0,2.2837283,2.8996567552,-3.3779843877
C,0,3.9538445134,3.2062266823,-6.3217631184
H,0,5.6154875066,1.9711146347,-6.9192535158
H,0,2.295261314,4.2609693847,-5.4383354953
H,0,3.9572147337,3.7984953006,-7.2312959756
C,0,5.133750048,0.2650403139,-2.155731109
C,0,6.3182470141,0.9941516033,-2.304872327
C,0,5.1539441565,-0.8635590064,-1.3257017844
C,0,7.4885188948,0.6056737577,-1.6522540906
H,0,6.3365033525,1.8811444143,-2.9288559679
C,0,6.3209730277,-1.2575975943,-0.6762309516
H,0,4.2511841305,-1.44213318,-1.1577184658
C,0,7.4953043508,-0.5232364173,-0.8361155533
H,0,8.3935098024,1.1910085986,-1.782495801
H,0,6.3087751166,-2.1361204816,-0.0388500244
H,0,8.4047579042,-0.826587591,-0.3271377817
H,0,4.4305306769,-1.1235215778,-4.4583359931
H,0,3.7015204688,-2.4166666926,-3.5156717311
H,0,2.91190776,-1.951234432,-6.1232346214
H,0,1.7235581851,-2.4535388212,-4.8883745901
H,0,2.3268488476,0.4184904746,-5.7432800007
H,0,0.7221503917,-0.3913156639,-5.6376783932
H,0,-2.032250523,-1.5706448201,-5.7775091911

Cartesian coordinates and computed total energies for the structures presents in Scheme 6.

TS-6a anti-down

M06-2X/6-31+G**, $E = -1580.20194445$ a.u.

Thermal correction to Gibbs Free Energy = 0.491655 a.u.

1 imaginary frequency = -87.33 cm⁻¹

SP at B2PLYP/6-311+G**, $E = -1579.6436445373$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1579.6729291521$ a.u.

0,1
C,0,-2.3328720964,3.6994883237,-6.1059544795
C,0,-2.1554798537,2.6122470661,-7.1223911507
H,0,-2.7449633832,4.6012779346,-6.5709159472
H,0,-1.4968611715,2.8335035201,-7.9651340783
H,0,-3.0034993225,3.3849442486,-5.3025112081
C,0,-2.7347524656,1.4120880205,-7.0669931802
C,0,-2.4591541513,0.3428441324,-8.089115918
H,0,-3.3944794511,1.1307890439,-6.2457794894
N,0,-3.7674319352,0.0756447231,-8.8848723285
C,0,-4.6080072737,1.2581126865,-9.2497400156
C,0,-3.7232132773,-0.848549523,-10.0860489673
C,0,-5.6888928939,0.6730390702,-10.1665151003
H,0,-5.0014179204,1.6934809935,-8.3321859327
H,0,-3.533878328,-1.8373721194,-9.6620226637
C,0,-2.5855639278,-0.5816319122,-11.1191882808
H,0,-4.3108932435,-0.498183717,-8.2096970563
O,0,-4.1494091098,-1.9872106045,-7.0744157223
O,0,-2.0636870072,-0.8475755893,-7.5465842835
H,0,-1.7359633074,0.7026918686,-8.8229690529
H,0,-2.9641292558,-1.4218613744,-7.2369146351
H,0,-5.8539982517,1.3290425186,-11.0224863964
H,0,-6.6348916263,0.5793691417,-9.6302703498
H,0,-3.9713655421,1.9931396468,-9.7473697244
C,0,-5.1724194108,-0.7223581937,-10.5967677954
H,0,-5.2388186296,-0.8788121733,-11.6731731721
H,0,-5.7716726975,-1.5051180567,-10.1234877079
C,0,-2.7104505822,-1.5428885212,-12.3173341997
C,0,-1.9694690593,-1.2536006023,-13.4699211729
C,0,-3.4080412771,-2.7532123496,-12.2617673016
C,0,-1.9255913792,-2.1447294448,-14.5372621385
H,0,-1.4095225475,-0.3241953795,-13.5250234756

C,0,-3.3652566678,-3.6505304426,-13.3305112632
H,0,-3.9951275197,-3.0233165722,-11.3894756615
C,0,-2.6242933602,-3.3508164656,-14.4708678797
H,0,-1.3407888032,-1.8996556209,-15.4183481027
H,0,-3.9147592772,-4.5844348033,-13.2655703613
H,0,-2.5913066585,-4.0494008608,-15.3009216453
C,0,-2.5820745829,0.8747654423,-11.6045825645
C,0,-1.5943111617,1.7666611207,-11.180465789
C,0,-3.5768267195,1.341381208,-12.4723254122
C,0,-1.6369726219,3.1093944798,-11.559075402
H,0,-0.7822336631,1.4042735327,-10.5605098683
C,0,-3.6244000227,2.6813495806,-12.8482231842
H,0,-4.31545812,0.6533924192,-12.8737321922
C,0,-2.6611279642,3.5762529612,-12.3793018325
H,0,-0.8633098723,3.7878360004,-11.2125496151
H,0,-4.4092546248,3.0240201341,-13.515427523
H,0,-2.6978039681,4.6212997379,-12.6702930817
O,0,-1.3469018656,-0.8175846349,-10.4833188295
Si,0,-0.5146229872,-2.2372673566,-10.0907470013
C,0,-1.5721555049,-3.564135705,-9.285440313
H,0,-2.099503977,-3.192921128,-8.4030812527
H,0,-2.2941402789,-3.9992365889,-9.9837846193
H,0,-0.903259927,-4.3734602308,-8.9679181154
C,0,0.260005128,-2.9837500874,-11.6326190575
H,0,0.982905836,-3.7518330006,-11.3331594947
H,0,-0.4874235934,-3.4547301162,-12.2803686103
H,0,0.7918241797,-2.2265960964,-12.2182641258
C,0,0.8208950651,-1.6190146927,-8.9408482605
H,0,0.3584222406,-1.161538331,-8.0617856819
H,0,1.4646878776,-2.4429121844,-8.6151718134
H,0,1.4481324798,-0.8754117039,-9.4437961718
H,0,-1.3699786652,3.9795588927,-5.6662026314
O,0,-4.8127148146,-1.0019879468,-6.2384582633
H,0,-4.5356262065,-1.2541013183,-5.3476684554

TS-6a syn-up

M06-2X/6-31+G**, $E = -1580.21182075$ a.u.

Thermal correction to Gibbs Free Energy = 0.491273 a.u.

1 imaginary frequency = -50.92 cm⁻¹

SP at B2PLYP/6-311+G**, $E = -1579.6538139190$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1579.6832403237$ a.u.

0,1
C,0,-6.4468396005,-2.1735223732,-6.2429058876
C,0,-5.3452827383,-1.1893709629,-6.4891939103
H,0,-7.3792881508,-1.8244634927,-6.7000954263
H,0,-5.4919743397,-0.1816208532,-6.0961716636
H,0,-6.2024600962,-3.15477042,-6.6574064495
C,0,-4.2215647002,-1.4597477344,-7.1550308573
C,0,-3.1572547509,-0.4363785497,-7.4020289689
H,0,-4.0303998255,-2.4635100057,-7.5371850707
N,0,-3.2405387343,0.1438519642,-8.8489510176
C,0,-4.3641553926,1.1178177372,-9.0170992174
C,0,-3.3882922849,-0.9190117749,-9.9028528614
C,0,-5.5138202381,0.339007974,-9.6684427726
H,0,-4.6134259179,1.5294674158,-8.037440082
H,0,-3.0150597945,-1.8440268934,-9.4569263274
C,0,-2.4494714428,-0.621323023,-11.1111010439
H,0,-2.2844904356,0.6244026963,-8.9056244098
O,0,-0.8497518541,1.084421101,-8.1545061566
O,0,-1.8964486736,-0.94955857,-7.2518482288
H,0,-3.3227689585,0.4571946974,-6.7875431203
H,0,-1.2656856505,-0.1406126933,-7.5416739477
H,0,-5.9505575698,0.9265218496,-10.4788633763
H,0,-6.3001484056,0.1300460803,-8.9398904879
H,0,-4.0094966358,1.9315906485,-9.6504231703
C,0,-4.8986784352,-0.9759771923,-10.1911514727
H,0,-5.0874929166,-1.1203662278,-11.2557987969
H,0,-5.333707223,-1.8325538808,-9.6691844169
C,0,-2.6087255465,-1.6616611354,-12.2278248256

C,0,-2.0570207631,-1.3759834911,-13.4828103006
C,0,-3.1666671664,-2.9257284532,-12.0175408563
C,0,-2.0604565868,-2.3251109107,-14.4997224721
H,0,-1.6083285634,-0.4019790793,-13.65784575
C,0,-3.1681337691,-3.8827495365,-13.0340023615
H,0,-3.6078924459,-3.1884185247,-11.0605974945
C,0,-2.6153718102,-3.5862992962,-14.2772395324
H,0,-1.6228776451,-2.0838048168,-15.463528631
H,0,-3.6052051366,-4.8591568219,-12.8496244927
H,0,-2.6170516151,-4.3306094907,-15.0674791916
C,0,-2.6960689368,0.7987116083,-11.6310136595
C,0,-1.8653729856,1.8444937116,-11.2190122538
C,0,-3.7925317569,1.0850589626,-12.4528733356
C,0,-2.1433943159,3.1573462637,-11.6032424719
H,0,-1.0224628602,1.6249357699,-10.5713524932
C,0,-4.0730739043,2.3965949645,-12.8295823867
H,0,-4.4269391163,0.2817593116,-12.8174961473
C,0,-3.2514956505,3.4397525557,-12.4000265957
H,0,-1.4933846347,3.9608027698,-11.2702666131
H,0,-4.9293269887,2.6023395598,-13.4646652434
H,0,-3.4694909878,4.4620400814,-12.6932721613
O,0,-1.12983373,-0.6633495281,-10.6035075278
Si,0,-0.0703462395,-1.9493433302,-10.3243921692
C,0,-0.8407257173,-3.3402805167,-9.3261476046
H,0,-1.2367389266,-2.9680970293,-8.3767903196
H,0,-1.6347984719,-3.8556420222,-9.8757705137
C,0,-0.0589452318,-4.0789950812,-9.1125579063
C,0,0.5804628387,-2.663374404,-11.9349303422
H,0,1.4561203593,-3.2862817863,-11.7173121328
H,0,-0.1669879992,-3.2881601578,-12.4359667331
H,0,0.8874935513,-1.8734996939,-12.6279307719
C,0,1.3050515856,-1.1308500364,-9.3629720801
H,0,2.0332770617,-1.8717521379,-9.016934272
H,0,1.8284746833,-0.3986842064,-9.9865800063
H,0,0.8933157819,-0.6012037222,-8.4979851181
H,0,-6.6390210426,-2.2833560049,-5.1709957536
O,0,-1.5391419237,2.0391254098,-7.3005549814
H,0,-0.8200486277,2.3818837285,-6.7552703565

TS-6c *syn-up*

M06-2X/6-31+G**, $E = -1619.50693908$ a.u.

Thermal correction to Gibbs Free Energy = 0.517706 a.u.

1 imaginary frequency = -51.86 cm^{-1}

SP at B2PLYP/6-311+G**, $E = -1618.9313570966$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1618.9616571939$ a.u.

0,1

C,0,-6.4419958271,-2.1804190159,-6.2394397922
C,0,-5.3443833385,-1.192085135,-6.4989762075
H,0,-7.3471605016,-1.8457146918,-6.7634313661
H,0,-5.501735315,-0.1820873627,-6.1115037509
H,0,-6.1668142174,-3.1524381528,-6.6633117558
C,0,-4.2125063093,-1.4630661625,-7.1508069912
C,0,-3.1501362383,-0.4376797764,-7.39954206
H,0,-4.0134232011,-2.4693633503,-7.5223117453
N,0,-3.2353812054,0.1425995018,-8.8459275255
C,0,-4.3590165527,1.1169402119,-9.0121604361
C,0,-3.3850425378,-0.9198002497,-9.8999793301
C,0,-5.5096292297,0.3390933254,-9.663134478
H,0,-4.6071854829,1.5279092826,-8.0319284172
H,0,-3.0112749116,-1.8451014951,-9.4550336778
C,0,-2.4485396964,-0.6216361794,-11.10987717
H,0,-2.2783987768,0.6234470439,-8.9030754283
O,0,-0.8467757365,1.084901007,-8.1583131302
O,0,-1.888759668,-0.9500800127,-7.250273645
H,0,-3.3160382954,0.455392848,-6.7845200334
H,0,-1.2592233365,-0.1419241579,-7.5415986789
H,0,-5.9459506644,0.9269547425,-10.4735230474
H,0,-6.2961570046,0.1310238087,-8.9345187058
H,0,-4.0047986248,1.9312400679,-9.6450661469

C,0,-4.8958845635,-0.9764968722,-10.1859017231
H,0,-5.0864017542,-1.1215798396,-11.2501531739
H,0,-5.3302395596,-1.8326592731,-9.6626759729
C,0,-2.610155169,-1.6616030879,-12.2266670544
C,0,-2.0621292946,-1.3751855477,-13.4830846598
C,0,-3.1668179759,-2.9260671063,-12.0152990842
C,0,-2.0679744613,-2.3239214781,-14.5003702193
H,0,-1.6144346922,-0.4008968272,-13.6590570832
C,0,-3.170693005,-3.8826869374,-13.0321247905
H,0,-3.6052247601,-3.1893414004,-11.0572264212
C,0,-2.6216159469,-3.5854661788,-14.2768205362
H,0,-1.6332916324,-2.0819714952,-15.4653281419
H,0,-3.6067820858,-4.8593767181,-12.846914413
H,0,-2.625268708,-4.3294412555,-15.0673687646
C,0,-2.6960583203,0.7985848843,-11.6289430615
C,0,-1.8640777801,1.8440800912,-11.2188543842
C,0,-3.7942142958,1.0853382597,-12.4484159429
C,0,-2.1425655527,3.1570557122,-11.6023273143
H,0,-1.0198200269,1.6242204935,-10.5731164106
C,0,-4.075196937,2.3969856205,-12.8244065187
H,0,-4.4297532181,0.2822960154,-12.8116377693
C,0,-3.2523644886,3.4398775268,-12.3965858336
H,0,-1.4915696358,3.9602797765,-11.27071509
H,0,-4.932805798,2.6030459914,-13.4575555392
H,0,-3.4707249906,4.4622621141,-12.6892270852
O,0,-1.1279270761,-0.6638799288,-10.60482421
Si,0,-0.0675309149,-1.9497288496,-10.3289931518
C,0,-0.8351796887,-3.3408255339,-9.3288332921
H,0,-1.2293290349,-2.9686773972,-8.3786658569
H,0,-1.6302718414,-3.8566045567,-9.8765811906
H,0,-0.052704705,-4.0792299115,-9.1167444971
C,0,0.5791004897,-2.6631322969,-11.9414673338
H,0,1.4550942861,-3.2864857654,-11.7265011589
H,0,-0.1698469018,-3.2872671876,-12.4410872819
H,0,0.8846209248,-1.8728590482,-12.6346872943
C,0,1.3101770526,-1.1312712213,-9.3708287918
H,0,2.039636862,-1.8720698823,-9.027190228
H,0,1.8315620824,-0.3984072326,-9.9953159542
H,0,0.9004613897,-0.6024833654,-8.504360297
O,0,-1.5344569059,2.0392394641,-7.3025746382
H,0,-0.8145569584,2.3804535395,-6.7573787055
C,0,-6.7502607788,-2.3177010049,-4.7448424279
H,0,-7.0435504285,-1.3535925685,-4.3177213558
H,0,-7.5675916783,-3.024229398,-4.5791661118
H,0,-5.8715858902,-2.6749544906,-4.2001811253

TS-6a *anti-up*

M06-2X/6-31+G**, $E = -1580.21110427$ a.u.

Thermal correction to Gibbs Free Energy = 0.491079 a.u.

1 imaginary frequency = -123.11 cm^{-1}

SP at B2PLYP/6-311+G**, $E = -1579.6539311294$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1579.6832509872$ a.u.

0,1

C,0,-5.5649182006,-3.7758113908,-7.5930468573
C,0,-4.3467975075,-2.9420303149,-7.8460524888
H,0,-5.3323240674,-4.6101881803,-6.923961751
H,0,-3.4836442695,-3.4562188817,-8.274650689
H,0,-6.3663102806,-3.1818227447,-7.1468865237
C,0,-4.2540988095,-1.6365447207,-7.5889068213
C,0,-3.0240651717,-0.8307084456,-7.8649051898
H,0,-5.0847662933,-1.0952800487,-7.1353365954
N,0,-3.1879244186,0.0533808612,-9.1277157776
C,0,-4.3469489965,0.9994586946,-9.039048947
C,0,-3.3580255967,-0.765553356,-10.3698121638
C,0,-5.507151651,0.3150839735,-9.7701128011
H,0,-4.5278217912,1.2125773562,-7.9845664855
H,0,-2.9889316222,-1.76663993,-10.1294837562
C,0,-2.4363719016,-0.2275559073,-11.5000081486
H,0,-2.2561711996,0.6178122991,-9.0679498283

O,0,-1.1551880051,1.3578954213,-8.161960108
O,0,-2.7180794949,-0.0066203466,-6.8132648146
H,0,-2.1864441758,-1.4852046365,-8.1501850514
H,0,-1.9454233753,0.5981613575,-7.1791895949
H,0,-6.0525919453,1.0444997262,-10.3732828694
H,0,-6.2128181274,-0.1226525088,-9.0602435804
H,0,-4.0423825906,1.9266459296,-9.5250279536
C,0,-4.872885772,-0.78591248,-10.6457952508
H,0,-5.0788416735,-0.6356952722,-11.7057290168
H,0,-5.2748680214,-1.7664621365,-10.3789292838
C,0,-2.5644940471,-1.0617010253,-12.780724944
C,0,-2.0219426029,-0.550007643,-13.9661697163
C,0,-3.0932221458,-2.355063931,-12.793646379
C,0,-2.0028580916,-1.3106140007,-15.1310318371
H,0,-1.6005270139,0.4516601267,-13.9696316804
C,0,-3.0725890291,-3.1230080687,-13.9598266823
H,0,-3.5330826895,-2.7888757509,-11.9006314338
C,0,-2.5260812295,-2.6044962774,-15.1308169776
H,0,-1.5738959726,-0.8959612167,-16.0379304285
H,0,-3.4875890133,-4.1259496263,-13.9473309431
H,0,-2.5107892568,-3.2013207046,-16.0372407182
C,0,-2.727736383,1.2537860903,-11.7678566492
C,0,-1.907473865,2.2400775248,-11.2149600706
C,0,-3.8410583579,1.6450009062,-12.5229185985
C,0,-2.2076759402,3.5913809994,-11.3970920188
H,0,-1.0440065023,1.9392472059,-10.630011896
C,0,-4.1476048875,2.9929764088,-12.6917138059
H,0,-4.4640246459,0.898570474,-13.0068051514
C,0,-3.3331759005,3.9732909416,-12.1235430512
H,0,-1.5568429244,4.348988474,-10.9696179562
H,0,-5.0156526478,3.2763548125,-13.2787398986
H,0,-3.5670262567,5.0245359678,-12.2595868149
O,0,-1.1154396587,-0.3138408518,-10.9958637035
Si,0,0.0233924092,-1.5577823774,-10.9564749148
C,0,-0.6460867223,-3.1331991389,-10.1747450583
H,0,-0.9207715015,-2.9985298883,-9.1238990922
H,0,-1.5059133015,-3.5412978436,-10.7163332761
H,0,0.1473162992,-3.8892728662,-10.2085402325
C,0,0.6666888279,-1.9763430603,-12.6657242608
H,0,1.5765358209,-2.579553442,-12.5661022882
H,0,-0.0627838523,-2.5501650589,-13.2474970875
H,0,0.916576959,-1.0715024157,-13.2284929812
C,0,1.3605383423,-0.8194584092,-9.8831834285
H,0,2.1531380098,-1.547562232,-9.6830071519
H,0,1.8090781311,0.0532131928,-10.368251837
H,0,0.9336961357,-0.4916869885,-8.9294289778
H,0,-5.9328197512,-4.2101983018,-8.528923177
O,0,-1.9034611385,2.5908199535,-7.9787121487
H,0,-1.4152639271,3.2051735725,-8.5416006446

TS-6c anti-up

M06-2X/6-31+G**, $E = -1619.50622184$ a.u.

Thermal correction to Gibbs Free Energy = 0.516864 a.u.

1 imaginary frequency = -122.85 cm^{-1}

SP at B2PLYP/6-311+G**, $E = -1618.9315443981$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1618.9617363033$ a.u.

0,1

C,0,-5.5632649431,-3.7878605766,-7.5797886681
C,0,-4.3493728444,-2.9494940345,-7.8504676945
H,0,-3.4861769811,-3.4717943109,-8.2729178224
H,0,-6.3656204661,-3.1528192026,-7.1888449409
C,0,-4.2536352245,-1.6437266548,-7.5955274168
C,0,-3.0227864717,-0.8386465751,-7.8707934877
H,0,-5.0843765321,-1.1006633433,-7.1440076938
N,0,-3.1868688702,0.0475870403,-9.1316425786
C,0,-4.346334953,0.9930459204,-9.0412496758
C,0,-3.3564990088,-0.7688696587,-10.3755154298
C,0,-5.5061237261,0.3097482871,-9.7739784076
H,0,-4.5274549419,1.2040131674,-7.9863739694

H,0,-2.9869030734,-1.7703309949,-10.1373628014
C,0,-2.4349988367,-0.227367941,-11.5041987612
H,0,-2.2552531471,0.6126404327,-9.0705639031
O,0,-1.1552641753,1.3515504754,-8.1638962428
O,0,-2.7163800149,-0.0168526337,-6.8174774106
H,0,-2.1857751124,-1.493452753,-8.1571328936
H,0,-1.9440133184,0.5889102469,-7.1824465349
H,0,-6.0515949777,1.0402217879,-10.3758337159
H,0,-6.2118660155,-0.1296299575,-9.0651797846
H,0,-4.0420403481,1.9213651648,-9.5252156159
C,0,-4.8713271746,-0.7893141237,-10.6517318361
H,0,-5.0771579242,-0.6370590196,-11.7113876986
H,0,-5.2729245904,-1.7705711502,-10.3869543495
C,0,-2.5621377792,-1.0580662524,-12.7872278693
C,0,-2.0196196317,-0.5425176395,-13.9710209968
C,0,-3.0896905985,-2.3518587092,-12.803918309
C,0,-1.9994251789,-1.2997660996,-15.1380168427
H,0,-1.5990628586,0.4595126187,-13.9714326935
C,0,-3.0678805236,-3.1164764443,-13.9722633487
H,0,-3.5294122155,-2.7884705324,-11.9121915507
C,0,-2.5214270683,-2.5941448819,-15.1415889732
H,0,-1.570510031,-0.8821708429,-16.0435875123
H,0,-3.4819203729,-4.1198467383,-13.9628358066
H,0,-2.5052640826,-3.1884230056,-16.0496727614
C,0,-2.7272490628,1.2544932639,-11.7683379799
C,0,-1.9070919663,2.2398668614,-11.213656675
C,0,-3.8411697477,1.6469639663,-12.5218626989
C,0,-2.2081553059,3.5914509383,-11.3922666495
H,0,-1.0430524597,1.9380795427,-10.6300568288
C,0,-4.1486126123,2.9951728316,-12.6870764961
H,0,-4.4640293663,0.9013579019,-13.0071652679
C,0,-3.3344032187,3.9745320735,-12.1169244718
H,0,-1.5574426844,4.3483700871,-10.9633852707
H,0,-5.017200413,3.27950408,-13.2728439336
H,0,-3.5690051015,5.0259822699,-12.2500709545
O,0,-1.1142104509,-0.3140738949,-10.9998444473
Si,0,0.0255238013,-1.5572480473,-10.9633165745
C,0,-0.6435489097,-3.1357637421,-10.1874539504
H,0,-0.9208393109,-3.0046206017,-9.1368411902
H,0,-1.5017312202,-3.5432978704,-10.7320818887
H,0,0.1508884214,-3.8907299548,-10.2217563271
C,0,0.6707791345,-1.9692700638,-12.6734106134
H,0,1.5813982627,-2.5715401376,-12.575217441
H,0,-0.0574285382,-2.542057717,-13.2577843896
H,0,0.9198614599,-1.0621382221,-13.2328522296
C,0,1.360951412,-0.8213088365,-9.8862105354
H,0,2.1540243217,-1.5493269351,-9.6876197246
H,0,1.809150962,0.0534126613,-10.3678976038
H,0,0.9327912882,-0.497086594,-8.9318298531
H,0,-5.9199835673,-4.2113492012,-8.5275634662
O,0,-1.9042193317,2.5833453343,-7.976064021
H,0,-1.4174274445,3.1996114746,-8.5380721005
C,0,-5.2631490124,-4.9290591802,-6.6020771701
H,0,-6.1519818256,-5.5434962867,-6.4369754353
H,0,-4.4704783492,-5.5767679267,-6.9895502525
H,0,-4.9342288826,-4.5337869699,-5.636817811

TS-6a syn-down

M06-2X/6-31+G**, $E = -1580.19584678$ a.u.

Thermal correction to Gibbs Free Energy = 0.492634 a.u.

1 imaginary frequency = -189.94 cm^{-1}

SP at B2PLYP/6-311+G**, $E = -1579.6385239149$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1579.6678624007$ a.u.

0,1

C,0,-1.1184174242,-2.963665333,-6.1786204876
C,0,-1.8743944218,-1.7106087126,-6.5080729113
H,0,-1.7116836436,-3.6188316206,-5.5319499206
H,0,-2.2183176787,-1.100410414,-5.6738954762
H,0,-0.8501395547,-3.5188888664,-7.0816177445

C,0,-2.1323064811,-1.30047232,-7.7512040785
C,0,-2.8470279613,0.0030578314,-8.036391459
H,0,-1.7731490902,-1.8734390454,-8.6005934783
N,0,-3.89840269,-0.2126596579,-9.1420392005
C,0,-4.7701916766,0.978640086,-9.4179952311
C,0,-3.5771793016,-0.8521099636,-10.4686441438
C,0,-5.6504031828,0.5016289196,-10.5813191332
H,0,-5.3285079078,1.1928346544,-8.50951603
H,0,-3.3231041399,-1.8856621258,-10.2323681427
C,0,-2.3523592271,-0.2669214138,-11.2460367159
H,0,-4.5672323009,-0.8566273317,-8.6513381524
O,0,-5.4521983616,-1.1171354387,-7.1344058518
O,0,-3.5319450771,0.4908221808,-6.9470250993
H,0,-2.1542971471,0.7585250095,-8.4173767629
H,0,-4.3143300951,-0.190517877,-6.8174433119
H,0,-5.7687903217,1.2952493519,-11.3202790925
H,0,-6.6430873921,0.2317047795,-10.2163633832
H,0,-4.1381390643,1.8304295613,-9.6701211194
C,0,-4.9412866299,-0.7436942822,-11.1736403235
H,0,-4.8312425162,-0.6973378457,-12.2574976817
H,0,-5.5176442559,-1.645230366,-10.9498936744
C,0,-2.1901190264,-1.0277110706,-12.5789883962
C,0,-1.5632672907,-0.4095771294,-13.6672989717
C,0,-2.5361134439,-2.3795501419,-12.6997670549
C,0,-1.2817120831,-1.117414458,-14.8348277194
H,0,-1.2894012426,0.638642531,-13.6098458146
C,0,-2.2674806868,-3.0870919538,-13.8698061483
H,0,-3.0167608364,-2.9107896244,-11.8855322378
C,0,-1.6341391619,-2.4609769886,-14.9418853005
H,0,-0.7891314132,-0.6131145977,-15.6602427085
H,0,-2.5500757141,-4.132923801,-13.9372234229
H,0,-1.4196057325,-3.0136971839,-15.8509346591
C,0,-2.4764471873,1.2463725388,-11.4718591846
C,0,-1.7239212723,2.1412883207,-10.7078060486
C,0,-3.371497791,1.766132402,-12.4161498779
C,0,-1.8874330647,3.5197225452,-10.8507491316
H,0,-1.0084440407,1.7607307766,-9.9877753899
C,0,-3.542998188,3.1405951118,-12.5564446848
H,0,-3.9357392186,1.0977004988,-13.059806425
C,0,-2.8073682544,4.0249264486,-11.7664940621
H,0,-1.2950800955,4.1944907739,-10.2407819823
H,0,-4.2484506467,3.5208191737,-13.2886133478
H,0,-2.9416294947,5.0964801161,-11.8750019367
O,0,-1.238776628,-0.5330891107,-10.4149640454
Si,0,0.4044418794,-0.808859985,-10.7138585483
C,0,0.6801352663,-2.4159591399,-11.6361201072
H,0,0.0875718043,-3.2240859418,-11.1942513614
H,0,0.4189947354,-2.3404145458,-12.6963092051
H,0,1.7387065356,-2.6904410827,-11.5620529
C,0,1.2211208914,0.6128801733,-11.6270092302
H,0,2.2711776194,0.3492321304,-11.8002980488
H,0,0.7643699988,0.8103059674,-12.6001918411
H,0,1.1995722614,1.5375117261,-11.0425405652
C,0,1.1085078516,-0.9250708205,-8.9834271221
H,0,0.7731407974,-1.8330172314,-8.4722336504
H,0,2.2029386178,-0.9411694451,-9.0243943107
H,0,0.7999968595,-0.0652778887,-8.3789875913
H,0,-0.1995352221,-2.7259700399,-5.6316099998
O,0,-5.0159917358,-2.4606669972,-7.5021266976
H,0,-4.2767141034,-2.6274418162,-6.8999646642

5a syn-up

M06-2X/6-31+G**, $E = -1428.70273040$ a.u.

Thermal correction to Gibbs Free Energy = 0.462456 a.u.

SP at B2PLYP/6-311+G**, $E = -1428.1656981590$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1428.1952609687$ a.u.

0,1
C,0,-1.5682174265,0.3540658157,0.3698880502
N,0,-1.5898986025,1.7349027227,0.814929672
C,0,-2.2695312981,1.9940685113,2.0890443532
C,0,-1.3653242266,3.0021482987,2.8221509314
C,0,-0.5038194492,3.6179078662,1.7126435336
C,0,-0.307102394,2.4422123771,0.7612454061
O,0,-1.2669185251,0.3914179971,-1.0167659426
H,0,-2.5840708912,-0.0291881566,0.5214618968
C,0,-3.7411783918,2.4721362426,1.8559887458
C,0,-4.5176938592,2.6395611941,3.17123239
C,0,-5.712449754,3.3724718998,3.176105778
C,0,-4.1517815125,1.9764667289,4.3476499522
C,0,-6.5243669869,3.4266603883,4.3064520572
H,0,-6.0146489561,3.9076293992,2.2807098588
C,0,-4.9580593971,2.0330151402,5.4854172687
H,0,-3.2342406104,1.4008298511,4.3985051746
C,0,-6.1512795734,2.751646111,5.468576168
H,0,-7.4478466347,3.9971133359,4.2781091175
H,0,-4.6507397267,1.5078079256,6.3846162062
H,0,-6.7807991799,2.7892258182,6.3521007878
C,0,-3.7361816427,3.7494751515,1.0163181638
C,0,-3.7132818831,3.6551386007,-0.3782061556
C,0,-3.6518372561,5.0183068231,1.6012261939
C,0,-3.606990161,4.7985947634,-1.1691597531
H,0,-3.7736973658,2.6739856974,-0.8360973648
C,0,-3.5406802374,6.1636102592,0.8135174552
H,0,-3.6766751247,5.1217218126,2.6825000842
C,0,-3.5162202103,6.0579053497,-0.5765287477
H,0,-3.5907244784,4.7036336459,-2.2508782824
H,0,-3.4763952314,7.1380360363,1.2884838626
H,0,-3.4332008802,6.9488825143,-1.1915824941
O,0,-4.3200135675,1.4089630108,1.1107167626
Si,0,-5.8731825527,0.8102522684,0.9076114877
C,0,-6.4946358875,-0.0345296285,2.464184227
H,0,-7.4454820492,-0.5382222303,2.255241514
H,0,-5.7789652161,-0.7911672755,2.8034826867
H,0,-6.6556424192,0.6755158908,3.2819874761
C,0,-7.0941639401,2.1233078852,0.333626284
H,0,-6.5840216003,2.9255967168,-0.2103850998
H,0,-7.8249801978,1.6677076949,-0.3437784681
H,0,-7.6428417053,2.5677372609,1.1688347195
C,0,-5.6206978087,-0.4599068618,-0.4477746407
H,0,-5.2417205576,0.0162818949,-1.3582587614
H,0,-4.8970795897,-1.2201372545,-0.1351365393
H,0,-6.5618561976,-0.9643437947,-0.690465833
H,0,-0.7262848085,2.459861802,3.5281545866
H,0,-1.9325142747,3.741821667,3.3936657978
H,0,0.4437860889,4.0142731627,2.08549408
H,0,-1.0427971572,4.4263021515,1.2098780214
H,0,-0.0893468908,2.7540406228,-0.2645898513
H,0,0.5229448302,1.8042059934,1.1055842633
H,0,-2.3567020547,1.0612141988,2.6596667706
C,0,-0.5970381938,-0.5217517838,1.1408621478
H,0,-0.8787098955,-0.7156633237,2.1778374429
C,0,0.5401205763,-1.0368305133,0.6711077014
H,0,0.8245582324,-0.8307111908,-0.3612757975
C,0,1.4859288507,-1.8866713672,1.4686549591
H,0,1.1174860142,-2.0418410728,2.4862037323
H,0,2.4745132424,-1.4186936469,1.5265290121
H,0,1.6251928321,-2.865525394,0.9978451746
H,0,-1.220295477,-0.5172286142,-1.3398716517

5a anti-up

M06-2X/6-31+G**, $E = -1428.70706043$ a.u.
Thermal correction to Gibbs Free Energy = 0.461596 a.u.
SP at B2PLYP/6-311+G**, $E = -1428.1695440981$ a.u.
SP at mPW2PLYP/6-311+G**, $E = -1428.1991741617$ a.u.

0,1
C,0,-1.2173208269,0.7501850181,0.0000610112
N,0,-1.3758451812,2.1111594009,0.4931121755
C,0,-1.9856926894,2.244583962,1.8227028909
C,0,-1.1583181285,3.3309545427,2.5334297731
C,0,-0.4704368136,4.0899393513,1.3914679697
C,0,-0.1945102047,2.9765447817,0.3863791086
O,0,-1.1379552472,0.7642962932,-1.412766084
H,0,-2.1223107543,0.216579089,0.3159316059
C,0,-3.5168778115,2.5422518431,1.7105963559
C,0,-4.2124834609,2.5309955905,3.0798820026
C,0,-5.5022501097,3.0676200037,3.1962679491
C,0,-3.6611025365,1.9015476183,4.2007391068
C,0,-6.2284183064,2.9565872287,4.3790346746
H,0,-5.9453284155,3.578391615,2.3462370337
C,0,-4.3810660863,1.7951474047,5.3916199348
H,0,-2.6624768915,1.4807205547,4.1675979886
C,0,-5.6703919493,2.3136794674,5.4842275014
H,0,-7.2289258289,3.374582053,4.4377155079
H,0,-3.9290373605,1.3014553696,6.2463916392
H,0,-6.2319193157,2.2255071687,6.4090859858
C,0,-3.7345452668,3.8589720616,0.9656184436
C,0,-3.813112446,3.8550111411,-0.4300651215
C,0,-3.7623761418,5.0898665546,1.6310116492
C,0,-3.9052365382,5.0485669865,-1.1452773624
H,0,-3.8019492196,2.9033465951,-0.950098476
C,0,-3.8502545709,6.2858565633,0.9195688311
H,0,-3.7204786257,5.1222449854,2.7161404363
C,0,-3.9173974218,6.2703533848,-0.4733840093
H,0,-3.9650587746,5.0227476714,-2.2293287802
H,0,-3.8701406342,7.2293471349,1.4566720975
H,0,-3.986792475,7.200986676,-1.0282872426
O,0,-4.0098737037,1.4683803927,0.9218117734
Si,0,-5.4472571065,0.609077644,0.8322020796
C,0,-5.7456678513,-0.4013178049,2.3846235913
H,0,-6.5850899424,-1.0870373848,2.221417503
H,0,-4.8619600742,-1.0005598817,2.6292838299
H,0,-5.9813669887,0.2295677287,3.2479524113
C,0,-6.9309970995,1.7061914183,0.4563806061
H,0,-6.6290568902,2.6021114185,-0.0972709954
H,0,-7.6429472849,1.1505577998,-0.1642676474
H,0,-7.4521114257,2.0210184007,1.3647748912
C,0,-5.1186076909,-0.5250155743,-0.6225853655
H,0,-4.9417039139,0.0575268212,-1.5332237203
H,0,-4.2355338876,-1.1464988698,-0.4405661019
H,0,-5.9709920443,-1.1881297435,-0.803661744
H,0,-0.4023927646,2.8496265292,3.1641411443
H,0,-1.7641743469,3.9727361456,3.1783306095
H,0,0.4428214508,4.5978997279,1.7106720393
H,0,-1.1471279916,4.8332188176,0.9586177314
H,0,-0.0792307435,3.3439839833,-0.6379964449
H,0,0.7266738945,2.437237254,0.6583663209
H,0,-1.9147069591,1.2877005398,2.3550036683
C,0,-0.0111023141,0.0268945347,0.5487276792
H,0,0.047175771,0.0100459012,1.6394141672
C,0,0.9342610772,-0.5765219785,-0.1712499506
H,0,0.8549649917,-0.54756681,-1.2568022549
C,0,2.1121155525,-1.3025310983,0.4104836858
H,0,2.1033087755,-1.2647642742,1.5033053237
H,0,3.0527537854,-0.8667707528,0.0570769468
H,0,2.1145649219,-2.3534108004,0.1016061064
H,0,-1.8616971634,1.3296512042,-1.7137384811

5a anti-down

M06-2X/6-31+G**, $E = -1428.70707613$ a.u.
Thermal correction to Gibbs Free Energy = 0.465239 a.u.
SP at B2PLYP/6-311+G**, $E = -1428.1672865131$ a.u.
SP at mPW2PLYP/6-311+G**, $E = -1428.1970532395$ a.u.

0,1
C,0,-3.0590027349,3.0830758668,-5.1703458563
C,0,-2.6867105416,2.2360393876,-6.3507862918
H,0,-3.3062442957,4.1026249725,-5.4846371338
H,0,-1.8339621681,2.5703793374,-6.9445982238
H,0,-3.9195847886,2.6658888928,-4.6409194816
C,0,-3.3198839227,1.1238381172,-6.7212262087
C,0,-2.9117244595,0.2918177951,-7.9051569407
H,0,-4.1818007936,0.7552292108,-6.1624342377
N,0,-4.0140602694,0.1988804028,-8.853709135
C,0,-4.5783506774,1.4544671584,-9.345185564
C,0,-3.9973594456,-0.7950128458,-9.9254867151
C,0,-5.6413976201,0.9988818712,-10.3602333987
H,0,-5.0154428572,2.0093625507,-9.4502595484
H,0,-4.0342975096,-1.7794377962,-9.4508103954
C,0,-2.7346759159,-0.8627189832,-10.8680035515
O,0,-2.5776158588,-0.996847236,-7.4297184954
H,0,-2.0192285096,0.7500479357,-8.3650446524
H,0,-2.1459513985,-1.4448074809,-8.1763088564
H,0,-5.6085527192,1.6116450613,-11.2641252998
H,0,-6.6429262042,1.0941805127,-9.9342927905
H,0,-3.824723907,2.1077975497,-9.8164469629
C,0,-5.3209372364,-0.4864370586,-10.655276407
H,0,-5.2667787654,-0.7038023505,-11.7240528096
H,0,-6.1005683323,-1.1312893057,-10.2416813002
C,0,-2.950464682,-1.8944504386,-11.9902815861
C,0,-2.3608671603,-1.7391128486,-13.2497783815
C,0,-3.6469535708,-3.0839889848,-11.7343959784
C,0,-2.4586652152,-2.736631636,-14.2210984495
H,0,-1.8148102118,-0.8310741083,-13.4835409642
C,0,-3.7566849861,-4.0771663149,-12.7042304802
H,0,-4.1063021651,-3.2579333443,-10.7673995575
C,0,-3.1588833739,-3.9103397731,-13.9533665616
H,0,-1.9864231297,-2.590431645,-15.1877400251
H,0,-4.3037706372,-4.9871594393,-12.4779049081
H,0,-3.2399086228,-4.6862560936,-14.7081285191
C,0,-2.3860624657,0.5285549522,-11.4010022074
C,0,-1.3431394408,1.2708187959,-10.8428814741
C,0,-3.1581286701,1.1269033415,-12.405533354
C,0,-1.0959257699,2.5827226723,-11.2469441295
H,0,-0.7230527038,0.8256968404,-10.0729901287
C,0,-2.9207729153,2.4387861185,-12.8077343405
H,0,-3.9556232853,0.5660753196,-12.8839280337
C,0,-1.8920528055,3.1779796471,-12.2225994706
H,0,-0.2819865289,3.1385438522,-10.7911255984
H,0,-3.5398745272,2.8819074275,-13.5819295852
H,0,-1.7073978791,4.2016001743,-12.5333016443
O,0,-1.6795156476,-1.3389593403,-10.0220172763
Si,0,-0.2154901392,-2.1194127792,-10.3745159979
C,0,-0.4799637296,-3.8731770471,-10.9750871139
H,0,-1.1939810739,-4.4029656694,-10.3364297276
H,0,-0.8498129375,-3.9074189852,-12.0049563835
H,0,0.4761348867,-4.4078812971,-10.9350543853
C,0,0.8340145082,-1.1729481451,-11.6084897991
H,0,1.7021049704,-1.7895187033,-11.8690229261
H,0,0.2936785914,-0.9496008435,-12.5323431354
H,0,1.2008861671,-0.2302768535,-11.1919913107
C,0,0.6127451402,-2.1263542437,-8.6961947111
H,0,0.0595486432,-2.7414395662,-7.9787034335
H,0,1.6270012825,-2.5316089354,-8.7740763425
H,0,0.6822343423,-1.1104632952,-8.2925826036
H,0,-2.2233063263,3.160026283,-4.4669839829

5a syn-down

M06-2X/6-31+G**, $E = -1428.69925146$ a.u.
Thermal correction to Gibbs Free Energy = 0.464553 a.u.
SP at B2PLYP/6-311+G**, $E = -1428.1592780921$ a.u.
SP at mPW2PLYP/6-311+G**, $E = -1428.1893218790$ a.u.

0,1

C,0,-0.7516762278,0.5585779212,0.7245903993
N,0,-1.4012568866,1.8420232754,0.6482394637
C,0,-2.0271769404,2.2922296945,1.8995987882
C,0,-1.2436701129,3.5566025958,2.2933001001
C,0,-0.7604416863,4.1397205079,0.9610762012
C,0,-0.5152787903,2.8946997114,0.1044610051
O,0,0.2957255448,0.6211836529,1.7010449537
H,0,-0.2972363186,0.3850798959,-0.2625744331
C,0,-3.5941227637,2.4717805635,1.7881502583
C,0,-4.1153909085,2.5221044104,3.2376962595
C,0,-4.0172586919,3.6435830869,4.0752175549
C,0,-4.5998873827,1.3372591347,3.8083271163
C,0,-4.4282298945,3.5927337119,5.4071516212
H,0,-3.6199523019,4.580625162,3.7049365904
C,0,-5.0113495269,1.2811102492,5.1391863162
H,0,-4.6376004822,0.4396484371,3.2027535497
C,0,-4.9353568797,2.4129495537,5.9473316026
H,0,-4.3477667788,4.4844630263,6.0215648689
H,0,-5.385916353,0.3449761967,5.5429207781
H,0,-5.2566824549,2.3754772601,6.9835073359
C,0,-3.9892177961,3.650567649,0.8825881815
C,0,-3.6554947847,3.5340418383,-0.4768003829
C,0,-4.7133600729,4.7764034178,1.2819222137
C,0,-3.9974954478,4.5224297262,-1.393408411
H,0,-3.12276765,2.6456880657,-0.8009842453
C,0,-5.0559813354,5.7735200042,0.3644444734
H,0,-5.0629615959,4.8800212654,2.3007678073
C,0,-4.6944635183,5.6574068384,-0.9741064822
H,0,-3.7247949287,4.4036506889,-2.4382453184
H,0,-5.6241739708,6.6350290272,0.7024775641
H,0,-4.9656886627,6.4313170137,-1.6857237989
O,0,-4.0550414095,1.280760029,1.175042107
Si,0,-5.5335338489,0.8911229124,0.4766849382
C,0,-6.0790553761,-0.7317521584,1.2507049713
H,0,-6.8543108592,-1.1970171381,0.6320182878
H,0,-5.2395129135,-1.4309322614,1.3233218226
H,0,-6.4923687394,-0.5885303083,2.2542425664
C,0,-6.8562862863,2.1935914484,0.7619405343
H,0,-6.7107258007,3.0716901783,0.1251328121
H,0,-7.836505695,1.7581225148,0.535805976
H,0,-6.8649411536,2.5256742687,1.8062533217
C,0,-5.268783945,0.6108262182,-1.3606478641
H,0,-5.1089566233,1.5533697695,-1.8923502751
H,0,-4.398881324,-0.0321118123,-1.5342156897
H,0,-6.1453799794,0.1178748558,-1.7952110964
H,0,-0.3833225253,3.2481019743,2.8956030961
H,0,-1.8174637729,4.2754232296,2.877719141
H,0,0.1466883861,4.738999598,1.0735231028
H,0,-1.5307042352,4.7752648429,0.5158466636
H,0,-0.7392874111,3.0714227808,-0.954723611
H,0,0.5314118495,2.578372356,0.1865406463
H,0,-1.9001606921,1.5100415811,2.6548403804
C,0,-1.7155025979,-0.5685897135,1.0008203997
H,0,-2.4711924973,-0.7153752945,0.2301745834
C,0,-1.6901182044,-1.354717535,2.0768301419
H,0,-0.9457862421,-1.1657199104,2.850072572
C,0,-2.6457581017,-2.4849271062,2.3254299343
H,0,-3.2731490699,-2.6743045457,1.4502985667
H,0,-3.299474141,-2.2619472478,3.1770188161
H,0,-2.1090994285,-3.4078068634,2.5682494261
H,0,0.8058811777,-0.1981252769,1.6640898938

TS-7a anti-down

M06-2X/6-31+G**, $E = -1580.19145651$ a.u.
Thermal correction to Gibbs Free Energy = 0.481259 a.u.
1 imaginary frequency = -256.75 cm⁻¹
SP at B2PLYP/6-311+G**, $E = -1579.6480360413$ a.u.
SP at mPW2PLYP/6-311+G**, $E = -1579.6762484515$ a.u.

0,1

C,0,-1.4511798653,-0.5646840827,-3.4929263021
C,0,-0.4865641009,0.3694767584,-3.5227935561
H,0,-0.6862344764,1.3761937209,-3.881614896
C,0,0.8392096195,0.0223669274,-3.0445423201
H,0,0.9830880317,-0.9655353289,-2.6239557688
N,0,1.7600904931,0.917276768,-2.7951082878
C,0,1.7580528398,2.2686940769,-3.380861235
C,0,3.0806119491,0.5092351278,-2.2904535138
C,0,3.1403675305,2.8316022871,-3.0443642002
C,0,4.0218105691,1.5869157001,-2.8407827625
H,0,0.9433416247,2.8627972654,-2.9581562563
H,0,3.0920446638,3.4292221571,-2.1316531491
H,0,1.6099443486,2.1718173258,-4.4626143709
H,0,3.513275995,3.4697947305,-3.8473276467
H,0,4.8677923952,1.7749911155,-2.174958526
H,0,4.4201410677,1.2460988136,-3.8008337728
H,0,3.2746448948,-0.4718008178,-2.7295252457
C,0,3.0524874721,0.3345933675,-0.7386316614
H,0,-1.1832878003,-1.563556281,-3.1455178351
O,0,0.5204708253,-3.041734778,-4.5023368303
O,0,0.628511268,-3.1333485313,-3.070761421
H,0,1.3640118006,-3.7501763834,-2.9538496155
H,0,1.0601011786,-2.0861904945,-4.7009122873
C,0,-2.8605641738,-0.3454105987,-3.928843564
H,0,-3.0262484354,0.6786985679,-4.2703373133
H,0,-3.1114723908,-1.0363873363,-4.7407417313
H,0,-3.5508477366,-0.5632531435,-3.1072361234
O,0,1.9973253705,-0.5850146312,-0.5291926491
Si,0,1.610150217,-1.6998557719,0.6719707914
C,0,1.5839807632,-0.930570527,2.38749015
H,0,1.2842521492,0.1223014911,2.3458439891
H,0,0.8521491984,-1.4644921232,3.0042735379
H,0,2.553337584,-0.9954852819,2.8891177461
C,0,2.7719828542,-3.1709746428,0.6194166527
H,0,3.7927481327,-2.8999241069,0.9088941896
H,0,2.4153331199,-3.9470654104,1.3061725886
H,0,2.8042614052,-3.5992298834,-0.3881383449
C,0,-0.1195843316,-2.2013886155,0.1652714898
H,0,-0.1228152382,-2.5700819268,-0.8664306635
H,0,-0.5077752893,-2.9899707637,0.818462801
H,0,-0.7996138136,-1.3441024377,0.2249207896
O,0,1.7091965529,-0.9508528478,-4.844005199
H,0,1.3171736473,-0.4729884053,-5.5851218749
C,0,2.7046666786,1.674522494,-0.0833986727
C,0,3.6892464053,2.6013784492,0.2779784556
C,0,1.3610088511,2.0347767359,0.0601032627
C,0,3.3393328381,3.8586809468,0.7671229337
H,0,4.7400940507,2.3453178296,0.1780040984
C,0,1.0083948348,3.2928959739,0.5478667213
H,0,0.5900771758,1.3203410686,-0.2134107865
C,0,1.9965202742,4.2109009374,0.9005612906
H,0,4.1183720933,4.5624807942,1.0436484361
H,0,-0.0404892029,3.5536981707,0.652150102
H,0,1.7231050261,5.1901406051,1.2810938206
C,0,4.3659168051,-0.2654533953,-0.2173910167
C,0,4.6721623619,-0.1630326898,1.1459246726
C,0,5.2078288876,-1.0359014139,-1.0262574117
C,0,5.7740286278,-0.8182293569,1.6893523157
H,0,4.0406216276,0.4376054385,1.7930118573
C,0,6.3171444972,-1.6886232187,-0.4869434095
H,0,5.0161826473,-1.1487329758,-2.0875724694
C,0,6.6021147205,-1.5879914597,0.8726068228
H,0,5.9842196617,-0.7260306314,-2.7505387798

H,0,6.9546702037,-2.2814501203,-1.1353128863
H,0,7.4623340249,-2.1002142318,1.2920242813

TS-7c anti-down

M06-2X/6-31+G**, $E = -1619.48659944$ a.u.
Thermal correction to Gibbs Free Energy = 0.507211 a.u.
1 imaginary frequency = -250.62 cm^{-1}
SP at B2PLYP/6-311+G**, $E = -1618.9254533923$ a.u.
SP at mPW2PLYP/6-311+G**, $E = -1618.9546097245$ a.u.

O,1
C,0,-1.4287539574,-0.5833527707,-3.4728825862
C,0,-0.478420236,0.3653677801,-3.5057904748
H,0,-0.700614724,1.3788975055,-3.8309750917
C,0,0.8595533598,0.024116303,-3.0582934281
H,0,1.017447015,-0.9692488995,-2.6562005482
N,0,1.7770078742,0.92125061,-2.808450045
C,0,1.7673319285,2.2783914679,-3.3799191881
C,0,3.0967475241,0.5165826445,-2.3011808455
C,0,3.1510542152,2.8417566069,-3.0468920079
C,0,4.0358080766,1.5984157985,-2.8458839728
H,0,0.9547540302,2.8666103474,-2.9449299042
H,0,3.1047573913,3.4395056037,-2.1341372903
H,0,1.610952508,2.1911176826,-4.4611840349
H,0,3.5211874405,3.4803263286,-3.8508233333
H,0,4.8798598263,1.7867573687,-2.177639487
H,0,4.4368299099,1.2616984903,-3.8062080396
H,0,3.296057103,-0.4635355017,-2.7400787356
C,0,3.0580793886,0.3400564974,-0.7488624556
H,0,-1.1384675088,-1.5875144463,-3.1557318409
O,0,0.5687897762,-3.0310442684,-4.5429535259
O,0,0.6961223363,-3.1321482524,-3.1133008063
H,0,1.4434312009,-3.7371378061,-3.0105206015
H,0,1.0899070402,-2.0628658986,-4.7420973062
C,0,-2.8631739968,-0.3782133948,-3.8345149322
H,0,-3.0285516444,0.6567973579,-4.1509058608
H,0,-3.099675127,-1.0250102851,-4.6889447523
O,0,1.9951408167,-0.5714100421,-0.5487246217
Si,0,1.5709052042,-1.6795859111,0.6447291798
C,0,1.5155029986,-0.9080868481,-2.3580183493
H,0,1.1971325584,0.1389908093,2.3122440861
H,0,0.7882161177,-1.4548056875,2.9689847674
H,0,2.4809936638,-0.9545948962,2.8690539406
C,0,2.7197804982,-3.1616504602,0.6181290984
H,0,3.7386685992,-2.8980975409,0.9210017556
H,0,2.3464001475,-3.9311021371,1.3033856486
H,0,2.7622248182,-3.5948693045,-3.3869184623
C,0,-0.1520682174,-2.1645966926,0.0987684832
H,0,-0.1295305662,-2.556910578,-0.92411161291
H,0,-0.5731998416,-2.9318847119,0.7569347292
H,0,-0.8192232503,-1.2951407099,0.1173329504
O,0,1.7140332611,-0.9176986824,-4.8880908425
H,0,1.3002063644,-0.4415671138,-5.6183830384
C,0,2.7154263598,1.68188255,-0.0948725307
C,0,3.7045078105,2.6004971753,0.2751855051
C,0,1.3735267305,2.0527269357,0.0376119453
C,0,3.3605852184,3.8607031347,0.7609990111
H,0,4.7540006841,2.3355458934,0.1844331787
C,0,1.0269553376,3.3138011288,0.5220091996
H,0,0.5991160695,1.3444835277,-0.2424777345
C,0,2.0195307961,4.2239664602,0.8824942363
H,0,4.1428311741,4.5582329756,1.0442161755
H,0,-0.0206039228,3.5832582504,0.6172307374
H,0,1.7509367687,5.2056722928,1.2600777715
C,0,4.3625807058,-0.2700631764,-0.2179279237
C,0,4.6535880727,-0.1766918844,1.1494566946
C,0,5.2093904224,-1.0403235592,-1.0214761907
C,0,5.74581598,-0.8403790411,1.7016597055
H,0,4.0176064077,0.4240302892,1.7922114614
C,0,6.3091046271,-1.7019844005,-0.4730822181

H,0,5.0296868086,-1.1457643321,-2.0856175611
C,0,6.5790213115,-1.6102616586,0.8900637168
H,0,5.9446817528,-0.7549761304,2.7655808092
H,0,6.9508410232,-2.2945804314,-1.1174923339
H,0,7.431659531,-2.1293151558,1.3164952201
C,0,-3.7881532992,-0.74010884,-2.6649548552
H,0,-3.6336635999,-1.77816528,-2.3552974514
H,0,-3.5921379018,-0.0965719804,-1.8024057557
H,0,-4.8360266511,-0.6218669257,-2.951352883

TS-7a syn-up

M06-2X/6-31+G**, $E = -1580.18342655$ a.u.
Thermal correction to Gibbs Free Energy = 0.485729 a.u.
1 imaginary frequency = -236.97 cm^{-1}
SP at B2PLYP/6-311+G**, $E = -1579.6343111970$ a.u.
SP at mPW2PLYP/6-311+G**, $E = -1579.6627034953$ a.u.

O,1
C,0,-0.728363111,0.2965646404,-1.277697026
C,0,0.4920389533,0.2103663543,-1.8297870486
H,0,1.381057185,0.1667807855,-1.2099182382
C,0,0.6253287336,0.2289167979,-3.2704722887
H,0,-0.2815058788,0.2515990851,-3.8632438055
N,0,1.7201800953,-0.0585804763,-3.920575304
C,0,1.7031088703,-0.250622556,-5.3862931392
C,0,3.0235782406,-0.3866690223,-3.3211857957
C,0,3.0298857478,-0.9540383239,-5.7059817604
C,0,3.605346918,-1.3776089303,-4.3396209531
H,0,1.6110345433,0.7244199546,-5.8712854195
H,0,3.7058264798,-0.2673696584,-6.218724834
H,0,0.8310242801,-0.8578884236,-5.6394849197
H,0,2.8717494812,-1.8175992669,-6.3539826888
H,0,4.6976695544,-1.3798839307,-4.3297024328
H,0,3.2662277677,-2.3845483363,-4.079970738
H,0,2.8143131911,-0.8639639318,-2.363594018
C,0,3.9059368035,0.8688186878,-3.0235651655
H,0,-1.5945362475,0.3948887057,-1.9311945554
O,0,-1.6035238024,2.8568380032,-2.1690351573
O,0,-1.6505670981,4.2858757068,-2.0056802516
H,0,-2.2843645609,4.5516389012,-2.684696644
H,0,-0.694374837,2.7133530459,-2.8424692844
C,0,-0.9876195002,0.33345755,0.1884481488
H,0,-0.0662179357,0.225409337,0.7658047512
H,0,-1.456606043,1.291558927,0.4393667198
H,0,-1.6898504986,-0.4538515079,0.4804689372
O,0,3.0577507423,1.7542227555,-2.3085772204
Si,0,3.2112552467,2.6791043404,-0.8986847334
C,0,4.4595303372,4.0740838353,-1.14914262796
H,0,4.5389688778,4.3806125691,-2.1405652562
H,0,4.1100929857,4.9403820537,-0.5187131359
H,0,5.4560337659,3.808834908,-0.7294368223
C,0,3.6359388129,1.6053600141,0.5826170666
H,0,4.6770543499,1.2677793591,0.5628553831
H,0,3.4836667884,2.1895791611,1.4975295953
H,0,2.9915436867,0.7210416949,0.6409195396
C,0,1.5203284363,3.4508894295,-0.6878263964
H,0,0.6947128849,2.7334294312,-0.7354854591
H,0,1.4851921423,3.9574922327,0.2839588518
H,0,1.3326882703,4.2077821617,-1.4574974933
O,0,0.3007706739,2.4877406823,-3.6216103285
C,0,4.3338803298,1.5395839453,-4.3353881197
C,0,5.5308502072,1.2068798258,-4.9819899281
C,0,3.4644622466,2.4423287407,-4.9542128512
C,0,5.847427254,1.7591229094,-6.2216271309
H,0,6.2260299202,0.5119202414,-4.5198931979
C,0,3.780428442,2.9943182366,-6.195432909
H,0,2.5200333137,2.6916307805,-4.4802489087
C,0,4.9711243634,2.6544351218,-6.8353167125
H,0,6.7806466936,1.4894007342,-6.7064859937
H,0,3.0885062125,3.689330198,-6.6615401179
H,0,5.2171019565,3.0854501937,-7.8009268236

C,0,5.1191317704,0.4732749893,-2.1655812875
C,0,6.1329776548,1.422747027,-1.9791712814
C,0,5.2264267053,-0.7444574287,-1.4869888409
C,0,7.1961227257,1.1844397069,-1.1140054465
H,0,6.0865197978,2.3641789443,-2.518492345
C,0,6.2974213473,-0.9930971327,-0.6264525442
H,0,4.4860637196,-1.5272230425,-1.6074176598
C,0,7.2796650292,-0.02725247,-0.4269696191
H,0,7.9601452909,1.9438845043,-0.9792592687
H,0,6.3556148164,-1.9457916346,-0.1095149282
H,0,8.1066014762,-0.2185230727,0.2495123365
H,0,1.0939742067,2.6820967032,-3.1071091881

TS-7a anti-up

M06-2X/6-31+G**, $E = -1580.18096395$ a.u.

Thermal correction to Gibbs Free Energy = 0.486444 a.u.

1 imaginary frequency = -225.15 cm^{-1}

SP at B2PLYP/6-311+G**, $E = -1579.6343368585$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1579.6627133634$ a.u.

0,1
C,0,-1.3670546425,0.0345725666,-4.2847657035
C,0,-0.6076245557,0.9168336638,-3.6197459677
H,0,-0.7498809229,1.9860074148,-3.7528773314
C,0,0.4407998932,0.4433219368,-2.7241371553
H,0,0.4690117198,-0.6133358387,-2.4750587012
N,0,1.5276051527,1.140112537,-2.5040620762
C,0,1.6792453392,2.5378908247,-2.9595310632
C,0,2.8042758135,0.5503664992,-2.0370248997
C,0,3.1679122666,2.8548112844,-2.7963420156
C,0,3.8513796214,1.4831257305,-2.6619003566
H,0,1.0361578293,3.1881165489,-2.3591628944
H,0,3.3295923782,3.461695222,-1.905601909
H,0,1.3691372192,2.5951892381,-4.0061327767
H,0,3.5461830695,3.4096060913,-3.6566646551
H,0,4.7629447309,1.5279181852,-2.0614400155
H,0,4.1233579465,1.0972842773,-3.6486069873
H,0,2.8430133687,-0.4524281165,-2.4642169289
C,0,2.9023078295,0.3768418445,-0.490200057
H,0,-1.2145809489,-1.0267182409,-4.0951859153
O,0,-2.2050990354,-1.4456535354,-1.6843117509
O,0,-1.1251059339,-2.2564241772,-2.1762075797
H,0,-0.8928120491,-2.783155493,-1.3987001546
H,0,-1.6696260351,-0.5286904679,-1.3624318955
C,0,-2.440438405,0.4077872628,-5.2531085791
H,0,-2.524378837,1.4907235076,-5.3702664352
H,0,-2.2492108901,-0.0409463484,-6.2332945624
H,0,-3.4022500272,0.0131859442,-4.9076975627
O,0,1.8559950253,-0.5326798173,-0.1884349663
Si,0,1.5440357768,-1.3795006051,1.2398701945
C,0,1.523328321,-0.24908099,2.7400544976
H,0,0.6980989669,0.4664722065,2.6725267759
H,0,1.3744819013,-0.8616943872,3.6370436321
H,0,2.4503131653,0.316900297,2.8678193368
C,0,2.7668896581,-2.7861660242,1.4832759008
H,0,3.7673424881,-2.4536098642,1.7723332689
H,0,2.3853649662,-3.4516954532,2.266790064
H,0,2.8536132303,-3.3710203494,0.560891911
C,0,-0.1542418244,-2.1230981983,0.9896338685
H,0,-0.0802973074,-3.0814545055,0.4623283069
H,0,-0.6193200758,-2.3252123737,1.9606911771
H,0,-0.7949570699,-1.4334626581,0.4306479344
O,0,-0.9729727222,0.5346659774,-0.9756440177
H,0,-1.5183701467,1.3033414906,-1.1890098683
C,0,2.6598484718,1.7356486035,0.1757863732
C,0,3.6896929349,2.645604058,0.4457324556
C,0,1.3371267166,2.1247623162,0.4092015335
C,0,3.4051206859,3.9089704578,0.9624764215
H,0,4.7238483414,2.3824263154,0.2434962978
C,0,1.0539982156,3.3907641665,0.9218067474

H,0,0.5311489897,1.4354105983,0.1572854586
C,0,2.0845674892,4.2862112662,1.2055892682
H,0,4.2177298621,4.5986763814,1.1696223539
H,0,0.0206281203,3.6766709856,1.0977941232
H,0,1.8635641296,5.269782204,1.6092960936
C,0,4.2473428859,-0.276616263,-0.1125947877
C,0,4.8483591763,-0.0468567273,1.1314336998
C,0,4.8255709102,-1.2444749517,-0.944422273
C,0,5.9933082669,-0.740987567,1.5218683859
H,0,4.4198526348,0.6738153506,1.8186900284
C,0,5.9695582063,-1.9404234338,-0.5594979223
H,0,4.3873009141,-1.4856049821,-1.9063987969
C,0,6.5622680164,-1.690468435,0.6767648094
H,0,6.4333085149,-0.5411535115,2.4941005064
H,0,6.3926892167,-2.6830021919,-1.2288037645
H,0,7.4522334351,-2.233531409,0.9787261848

TS-7a syn-down

M06-2X/6-31+G**, $E = -1580.18762406$ a.u.

Thermal correction to Gibbs Free Energy = 0.481935 a.u.

1 imaginary frequency = -264.44 cm^{-1}

SP at B2PLYP/6-311+G**, $E = -1579.6432932437$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1579.6713069120$ a.u.

0,1
C,0,-0.7523539238,0.7845948,-0.9519088856
C,0,0.3814550489,0.3839347778,-1.5441579855
H,0,1.2725742405,0.1739812315,-0.9615913242
C,0,0.4185089238,0.2476675343,-2.9916005133
H,0,-0.4869659457,0.4907727492,-3.5422941143
N,0,1.4979302974,0.1234993032,-3.7175798424
C,0,1.3505384855,-0.0718256598,-5.1798338705
C,0,2.7895463929,-0.363226679,-3.2088281483
C,0,2.612955013,-0.8270874284,-5.6115356109
C,0,3.2437590098,-1.3390315042,-4.3025283215
H,0,2.5829477434,-0.8824772581,-2.2727324302
C,0,3.7690685502,0.8073916355,-2.8853030978
H,0,-1.6198038242,0.9999042538,-1.577159287
O,0,-1.7258163389,-1.6085688386,-5.0760214387
O,0,-2.0566039792,-0.2112996529,-4.9753683587
H,0,-2.9780422156,-0.237666381,-4.6848703941
H,0,-1.1067212268,-1.7545295774,-4.1598518651
C,0,-0.9229128347,0.9605974557,0.5211071291
H,0,-0.0070052826,0.7146180426,1.0642987415
H,0,-1.2063628646,1.99291787,0.7540743372
H,0,-1.7323740413,0.3208472888,0.8884367462
O,0,3.0377609799,1.6325939534,-1.9956855514
Si,0,3.4742252273,2.6869646171,-0.7551188127
C,0,4.7204602721,3.9836851239,-1.312056601
H,0,4.6808311258,4.13159329,-2.3968623207
H,0,4.4810869871,4.9401656745,-0.834613961
H,0,5.7449567936,3.7181678592,-1.0369627916
C,0,4.1000941206,1.7348444111,0.7341292473
H,0,5.0703557744,1.2630840227,0.5475909874
H,0,4.2073100664,2.4143691193,1.5872940447
H,0,3.3861889256,0.9519727264,1.014515206
C,0,1.848281878,3.5194296784,-0.3466723014
H,0,1.1126756033,2.7918358395,0.008316068
H,0,1.9909840177,4.2736573057,0.4344125963
H,0,1.4344445214,4.0156417249,-1.2309637163
O,0,-0.3031569125,-1.8460227464,-3.126286216
H,0,-0.8071078093,-2.0205569543,-2.322782239
C,0,4.0867788595,1.5901913348,-4.1633764395
C,0,5.1528667597,1.2366691258,-4.9992058286
C,0,3.2473585849,2.6372215249,-4.5540978882
C,0,5.3710081726,1.9092147489,-6.1994034502
H,0,5.823566769,0.4309154534,-4.7148844775
C,0,3.4629982738,3.3116356586,-5.7564497182
H,0,2.4203829899,2.9196467029,-3.909139134
C,0,4.5237288677,2.9481113632,-6.5847647188

H,0,6.2045907343,1.6207911267,-6.8321438081
H,0,2.800159748,4.1219908005,-6.0443260502
H,0,4.6929115664,3.4726954244,-7.519902003
C,0,5.0371928402,0.2858776149,-2.1878462587
C,0,6.1675695943,1.1120229387,-2.1263302055
C,0,5.0746747222,-0.929448844,-1.4964530768
C,0,7.2877714631,0.7515646524,-1.3823566955
H,0,6.173893744,2.0537070041,-2.6659271621
C,0,6.1989160001,-1.2991127293,-0.7559916399
H,0,4.2342245557,-1.6141952175,-1.5163061439
C,0,7.3066452169,-0.4579201674,-0.6885959709
H,0,8.1457220498,1.4159486497,-1.3479406196
H,0,6.2015250345,-2.2480086144,-0.2288554724
H,0,8.1776753515,-0.743779755,-0.1075578088
H,0,4.3327286777,-1.4112914777,-4.3599382229
H,0,2.8535608825,-2.3310462013,-4.0608785269
H,0,3.2944752285,-0.1602686419,-6.1422740434
H,0,2.3626973411,-1.6533332506,-6.2792642649
H,0,1.2542696665,0.9014091156,-5.6680345229
H,0,0.4382955065,-0.6526499493,-5.3414779532

TS-7c *syn-down*

M06-2X/6-31+G**, $E = -1619.48276064$ a.u.

Thermal correction to Gibbs Free Energy = 0.508544 a.u.

1 imaginary frequency = -261.73 cm^{-1}

SP at B2PLYP/6-311+G**, $E = -1618.9209134502$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1618.9498072892$ a.u.

0,1
C,0,-0.7487982125,0.7955865459,-0.9484191888
C,0,0.3825175473,0.3963088538,-1.5460932373
H,0,1.2748608178,0.1843127831,-0.9661106587
C,0,0.4167626212,0.2617370263,-2.9939491201
H,0,-0.4886860591,0.5070669914,-3.5436972655
N,0,1.4945147703,0.1310026525,-3.7207113603
C,0,1.3450148977,-0.067542747,-5.1824854079
C,0,2.7848595553,-0.3592523242,-3.2116147782
C,0,2.6097457372,-0.8181208693,-5.6146448167
C,0,3.2367036981,-1.3352830271,-4.305968122
H,0,2.5759707397,-0.8790471385,-2.2764333644
C,0,3.7674397741,0.8086895121,-2.8868325519
H,0,-1.6230482167,1.0094502103,-1.5671546236
O,0,-1.7335216165,-1.5904849087,-5.0747493707
O,0,-2.0558323868,-0.1908046117,-4.9794029531
H,0,-2.9786994221,-0.2105245809,-4.6928973352
H,0,-1.1176040122,-1.7376646378,-4.1560523482
C,0,-0.9252907543,0.9419170653,0.5295590128
H,0,0.0251478535,0.7446140197,1.037620409
H,0,-1.2078201258,1.9785275322,0.7540597429
O,0,3.0357086761,1.6391844091,-2.0025408212
Si,0,3.4704764246,2.6989424749,-0.7659001261
C,0,4.7244503658,3.9875782407,-1.3241786699
H,0,4.6889320219,4.1314860537,-2.4096610223
H,0,4.4879618077,4.9470126591,-0.8512374472
H,0,5.7468263518,3.7185688066,-1.0446907089
C,0,4.0860500294,1.7525960235,0.7312746668
H,0,5.0559604803,1.2773423647,0.551953519
H,0,4.1909872696,2.4362887208,1.5813924553
H,0,3.3686632403,0.9731413343,1.0123406203
C,0,1.8466556873,3.5413309927,-0.368829198
H,0,1.1060741984,2.8199428739,-0.0113568761
H,0,1.9907611085,4.3000431081,0.4076695576
H,0,1.4383041797,4.0339108189,-1.257697843
O,0,-0.3173375158,-1.8312405991,-3.120869903
H,0,-0.8251481647,-1.9949444369,-2.3173546716
C,0,4.0928932431,1.5867773382,-4.165832195
C,0,5.1626048245,1.2300880846,-4.995662277
C,0,3.2552331533,2.6323972576,-4.5640761874
C,0,5.3861021102,1.8985640667,-6.1971996127
H,0,5.8317623976,0.4250188401,-4.7058487603

C,0,3.4760611471,3.3024726447,-5.7678563519
H,0,2.4254024217,2.9170691012,-3.9237936246
C,0,4.5405393014,2.9360550136,-6.5900764367
H,0,6.2224494646,1.6079225912,-6.825259438
H,0,2.8143954718,4.1116566622,-6.0616417567
H,0,4.7138667762,3.4572551525,-7.5263393766
C,0,5.0305163335,0.2843236424,-2.1822388881
C,0,6.1638720428,1.1063077411,-2.1187984774
C,0,5.0601140688,-0.928274761,-1.4856679385
C,0,7.2792477495,0.7445057216,-1.3682958876
H,0,6.1761123002,2.0461010799,-2.6615702257
C,0,6.179532849,-1.2992795955,-0.7385404947
H,0,4.2170933445,-1.6097953115,-1.5061970045
C,0,7.2902772585,-0.46220402,-0.669566674
H,0,8.1395826102,1.4057313102,-1.3326458066
H,0,6.1758625531,-2.2459242682,-0.2073923017
H,0,8.1575516319,-0.7490563808,-0.0834240758
H,0,4.3254426303,-1.4123357201,-4.3616983568
H,0,2.8412303352,-2.3258494238,-4.0667243918
H,0,3.2919037044,-0.1472212023,-6.1393671505
H,0,2.363027484,-1.641218334,-6.287557198
H,0,1.2431112258,0.9043510753,-5.6721696342
H,0,0.4350198274,-0.6529226144,-5.3407849031
C,0,-2.0163440811,0.0002670215,1.0563128197
H,0,-2.1566148697,0.1370774036,2.1313690515
H,0,-2.9720564252,0.1953979539,0.5607090262
H,0,-1.7464678417,-1.0437655931,0.8737394548

6a *trans*

M06-2X/6-31+G**, $E = -1580.19778703$ a.u.

Thermal correction to Gibbs Free Energy = 0.483830 a.u.

SP at B2PLYP/6-311+G**, $E = -1579.6547949296$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1579.6834777405$ a.u.

0,1
C,0,-1.4811139696,-0.4893996634,-3.5544634466
C,0,-0.6204147838,0.5417756112,-3.4152454319
H,0,-0.9148162843,1.5667960463,-3.6251545318
C,0,0.710173212,0.2271139038,-2.9722629861
H,0,0.9378551045,-0.8165033916,-2.7390252064
N,0,1.6637078491,1.0933303397,-2.8355470854
C,0,1.5752014685,2.5183938439,-3.2199827881
C,0,3.0078594381,0.7015719336,-2.3632985408
C,0,2.9820625412,3.075771259,-2.9718097102
C,0,3.8959995298,1.837938406,-2.8736874702
H,0,0.8095574184,3.0130004229,-2.6163774209
H,0,2.9976030469,3.6505589521,-2.0441055521
H,0,1.2861275479,2.5644616215,-4.2735511783
H,0,3.287278028,3.7379409711,-3.783578912
H,0,4.7580074979,2.0052505503,-2.2238604043
H,0,4.2748833858,1.5674189184,-3.8634187682
H,0,3.220577823,-0.249626946,-2.8513806613
C,0,2.9907001078,0.448404339,-0.8137692094
H,0,-1.0993831075,-1.490996937,-3.3345853345
O,0,0.7772764396,-2.7707806845,-3.2502606339
O,0,1.0204989709,-4.0048458467,-2.5284314765
H,0,0.7182618324,-4.670937565,-3.158295097
H,0,2.0838036423,-2.3939711806,-3.6410119124
C,0,-2.8939483688,-0.3558559879,-4.0002455614
H,0,-3.1673844369,0.6816541621,-4.2015660914
H,0,-3.0552739323,-0.953034856,-4.9042803718
H,0,-3.5648260325,-0.7646707945,-3.2370080578
O,0,1.9022153688,-0.4265104541,-0.6284810984
Si,0,1.5146666622,-1.6378986773,0.4804610101
C,0,1.5128882772,-0.9564905191,2.232619001
H,0,0.9855839081,0.0022153991,2.2814543261
H,0,0.9959055695,-1.6614541882,2.8939072947
H,0,2.5239013169,-0.8131414617,2.6244084944
C,0,2.6676309419,-3.1023377921,0.3283557298
H,0,3.6673899387,-2.8932006168,0.7227650875

H,0,2.247874574,-3.9517801312,0.8802115994
H,0,2.7465568356,-3.3913206772,-0.7256728351
C,0,-0.2151517841,-2.0825046557,-0.0658857013
H,0,-0.1651380009,-2.4408453756,-1.1018432002
H,0,-0.6408574832,-2.8719742368,0.5626808766
H,0,-0.8745012493,-1.2081878647,-0.0159465375
O,0,3.0486866098,-2.0275629666,-3.9051876265
H,0,3.312039087,-2.4815259776,-4.7120102563
C,0,2.7100340372,1.76861838,-0.0893484338
C,0,3.7281070242,2.6665168546,0.2557770795
C,0,1.3820643154,2.1493895839,0.1292731178
C,0,3.4251391077,3.9129925994,0.7994372831
H,0,4.7682509366,2.3966981875,0.0983462097
C,0,1.0759864905,3.3991224973,0.6680667358
H,0,0.5848977548,1.4579974641,-0.1293313585
C,0,2.0966035966,4.2871039024,1.0029329868
H,0,4.2297798942,4.5930393255,1.0614934317
H,0,0.0381173115,3.6757757326,0.8273777755
H,0,1.8613093034,5.2594285805,1.4244663814
C,0,4.2907624403,-0.2436696577,-0.3751271522
C,0,4.7384303341,-0.1263038342,0.9470948459
C,0,4.9589885903,-1.1350694823,-1.2246863483
C,0,5.8317330865,-0.8590293988,1.4054843364
H,0,4.225915972,0.5385788573,1.6351222682
C,0,6.0611614839,-1.8586465858,-0.7694828918
H,0,4.6072766054,-1.3223028273,-2.2351287317
C,0,6.5042287424,-1.724381925,0.5443439643
H,0,6.1546950873,-0.7520884761,2.4365319726
H,0,6.5613225831,-2.5453569199,-1.4456319878
H,0,7.3581227616,-2.2951260909,0.8961891923

6c trans

M06-2X/6-31+G**, $E = -1619.49255105$ a.u.

Thermal correction to Gibbs Free Energy = 0.509953 a.u.

SP at B2PLYP/6-311+G**, $E = -1618.9321211529$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1618.9616804057$ a.u.

0,1
C,0,-1.47651,-0.485001,-3.550893
C,0,-0.612173,0.544201,-3.421042
H,0,-0.905247,1.569193,-3.633309
C,0,0.71894,0.229109,-2.978576
H,0,0.946467,-0.814713,-2.746277
N,0,1.671933,1.095414,-2.839697
C,0,1.583562,2.521166,-3.221783
C,0,3.014956,0.703754,-2.364295
C,0,2.989876,3.078632,-2.970453
C,0,3.904044,1.841039,-2.870908
H,0,0.816862,3.014392,-2.618392
H,0,3.003341,3.653056,-2.042503
H,0,1.296043,2.568966,-4.275681
H,0,3.296641,3.741224,-3.781288
H,0,4.763941,2.008089,-2.218228
H,0,4.286112,1.571729,-3.859738
H,0,3.229169,-0.247025,-2.852626
C,0,2.993257,0.449293,-0.81491
H,0,-1.096482,-1.489075,-3.333118
O,0,0.786245,-2.770039,-3.256566
O,0,1.028518,-4.005671,-2.537039
H,0,0.725806,-4.670209,-3.168311
H,0,2.09266,-2.392201,-3.644153
C,0,-2.891585,-0.357487,-4.000804
H,0,-3.139268,0.691862,-4.188606
H,0,-3.53875,-0.710188,-3.187254
O,0,1.904582,-0.426105,-0.633453
Si,0,1.513571,-1.638143,0.47354
C,0,1.506123,-0.957856,2.226163
H,0,0.980672,0.001945,2.273471
H,0,0.984711,-1.662145,2.884691
H,0,2.515723,-0.816985,2.622474

C,0,2.666837,-3.102641,0.324147
H,0,3.665692,-2.893854,0.721033
H,0,2.245521,-3.952019,0.874926
H,0,2.748198,-3.391708,-0.729663
C,0,-0.214445,-2.082579,-0.078503
H,0,-0.160713,-2.440983,-1.114262
H,0,-0.642352,-2.871989,0.548655
H,0,-0.874034,-1.208288,-0.031103
O,0,3.058335,-2.024896,-3.905652
H,0,3.319288,-2.470642,-4.717797
C,0,2.710066,1.768777,-0.090048
C,0,3.726871,2.666509,0.259176
C,0,1.38136,2.148804,0.125497
C,0,3.421983,3.912102,0.803773
H,0,4.767532,2.397162,0.104399
C,0,1.07338,3.397644,0.665194
H,0,0.585128,1.457527,-0.136395
C,0,2.092772,4.285464,1.004165
H,0,4.225667,4.592,1.069136
H,0,0.034983,3.673708,0.822064
H,0,1.85597,5.257062,1.42653
C,0,4.292213,-0.242729,-0.372919
C,0,4.735301,-0.126697,0.950957
C,0,4.963728,-1.132835,-1.221229
C,0,5.827303,-0.859487,1.412276
H,0,4.220139,0.537174,1.637976
C,0,6.064659,-1.856447,-0.763056
H,0,4.615616,-1.319055,-2.233109
C,0,6.503129,-1.72355,0.552445
H,0,6.146591,-0.753662,2.444584
H,0,6.567517,-2.542109,-1.438268
H,0,7.356025,-2.294371,0.906589
C,0,-3.157916,-1.210834,-5.249279
H,0,-2.929039,-2.262793,-5.057326
H,0,-4.207739,-1.136565,-5.542166
H,0,-2.541727,-0.875821,-6.087825

6a cis

M06-2X/6-31+G**, $E = -1580.19519936$ a.u.

Thermal correction to Gibbs Free Energy = 0.481493 a.u.

SP at B2PLYP/6-311+G**, $E = -1579.6502660323$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1579.6786955979$ a.u.

0,1
C,0,2.9275773146,1.6325159461,2.764636266
C,0,1.6388829929,1.6031529513,2.3682123181
H,0,0.8859548466,2.2545581816,2.7964177551
C,0,1.3038856347,0.6646761471,1.3319549499
H,0,2.103962962,0.0216029118,0.9648714642
N,0,0.158494628,0.5231617861,0.7463584134
C,0,0.0047942637,-0.3272480246,-0.4514704349
C,0,-1.0595498389,1.3360398745,0.9590356143
C,0,-0.7819202984,0.5982430972,-1.3718059617
H,0,0.9965514785,-0.5972606325,-0.8139860077
H,0,-0.5656389559,-1.2208683631,-0.1751973936
C,0,-1.7518835531,1.3238060073,-0.4204234799
H,0,-0.728202071,2.3369182023,1.2425159137
H,0,-0.0812435236,1.3048570543,-1.8241491619
H,0,-1.3025812107,0.0534719296,-2.1611475896
H,0,-1.9688726299,2.3410516998,-0.7512804319
H,0,-2.7043284621,0.7936898623,-0.3629162063
C,0,3.4661735142,2.5510418664,3.8049125259
H,0,3.8523866303,1.9687317565,4.6495136866
H,0,4.3130158359,3.1176259336,3.4040578505
H,0,2.7092125374,3.2475748255,4.1709695656
H,0,3.6214313032,0.9439806414,2.2759426492
O,0,4.0932119847,-0.048422336,0.1676874835
O,0,3.3803641166,-1.3074041771,-0.0101883857
H,0,3.6786195541,-1.6008432684,-0.8800769738
H,0,3.2431303437,0.8370961049,-0.5965921306

O,0,2.5344712212,1.4352742737,-1.0980871799
H,0,2.9255511588,1.6794668515,-1.9428805643
C,0,-1.9037215642,0.7743455222,2.154855899
O,0,-1.0999952977,1.0502952994,3.2866507703
C,0,-2.0631671031,-0.7408746192,1.98422271
C,0,-3.0495292689,-1.2993634111,1.1610826377
C,0,-1.1174415078,-1.5945789009,2.5615059282
C,0,-3.0807143212,-2.6708757065,0.9127943105
C,0,-1.146513155,-2.9663007333,2.315092759
C,0,-2.1251413975,-3.5097294251,1.484280098
H,0,-3.8120728119,-0.66882362,0.7145253626
H,0,-0.3429227739,-1.1785990156,3.1981859061
H,0,-3.8545190394,-3.0810116112,0.2714866466
H,0,-0.3977894726,-3.608349291,2.7686769184
H,0,-2.1461345985,-4.57692034,1.2876175045
C,0,-3.2336821912,1.5310416833,2.2763165649
C,0,-3.3010334821,2.8975597974,1.9782671788
C,0,-4.3651504598,0.918211719,2.8261202241
C,0,-4.4645787583,3.6266644071,2.2132258933
C,0,-5.5297926701,1.6456588354,3.0679787386
C,0,-5.5848440736,3.0036119915,2.7613527358
H,0,-2.4404662172,3.4186527326,1.5707482113
H,0,-4.3445584654,-0.1375209333,3.0755236449
H,0,-4.4910070112,4.6847443663,1.9724810817
H,0,-6.3923114736,1.1470887768,3.4991209631
H,0,-6.4907406826,3.5711159997,2.9493445267
Si,0,-1.4593286436,1.1538323339,4.9353783932
C,0,-2.4853904576,2.6754949832,5.3182629469
H,0,-3.5180142593,2.5819898673,4.9680975949
H,0,-2.5029071562,2.8339671425,6.4025418714
H,0,-2.0462534399,3.5638566274,4.8521818174
C,0,-2.3068314062,-0.3930622337,5.5720542053
H,0,-3.2605761875,-0.5858502219,5.0729552394
H,0,-1.672077743,-1.275508861,5.4462533552
H,0,-2.5089608623,-0.2680204243,6.6420809618
C,0,0.2440757607,1.3195594241,5.6935114301
H,0,0.1864149645,1.2729750221,6.7860056013
H,0,0.9035436697,0.516488959,5.3475499353
H,0,0.7010627727,2.2762144161,5.4196215566

6c cis

M06-2X/6-31+G**, $E = -1619.49005544$ a.u.

Thermal correction to Gibbs Free Energy = 0.508250 a.u.

SP at B2PLYP/6-311+G**, $E = -1618.9276557912$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1618.9569696394$ a.u.

0,1
C,0,2.9238583018,1.6399512259,2.7675861351
C,0,1.636510192,1.6043910983,2.3680632954
H,0,0.8817175022,2.2572079119,2.7908961818
C,0,1.3043026661,0.6598655251,1.3357660514
H,0,2.1062208344,0.0169656334,0.9722251568
N,0,0.1598526473,0.5159551056,0.7491679956
C,0,0.0074220258,-0.3360750079,-0.4477183779
C,0,-1.0581258729,1.3295538338,0.9589688139
C,0,-0.7771882842,0.5889544968,-1.3705109312
H,0,0.9995841343,-0.6079326648,-0.8078358397
H,0,-0.5643351096,-1.2287254127,-0.1710806091
C,0,-1.7478074754,1.3172386453,-0.4216942579
H,0,-0.7267025412,2.3303518247,1.2423033363
H,0,-0.0751486267,1.2941114377,-1.8229595007
H,0,-1.2973306257,0.0434092219,-2.1596587484
H,0,-1.9619582764,2.3346317713,-0.7539762566
H,0,-2.7013979299,0.7891398148,-0.3655551541
C,0,3.4659527039,2.5772969591,3.7931901096
H,0,3.8031872071,1.9826964399,4.6530338405
H,0,2.6762349396,3.246504349,4.1494549435
H,0,3.62445407,0.9528276895,2.2835816475
O,0,4.0887051718,-0.0551773694,0.1727935755
O,0,3.3768328599,-1.3129435624,-0.0179201578

H,0,3.6813289974,-1.6010258161,-0.8874320556
H,0,3.2418205347,0.8347375047,-0.590239839
O,0,2.5349958397,1.4348905794,-1.0919948277
H,0,2.9324893474,1.6883282346,-1.931057413
C,0,-1.9038903991,0.7687798363,2.1538942322
O,0,-1.0980398681,1.0386114339,3.2855523594
C,0,-2.0701564084,-0.7454100503,1.9805152435
C,0,-3.0594024602,-1.2979777887,1.1568500737
C,0,-1.1283912902,-1.6044548252,2.5563921628
C,0,-3.0969253173,-2.6688918027,0.9062072133
C,0,-1.1639779475,-2.9756400981,2.30782255
C,0,-2.1451490342,-3.5131255665,1.4761790418
H,0,-3.8193292821,-0.6631249881,0.7119142198
H,0,-0.3518123255,-1.1932300039,3.1935964004
H,0,-3.8727690133,-3.0743825313,0.2644100532
H,0,-0.4182952075,-3.6219759065,2.7603118984
H,0,-2.1711497134,-4.5798796451,1.2777460931
C,0,-3.2304330377,1.5310283754,2.2778187439
C,0,-3.2931162879,2.8978962109,1.9804456378
C,0,-4.3631449283,0.922322208,2.8297134755
C,0,-4.4531887056,3.631524481,2.2186417704
C,0,-5.5242696979,1.6542795935,3.0747729688
C,0,-5.5745474148,3.0126862595,2.7692456539
H,0,-2.4316261661,3.4158506909,1.5709631697
H,0,-4.3461916909,-0.1337092825,3.0781983541
H,0,-4.4759716514,4.6898250736,1.9784984373
H,0,-6.3877881028,1.158908752,3.5075838714
H,0,-6.4776292073,3.5837596213,2.9599441589
Si,0,-1.4545473774,1.1429546957,4.9347900858
C,0,-2.4701474284,2.6711605447,5.31977735
H,0,-3.5035462553,2.5851715322,4.9699007607
H,0,-2.4861036587,2.8286633846,6.4042240464
H,0,-2.0250491717,3.5570035217,4.8544993816
C,0,-2.3110248303,-0.3988225494,5.5717720542
H,0,-3.2692823742,-0.582572014,5.0779605799
H,0,-1.6841079006,-1.2860164941,5.4401968342
H,0,-2.5059126409,-0.2748821115,6.6432884748
C,0,0.2506627977,1.296914591,5.6912638357
H,0,0.1936126858,1.2505281128,6.7838196959
H,0,0.9043601499,0.4894127849,5.3446733189
H,0,0.7141869191,2.2503133584,5.4169512864
C,0,4.6518335992,3.3833242551,3.2469152791
H,0,5.0553268413,4.0405872479,4.020762773
H,0,5.452185631,2.7183830721,2.9100579212
H,0,4.3432359377,3.9993805512,2.3980234249

Cartesian coordinates and computed total energies for the structures presents in Scheme 7.

TS-8 trans-down

M06-2X/6-31+G**, $E = -1504.17871301$ a.u.

Thermal correction to Gibbs Free Energy = 0.474552 a.u.

1 imaginary frequency = -671.82 cm⁻¹

SP at B2PLYP/6-311+G**, $E = -1503.6801172989$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1503.7019941568$ a.u.

0,1
C,0,-0.8589708123,-1.2224579258,-3.5525378614
C,0,0.2495840224,-0.2729902068,-3.687246596
H,0,0.039930406,0.6984913594,-4.1201671619
C,0,1.554098024,-0.6281188908,-3.2604515797
H,0,1.7215227374,-1.5827619732,-2.7663109553
N,0,2.594104528,0.1493717207,-3.3782245728
C,0,2.5825154245,1.4609204858,-4.0547131676
C,0,3.8979600235,-0.1626776795,-2.7663619335
C,0,4.0594581859,1.8683169621,-4.1706214688
C,0,4.8813980992,0.7255792652,-3.5339978453
H,0,2.0013018501,2.1632716075,-3.4468947666
H,0,4.2254642692,2.8128497955,-3.6525013602

H,0,2.0963133627,1.3406960536,-5.0258446672
H,0,4.336303355,2.0080870134,-5.2160263374
H,0,5.6689417061,1.1005613848,-2.878172008
H,0,5.3642387039,0.1258781443,-4.3083291001
H,0,4.0809473062,-1.2268512377,-2.926463393
C,0,3.8028526612,0.0381382308,-1.210671152
H,0,-0.6740136974,-2.0763518867,-2.8995302927
O,0,-0.4947598887,-1.5688448352,-4.9320151311
O,0,-1.4162116507,-3.1506955303,-5.6051497849
H,0,-1.7886681998,-2.7096299144,-6.3825908058
H,0,0.1086200063,-2.3407710051,-4.9733140955
C,0,-2.268324437,-0.7084451292,-3.5171303179
H,0,-2.3991567763,0.1067835493,-4.2323909204
H,0,-2.9568579814,-1.5194753025,-3.758928794
H,0,-2.4847393027,-0.3403951432,-2.5118312373
C,0,3.2142015397,1.4223416115,-0.9200985535
C,0,1.8447123145,1.5635941867,-0.6755996208
C,0,4.0048294596,2.5755526831,-0.9919977453
C,0,1.2766886834,2.826615862,-0.5073377275
C,0,3.4389138492,3.8384043462,-0.8294473776
C,0,2.0712972635,3.9687095866,-0.5880863961
H,0,1.2173561092,0.6792045392,-0.621482427
H,0,5.0743966944,2.4921011528,-1.1652876529
H,0,0.2121064501,2.9148734244,-0.313947852
H,0,4.0698331498,4.7198522252,-0.8845673678
H,0,1.6310214892,4.9519114908,-0.4566729553
C,0,5.1671963581,-0.1990313742,-0.5514244936
C,0,5.4812572697,0.42355187,0.6611943059
C,0,6.0630443074,-1.1446153064,-1.0654839179
C,0,6.6536502454,0.1079908537,1.3463845087
C,0,7.2402105925,-1.4551943702,-0.3876566789
C,0,7.5381138767,-0.8332689696,0.8238794328
H,0,4.8064498316,1.1611573856,1.0827685765
H,0,5.8552582711,-1.6637937295,-1.9958924112
H,0,6.8718801683,0.6004403664,2.2886387996
H,0,7.9208773849,-2.1900647886,-0.8054184773
H,0,8.4519152799,-1.0797765704,1.3548169907
O,0,2.8924658012,-0.9705279083,-0.818022331
Si,0,2.6270735058,-1.7660944856,0.6568464752
C,0,2.2855479577,-0.5670045982,2.0552579487
H,0,3.136284817,0.0850579377,2.2708033858
H,0,1.4151936415,0.0616032698,1.8447699373
H,0,2.0734620783,-1.1451040654,2.962188386
C,0,4.0563531507,-2.8968018253,1.0839330857
H,0,4.9410181957,-2.3390008924,1.4076764822
H,0,3.7563029293,-3.5655349933,1.8984556802
H,0,4.3367524515,-3.5130762618,0.2236653057
C,0,1.0876379268,-2.7501999603,0.251461778
H,0,1.2763678527,-3.450023952,-0.5693843343
H,0,0.7530682327,-3.3284486318,1.1185540352
H,0,0.2717181724,-2.0818764489,-0.0453400092

TS-8 *trans-up*

M06-2X/6-31+G**, $E = -1504.18006380$ a.u.

Thermal correction to Gibbs Free Energy = 0.475016 a.u.

1 imaginary frequency = -651.12 cm⁻¹

SP at B2PLYP/6-311+G**, $E = -1503.6801025063$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1503.7023935903$ a.u.

0,1
C,0,-0.893837893,-1.0456779256,-3.5380360026
C,0,0.2513372385,-0.1657876326,-3.7824714832
H,0,0.0730328565,0.7941643144,-4.2568345762
C,0,1.5389729526,-0.5310575894,-3.3096714559
H,0,1.6717499028,-1.4815285843,-2.7988370871
N,0,2.5969559085,0.2196516987,-3.4219158598
C,0,2.6137148003,1.5331809878,-4.096839614
C,0,3.894068788,-0.1208645023,-2.8038960478
C,0,4.0910402519,1.95009455,-4.1412846094
C,0,4.8930926008,0.7760895472,-3.5403875603

H,0,1.9984160011,2.2290056155,-3.5148383615
H,0,4.2364633198,2.8635675894,-3.5649430921
H,0,2.1770013824,1.4145903294,-5.0910495867
H,0,4.4024625741,2.1493230876,-5.1670859508
H,0,5.6850602199,1.118554458,-2.8719853781
H,0,5.3678330041,0.1937078812,-4.3329199104
H,0,4.0704975306,-1.1817729556,-2.9895182463
C,0,3.7828683946,0.0419251348,-1.2447238619
O,0,-0.9431703456,-0.3217763528,-2.2559400896
O,0,-2.6027045137,-0.5764533249,-1.2654018994
H,0,-2.1838323912,-0.8388146374,-0.4324486459
H,0,-1.4968454713,0.4860261937,-2.3254808257
C,0,-2.1441128674,-0.9090175962,-4.3575949806
H,0,-2.3527684081,0.1379841337,-4.5945059043
H,0,-2.0089380046,-1.4556524448,-5.2933003313
H,0,-2.9867831239,-1.3341644427,-3.8106132343
C,0,3.176555626,1.4129843632,-0.9271376702
C,0,1.8002421892,1.5349341394,-0.7110558024
C,0,3.957079754,2.5748505911,-0.9493035335
C,0,1.2163985897,2.7871469111,-0.5203260267
C,0,3.3755990269,3.8274654473,-0.7625972559
C,0,2.0018616679,3.9385336581,-0.5487037553
H,0,1.178960225,0.6446588446,-0.6976907235
H,0,5.03078038,2.5060137468,-1.1023470453
H,0,0.1466194423,2.8596933955,-0.3485567688
H,0,3.9991392386,4.7156691557,-0.7786752263
H,0,1.5495576103,4.9136220383,-0.3987998764
C,0,5.1410543974,-0.2030118069,-0.5754807658
C,0,5.4501296056,0.4045964151,0.6459168564
C,0,6.0351454656,-1.148793711,-1.0927802872
C,0,6.6172552085,0.0765620665,1.3346285765
C,0,7.2063179909,-1.4724219595,-0.4110496799
C,0,7.500346834,-0.8635427492,0.8081917596
H,0,4.7762069413,1.1396492164,1.073074725
H,0,5.8290820881,-1.6579975068,-2.0291797438
H,0,6.8314967736,0.5579588848,2.2834918835
H,0,7.8853683811,-2.2072629801,-0.8315368876
H,0,8.409581962,-1.1199378638,1.3422810437
O,0,2.8787459024,-0.9855750301,-0.8852277
Si,0,2.5834230784,-1.7859723646,0.5809370917
C,0,2.19410507,-0.5857261903,1.9660357079
H,0,2.9937847752,0.1419177673,2.1288994816
H,0,1.2682050446,-0.036032424,1.7716700642
H,0,2.0637680178,-1.1515955902,2.8955682264
C,0,4.0128823681,-2.90270942,1.0436773527
H,0,4.885648226,-2.3392822231,1.3889687522
H,0,3.6979513615,-3.5747395501,1.8499042809
H,0,4.3177035574,-3.5160691396,0.1895372567
C,0,1.0679996623,-2.7890447413,0.1343498935
H,0,1.2962359147,-3.5067076866,-0.6605741363
H,0,0.6975066562,-3.3482231205,0.9993286022
H,0,0.2641288874,-2.1321515789,-0.2161892405
H,0,-0.6422056276,-2.0725915369,-3.2742078351

TS-8 *cis-up*

M06-2X/6-31+G**, $E = -1504.17668621$ a.u.

Thermal correction to Gibbs Free Energy = 0.477468 a.u.

1 imaginary frequency = -621.66 cm⁻¹

SP at B2PLYP/6-311+G**, $E = -1503.6774147286$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1503.6996244786$ a.u.

0,1
C,0,0.4553907235,-2.7404899601,-3.1988892661
C,0,1.6458221509,-1.932976334,-2.9204942666
H,0,2.3942896911,-2.3112474924,-2.2341967284
C,0,1.7666853057,-0.6450441716,-3.4990053454
H,0,0.945609353,-0.2771357456,-4.1132105332
N,0,2.7892420592,0.1586397243,-3.4102221682
C,0,2.8553598055,1.425801051,-4.1652644409
C,0,4.0966843732,-0.1221792466,-2.7660094531

C,0,4.2817444655,1.3980382391,-4.702076998
C,0,5.0870677343,0.7607638089,-3.5572608937
H,0,2.6958422443,2.2494812792,-3.4598325747
H,0,4.6393487614,2.3964888146,-4.9565553148
H,0,2.0765259635,1.4409853516,-4.927858179
H,0,4.3213781563,0.7749303895,-5.599262856
H,0,5.5044897959,1.530058688,-2.9066164288
H,0,5.9223532988,0.1638063301,-3.9259152309
H,0,4.2922805499,-1.1877882771,-2.9047262464
C,0,4.0603759353,0.1466151445,-1.2169528094
H,0,-0.147597303,-2.4358743184,-4.0546674107
O,0,-0.0499529675,-2.0868039152,-1.9808954788
O,0,-1.928089798,-2.4334711855,-1.5989074286
H,0,-1.7561021921,-2.8462545963,-0.7398030789
H,0,-0.5757072377,-1.2859566089,-2.1847173321
C,0,0.5110790363,-4.2244824574,-2.9838209541
H,0,1.0768871358,-4.4613527019,-2.080239959
H,0,-0.5024635147,-4.6173248201,-2.8913772816
H,0,1.0000923733,-4.6879957841,-3.8433009567
C,0,3.3467787719,1.4812362937,-0.9752386674
C,0,1.9629748843,1.4775622493,-0.7687455002
C,0,3.9994640006,2.7153948048,-1.0919564371
C,0,1.2468131268,2.6707568028,-0.6888408049
C,0,3.2849161609,3.9103254991,-1.0132544494
C,0,1.9048901728,3.8930245541,-0.8171963937
H,0,1.4435467869,0.5286589859,-0.6729804105
H,0,5.0746334783,2.7587362937,-1.2336967383
H,0,0.1739679645,2.643369216,-0.5257504025
H,0,3.8118782438,4.8548084069,-1.1033975293
H,0,1.3496004699,4.8234912906,-0.7570347041
C,0,5.4830716149,0.0686897024,-0.6462386582
C,0,5.8668154809,0.8352166764,0.4588204407
C,0,6.3793572025,-0.8941293924,-1.1285074948
C,0,7.1117719442,0.6513457519,1.0611843312
C,0,7.6255448389,-1.0749309178,-0.5346820492
C,0,7.997042753,-0.3024681996,0.5654914609
H,0,5.1929083568,1.5803618718,0.8672493471
H,0,6.1124898988,-1.5332902033,-1.9646928676
H,0,7.3838950179,1.2555532786,1.9206829053
H,0,8.3027081623,-1.8266322618,-0.9273888312
H,0,8.9662394907,-0.4458718099,1.0322276486
O,0,3.2887028629,-0.9203422407,-0.6942275588
Si,0,3.1812552434,-1.508053517,0.8998088381
C,0,2.8096192676,-0.1514276317,2.1379151362
H,0,3.6035100717,0.5977497831,2.2007424792
H,0,1.8701223366,0.3606475123,1.9107587026
H,0,2.7121668059,-0.613921101,3.1271106691
C,0,4.726835395,-2.4471272912,1.3872575448
H,0,5.5787493792,-1.7898953259,1.5864770068
H,0,4.5162502523,-3.0195889407,2.2978903762
H,0,5.0154003846,-3.1542353653,0.6025822051
C,0,1.7352245256,-2.6886319099,0.7861251494
H,0,1.9433148932,-3.500393173,0.0808971134
H,0,1.5437981156,-3.1403379297,1.7651876288
H,0,0.8265238141,-2.1739180585,0.4600824748
C,0,3.0336908831,0.6331841879,-1.8504737658
C,0,3.4615402815,-0.0019265436,-4.1570585555
C,0,3.9675380078,1.7040602432,-2.4262569927
C,0,4.1937215646,1.3317049452,-3.9099583483
H,0,3.5796552167,-0.1105687021,-1.2641874951
H,0,4.9083156725,1.724376285,-1.8741755437
H,0,2.2049215261,1.0334156402,-1.2658099104
H,0,3.5112732465,2.6914966962,-2.343269812
H,0,5.2546964114,1.2332898676,-4.1382496322
H,0,3.7790272137,2.0981034561,-4.56826089
H,0,2.9140761206,-0.0136988916,-5.102147682
C,0,4.4073288744,-1.2513021751,-4.0833438517
O,0,-1.1323186934,-0.4169595558,-4.1925289846
O,0,-3.0514312254,-0.2723109955,-4.5083302319
H,0,-3.2173332114,0.3458458707,-3.7817136276
H,0,-1.261470422,-0.2097176896,-5.1417658724
C,0,-1.1736073299,-2.747456226,-5.0526121594
H,0,-0.8295384101,-2.4667839166,-6.0526730776
H,0,-0.8037847627,-3.7497973036,-4.8276788151
H,0,-2.264528496,-2.7493956832,-5.0256211808
C,0,5.3591535035,-1.3086231216,-5.2849333026
C,0,6.187303491,-2.4345756753,-5.3744499436
C,0,5.4646847756,-0.3234570515,-6.2692128055
C,0,7.1372570951,-2.5501570254,-6.38258862
C,0,6.4090423562,-0.4429228639,-7.2925224041
C,0,7.2572051585,-1.5452758911,-7.3443277131
H,0,6.0770933165,-3.2330641939,-4.6458562077
H,0,4.8247741635,0.5524650817,-6.2646453576
H,0,7.7757529529,-3.4271085983,-6.4228127838
H,0,6.4795007575,0.3348363698,-8.0462141765
H,0,7.9960783528,-1.63021767,-8.1346216297
C,0,3.5559386597,-2.5246972626,-4.0353729985
C,0,3.0163281738,-3.06366028,-5.2095257897
C,0,3.2477505537,-3.1212067391,-2.8109869461
C,0,2.1708994783,-4.1696010013,-3.1570806891
C,0,2.4014364273,-4.2304525494,-2.7578150986
C,0,1.8574740183,-4.7544520232,-3.929143887
H,0,3.2634824969,-2.6227349288,-6.1728820176
H,0,3.6791486403,-2.7171321152,-1.9002701429
H,0,1.7615603894,-4.577286416,-6.0764525427
H,0,2.1739835242,-4.6868284779,-1.7994024239
H,0,1.2030271291,-5.6197182634,-3.8888182288
O,0,5.099450947,-1.1170560596,-2.8622201105
Si,0,6.704575089,-1.0873300294,-2.3316344326
C,0,7.7266749623,0.1620885959,-3.2821135819
H,0,7.3436233076,1.1804870832,-3.158159813
H,0,8.7513552443,0.1453424889,-2.8937440373
H,0,7.7682501944,-0.069903523,-4.3516502757
C,0,7.5071958383,-2.7834543279,-2.381267674
H,0,8.0302754978,-2.9745848364,-3.3217817756
H,0,8.2400829657,-2.8485790759,-1.5694029545
H,0,6.7655933888,-3.5747283404,-2.2264483131
C,0,6.4978854824,-0.5821979858,-0.5405906439
H,0,5.8685112119,-1.3080803671,-0.014112275
H,0,7.4713758925,-0.5564183639,-0.0399563766
H,0,6.0414721454,0.4067470693,-0.4358542042
H,0,-0.9241266473,-2.060296145,-2.991316395

TS-8 *cis-down*

M06-2X/6-31+G**, $E = -1504.17632963$ a.u.

Thermal correction to Gibbs Free Energy = 0.476332 a.u.

1 imaginary frequency = -596.56 cm^{-1}

SP at B2PLYP/6-311+G**, $E = -1503.6753327064$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1503.6976323245$ a.u.

0,1

C,0,-0.6546795443,-1.7954307087,-4.0131580262
C,0,0.6707343682,-1.1915296271,-4.1779400535
H,0,1.1026057309,-1.1737344118,-5.1719444557
C,0,1.3076754352,-0.5847689239,-3.0665044691
H,0,0.7573231847,-0.5431354311,-2.1274106929
N,0,2.4921059733,-0.0437340831,-3.0473022827

Cartesian coordinates and computed total energies for the structures presents in Scheme 8.

TS-9a anti-anti-down

M06-2X/6-31+G**, $E = -1580.18878436$ a.u.

Thermal correction to Gibbs Free Energy = 0.482739 a.u.

1 imaginary frequency = -106.53 cm⁻¹

SP at B2PLYP/6-311+G**, $E = -1579.6490013193$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1579.6767257956$ a.u.

0,1
C,0,3.0128583632,-0.6669306968,2.0379104814
C,0,1.8611068465,-0.9427432073,1.3594252486
H,0,1.8090945442,-1.782550034,0.6745735795
C,0,0.80549113,-0.0075989259,1.4278664049
H,0,0.865336504,0.8073384271,2.1449739551
N,0,-0.263247133,-0.0305436975,0.6788155008
C,0,-0.4323310825,-0.9609087521,-0.4534877118
C,0,-1.3574987756,0.945074801,0.7998313779
C,0,-1.7354916311,-0.5218841329,-1.1317552457
H,0,0.4497269807,-0.8408405817,-1.0901354339
H,0,-0.4820316451,-1.9878462584,-0.0784745064
C,0,-2.0417795748,0.8798363896,-0.5696482306
H,0,-0.8979575695,1.9169497923,0.9907433518
H,0,-1.621020136,-0.4980625441,-2.2166209002
H,0,-2.5388522835,-1.2204016032,-0.8940023156
H,0,-1.608874334,1.6498217078,-1.213825165
H,0,-3.1142925356,1.074055906,-0.4955289427
C,0,4.2192537851,-1.5319315583,2.0145452782
H,0,4.056085172,-2.4327106384,1.4187193914
H,0,5.0415552138,-0.9547588742,1.5750430866
H,0,4.5056528842,-1.8162906882,3.0323507866
H,0,3.023896884,0.1820363535,2.7162056154
O,0,3.9464148495,1.05425545,0.6527826947
O,0,5.2578928993,0.7476581687,0.1264604706
H,0,5.7854494367,1.4918803261,0.4416110106
H,0,3.0723638502,0.6775632647,-0.4969074086
O,0,2.4415244566,0.4100743016,-1.2765718436
H,0,2.7958211117,0.8396559209,-2.0619859659
C,0,-2.2443076504,0.6205121225,2.0484818554
O,0,-1.325008757,0.6989095443,3.1210605346
C,0,-2.7861623791,-0.8072538963,1.9332060921
C,0,-3.9803059089,-1.0911608227,1.2600555924
C,0,-2.0270179194,-1.8719396227,2.4282155827
C,0,-4.4030323874,-2.4072201393,1.08403171
C,0,-2.4471176929,-3.1900592822,2.251953343
C,0,-3.635975186,-3.4627062355,1.5771916585
H,0,-4.5900664481,-0.2815936819,0.868313305
H,0,-1.0994791226,-1.6636445919,2.953775218
H,0,-5.3332109691,-2.606313655,0.5609791503
H,0,-1.8427351689,-4.0028564084,2.6430400755
H,0,-3.9654551786,-4.487918663,1.4405152776
C,0,-3.3473016217,1.6704307461,2.2375728716
C,0,-3.2118611035,2.9789027288,1.761531584
C,0,-4.4634943248,1.3667935118,3.027849062
C,0,-4.1601273733,3.9544186453,2.0676072604
C,0,-5.4094013421,2.3399408191,3.3412103982
C,0,-5.2604094721,3.6410813552,2.8626658896
H,0,-2.3649168479,3.2661944911,1.1480353392
H,0,-4.5977073621,0.3575901608,3.4049845877
H,0,-4.03268846,4.9616972556,1.6839091442
H,0,-6.2632798292,2.07862066,3.9585199376
H,0,-5.9965036482,4.4016788921,3.10319
Si,0,-1.4451458036,1.0232921358,4.7720411231
C,0,-1.8941125358,2.8164003358,5.0773766941
H,0,-2.9266518842,3.0378266995,4.7882506485
H,0,-1.779594188,3.0465196947,6.1426656026
H,0,-1.2302329311,3.4800745799,4.513522294
C,0,-2.6477767599,-0.1270479677,5.6394856069
H,0,-3.6843738804,0.2081968423,5.5482378166

H,0,-2.5762144867,-1.1468078872,5.2475440428
H,0,-2.400862533,-0.1567554057,6.7068378649
C,0,0.3063154186,0.6702674469,5.3312344462
H,0,0.411399726,0.8049923153,6.4126000228
H,0,0.5848589952,-0.3606876619,5.0864915035
H,0,1.0154898056,1.3418283221,4.8356603001

TS-9c anti-anti-down

M06-2X/6-31+G**, $E = -1619.48355378$ a.u.

Thermal correction to Gibbs Free Energy = 0.509466 a.u.

1 imaginary frequency = -95.00 cm⁻¹

SP at B2PLYP/6-311+G**, $E = -1618.9261733920$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1618.9547911751$ a.u.

0,1
C,0,3.0041290314,-0.6472170473,2.0412540796
C,0,1.8572884472,-0.9338863213,1.3595187966
H,0,1.8073981032,-1.7849834814,0.6885170388
C,0,0.8000379446,0.000933531,1.4145000092
H,0,0.858793353,0.822896041,2.1235185959
N,0,-0.269153104,-0.0305249242,0.6670144393
C,0,-0.4382786317,-0.9663673361,-0.4606405311
C,0,-1.3657051915,0.9424280655,0.7869433302
C,0,-1.7444747528,-0.533288161,-1.1373710589
H,0,0.4421152846,-0.8465571584,-1.0995668962
H,0,-0.4843876957,-1.9918784176,-0.0814871628
C,0,-2.0531681352,0.8701766307,-0.5803418389
H,0,-0.9080307427,1.9159646763,0.973292362
H,0,-1.6328253926,-0.5136773931,-2.2226114969
H,0,-2.5454280321,-1.2329934063,-0.8948234498
H,0,-1.6238242999,1.6385176301,-1.2288165578
H,0,-3.1260158806,1.0618747312,-0.504271897
C,0,4.209817127,-1.5183646475,2.06634137
H,0,4.0224696483,-2.4281907394,1.486588869
H,0,5.0085714904,-0.9605639903,1.5606036337
H,0,3.0101524615,0.2129556746,2.7078358588
O,0,3.950472462,1.0566797988,0.641319526
O,0,5.2548183197,0.7388143253,0.1037541733
H,0,5.794147768,1.471468008,0.4257694507
H,0,3.0676694183,0.6783172413,-0.5026109814
O,0,2.4333650443,0.4108774267,-1.2791946147
H,0,2.7904290645,0.8324679684,-2.0677122509
C,0,-2.248316456,0.6188246135,2.0392333413
O,0,-1.3237682003,0.6905224685,3.1075011659
C,0,-2.7967224849,-0.8063383201,1.9226472275
C,0,-3.996655879,-1.0836271973,1.2570277887
C,0,-2.037435156,-1.8755573785,2.4076531143
C,0,-4.4248229813,-2.3975916262,1.0785390749
C,0,-2.4629766874,-3.1915701318,2.2288590392
C,0,-3.6575229543,-3.4576131878,1.5616061214
H,0,-4.6067274356,-0.2705309858,0.8732548122
H,0,-1.104938846,-1.6726008697,2.9266069931
H,0,-5.3595034746,-2.5914479796,0.5615906383
H,0,-1.8582568726,-4.0079844707,2.6118175346
H,0,-3.9912388058,-4.4811854116,1.4229558844
C,0,-3.3458308332,1.6732875661,2.236155196
C,0,-3.2074508828,2.9823949347,1.7627652007
C,0,-4.4590183853,1.3725630137,3.0318979645
C,0,-4.1497034406,3.9612651331,2.0768841141
C,0,-5.3988782978,2.3489284288,3.3531042741
C,0,-5.24676635,3.6507462013,2.877360133
H,0,-2.3628820786,3.2680809657,1.1453294682
H,0,-4.5957773227,0.3629655202,3.407019603
H,0,-4.0199209686,4.9690001869,1.6951713532
H,0,-6.2504363802,2.0896389834,3.9744628149
H,0,-5.9779706742,4.4139889538,3.124355209
Si,0,-1.4310658047,1.0001960828,4.7617988989
C,0,-1.8725449321,2.7922078432,5.0836487721
H,0,-2.9057232669,3.0185137707,4.800902091
H,0,-1.7521827374,3.0145588254,6.1498925423

H,0,-1.2093843493,3.4576739097,4.5210662706
C,0,-2.6312308268,-0.1540145479,5.6270985043
H,0,-3.6686339492,0.1788050588,5.535955417
H,0,-2.5569682133,-1.1728835786,5.2333922324
H,0,-2.3846983387,-0.1847285319,6.6945038802
C,0,0.3233550718,0.637346056,5.306393062
H,0,0.4335299992,0.7535887614,6.3894249496
H,0,0.6012613201,-0.389265295,5.0427690158
H,0,1.0303729351,1.3174372963,4.8193921542
C,0,4.6303117535,-1.8625314336,3.500628631
H,0,5.5314548696,-2.4805882474,3.4964706639
H,0,4.8467500819,-0.9532228879,4.0698979784
H,0,3.842763836,-2.4118852173,4.0251326131

TS-9a anti-anti-up

M06-2X/6-31+G**, $E = -1580.18910043$ a.u.

Thermal correction to Gibbs Free Energy = 0.486715 a.u.

1 imaginary frequency = -29.82 cm^{-1}

SP at B2PLYP/6-311+G**, $E = -1579.6430789823$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1579.6718617202$ a.u.

0,1
C,0,2.6804070697,-1.1733445188,1.8450996829
C,0,1.7303813521,-1.038259134,0.8838293986
H,0,1.6434897099,-1.7602816083,0.0785225455
C,0,0.7409735178,-0.039411753,1.0792275539
H,0,0.8570119559,0.6629302866,1.901155639
N,0,-0.3549691435,0.0758975443,0.3861352693
C,0,-0.715201454,-0.8207409165,-0.7270533401
C,0,-1.4540683,0.9861080783,0.7594806406
C,0,-1.9718369552,-0.200915107,-1.3562457955
H,0,0.1259008578,-0.8741375632,-1.4212840793
H,0,-0.9037958941,-1.8194056247,-0.3150826771
C,0,-2.3331898034,1.0326597458,-0.4966866506
H,0,-1.0087592038,1.956332862,0.9882995124
H,0,-1.7795998118,0.0924152683,-2.3892526702
H,0,-2.7831742449,-0.9298753845,-1.363117333
H,0,-2.1174798169,1.9534520043,-1.0432700707
H,0,-3.3929554115,1.055933337,-0.2361436705
C,0,3.7268327407,-2.2228376596,1.8569986239
H,0,4.7145250865,-1.7570222287,1.7586372499
H,0,3.6951855003,-2.7182664969,2.8318516121
H,0,3.5904462058,-2.9491403403,1.0535139514
H,0,2.7096139829,-0.4522999712,2.6590402625
O,0,1.423499321,-2.1413124339,3.8809894442
O,0,2.5609508188,-2.1382081051,4.7836730221
H,0,2.3317817211,-1.4444940997,5.4180874691
H,0,0.5234703016,-3.0094424702,4.6728165837
O,0,-0.0812724446,-3.6084078029,5.2715295982
H,0,0.5291496986,-4.1047019679,5.8262470417
C,0,-2.1279111851,0.4864400316,2.0897310777
O,0,-1.1369379572,0.7500890736,3.0642810854
C,0,-2.3781588222,-1.0195871596,1.9741132227
C,0,-3.4598998181,-1.5205327905,1.2395973521
C,0,-1.4431994365,-1.9206118439,2.4958477193
C,0,-3.5999475699,-2.8903599707,1.0230560522
C,0,-1.5883125354,-3.2925340727,2.288236966
C,0,-2.6620955041,-3.7819120627,1.5461325909
H,0,-4.2048794685,-0.8408755769,0.833297743
H,0,-0.5805854635,-1.5662675577,3.0573698182
H,0,-4.4457758645,-3.2586816673,0.450297248
H,0,-0.8579574457,-3.9662702603,2.726219154
H,0,-2.7749300329,-4.8492621229,1.3822236499
C,0,-3.3795359952,1.3134029093,2.4088363923
C,0,-3.3959731179,2.6894307293,2.1480737783
C,0,-4.459884935,0.7570119074,3.1002965404
C,0,-4.4624540154,3.4844273651,2.559764913
C,0,-5.5267039167,1.5517203667,3.5213310728
C,0,-5.5326769712,2.9183183141,3.2525325038
H,0,-2.566868593,3.1638689026,1.6321131713

H,0,-4.4722899477,-0.3047440777,3.3226833959
H,0,-4.4522056815,4.5486140587,2.3458912294
H,0,-6.3511017063,1.0967636271,4.0614884391
H,0,-6.3621823047,3.5375469208,3.5789279842
Si,0,-1.1951301987,0.8264242639,4.7537882339
C,0,-2.0416012588,2.4099677815,5.3019622694
H,0,-3.1185451664,2.3939510847,5.1033710935
H,0,-1.8942749215,2.5467368515,6.3794673603
H,0,-1.6123531056,3.2766107288,4.7881662056
C,0,-2.036755293,-0.6595682317,5.5236973986
H,0,-3.0456064164,-0.811503779,5.1278910386
H,0,-1.4595648244,-1.5785537306,5.3704817355
H,0,-2.125920628,-0.486826182,6.6031654392
C,0,0.6275777812,0.8442643548,5.1692199108
H,0,0.7952872918,0.7618744071,6.2483843147
H,0,1.0748520935,-0.0235203048,4.6656892699
H,0,1.112789578,1.7589397719,4.812693816

TS-9c anti-anti-up

M06-2X/6-31+G**, $E = -1619.48390874$ a.u.

Thermal correction to Gibbs Free Energy = 0.512054 a.u.

1 imaginary frequency = -38.70 cm^{-1}

SP at B2PLYP/6-311+G**, $E = -1618.9206881587$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1618.9503112498$ a.u.

0,1
C,0,2.6892385623,-1.1731635175,1.834821996
C,0,1.7328593583,-1.0412394056,0.8785034643
H,0,1.647371242,-1.7617676275,0.0715881516
C,0,0.739493448,-0.0478399486,1.0788486895
H,0,0.8559006899,0.6549419356,1.9003985746
N,0,-0.3589379526,0.0647779257,0.3887346294
C,0,-0.7194826084,-0.8318429847,-0.7241487514
C,0,-1.4562405227,0.9774176171,0.760301072
C,0,-1.9754409187,-0.2111356857,-1.3539511721
H,0,0.1216805346,-0.8859044512,-1.4182715915
H,0,-0.9086399446,-1.8304161002,-0.3122596398
C,0,-2.3331687078,1.0255212039,-0.4973653535
H,0,-1.0088573862,1.9467580313,0.988790578
H,0,-1.7834743554,0.0789459544,-2.3879321648
H,0,-2.7883722451,-0.9383238053,-1.3581778982
H,0,-2.1121524929,1.9442840598,-1.0452602349
H,0,-3.3933201021,1.0541019328,-0.2389320182
C,0,3.7619894982,-2.2005284228,1.8277430303
H,0,3.6665400608,-2.7510090721,2.7695746677
H,0,3.617647706,-2.8961845964,0.9952501618
H,0,2.7257570284,-0.4503133688,2.6483841899
O,0,1.4740097456,-2.1451008869,3.8509148656
O,0,2.6094506894,-2.1244490499,4.7551771476
H,0,2.3842472224,-1.4114349513,5.3695124215
H,0,0.5618199202,-2.9871582904,4.6548472565
O,0,-0.0593558749,-3.5627474896,5.2594740921
H,0,0.5346827959,-4.0484279151,5.8407316551
C,0,-2.1332171383,0.4812751725,-2.0897933151
O,0,-1.1422234107,0.7407967064,3.0653463937
C,0,-2.3910020991,-1.0236080653,1.9759050745
C,0,-3.4735952648,-1.5194386016,1.2390900658
C,0,-1.4661136093,-1.9299067264,2.5063797371
C,0,-3.6245324364,-2.8890199769,1.0289756879
C,0,-1.6233078399,-3.3017545649,2.3070721183
C,0,-2.6976265109,-3.785841683,1.8623808042
H,0,-4.2117162883,-0.8357876817,0.0271074477
H,0,-0.6035567943,-1.5793617999,3.0701041186
H,0,-4.4707808926,-3.2529340906,0.4540454549
H,0,-0.9025069896,-3.9798649714,2.7537984216
H,0,-2.819406027,-4.8531381271,1.4046717764
C,0,-3.3817182774,1.3139722324,2.407128711
C,0,-3.3915774396,2.6900765351,2.1463077459
C,0,-4.4660709181,0.7624782702,3.0962403673
C,0,-4.4556415241,3.4897182157,2.5553043887

C,0,-5.5304655665,1.5618304873,3.5146077646
C,0,-5.5300013548,2.9283611458,3.2454891769
H,0,-2.5592995169,3.1610086264,1.632294556
H,0,-4.4837942936,-0.2991654027,3.3187369144
H,0,-4.4403095724,4.5538049789,2.3412238182
H,0,-6.3581323398,1.1104615107,4.0527761644
H,0,-6.3577050786,3.551142209,3.5696779811
Si,0,-1.2020795053,0.8170707924,4.7584694814
C,0,-2.0396829427,2.4054480501,5.3020707502
H,0,-3.1165946853,2.3946272749,5.1028185489
H,0,-1.8923685479,2.5420317482,6.3795788193
H,0,-1.6058087235,3.2695294274,4.7878892045
C,0,-2.0509105744,-0.6650223915,5.5243767303
H,0,-3.054899595,-0.8217951069,5.11825972
H,0,-1.4693147299,-1.583487083,5.3834874051
H,0,-2.1525069107,-0.485377296,6.6016454423
C,0,0.6209716788,0.8206440071,5.1697559464
H,0,0.7893881085,0.7271732981,6.2478523018
H,0,1.061364581,-0.045858586,6.6576297789
H,0,1.1125998769,1.7345094379,4.820058413
C,0,5.1500233522,-1.5466414603,1.7589154341
H,0,5.3009609538,-0.870322106,2.6057542378
H,0,5.9286237731,-2.3124267323,1.7944102287
H,0,5.2750296227,-0.9736987998,0.8355487055

TS-9a *syn-anti-down*

M06-2X/6-31+G**, $E = -1580.18682615$ a.u.

Thermal correction to Gibbs Free Energy = 0.484554 a.u.

1 imaginary frequency = -150.32 cm⁻¹

SP at B2PLYP/6-311+G**, $E = -1579.6462435044$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1579.6741107521$ a.u.

0,1
C,0,2.9476763177,1.0930306966,2.198306999
C,0,1.5932035669,0.9277471047,2.1233877021
H,0,0.9161344694,1.5763136737,2.6654215151
C,0,1.0984215043,0.0260722657,1.1596525708
H,0,1.8089823486,-0.6468752627,0.6800925646
N,0,-0.1298229161,-0.0673264179,0.7193748534
C,0,-0.5016454212,-0.8955517778,-0.4383966258
C,0,-1.2153589334,0.8797439881,1.0425599078
C,0,-1.2874537216,0.0943569521,-1.2947766099
C,0,-2.0330839261,0.9635879908,-0.2644853481
H,0,-0.7266234287,1.8312389756,1.2571151252
C,0,3.6093853932,2.0763570073,3.0945174236
H,0,4.2624911018,1.5614595128,3.807747778
H,0,4.2252732557,2.743492057,2.4813825552
H,0,2.8775279502,2.6731249127,3.6437270095
H,0,3.5913148206,0.3917554042,1.6741259349
O,0,3.3288036574,2.2711166402,0.2103481148
O,0,4.0022347381,3.5431665747,0.337179888
H,0,4.8011448679,3.4071756562,-0.1871114672
H,0,1.8839623804,2.6818331804,0.0601714187
O,0,0.8833897834,2.9223394005,-0.0379804045
H,0,0.8444919143,3.6098368391,-0.7110281118
C,0,-2.0131584347,0.430670848,2.3100464405
O,0,-1.0870092633,0.5839453675,3.3705716144
C,0,-2.392573312,-1.0473467627,2.1651943211
C,0,-3.5155738311,-1.4641298691,1.4387194629
C,0,-1.523396642,-2.0239229483,2.6634036831
C,0,-3.7566092204,-2.8182768954,1.2091337117
C,0,-1.7637218498,-3.3786307566,2.4378836685
C,0,-2.8790493223,-3.7817601494,1.7045232946
H,0,-4.2221598078,-0.7341107529,1.0564444388
H,0,-0.6440441942,-1.7155239491,3.2201890995
H,0,-4.6345517347,-3.1168711457,0.6448158519
H,0,-1.0744590931,-4.118459812,2.8333249178
H,0,-3.0665509954,-4.8358505523,1.5258385768
C,0,-3.2094913926,1.3632514514,2.5446215393
C,0,-3.1084207164,2.7273968559,2.2437940506

C,0,-4.3619537147,0.9134690699,3.1975503081
C,0,-4.1320620208,3.6119164072,2.5757828984
C,0,-5.3864546752,1.7968508335,3.5367928517
C,0,-5.2762025557,3.1503394628,3.2253443586
H,0,-2.2193497408,3.1226102882,1.762328309
H,0,-4.4654449017,-0.1362668929,3.5129599112
H,0,-4.029205639,4.6649281261,2.3329410256
H,0,-6.2694567169,1.4232872718,4.0461178976
H,0,-6.072567924,3.8395905081,3.4880598449
Si,0,-1.2772644248,0.7533728657,5.0380067937
C,0,-2.0154213519,2.41759051,5.4828397426
H,0,-3.0773439247,2.4865817598,5.2252579448
H,0,-1.9124134617,2.5816718917,6.5616669806
H,0,-1.4853885135,3.2238525339,4.9648342648
C,0,-2.2959169823,-0.6371009288,5.7794122418
H,0,-3.3202436957,-0.6600021943,5.3969386491
H,0,-1.8379914345,-1.6126318051,5.5887793192
H,0,-2.349155635,-0.4932287448,6.8649356438
C,0,0.488949891,0.6447063553,5.6492538047
H,0,0.5197399673,0.6616071727,6.7437578613
H,0,0.9592514352,-0.2829374549,5.3062156805
H,0,1.0863674896,1.4844403192,5.2796277005
H,0,-2.1069066236,2.0016999208,-0.5937718496
H,0,-3.0494641269,0.596406146,-0.1113696921
H,0,-0.5886515692,0.706171004,-1.8706990193
H,0,-1.9654654268,-0.4097561723,-1.986064305
H,0,0.3973239589,-1.2905538152,-0.9132383171
H,0,-1.1273596657,-1.7275595921,-0.0969416545

TS-9c *syn-anti-down*

M06-2X/6-31+G**, $E = -1619.48207317$ a.u.

Thermal correction to Gibbs Free Energy = 0.510933 a.u.

1 imaginary frequency = -118.50 cm⁻¹

SP at B2PLYP/6-311+G**, $E = -1618.9232591533$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1618.9521318916$ a.u.

0,1
C,0,2.929858405,1.0757812729,2.2088737741
C,0,1.577939611,0.9233056783,2.1107302821
H,0,0.8995056297,1.5763324655,2.6451003956
C,0,1.0847524893,0.0238281459,1.1416284189
H,0,1.7944094923,-0.6529954766,0.6663104316
N,0,-0.1407620747,-0.0619179348,0.695981968
C,0,-0.5147816675,-0.8895176195,-0.4618025053
C,0,-1.2272094787,0.8837400643,1.0229599318
C,0,-1.3035353033,0.1009261816,-1.3144114645
C,0,-2.0515880779,0.9630128153,-0.2799913667
H,0,-0.7390299112,1.8365358093,1.2336930265
C,0,3.5889485908,2.0384221155,3.1335082459
H,0,4.2250029773,2.6896207723,2.5222976385
H,0,2.8313292142,2.6715252134,3.6079780595
H,0,3.5810493897,0.3743766536,1.6907623922
O,0,3.3486953332,2.2877519921,0.218672077
O,0,4.0097231522,3.5662545278,0.3600302897
H,0,4.8100251196,3.4428680687,-0.1649889933
H,0,1.9083096331,2.682776745,0.0592283737
O,0,0.9033424006,2.9130088192,-0.0472069867
H,0,0.8620036152,3.5962368719,-0.7244839683
C,0,-2.0155609814,0.4324854526,2.2962746132
O,0,-1.0814337406,0.5875305847,3.3483075889
C,0,-2.3926852826,-1.0465383177,2.1551367021
C,0,-3.5217208434,-1.4650904584,1.4392102813
C,0,-1.5188946819,-2.0215618781,2.6482624684
C,0,-3.763986833,-2.8197153558,1.2141166622
C,0,-1.7605796765,-3.3768358585,2.4272244324
C,0,-2.8817493184,-3.7818127952,1.7039585603
H,0,-4.2322115603,-0.7358634619,1.0626284464
H,0,-0.6353132546,-1.7119885759,3.1977377584
H,0,-4.6465537099,-3.1198735457,0.6578954086

H,0,-1.0679700011,-4.1156500152,2.8186828271
H,0,-3.0702671901,-4.8363324392,1.5289413686
C,0,-3.2132250391,1.3600237549,2.5416602396
C,0,-3.1263291455,2.7228456651,2.2314854618
C,0,-4.3516892564,0.9058132799,3.2159998771
C,0,-4.1509635194,3.6020832344,2.5749005163
C,0,-5.376929655,1.7837982358,3.5663496988
C,0,-5.2812297451,3.1362315941,3.245182833
H,0,-2.2479910115,3.1216195646,1.7335545887
H,0,-4.4427524001,-0.1431403393,3.4787352972
H,0,-4.0596453493,4.6543565875,2.3244035638
H,0,-6.2488999608,1.4072702959,4.0922452499
H,0,-6.0781520093,3.8213614918,3.5167883612
Si,0,-1.2372113631,0.7730590419,5.0168090688
C,0,-1.9906468016,2.4299538732,5.4619310243
H,0,-3.0563204173,2.4854902059,5.2171257652
H,0,-1.8757690973,2.6013535639,6.5384107686
H,0,-1.4758340568,3.2388936143,4.9328295843
C,0,-2.2166148619,-0.627847515,5.7906028241
H,0,-3.2454223002,-0.6741612807,5.4221642066
H,0,-1.7429831477,-1.5963248762,5.6022535992
H,0,-2.2576522946,-0.4746883344,6.8752410007
C,0,0.5465456196,0.7007678063,5.5832075576
H,0,0.6080377403,0.705329406,6.6765824368
H,0,1.0308586122,-0.2097431058,5.214083276
H,0,1.1129545366,1.5599852144,5.2078132588
H,0,-2.1363917789,2.000688758,-0.6079621549
H,0,-3.0639716451,0.5865815465,-0.1226727027
H,0,-0.6065143234,0.7171141468,-1.8878678433
H,0,-1.9800240181,-0.4026437922,-2.0074863232
H,0,0.383256466,-1.2836724106,-0.9389327092
H,0,-1.1395535907,-1.7215400139,-0.1185265631
C,0,4.4240696114,1.311282534,4.1962343171
H,0,5.193838956,0.6888228252,3.7296464421
H,0,4.9225286022,2.0333069757,4.8480502737
H,0,3.7961214777,0.6666676676,4.819039497

TS-9a *syn-anti-up*

M06-2X/6-31+G**, $E = -1580.18670621$ a.u.

Thermal correction to Gibbs Free Energy = 0.487107 a.u.

1 imaginary frequency = -185.91 cm⁻¹

SP at B2PLYP/6-311+G**, $E = -1579.6416176415$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1579.6701058376$ a.u.

0,1

C,0,2.2775115756,0.3531898148,3.4766255302
C,0,1.0399166285,0.5536789218,2.9263438752
H,0,0.3246192023,1.2399177755,3.3641087437
C,0,0.7014845072,-0.2411117966,1.8123879724
H,0,1.4472471559,-0.9587521585,1.4759907497
N,0,-0.385797165,-0.2249679508,1.0829257644
C,0,-0.4468628342,-1.0308549163,-0.1606025545
C,0,-1.5365957049,0.6845171797,1.2311027651
C,0,-1.7187685207,-0.5662383084,-0.8717763054
H,0,0.452484323,-0.8183945947,-0.744235102
H,0,-0.463137001,-2.0920002485,0.0992166746
C,0,-2.0826914985,0.7715064244,-0.2028659949
H,0,-1.1422500872,1.6383278465,1.5907159197
H,0,-1.5489202697,-0.4448622895,-1.9428855911
H,0,-2.5153778486,-1.2985933024,-0.7367821829
H,0,-1.5911560054,1.6016806598,-0.7183147993
H,0,-3.1584584457,0.9605802495,-0.2161752297
C,0,2.85985611,1.2181210108,4.5384650803
H,0,2.0827942457,1.7031603219,5.1336449177
H,0,3.5101825749,0.6275839701,5.1846183043
H,0,3.4666885408,2.0000894115,4.0638313574
H,0,2.9596108618,-0.3431260936,2.9954871892
O,0,2.2494532728,-1.5436160276,4.8422370623
O,0,3.6033872396,-1.9565614188,4.5425428713
H,0,4.001928291,-1.9945277782,5.4205734252

H,0,1.4728030313,-2.280429313,3.8334709031
O,0,0.9130959529,-2.7450375248,3.0878000835
H,0,0.8535824617,-3.6734912782,3.3368798175
C,0,-2.5642657123,0.1867815519,2.3005225684
O,0,-1.8108632533,0.1423186356,3.4959137766
C,0,-3.0518372665,-1.215908594,1.9217471494
C,0,-4.2263359811,-1.4338525346,1.192846551
C,0,-2.2341107028,-2.3088580807,2.2298691812
C,0,-4.5831994873,-2.719665226,0.7878732278
C,0,-2.590402437,-3.593563965,1.8221499183
C,0,-3.7655210883,-3.8052080711,1.1014945863
H,0,-4.8680038012,-0.5983683364,0.9287838076
H,0,-1.3003054232,-2.1585973246,2.7688443657
H,0,-5.4998887391,-2.8704051292,0.22591779
H,0,-1.9416721633,-4.4297872206,2.0674102452
H,0,-4.0431989254,-4.8065110682,0.7866873803
C,0,-3.7108312666,1.1993768826,2.4625289818
C,0,-3.6025748777,2.5345170274,2.0587866259
C,0,-4.8752292384,0.8104340877,3.1360833764
C,0,-4.6265374385,3.4475991431,2.3137687733
C,0,-5.9002305634,1.7167446839,3.928527321
C,0,-5.7799317398,3.0432160465,2.9812462284
H,0,-2.7246856038,2.8908726427,1.5305959997
H,0,-4.9856512647,-0.2184131111,3.4678631481
H,0,-4.5178118447,4.4765161442,1.9852986866
H,0,-6.7902209513,1.3857884883,3.9194179372
H,0,-6.5767479563,3.7536987035,3.1774479744
Si,0,-2.1770237373,-0.1303100128,5.1209996477
C,0,-3.2091457706,1.261741919,5.8566090704
H,0,-4.2839819553,1.0782287148,5.7883250409
H,0,-2.9473598985,1.3674757416,6.9158928623
H,0,-2.9967799982,2.2144353431,5.35858522
C,0,-3.03850095,-1.7778624174,5.3828295431
H,0,-3.9616062355,-1.8712757145,4.8013757011
H,0,-2.3841013395,-2.6114150378,5.1098807949
H,0,-3.2957000176,-1.875106067,6.4440735608
C,0,-0.5012139603,-0.1153337432,5.9424485022
H,0,-0.5956813314,-0.437324954,6.9859813428
H,0,0.223541597,-0.7661260703,5.4421106156
H,0,-0.0913862709,0.9011783363,5.9461608396

TS-9c *syn-anti-up*

M06-2X/6-31+G**, $E = -1619.48175793$ a.u.

Thermal correction to Gibbs Free Energy = 0.513253 a.u.

1 imaginary frequency = -156.11 cm⁻¹

SP at B2PLYP/6-311+G**, $E = -1618.9189465441$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1618.9482939149$ a.u.

0,1

C,0,2.274263364,0.351005476,3.4764046488
C,0,1.0400308472,0.554725625,2.9228536097
H,0,0.3263014984,1.2445704522,3.3583833472
C,0,0.700209061,-0.2415535753,1.8085568847
H,0,1.4454197597,-0.9603741862,1.4736397025
N,0,-0.3864093547,-0.2245730822,1.0796132216
C,0,-0.449418715,-1.032610428,-0.1627483824
C,0,-1.5376638038,0.6847798519,1.2280894351
C,0,-1.7214167665,-0.5679718295,-0.8736802006
H,0,0.4498649201,-0.8218986323,-0.7469861792
H,0,-0.466487922,-2.0931388292,0.0993642526
C,0,-2.0849758429,0.7702448458,-0.2054592112
H,0,-1.1432675428,1.6389177259,1.5865340987
H,0,-1.5517607334,-0.44711238,-1.9448617359
H,0,-2.5180749302,-1.3001330807,-0.7381505561
H,0,-1.5942507788,1.6001482891,-0.7220763232
H,0,-3.1607961678,0.9589673496,-0.2177757118
C,0,2.8647298915,1.2279389969,4.5280566678
H,0,2.0692692266,1.6747420029,5.1329920898
H,0,3.4877993784,0.6108532004,5.1790742005
H,0,2.9575308894,-0.349194662,3.0001877905

O,0,2.2532855624,-1.5579861868,4.8560772603
O,0,3.6067727541,-1.9626750531,4.5406775625
H,0,4.017146673,-1.9907631152,5.4135451076
H,0,1.4756755592,-2.2806144783,3.8421594823
O,0,0.9136845231,-2.738048307,3.0919940195
H,0,0.8515375676,-3.6682723188,3.3337616513
C,0,-2.5638360051,0.1870454854,2.298993142
O,0,-1.8091976567,0.1438422063,3.4935767237
C,0,-3.0509586621,-1.2162921178,1.9218725109
C,0,-4.2256931486,-1.4356979072,1.1937964607
C,0,-2.2327370609,-2.3084761354,2.231399799
C,0,-4.5823101412,-2.7222799306,0.7910542438
C,0,-2.5887781972,-3.5939351936,1.8258505261
C,0,-3.7641567105,-3.8070713025,1.1060732347
H,0,-4.8678032286,-0.6008387893,0.9288099027
H,0,-1.2989375721,-2.1570357008,2.7701646644
H,0,-5.4992238096,-2.8742455185,0.229807078
H,0,-1.9397884835,-4.4296106644,2.0722809437
H,0,-4.0417076446,-4.8089781853,0.7930869019
C,0,-3.7107299646,1.1993438887,2.4609553732
C,0,-3.6029876504,2.5343419413,2.0565666986
C,0,-4.8748820589,0.8103321986,3.1348957667
C,0,-4.6272386249,3.4471852067,2.311186099
C,0,-5.9001468266,1.7164478371,3.3913500226
C,0,-5.7803798023,3.0427467359,2.9790588584
H,0,-2.7253674613,2.8908248164,1.5280057091
H,0,-4.9850142627,-0.2183627884,3.4671482875
H,0,-4.5189355173,4.4759498449,1.9821131052
H,0,-6.789955883,1.3854264544,3.9181713157
H,0,-6.5774321709,3.7530377482,3.174975231
Si,0,-2.1749317048,-0.1286408639,5.1190710619
C,0,-3.2035037595,1.2662038666,5.854284191
H,0,-4.2788346207,1.0859866493,5.7850046461
H,0,-2.9423207025,1.3709636861,6.9138105155
H,0,-2.9877382882,2.2183539911,5.3566596386
C,0,-3.0401834399,-1.7741082229,5.3814811781
H,0,-3.9629634608,-1.8667925438,4.799448616
H,0,-2.3870130194,-2.6092150126,5.110367691
H,0,-3.2984161055,-1.8693736572,6.4426673421
C,0,-0.499038378,-0.1183424734,5.9401090463
H,0,-0.5940597338,-0.4434271766,6.982637277
H,0,0.2249080884,-0.7685730862,5.4377862809
H,0,-0.0875688267,0.8974607495,5.9468852084
C,0,3.7148225249,2.332997042,3.8789870193
H,0,4.1862763133,2.9484881855,4.6496078617
H,0,4.5062489727,1.9026332947,3.2576004521
H,0,3.1009431171,2.9817605788,3.2477139104

7a anti-syn-up

M06-2X/6-31+G**, $E = -1503.82150864$ a.u.

Thermal correction to Gibbs Free Energy = 0.464970 a.u.

SP at B2PLYP/6-311+G**, $E = -1503.2759750843$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1503.3047953623$ a.u.

O,1
C,0,-1.7634186016,-1.5293295809,-4.1603802176
C,0,-0.6265178408,-0.760920077,-3.5638039477
H,0,0.2729314959,-0.692930428,-4.169093768
C,0,-0.6940540833,-0.1320926593,-2.3663813003
H,0,-1.6026316883,-0.1609806561,-1.7716009702
N,0,0.3173444078,0.5701093723,-1.7876203139
C,0,1.6510796519,0.5960132199,-2.3655523035
C,0,0.2173866162,1.211630379,-0.4856214602
C,0,2.5026854094,1.3686127143,-1.3497490884
C,0,1.6832042954,1.342152306,-0.0457692056
H,0,1.6394114653,1.0852318629,-3.3493435883
H,0,2.6514320819,2.3944438018,-1.6911694852
H,0,2.0029183969,-0.4363772237,-2.5104926775
H,0,3.4863309187,0.9126943307,-1.2195333294
H,0,1.8553467967,2.2254018338,0.5756183927

H,0,1.9497259437,0.4640523935,0.5500335298
H,0,-0.3497115921,0.5496977806,0.1761445808
C,0,-0.5935128494,2.5524548139,-0.5424125648
H,0,-1.3801033225,-2.4381804165,-4.6461621423
O,0,-2.2623192727,-0.6808323135,-5.2262044421
O,0,-3.1695636936,-1.4474957798,-6.0246391902
H,0,-2.626817375,-1.6530729976,-6.8010859564
C,0,-2.8995331424,-1.8992856609,-3.2205119099
H,0,-3.3439554353,-1.0029689585,-2.7795741118
H,0,-3.6774621995,-2.4278193631,-3.7749042803
H,0,-2.5375906358,-2.5488515459,-2.4189377577
O,0,-1.8744905254,2.13237546,-0.9917238529
Si,0,-3.390373687,2.8585134503,-0.999362013
C,0,-3.3599672351,4.5525465007,-1.805540107
H,0,-3.000491749,4.4832011338,-2.8370325122
H,0,-4.3769193624,4.9608863792,-1.8241550916
H,0,-2.7224752007,5.2636245058,-1.2728575897
C,0,-4.108999248,2.9390679172,0.7320266388
H,0,-3.586325078,3.6576760617,1.3705754802
H,0,-5.1655344252,3.2261021399,0.6822366011
H,0,-4.0473067256,1.9540345487,1.2072526919
C,0,-4.3943703538,1.6729634799,-2.0435601917
H,0,-4.488609422,0.7037454766,-1.5423827785
H,0,-5.4030267514,2.0625708496,-2.2171918025
H,0,-3.9164885141,1.5110265392,-3.0162735547
C,0,0.0502620859,3.4756466031,-1.5781639101
C,0,-0.2948303429,3.3285494163,-2.925635195
C,0,1.064076893,4.3809577309,-1.2438632679
C,0,0.3485163007,4.0736175536,-3.9130530027
C,0,1.7076067838,5.1294988415,-2.2284215503
C,0,1.3530493034,4.9773067567,-3.5682788199
H,0,-1.0696829354,2.6174431286,-3.1985382562
H,0,1.3642180861,4.5031868787,-0.2070199281
H,0,0.0656980277,3.9425536324,-4.9533259713
H,0,2.4895535873,5.8278651626,-1.24386350271
H,0,1.8541899495,5.5581978768,-4.336488751
C,0,-0.7409010065,3.193605413,0.8471636838
C,0,-0.9933439381,4.5651508824,0.9802241729
C,0,-0.7706000107,2.4098162567,2.0076396711
C,0,-1.2643083514,5.1356000134,2.224788433
C,0,-1.0386330788,2.9757651582,3.2534920309
C,0,-1.2891541339,4.3416136917,-3.3677145266
H,0,-0.9818950364,5.2031677879,0.1030286677
H,0,-0.5913470033,1.3414721958,1.9607989821
H,0,-1.4584726672,6.2015812487,2.2914477106
H,0,-1.0533798075,2.3431766475,4.1356158951
H,0,-1.4992324984,4.7822275328,4.3373104102

7a anti-anti-down

M06-2X/6-31+G**, $E = -1503.82287528$ a.u.

Thermal correction to Gibbs Free Energy = 0.464933 a.u.

SP at B2PLYP/6-311+G**, $E = -1503.2777847952$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1503.3064955904$ a.u.

O,1
C,0,-0.6839294661,-1.3005711052,-4.5917840166
C,0,0.3032698538,-0.2260562214,-4.2821861018
H,0,-0.0050277647,0.8032397346,-4.4501062222
C,0,1.5295556438,-0.5276123531,-3.7938543962
H,0,1.7902486113,-1.5655278654,-3.600054445
N,0,2.5122262292,0.3588850462,-3.4879662581
C,0,2.4090620892,1.7657178362,-3.841353736
C,0,3.781079587,-0.016194004,-2.8847720239
C,0,3.7505501534,2.3744087768,-3.4091023032
C,0,4.6939188773,1.1696028334,-3.2274420689
H,0,1.5611227594,2.2371404862,-3.3259067409
H,0,3.6293468808,2.9144289569,-2.468049064
H,0,2.2328468306,1.8547957729,-4.923220311
H,0,4.1314998338,3.0782348962,-4.151898806
H,0,5.4529336025,1.3441362919,-2.4598400916

H,0,5.2150287501,0.9520958248,-4.1646008205
H,0,4.1192774807,-0.9444332942,-3.3565207394
C,0,3.6353744331,-0.3414337655,-1.358051137
H,0,-0.3340660521,-2.2638266301,-4.1954809629
O,0,-0.6897708723,-1.4151021527,-6.03775354
O,0,-1.5186408571,-2.5219669397,-6.4052047608
H,0,-2.3316637452,-2.0848743243,-6.7008325782
C,0,-2.0819962846,-0.9904433985,-4.0749792384
H,0,-2.4310578662,-0.0363367267,-4.4843725347
H,0,-2.7933214298,-1.7757711387,-4.3423652573
H,0,-2.0569660329,-0.9091307101,-2.9849214513
O,0,2.6890428907,-1.3972599724,-1.347335835
Si,0,2.2603485287,-2.6189627804,-0.2811172893
C,0,1.8241655763,-1.9706925203,1.426162464
H,0,1.1719557862,-1.0938294166,1.3585583993
H,0,1.2853023105,-2.7527656068,1.9734577698
H,0,2.7047365818,-1.7011945937,2.0153226156
C,0,3.5972987166,-3.9304348879,-0.180820935
H,0,4.5212727479,-3.5446626468,0.2615122238
H,0,3.2492035122,-4.7720268699,0.4286094344
H,0,3.8306147347,-4.310926519,-1.1810954908
C,0,0.7270278368,-3.3149960493,-1.103263783
H,0,0.9713936883,-3.7291030674,-2.0874235371
H,0,0.2789925743,-4.1119872675,-0.5008041812
H,0,-0.0216030706,-2.5268845003,-1.2438661871
C,0,3.0584117709,0.8799080837,-0.6411105134
C,0,1.6739170814,1.0785670091,-0.6432315692
C,0,3.8753911372,1.8692122421,-0.081438526
C,0,1.1187122972,2.235694478,-0.0982816352
C,0,3.3229696766,3.0264619474,0.4654717674
C,0,1.9413245318,3.2156308929,0.4568451322
H,0,1.0319031685,0.3223461234,-1.0865211624
H,0,4.9543750457,1.7432849455,-0.0741604328
H,0,0.0414821533,2.372597956,-0.1122504212
H,0,3.9752002553,3.7805818591,0.895326888
H,0,1.5102852423,4.1171683823,0.8811418642
C,0,4.9492959962,-0.8398546894,-0.739484459
C,0,5.1136799124,-0.8222741698,0.6521414346
C,0,5.9463029209,-1.4490067598,-1.5092128492
C,0,6.2278509411,-1.3994601011,1.2569093056
C,0,7.066345414,-2.0250929618,-0.9085908098
C,0,7.2104001915,-2.0079747285,0.4767913897
H,0,4.3605476155,-0.3503130549,1.2755099038
H,0,5.8683990595,-1.4907060665,-2.5898811982
H,0,6.3257512014,-1.3737885671,2.3379122007
H,0,7.8248418317,-2.4912560624,-1.5299536507
H,0,8.0795972587,-2.4607621982,0.9433544381

7a anti-syn-down

M06-2X/6-31+G**, $E = -1503.82248554$ a.u.
Thermal correction to Gibbs Free Energy = 0.466353 a.u.
SP at B2PLYP/6-311+G**, $E = -1503.2758235097$ a.u.
SP at mPW2PLYP/6-311+G**, $E = -1503.3047314920$ a.u.

0,1
C,0,-2.031737601,-0.4751857189,-4.1652646375
C,0,-0.7197021132,-0.6890523754,-4.8615938645
H,0,-0.767841677,-0.7428359136,-5.9465192382
C,0,0.4663247377,-0.8371347246,-4.2231459874
H,0,0.5329920935,-0.7374004332,-3.1422875677
N,0,1.6606279276,-1.092685819,-4.825410827
C,0,1.7232031742,-1.4554852893,-6.2336020132
C,0,2.879907862,-1.3897049683,-4.0842715466
C,0,3.1799136271,-1.8670396414,-6.4629757199
C,0,3.6917360652,-2.2514151609,-5.0636033625
H,0,1.4250795711,-0.6100671225,-6.8671670716
H,0,3.7469001037,-1.025313274,-6.8658768522
H,0,1.0213618252,-2.281845522,-6.4281553337
H,0,3.2589409861,-2.6953615873,-7.1701038325
H,0,4.7693638164,-2.1033980451,-4.9528061199

H,0,3.4817025837,-3.3064469413,-4.8621113954
H,0,2.6031292023,-1.9479292459,-3.1848381562
C,0,3.5970271598,-0.0915342588,-3.5778390662
H,0,-2.5970692615,0.3145457381,-4.6766836596
O,0,-2.9080600384,-1.6061337257,-4.408683061
O,0,-2.3449018345,-2.7649793754,-3.033659644
H,0,-1.5390593502,-2.9042053724,-4.3334378042
C,0,-1.9709983005,-0.1633832626,-2.6784920984
H,0,-1.4417515347,0.7774907305,-2.5102785253
H,0,-2.9868396591,-0.0674163391,-2.2876117564
H,0,-1.4645567514,-0.9567096431,-2.123379805
O,0,2.6163353445,0.5172051765,-2.7484433127
Si,0,2.7005453219,1.6610957874,-1.5181533413
C,0,0.8906410607,2.0219506125,-1.2035439664
H,0,0.3666531013,1.1153144087,-0.883111285
H,0,0.7692454934,2.7795327368,-0.4224484824
H,0,0.4097926382,2.3906342053,-2.1162558467
C,0,3.5705722726,3.2337348321,-2.0612561295
H,0,3.1986411975,3.5697175102,-3.0344986869
H,0,3.3664186314,4.0221711551,-1.327618632
H,0,4.655320546,3.1174824505,-2.1295981181
C,0,3.4845293399,0.9562936899,0.0332580753
H,0,4.5524371992,0.7527200169,-0.0908651997
H,0,3.3632305029,1.6690443448,0.857063938
H,0,2.9887557685,0.0222229981,0.3186372933
C,0,3.8967081616,0.8055465789,-4.7787870056
C,0,5.0955111293,0.7174563477,-5.4961090782
C,0,2.892409927,1.6522641122,-5.2601176098
C,0,5.2893729626,1.4609860492,-6.6593882146
C,0,3.0823058408,2.3953566103,-6.4245302954
C,0,4.2818289476,2.3021258341,-7.1298998079
H,0,5.8872872871,0.0570605206,-5.1544934224
H,0,1.9536691299,1.7173401164,-4.7178384949
H,0,6.2284658933,1.3785614076,-7.1981012368
H,0,2.2891447508,3.0452545408,-6.7820930439
H,0,4.4311337693,2.8801131473,-8.0367958837
C,0,4.8368733463,-0.4161098563,-2.7292505696
C,0,5.8513528166,0.5357064087,-2.5594755076
C,0,4.9233370341,-1.6007638146,-1.9877153664
C,0,6.9087823941,0.3183446828,-1.6782499991
C,0,5.9809589513,-1.8247814424,-1.1070671893
C,0,6.9774482909,-0.8646352529,-0.9442981941
H,0,5.8188574665,1.4640731566,-3.1201578063
H,0,4.1638686425,-2.3695091778,-2.0766148376
H,0,7.6765022963,1.07754979,-1.5646028871
H,0,6.0200620881,-2.7523571502,-0.5443756421
H,0,7.7977134648,-1.0367470665,-0.2545598768

7a anti-anti-up

M06-2X/6-31+G**, $E = -1503.82382256$ a.u.
Thermal correction to Gibbs Free Energy = 0.466039 a.u.
SP at B2PLYP/6-311+G**, $E = -1503.2764945488$ a.u.
SP at mPW2PLYP/6-311+G**, $E = -1503.3055494308$ a.u.

0,1
C,0,-0.8080925224,-1.2114405871,-4.2797229955
C,0,0.2163925279,-0.137349803,-4.12690079
H,0,-0.0813691402,0.8857616989,-4.3428249026
C,0,1.4499601844,-0.4428411524,-3.6588996155
H,0,1.692078686,-1.4788785839,-3.4366214688
N,0,2.464090215,0.4264152791,-3.4133752924
C,0,2.3639606195,1.8358984851,-3.7572371904
C,0,3.7634094866,0.0244069981,-2.8937531015
C,0,3.7000313468,2.4330026735,-3.3030545268
C,0,4.6565860394,1.2287715621,-3.2323171686
H,0,1.5090922989,2.2990787784,-3.2461510866
H,0,3.5862409135,2.8912847559,-2.3173088384
H,0,2.2025597995,1.9401098777,-4.840709354
H,0,4.0587281427,3.1994408672,-3.9930654201
H,0,5.4538244563,1.3749800928,-2.4985252939

H,0,5.1256182904,1.0594908298,-4.2066625064
H,0,4.0787916559,-0.8848488594,-3.4175541712
C,0,3.7085258467,-0.3543853535,-1.3724356342
H,0,-0.3250476893,-2.1980882602,-4.2271314526
O,0,-1.6587385253,-1.101699612,-3.1077209864
O,0,-2.5144495095,-2.2461678873,-3.0626020528
H,0,-2.0380518073,-2.8197926787,-2.4394082705
C,0,-1.6510667542,-1.096168033,-5.5400029034
H,0,-1.0238344144,-1.2485617595,-6.4226261944
H,0,-2.4496686178,-1.8417586185,-5.5422128497
H,0,-2.0980172953,-0.098635151,-5.5992803726
O,0,2.7269424085,-1.3740167853,-1.3229563096
Si,0,1.9819911957,-2.3446423832,-0.1764733925
C,0,1.5001479797,-1.4412283423,1.3993177749
H,0,0.7072949519,-0.7118012713,1.2081799336
H,0,1.1190795955,-2.1787543158,2.1154809756
H,0,2.3317705135,-0.912564831,1.8740011294
C,0,3.0494998987,-3.833703264,0.2298325536
H,0,3.8884177332,-3.577054766,0.8825303405
H,0,2.4424839234,-4.5927750862,0.7361444536
H,0,3.4535813614,-4.2771573721,-0.6862544793
C,0,0.4265549768,-2.8861323325,-1.0751855692
H,0,0.676367068,-3.4789923937,-1.9626009134
H,0,-0.2113676104,-3.4931837985,-0.423486229
H,0,-0.1330984653,-1.9996760357,-1.3988336558
C,0,3.2540535156,0.8663477649,-0.5727117892
C,0,1.8950971014,1.2018217748,-0.5697756052
C,0,4.1597673904,1.7314967738,0.0498214507
C,0,1.4520499953,2.3743510637,0.037561258
C,0,3.7184288661,2.9061448324,0.6594384961
C,0,2.3633282057,3.2336445734,0.6524444474
H,0,1.1834197021,0.5413269943,-1.0590917259
H,0,5.2200553694,1.4962497128,0.0555675153
H,0,0.3938234885,2.6181290947,0.026861502
H,0,4.4368011538,3.5659473817,1.1363575751
H,0,2.0194921303,4.1489584755,1.124413184
C,0,5.043771581,-0.9269065469,-0.8755747168
C,0,5.2054476546,-1.1597273003,0.4966632388
C,0,6.084163414,-1.3026423933,-1.7302712476
C,0,6.3581859223,-1.7526558924,1.0015566805
C,0,7.2460993996,-1.8944325427,-1.2291205233
C,0,7.3875569653,-2.1249238456,0.1361916153
H,0,4.4186564943,-0.8624120875,1.1849868754
H,0,6.0162281087,-1.1369883854,-2.7997716899
H,0,6.4534027445,-1.9214432038,2.0699215537
H,0,8.040365037,-2.1741433762,-1.9143626327
H,0,8.291010896,-2.5846922775,0.5243263564

7a *syn-anti-down*

M06-2X/6-31+G**, $E = -1503.81749158$ a.u.

Thermal correction to Gibbs Free Energy = 0.465549 a.u.

SP at B2PLYP/6-311+G**, $E = -1503.2724315962$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1503.3011482088$ a.u.

O,1
C,0,0.510557005,-2.5381101627,-4.6730125005
C,0,1.4290139613,-1.7195795868,-3.8248291089
H,0,2.070204644,-2.2357469919,-3.1161259091
C,0,1.4663846566,-0.3764838265,-3.9607979474
H,0,0.7520251334,0.0887166608,-4.6421855808
N,0,2.2997472783,0.5328225876,-3.3640293518
C,0,2.2924252429,1.9116648387,-3.8743957665
C,0,3.5915778479,0.1451980377,-2.8064687401
C,0,3.6784065723,2.4734383734,-3.5375456823
C,0,4.5546204357,1.2286617672,-3.3184811589
H,0,1.4915991723,2.4944309688,-3.4057245187
H,0,3.632832918,3.0810012609,-2.6317709428
H,0,2.1200815415,1.9003741585,-4.9581298057
H,0,4.0596657552,3.1036531252,-4.3440038403
H,0,5.384291491,1.4129361176,-2.6301675387

H,0,4.9810078122,0.8952977408,-4.2697670007
H,0,3.8331523403,-0.8401002996,-3.2190060078
C,0,3.5576429682,-0.0236045171,-1.2523339377
H,0,-0.2550465971,-1.8962423673,-5.1329663144
O,0,1.342281287,-3.043251195,-5.7489077182
O,0,0.5128916996,-3.7643061267,-6.6655330941
H,0,0.4113441308,-3.1234165166,-7.385839755
C,0,-0.1429529416,-3.6928815235,-3.9301709784
H,0,-0.8178667042,-3.3024314087,-3.1634740506
H,0,-0.7156461138,-4.3222366617,-4.6144098063
H,0,0.6227053304,-4.3058659573,-3.4426134439
O,0,2.5371084222,-0.9843613478,-1.0328713665
Si,0,2.1990040036,-2.0407300994,0.23028480345
C,0,2.1414498429,-1.1922108411,1.9093496477
H,0,1.7969473471,-0.1561644538,1.8234969437
H,0,1.4340596669,-1.7301842035,2.5508230727
H,0,3.1123372011,-1.1932581652,2.4119891588
C,0,3.4081660542,-3.4756610137,0.2525000503
H,0,4.4214971998,-3.1617627784,0.5238353974
H,0,3.0746114593,-4.2267791504,0.9778712877
H,0,3.4490402088,-3.9528007833,-0.7330735398
C,0,0.4915382525,-2.6655803421,-0.2137685113
H,0,0.5189008809,-3.2115079238,-1.1614654671
H,0,0.1107116233,-3.3406238882,0.5599930614
H,0,-0.2125728661,-1.8339434888,-0.3240737761
C,0,3.1550495226,1.3070350267,-0.6109340213
C,0,1.7965379338,1.6230741134,-0.5061592492
C,0,4.0961416319,2.2680324975,-0.2242790638
C,0,1.3881451723,2.8670947506,-0.0262638359
C,0,3.6912216543,3.5118915136,0.258221726
C,0,2.334317845,3.8173874211,0.3568149604
H,0,1.0626853286,0.8832177456,-0.8109501196
H,0,5.1577228141,2.0517204515,-0.3023250397
H,0,0.3285319561,3.0936440156,0.0466137919
H,0,4.4383784928,4.2415154505,0.5557644913
H,0,2.016846532,4.7854624621,0.7319417428
C,0,4.8877002468,-0.5740982814,-0.7104591754
C,0,5.2041317291,-0.4232050127,0.6460933411
C,0,5.7426726,-1.3546103783,-1.4974752308
C,0,6.3248057345,-1.0357963525,1.2022836997
C,0,6.8692928177,-1.9662478598,-0.9468590747
C,0,7.1639978087,-1.8142201055,0.4061328322
H,0,4.5646648721,0.1810804519,1.2812412007
H,0,5.5454996942,-1.5078279185,-2.5523803473
H,0,6.5396800728,-0.9035190675,2.2583885885
H,0,7.5134249072,-2.5673773291,-1.5811445798
H,0,8.0383399481,-2.2936282953,0.8350530593

7a *syn-syn-up*

M06-2X/6-31+G**, $E = -1503.81457960$ a.u.

Thermal correction to Gibbs Free Energy = 0.466827 a.u.

SP at B2PLYP/6-311+G**, $E = -1503.2674386216$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1503.2964446697$ a.u.

O,1
C,0,-1.1342727687,-0.9651882125,-2.034611407
C,0,0.2054879286,-0.8521075061,-2.6993799043
H,0,1.045672213,-0.6476349184,-2.0428504823
C,0,0.3921469838,-0.9582568284,-4.028728895
H,0,-0.473197951,-1.0997184408,-4.6754184948
N,0,1.5749201811,-0.9378545953,-4.7384892805
C,0,1.5207399325,-1.426588884,-6.1255980965
C,0,2.8508839457,-1.2464968605,-4.0962189497
C,0,2.95739928,-1.8270332817,-6.4577368106
C,0,3.5533824679,-2.1878855205,-5.0890949212
H,0,1.1387063041,-0.6484960736,-6.7953366305
H,0,3.4933878899,-0.987606372,-6.9074109582
H,0,0.8493370698,-2.2945377635,-6.1906553946
H,0,2.9903392937,-2.6646911332,-7.158039901
H,0,4.6426732775,-2.096251023,-5.0606917441

H,0,3.3020707782,-3.2226330324,-4.8333279935
H,0,2.6206416927,-1.7523418742,-3.1521969885
C,0,3.6739362661,0.0291053118,-3.7174673781
H,0,-1.0440938983,-1.6360161103,-1.1691289996
O,0,-1.4893808103,0.2585143171,-1.3445073878
O,0,-1.7462141077,1.2767666102,-2.309240718
H,0,-2.714622579,1.3176517157,-2.30080541
C,0,-2.2932428044,-1.440990238,-2.8989917291
H,0,-2.0997235953,-2.4497626219,-3.2720054782
H,0,-3.2082470247,-1.4634092276,-2.3007601242
H,0,-2.4549880417,-0.7812261484,-3.7549055363
O,0,2.7857040556,0.7924318807,-2.9207625771
Si,0,2.9939238435,1.9338694495,-1.7055822535
C,0,1.2665559817,2.6085801622,-1.4732252878
H,0,0.5471199496,1.8092997677,-1.2681141623
H,0,1.2428883588,3.325392713,-0.6447837793
H,0,0.933410523,3.1247789216,-2.3803129808
C,0,4.15091477,3.3316392653,-2.2175425836
H,0,4.1974686898,3.4211219281,-3.3087615458
H,0,3.7717419929,4.2791114988,-1.8188716867
H,0,5.1673491699,3.189776869,-1.8395206053
C,0,3.5918199366,1.1202728456,-0.1224765624
H,0,4.6208337444,0.7561338979,-0.2083793996
H,0,3.5495667028,1.8402284563,0.7028842996
H,0,2.9488860646,0.2715647786,0.1362356263
C,0,4.0105807407,0.8092002615,-4.9896958207
C,0,5.1863668378,0.5872586729,-5.7150958803
C,0,3.0588814748,1.6923121224,-5.5112295145
C,0,5.4058124004,1.2279438157,-6.9339415232
C,0,3.2756975843,2.3342725372,-6.730303956
C,0,4.448603988,2.1018035333,-7.4484728713
H,0,5.9397505975,-0.0962170895,-5.3343850043
H,0,2.143585855,1.8640915309,-4.9535796545
H,0,6.3252484058,1.0410922649,-7.4804502008
H,0,2.5252256662,3.015450254,-7.1203755259
H,0,4.6173833316,2.600118863,-8.3981812936
C,0,4.9206946303,-0.3311267325,-2.8900834307
C,0,5.9621189321,0.5982407642,-2.7617327737
C,0,5.0038611688,-1.5097268241,-2.1393872556
C,0,7.0347390481,0.3724027636,-1.9022514119
C,0,6.0793436577,-1.7445626618,-1.2823369713
C,0,7.0968969401,-0.8023610524,-1.1534842375
H,0,5.9357172274,1.5168779835,-3.3395457715
H,0,4.2311354069,-2.2674385724,-2.2020812678
H,0,7.8211309104,1.1165188796,-1.8184836986
H,0,6.114824819,-2.6672842008,-0.7114281425
H,0,7.9299994484,-0.982483533,-0.4812918788

7a *syn-anti-up*

M06-2X/6-31+G**, $E = -1503.81754871$ a.u.
Thermal correction to Gibbs Free Energy = 0.465524 a.u.
SP at B2PLYP/6-311+G**, $E = -1503.2727067423$ a.u.
SP at mPW2PLYP/6-311+G**, $E = -1503.3014478342$ a.u.

0,1
C,0,-0.295870729,-1.8367853545,-5.3387886107
C,0,1.0557891063,-1.2995101283,-4.9979310749
H,0,1.8282111153,-1.3689800472,-5.7585608145
C,0,1.3093146375,-0.7632317714,-3.7863752189
H,0,0.5130163797,-0.7742298956,-3.0404323925
N,0,2.4530365996,-0.1529227845,-3.3321646336
C,0,2.3428434089,0.6654055258,-2.1143959101
C,0,3.4664418844,0.3551888347,-4.2541725268
C,0,3.5287463937,1.6295100048,-2.1787794811
C,0,3.8375994206,1.7321028652,-3.6808177198
H,0,2.3703583859,0.0333247749,-1.220220433
H,0,4.3826225488,1.2217017274,-1.6329629692
H,0,1.3910909997,1.2139197183,-2.1190777289
H,0,3.2815052554,2.5994511034,-1.7415791073
H,0,4.8768675668,2.0059307195,-3.8831203317

H,0,3.198712394,2.4911284998,-4.1438735397
H,0,2.9910098991,0.4411233791,-5.2371890851
C,0,4.6695068298,-0.6284677364,-4.4316726777
H,0,-1.0174273316,-1.5978276909,-4.544329889
O,0,-0.144167183,-3.2758582817,-5.3639337238
O,0,-1.4242855426,-3.8619251179,-5.6176356664
H,0,-1.6722262537,-4.178924051,-4.7358250615
C,0,-0.8017252879,-1.338626312,-6.6861222672
H,0,-0.062884753,-1.5599038259,-7.4634014116
H,0,-1.7480925398,-1.814398069,-6.9510694247
H,0,-0.9496113768,-0.2561132837,-6.6459379004
O,0,4.0599262319,-1.845058854,-4.8242407591
Si,0,4.5830407027,-3.2010571907,-5.6665006994
C,0,6.2093448709,-3.8911143419,-5.0074702652
H,0,6.3649605439,-3.6041107675,-3.9615824476
H,0,6.1794269117,-4.9854052463,-5.0545314511
H,0,7.0705802313,-3.5530845097,-5.5905018247
C,0,4.7166573688,-2.8212816249,-7.500265295
H,0,5.5299963248,-2.1200195481,-7.716611456
H,0,4.9011663923,-3.7448909183,-8.0606892023
H,0,3.7809594047,-2.3844359669,-7.8668751492
C,0,3.2113074977,-4.4325294591,-5.3512854602
H,0,2.2381227307,-4.0247732233,-5.6431488634
H,0,3.3873777296,-5.358085428,-5.9103665263
H,0,3.1635655515,-4.6821362014,-4.2854291942
C,0,5.3668871839,-0.8192397814,-3.0824652748
C,0,4.8509207835,-1.759901923,-2.1846688725
C,0,6.4334614773,-0.0136066877,-2.6679845973
C,0,5.3851641301,-1.8903367159,-0.9032393104
C,0,6.9709494208,-0.1429342353,-1.3878576237
C,0,6.4464360944,-1.0804434646,-0.4986488553
H,0,4.0218704432,-2.3844348968,-2.5019543657
H,0,6.8524147385,0.7255983421,-3.3446922533
H,0,4.9708412184,-2.6254459155,-0.2196779858
H,0,7.8009660431,0.489379358,-1.0877104592
H,0,6.8650387908,-1.1831286392,0.4977985858
C,0,5.6283798913,-0.1625601773,-5.5405686253
C,0,6.924411859,-0.6920764349,-5.6035166131
C,0,5.2134460652,0.6728715244,-6.5838037497
C,0,7.7704335118,-0.4137881361,-6.6745375391
C,0,6.0592774922,0.9607041163,-7.6558134084
C,0,7.3390846237,0.4142341337,-7.7103151663
H,0,7.2787290984,-1.3362049217,-4.8049158134
H,0,4.2226192865,1.1125299154,-6.5864933618
H,0,8.7667040883,-0.8451665561,-6.6980697353
H,0,5.7098674283,1.6119081166,-8.4511111816
H,0,7.9944090112,0.6342444563,-8.5473065998

7a *syn-syn-down*

M06-2X/6-31+G**, $E = -1503.81636002$ a.u.
Thermal correction to Gibbs Free Energy = 0.467176 a.u.
SP at B2PLYP/6-311+G**, $E = -1503.2707736508$ a.u.
SP at mPW2PLYP/6-311+G**, $E = -1503.2995439738$ a.u.

0,1
C,0,-2.8416968404,-1.6252110404,-2.3314173896
C,0,-1.9250803536,-0.5571469725,-1.81886565
H,0,-2.3104472009,0.054216817,-1.009958848
C,0,-0.7093875515,-0.3043378621,-2.3436234465
H,0,-0.3689956322,-0.8898172899,-3.196485355
N,0,0.2166415106,0.6353957329,-1.9580181623
C,0,1.5875729581,0.4740770503,-2.4656121213
C,0,0.1780183701,1.2866545103,-0.6504760076
C,0,2.4553351154,1.3021938658,-1.518816873
C,0,1.6509891706,1.323264271,-0.2099930933
H,0,1.6584706399,0.819382757,-3.5030464501
H,0,2.5852384065,2.3127937406,-1.9106491409
H,0,1.874904897,-0.5859235554,-2.4352539859
H,0,3.4450040739,0.8590702618,-1.3884218183
H,0,1.8819100237,2.1892065347,0.4165827183

H,0,1.8667291053,0.4242606321,0.3763561108
H,0,-0.428139061,0.6574052831,0.0107368336
C,0,-0.5256061822,2.6852794418,-0.6935547914
H,0,-3.8350428381,-1.1949209529,-2.5313081467
O,0,-3.0106097475,-2.5256364257,-1.2094553723
O,0,-4.1056178718,-3.3983966607,-1.4960745456
H,0,-4.8170157787,-3.0072084563,-0.9659713005
C,0,-2.376289845,-2.4012174954,-3.5521148625
H,0,-1.4062922476,-2.8715000215,-3.3656058128
H,0,-3.1018009805,-3.184050782,-3.7815456045
H,0,-2.2925567175,-1.7419677537,-4.4206925178
O,0,-1.8142741843,2.4034512529,-1.2105981326
Si,0,-3.3311658268,3.1053701553,-1.0781114136
C,0,-3.3517181364,4.883645795,-1.6849435495
H,0,-2.7791815534,4.985684671,-2.6129730701
H,0,-4.3868045754,5.1792530164,-1.8911631884
H,0,-2.9461621357,5.5845261713,-0.9506031581
C,0,-3.9994028981,2.9808150735,0.6715404381
H,0,-3.4729555235,3.6386539541,1.3701432815
H,0,-5.062631258,3.2470080882,0.6799940924
H,0,-3.905259672,1.9516093449,1.0356499276
C,0,-4.3704735092,2.038839272,-2.2164873891
H,0,-4.4906029423,1.0348671063,-1.7965761703
H,0,-5.3663872235,2.4724051152,-2.3559387062
H,0,-3.8941544174,1.9377949087,-3.1973438041
C,0,0.2223127523,3.598082155,-1.6677230995
C,0,-0.0772049456,3.5162333037,-3.031389884
C,0,1.2703861288,4.4321463009,-1.2617130109
C,0,0.6535562195,4.2471140368,-3.9674491248
C,0,2.000903499,5.1665774875,-2.1949163268
C,0,1.6972355539,5.0743391669,-3.5528366411
H,0,-0.8865087843,2.866355359,-3.3488956854
H,0,1.5279690982,4.5098329828,-0.2092307694
H,0,0.4073736613,4.1687635811,-5.0222952704
H,0,2.8090532409,5.8091160598,-1.5888252163
H,0,2.2662166995,5.6449504461,-4.2804636538
C,0,-0.6658812457,3.2970305345,0.7100800028
C,0,-0.9070688189,4.670181915,0.851252493
C,0,-0.6953697799,2.5064856546,1.8648617716
C,0,-1.1770122379,5.234952995,2.095467328
C,0,-0.9612648176,3.0675050119,3.1142581344
C,0,-1.2074272097,4.4330167363,3.2359914397
H,0,-0.8836517363,5.3107097885,-0.0246144629
H,0,-0.5158871519,1.438391186,1.8134569103
H,0,-1.3633954675,6.3018817652,2.1718730954
H,0,-0.9771472367,2.4302827778,3.9930143188
H,0,-1.4159964409,4.8686774049,4.2081761796

TS-10a anti-syn-up

M06-2X/6-31+G**, $E = -1580.19196516$ a.u.

Thermal correction to Gibbs Free Energy = 0.486613 a.u.

1 imaginary frequency = -640.89 cm^{-1}

SP at B2PLYP/6-311+G**, $E = -1579.6664049052$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1579.6918398164$ a.u.

0,1

C,0,-1.4205323455,-1.089361201,-3.3703247154
C,0,-0.1954740586,-0.2531690515,-3.5447154758
H,0,-0.3336971994,0.7880869572,-3.8074787648
C,0,1.0601017995,-0.7405511021,-3.1852039812
H,0,1.1522594028,-1.7492935978,-2.7946189633
N,0,2.1862225803,-0.0508276514,-3.2106625309
C,0,2.3283442051,1.3023162364,-3.7528864788
C,0,3.4356682245,-0.5142601504,-2.5814996998
C,0,3.8037387588,1.341942336,-4.1486789792
C,0,4.5033699026,0.4709462328,-3.090625107
H,0,3.6155228647,-1.5374905357,-2.9220978431
C,0,3.2700028649,-0.5828459935,-1.0206567364
O,0,-1.2215470912,-0.6372856323,-2.0702892851
O,0,-2.7170206165,-1.1893216844,-1.047644072

H,0,-2.2163052893,-1.568911446,-0.3134948692
H,0,-2.8490162452,0.4430426404,-0.8873570491
O,0,2.3530342463,-1.646948722,-0.8417657491
O,0,-2.8490177056,1.4428334788,-0.895299664
H,0,-2.1631135475,1.6508883563,-1.5391868058
C,0,2.6546820455,0.7343639709,-0.5293700238
C,0,3.432316478,1.8741882469,-0.285472496
C,0,1.2635166364,0.8491192096,-0.4319951479
C,0,2.8360964052,3.0936450908,0.033900275
H,0,4.5159374385,1.8170775877,-0.3229990418
C,0,0.6640502978,2.0663454198,-0.1105488234
H,0,0.6329286844,-0.0130588149,-0.6261446327
C,0,1.4483459259,3.1963277281,0.1177244114
H,0,3.4609870215,3.9610449829,0.2232074359
H,0,-0.4190988944,2.121982608,-0.0403300227
H,0,0.9838315583,4.145429423,0.3667539754
C,0,4.5950918744,-0.9472021394,-0.3388796524
C,0,4.8675506912,-0.5405960395,0.9721177543
C,0,5.4892623657,-1.830472571,-0.9562477371
C,0,5.9990373628,-0.9988573021,1.6459652746
H,0,4.1904648447,0.1372920433,1.4809474924
C,0,6.6245045522,-2.2854521206,-0.288759088
H,0,5.3041487883,-2.190199293,-1.9633837605
C,0,6.883123647,-1.8732369938,1.0177093237
H,0,6.1850594825,-0.6714229382,2.664149579
H,0,7.3026364682,-2.9695706857,-0.7893799637
H,0,7.7646169013,-2.2309373892,1.5404958985
Si,0,1.8977395249,-2.5673981074,0.4990737175
C,0,3.2458942606,-3.7930218592,0.9383586236
H,0,4.1288361801,-3.299771105,1.3588240488
H,0,2.8680387681,-4.5083103553,1.6775154499
H,0,3.559040483,-4.3541840787,0.0517377081
C,0,1.4573791914,-1.5149887043,1.9884817381
H,0,2.2769750691,-0.8594682061,2.2960408737
H,0,0.5784190929,-0.8929918738,1.7934204895
H,0,1.225575317,-2.1784056443,2.8297135774
C,0,0.3749097974,-3.4288048923,-0.1621789
H,0,0.63872585,-4.1513917984,-0.9421318586
H,0,-0.1614921277,-3.9626996465,0.6287877538
H,0,-0.3027268136,-2.6875782929,-0.6038353703
C,0,-1.3998751765,-2.587348103,-3.5562272341
H,0,-1.4086487009,-2.8346824303,-4.6210148476
H,0,-0.5237231036,-3.0426667607,-3.0894580174
H,0,-2.2916942434,-3.0053923057,-3.0837966886
H,0,-2.2943730221,-0.6231094871,-3.8371830256
H,0,5.3626932107,-0.0616523515,-3.5017578934
H,0,4.8698676904,1.0886140804,-2.2694273383
H,0,4.1935870332,2.3607657549,-4.1751957845
H,0,3.922504992,0.9027272418,-5.1429809376
H,0,2.08409072,2.0384146895,-2.974442023
H,0,1.6515482713,1.4364028226,-4.5986368318

TS-10c anti-syn-up

M06-2X/6-31+G**, $E = -1619.48791920$ a.u.

Thermal correction to Gibbs Free Energy = 0.512725 a.u.

1 imaginary frequency = -637.96 cm^{-1}

SP at B2PLYP/6-311+G**, $E = -1618.9445197475$ a.u.

SP at mPW2PLYP/6-311+G**, $E = -1618.9708354011$ a.u.

0,1

C,0,-1.4328577028,-1.0881097812,-3.3768036561
C,0,-0.2099853913,-0.2450654748,-3.537131448
H,0,-0.3484217792,0.7971566978,-3.7957629037
C,0,1.0452376716,-0.7351889323,-3.1806754406
H,0,1.136391562,-1.7463163525,-2.7951881203
N,0,2.1725178714,-0.0474237449,-3.2069712538
C,0,2.316541546,1.3064845697,-3.7467773579
C,0,3.4225237779,-0.5157716136,-2.5834396451
C,0,3.7904641272,1.3422973895,-4.1489274497
C,0,4.4923507539,0.4644535054,-3.0978058668

H,0,3.5963105404,-1.5399768479,-2.9241823682
C,0,3.2630525239,-0.5825081649,-1.0218582675
O,0,-1.2509626645,-0.641735781,-2.0745976021
O,0,-2.7545018658,-1.2085956327,-1.0696968892
H,0,-2.2593689737,-1.6181789642,-0.3479990384
H,0,-2.8655962666,0.4196621574,-0.8589013387
O,0,2.3428621578,-1.6430011809,-0.8377749331
O,0,-2.8541649546,1.4192199415,-0.8389547675
H,0,-2.1797538783,1.6374114143,-1.4915373273
C,0,2.6542574613,0.7373925663,-0.5298726125
C,0,3.4367279924,1.8750318941,-0.2915467979
C,0,1.2637532031,0.8571483632,-0.4273420835
C,0,2.8460455785,3.0972087652,0.0277534331
H,0,4.5199504293,1.8141396081,-0.3338831743
C,0,0.6699823022,2.0769391597,-0.1051550091
H,0,0.6293321917,-0.003226223,-0.6179580883
C,0,1.459083477,3.2046765011,0.1176100895
H,0,3.4747155298,3.9628934401,0.2123537387
H,0,-0.4125246879,2.136355082,-0.0291737284
H,0,0.9988384103,4.1557586969,0.3669968518
C,0,4.5900091788,-0.9514986592,-0.3461412137
C,0,4.8740636573,-0.5415227277,0.9612871144
C,0,5.4744184462,-1.8427715017,-0.9661598428
C,0,6.0074276567,-1.0043527722,1.6289940729
H,0,4.204736298,0.1423397551,1.4723552913
C,0,6.6113837637,-2.3022917486,-0.304938825
H,0,5.2798678521,-2.2054023271,-1.9704409577
C,0,6.8816457096,-1.8866768925,0.9981239246
H,0,6.2025127217,-0.6742600232,2.6446192696
H,0,7.2816260981,-2.9926470125,-0.8076201335
H,0,7.7644292596,-2.2480015718,1.5162110396
Si,0,1.8927559909,-2.5583047839,0.5086663665
C,0,3.2376634514,-3.7900155991,0.940982422
H,0,4.1262969812,-3.3008266522,1.3541811057
H,0,2.8610731284,-4.5016221336,1.684344181
H,0,3.5414776874,-4.3548850779,0.0534771535
C,0,1.4688668038,-1.5009663997,1.9991691098
H,0,2.296211346,-0.8534820303,2.3028726302
H,0,0.5949663323,-0.8706918395,1.8081691121
H,0,1.2347544369,-2.1621206058,2.8415616389
C,0,0.3608143268,-3.4135418125,-0.1391383425
H,0,0.6147810375,-4.1402069897,-0.9185353208
H,0,-0.1737573128,-3.9411549428,0.65722178
H,0,-0.3143844999,-2.6691735578,-0.579123698
C,0,-1.3940665258,-2.5859544016,-3.5876531205
H,0,-0.5510752279,-3.0171569376,-3.0380311465
H,0,-2.3033423657,-2.9921976678,-3.1333891651
H,0,-2.3048806491,-0.627404623,-3.8560930719
H,0,5.345289613,-0.0724224164,-3.5166532972
H,0,4.869080059,1.0776237924,-2.2778801502
H,0,4.1837377102,2.3598681282,-4.1731005424
H,0,3.9032116266,0.9068477832,-5.1455760145
H,0,2.0779304267,2.0416939498,-2.9658197486
H,0,1.6364848279,1.4443150443,-4.5893132264
C,0,-1.3173581288,-2.9423441848,-5.0703646774
H,0,-0.3896018364,-2.569272016,-5.5162344751
H,0,-1.3514799659,-4.024926834,-5.2138011816
H,0,-2.1553485006,-2.5043806903,-5.6222958907
H,0,-1.2417210434,0.5149789111,2.3484925107
O,0,-7.2922386364,0.8098482733,-2.1281055594
H,0,-8.2345102118,0.9183257365,-1.9660469491
C,0,1.650709762,-0.6058149771,-1.088208893
C,0,2.7710507309,-0.7558995629,-1.9143370303
C,0,1.1499989161,0.6812594598,-0.8676243255
C,0,3.3754730995,0.3525767711,-2.503865745
H,0,3.1788612499,-1.7447269887,-2.1043127486
C,0,1.7517107047,1.7921904459,-1.4585403194
H,0,0.2806001881,0.8105707442,-0.2285671145
C,0,2.8656254396,1.6315828556,-2.2807711992
H,0,4.2445726172,0.2145558517,-3.1397149809
H,0,1.3461985711,2.7827627629,-1.2762118545
H,0,3.3359625472,2.4950001914,-2.7407063506
C,0,1.8139175464,-2.9831921822,-0.1415170443
C,0,1.3613850458,-4.3075898293,-0.1605282046
C,0,3.0888628002,-2.7317783512,0.3811348176
C,0,2.156375861,-5.3448840142,0.3265225287
H,0,0.3796041274,-4.5595787005,-0.5459558796
C,0,3.8841627269,-3.7641518272,0.8735330965
H,0,3.4697772662,-1.7162173627,0.406234002
C,0,3.4193339988,-5.0780887746,0.849899152
H,0,1.7806240167,-6.3628662735,0.2994426076
H,0,4.8666147042,-3.5387659034,1.2768218128
H,0,4.0356216348,-5.8852619484,1.2329387513
C,0,-4.0089910521,0.5588236631,-0.1127637322
C,0,-2.9872743708,0.26324906,-1.1568624378
H,0,-2.9944740754,0.8562243998,-2.063100549
C,0,-2.0891646866,-0.7819649243,-0.9526413106
H,0,-2.1394804083,-1.346884575,-0.025618538
N,0,-1.155043914,-1.1636398977,-1.8037788437
C,0,-1.0284428395,-0.600063175,-3.1544026713
C,0,-0.21125452,-2.2552040667,-1.5322243511
C,0,0.1086280925,-1.3968968858,-3.8046470188
C,0,0.2688186524,-2.6561888447,-2.9319922526
H,0,-0.809960293,0.471032848,-3.0931328279
H,0,1.0248895331,-0.8049636917,-3.8064720753
H,0,-1.9859353467,-0.7324294174,-3.6706305974
H,0,-0.1297363366,-1.6515294817,-4.8385202376
H,0,1.2963125244,-3.0277720361,-2.9194307041
H,0,-0.3702651015,-3.460932248,-3.3057213589
H,0,-0.7750346771,-3.0516460613,-2.0423925007
C,0,0.8963001973,-1.8098835746,-0.5179346108
H,0,-3.7414551763,0.2203659873,0.8956470212
O,0,-4.6630550533,-0.4169535196,-0.8444127395
O,0,-6.3925901992,-0.5559850998,-0.0713969237
H,0,-6.4664280457,-1.5087911653,-0.2102598097
H,0,-6.9461619853,0.2798086804,-1.350035585
O,0,0.1501841157,-1.4170111061,0.6194237558
Si,0,0.5060387548,-1.2401382713,2.2584336743
C,0,1.9792336256,-0.1175169722,2.5539516948
H,0,1.897816867,0.8058957361,1.9720992147
H,0,2.0055161674,0.1523380163,3.6160773518
H,0,2.9314538336,-0.5960513229,2.3103442883
C,0,0.7527505476,-2.9059630677,3.0807550037
H,0,1.6728155763,-3.3993157357,2.7513124884
H,0,0.8040835291,-2.7731119359,4.1672807473
H,0,-0.0899919106,-3.5695442045,2.8600352249
C,0,-4.6512118671,1.9237588701,-0.1337261522
H,0,-4.8986108561,2.2091069362,-1.1593975083
H,0,-5.5758468228,1.888642918,0.4465836719
H,0,-3.9766541555,2.6648414814,0.3036071199

TS-10a anti-anti-down

M06-2X/6-31+G**, E = -1580.19212123 a.u.

Thermal correction to Gibbs Free Energy = 0.483017 a.u.

1 imaginary frequency = -659.83 cm⁻¹

SP at B2PLYP/6-311+G**, E = -1579.6690552127 a.u.

SP at mPW2PLYP/6-311+G**, E = -1579.6938354977 a.u.

0,1

C,0,-1.0571156235,-0.4223818287,2.8850994452

H,0,-1.9241943487,-1.0757918693,2.739949748

H,0,-0.9817134732,-0.1939643124,3.9531057588

TS-10b anti-anti-down

M06-2X/6-31+G**, E = -1619.49345419 a.u.
Thermal correction to Gibbs Free Energy = 0.510820 a.u.
1 imaginary frequency = -671.21 cm⁻¹
SP at B2PLYP/6-311+G**, E = -1618.9494616335 a.u.
SP at mPW2PLYP/6-311+G**, E = -1618.9755248329 a.u.

O,1
C,0,-0.696145196,-4.0683189317,-0.0748408434
H,0,-1.242459124,-4.0579667535,-1.0236162758
H,0,-0.4553989525,-5.1086229661,0.167578758
H,0,-1.3598581364,-3.6836382585,0.7057160786
O,0,-7.4247764671,-2.9587214861,0.0769636512
H,0,-8.0674945577,-3.4342416839,-0.4587684024
C,0,0.9243960398,0.3988856291,0.665062531
C,0,1.7375543599,1.5007542071,0.9621712097
C,0,0.0014439611,-0.0196573104,1.6295797685
C,0,1.6226160888,2.1676620836,2.1818107442
H,0,2.4821310466,1.8417991483,0.2496285469
C,0,-0.1166600632,0.6447602857,2.84876208
H,0,-0.6413139226,-0.8684042805,1.4172385511
C,0,0.6907022591,1.7462438519,3.1287869926
H,0,2.26661463,3.0165331344,2.3895482203
H,0,-0.8440360135,0.3000679068,3.577590626
H,0,0.599410458,2.2664340315,4.0770789509
C,0,2.2935221318,-0.434804363,-1.3552305242
C,0,2.4096124989,-0.6241973308,-2.7384377748
C,0,3.4483891287,-0.5488072717,-0.574299316
C,0,3.6413661549,-0.9055664127,-3.323663228
H,0,1.533635461,-0.5748740475,-3.3773187693
C,0,4.6828796117,-0.8389524639,-1.1553396563
H,0,3.3925322032,-0.4159049252,0.5008419359
C,0,4.7850188059,-1.0164431799,-2.5331738261
H,0,3.7042814712,-1.0479324053,-4.3979682947
H,0,5.5633122532,-0.9251952905,-0.5263379424
H,0,5.7450986231,-1.2400450391,-2.9875749292
C,0,-4.4289887917,-0.7796947474,0.262887722
C,0,-3.3699047135,0.2588688539,0.0450004715
H,0,-3.5448211232,1.2299248019,0.491406669
C,0,-2.2325897951,0.0164836316,-0.7177536173
H,0,-2.0507879944,-0.9717823885,-1.1317852083
N,0,-1.2950773482,0.9094014395,-0.9917408805
C,0,-1.3622949144,2.3286983776,-0.6398228281
C,0,-0.0279796968,0.578489352,-1.6607628577
C,0,-0.5419520304,2.9828130253,-1.7513141333
C,0,0.5400027245,1.9442519688,-2.0928831814
C,0,0.9075356821,-0.2628537424,-0.7193974755
O,0,-4.8382713363,-0.2433028545,-0.9557246917
O,0,-6.46359764,-1.0606296698,-1.4297872989
H,0,-6.9838430772,-0.2520729021,-1.3400582214
H,0,-7.0650251636,-2.2238822733,-0.5095279049
O,0,0.2641213384,-1.5263305555,-0.6462923213
Si,0,0.8626139738,-3.0428761147,-0.1904562325
C,0,1.7277829782,-2.9863887783,1.473048555
H,0,1.0442081591,-2.6857315877,2.2725783926
H,0,2.1047341421,-3.9889662497,1.7063184753
H,0,2.5796538597,-2.3009383924,1.4771821276
C,0,2.0086888111,-3.7498895762,-1.4951653376
H,0,2.9770270762,-3.2395813955,-1.5187992475
H,0,2.1845947918,-4.8101682394,-1.2807536562
H,0,1.5585054079,-3.6742323514,-2.4904445344
C,0,-4.0559207822,-2.2475152968,0.2011390356
H,0,-3.5001898206,-2.5307884078,1.09986302
H,0,-4.9755222329,-2.8377406589,0.1542886019
H,0,-3.4553007887,-2.4779109978,-0.6810470357
C,0,-5.3627789598,-0.4580555055,1.4158018872
H,0,-5.6463062747,0.597734814,1.3938158187
H,0,-6.2636833023,-1.0717584999,1.3308489314
H,0,-4.8731639096,-0.676895374,2.369198877
H,0,-0.2657435329,-0.0619285303,-2.5143632515
H,0,1.4643587441,2.1602276628,-1.5553593701

H,0,0.7839572873,1.9435130047,-3.1566917236
H,0,-0.1181826246,3.9387498772,-1.4385519546
H,0,-1.1872046072,3.160142596,-2.615870845
H,0,-0.9230870336,2.4836172764,0.3547879492
H,0,-2.4021084962,2.6592143297,-0.6277929572

TS-10c anti-anti-down

M06-2X/6-31+G**, E = -1619.48853268 a.u.
Thermal correction to Gibbs Free Energy = 0.510178 a.u.
1 imaginary frequency = -657.47 cm⁻¹
SP at B2PLYP/6-311+G**, E = -1618.9469335254 a.u.
SP at mPW2PLYP/6-311+G**, E = -1618.9727382958 a.u.

O,1
C,0,-1.1117716091,-0.430653083,2.8403958396
H,0,-1.9649835575,-1.1059357356,2.7143650867
H,0,-1.0464793152,-0.1631620606,3.8999315598
H,0,-1.3128256033,0.4834427406,2.2697275311
O,0,-7.2780641219,1.0146033868,-2.0565885271
H,0,-8.2334329733,1.058558578,-1.9500566359
C,0,1.6290168123,-0.6083644491,-1.0962782016
C,0,2.7580935363,-0.7429644964,-1.9129598221
C,0,1.1048974135,0.6711779106,-0.8849525972
C,0,3.3483277334,0.3730946275,-2.5026468516
H,0,3.1835571809,-1.7257794748,-2.0953307142
C,0,1.6921927233,1.7895237114,-1.4762432195
H,0,0.2276297466,0.7890699826,-0.253990168
C,0,2.8150880101,1.6442176044,-2.2891361196
H,0,4.2247555129,0.2474973692,-3.1309610956
H,0,1.268515412,2.7739085281,-1.3015099684
H,0,3.2743309533,2.5135818199,-2.7490918053
C,0,1.8255830034,-2.9793813483,-0.140207563
C,0,1.3985329693,-4.3120622823,-0.1636676127
C,0,3.0900414794,-2.703480629,0.39558537
C,0,2.208354708,-5.3339709985,0.3316499146
H,0,0.4261216371,-4.5830503591,-0.5597944107
C,0,3.8997993103,-3.7203282935,0.8963320209
H,0,3.450805284,-1.6806619874,0.4237875865
C,0,3.4603796514,-5.0429800782,0.8681305293
H,0,1.8526430478,-6.3590183574,0.3007959257
H,0,4.8735786646,-3.4760368544,1.3095585263
H,0,4.0881630086,-5.8380305158,1.2577586793
C,0,-4.0034837317,0.5110901517,-0.1096474291
C,0,-2.988117666,0.2147313021,-1.1596879493
H,0,-2.9824561244,0.828028908,-2.0526974879
C,0,-2.0994757984,-0.8406666709,-0.969480002
H,0,-2.1554035647,-1.4179042358,-0.0503376452
N,0,-1.1626935185,-1.2132172092,-1.8216916534
C,0,-1.0300500419,-0.6377897541,-3.1666124078
C,0,-0.2037097865,-2.2896325381,-1.5462206614
C,0,0.1148681585,-1.4246739757,-3.8165087226
C,0,0.2897876658,-2.6821160565,-2.9434098201
H,0,-0.8152737907,0.4334951829,-3.095656781
H,0,1.0249106419,-0.8232655686,-3.8199919681
H,0,-1.9841073728,-0.768911169,-3.6892158644
H,0,-0.1216664104,-1.6828727499,-4.8499134544
H,0,1.3230496648,-3.037276407,-2.9256143645
H,0,-0.3343837757,-3.4967833517,-3.320723887
H,0,-0.7566432282,-3.0947144272,-1.0580597269
C,0,0.8908918628,-1.8231137362,-0.526625249
H,0,-3.7462880729,0.1382568803,0.8912009486
O,0,-4.6869550593,-0.4191227672,-0.8682002453
O,0,-6.4257726314,-0.5208254903,-0.106039819
H,0,-6.5373964054,-1.4591186336,-0.3046612982
H,0,-6.9529782114,0.4167553757,-1.3188769197
O,0,0.1316892425,-1.438759055,0.6043129685
Si,0,0.4700912064,-1.2351582073,2.2434758141
C,0,1.923154819,-0.0871639522,2.540586834
H,0,1.8294783131,0.8324622189,1.9546414401
H,0,1.9396135492,0.1874365951,3.6016981163

H,0,2.884287689,-0.5509904229,2.3038110163
C,0,0.7351197773,-2.8884554356,3.0847283184
H,0,1.6610785291,-3.3737114656,2.7593683388
H,0,0.7853263712,-2.7446503973,4.1698390471
H,0,-0.0995278779,-3.5643227833,2.8706924183
C,0,-4.5763225031,1.9096585948,-0.0844189983
H,0,-4.8317976017,-2.1989875061,-1.1095193473
H,0,-5.5140005865,1.8684938097,0.4791102486
C,0,-3.5971123654,2.8956646623,0.548036436
H,0,-3.3483107534,2.5999055446,1.5727525925
H,0,-2.6639454898,2.9430332635,-0.0238810992
H,0,-4.0226761908,3.9013991685,0.5843979728

TS-10a anti-syn-down

M06-2X/6-31+G**, E = -1580.19079392 a.u.

Thermal correction to Gibbs Free Energy = 0.484065 a.u.

1 imaginary frequency = -664.56 cm⁻¹

SP at B2PLYP/6-311+G**, E = -1579.6658707063 a.u.

SP at mPW2PLYP/6-311+G**, E = -1579.6908425624 a.u.

0,1
C,0,-0.2921828677,-3.7534399928,0.6584818867
H,0,-0.8323462489,-3.9672500795,-0.2696721248
H,0,0.0209242613,-4.7071787677,1.0960492666
H,0,-0.9858400596,-3.2715983615,1.3550388314
O,0,-7.3021018264,-1.8837450796,0.9778048225
H,0,-7.9704674065,-2.575810783,0.9577979533
C,0,1.0244992016,0.8941863296,0.5733699685
C,0,1.7555648304,2.0875229574,0.5959746037
C,0,0.1993396077,0.5962649445,1.6625193058
C,0,1.6660065182,2.9598033854,1.6793151089
H,0,2.4054175826,2.3430978792,-0.2368637705
C,0,0.1095719712,1.4654515327,2.7492744054
H,0,-0.385654674,-0.3183583359,1.6528565315
C,0,0.8408521639,2.6522814717,2.7607009875
H,0,2.2440001845,3.8786934057,1.6768030799
H,0,-0.536753223,1.2145550417,3.5847647309
H,0,0.7719994355,3.3302632789,3.6055509502
C,0,2.3952342867,-0.1939747183,-1.3060521094
C,0,2.5059205442,-0.5842627623,-2.6466123787
C,0,3.5659744152,-0.1153587478,-0.5435591585
C,0,3.7455268185,-0.8793131734,-3.2090132295
H,0,1.6231874974,-0.6764276131,-3.271334897
C,0,4.8082310885,-0.4174448938,-1.1006921743
H,0,3.5161293464,0.180786334,0.4991309251
C,0,4.9038099677,-0.7996431558,-2.4367570925
H,0,3.8029377179,-1.1789678699,-4.2507650224
H,0,5.7004372594,-0.3542508651,-0.4855325076
H,0,5.8700355943,-1.0332801594,-2.8727092939
C,0,-4.3127853506,-0.9869167426,0.2901146164
C,0,-3.3489621024,0.1158025651,-0.0027141108
H,0,-3.6330638236,1.1160012411,0.2968474677
C,0,-2.1637768763,-0.1149627859,-0.6973996321
H,0,-1.8836639632,-1.1244184096,-0.9848501381
N,0,-1.3086088495,0.8275663725,-1.0541162125
C,0,-1.5399367532,2.2562022341,-0.8122672267
C,0,-0.0196893296,0.5532175837,-1.6966239948
C,0,-0.4545650618,2.9842926605,-1.6216268619
C,0,0.3301140516,1.8863058336,-2.3711451155
H,0,-0.1813409323,-0.243924909,-2.4260495393
C,0,1.0142091461,-0.0110239881,-0.6611519915
O,0,-4.6994506536,-0.6499660836,-0.9983460295
O,0,-6.2138434104,-1.7220770704,-1.3848001918
H,0,-6.6439061599,-1.0549480815,-1.9345984235
H,0,-6.9244024456,-1.8296617935,0.0460422258
O,0,0.4761271705,-1.2815292601,-0.329215784
Si,0,1.1911725928,-2.6621024927,0.3362455001
C,0,2.0805374626,-2.3014823556,1.9483441694
H,0,1.3997902758,-1.8833942024,2.695926019
H,0,2.4813376147,-3.2429430417,2.3419096937

H,0,2.9185007854,-1.6103980319,1.8235808514
C,0,2.3516062479,-3.4950767695,-0.8773184892
H,0,3.28660148,-2.9420544016,-1.0123966882
H,0,2.5966255108,-4.4964332118,-0.5048839825
H,0,1.8746074623,-3.6048416284,-1.8566948648
H,0,-5.0518426358,-0.6869061503,1.0397340725
C,0,-3.8609566877,-2.4143076762,0.4793699118
H,0,-3.4144799643,-2.5405169816,1.4694265844
H,0,-4.73694352,-3.0626309783,0.401958408
H,0,-3.1409339461,-2.7188756181,-0.283477578
H,0,1.4064055143,2.0705535064,-2.3699382943
H,0,0.0121086734,1.8396601175,-3.4156676958
H,0,0.1966053539,3.5481343915,-0.9532387353
H,0,-0.9015095463,3.6904526919,-2.323013716
H,0,-1.4650990725,2.4637094046,0.2624056572
H,0,-2.5520267248,2.5045272096,-1.1457329608

TS-10c anti-syn-down

M06-2X/6-31+G**, E = -1619.48530293 a.u.

Thermal correction to Gibbs Free Energy = 0.511943 a.u.

1 imaginary frequency = -651.00 cm⁻¹

SP at B2PLYP/6-311+G**, E = -1618.9415269254 a.u.

SP at mPW2PLYP/6-311+G**, E = -1618.9675504557 a.u.

0,1
C,0,-0.2839377852,-3.8162609051,0.5652075961
H,0,-0.8358003276,-3.9811080468,-0.3660826019
H,0,0.0502739744,-4.7899668559,0.9386010575
H,0,-0.9728268055,-3.389891292,1.3008400498
O,0,-7.5849990744,-1.1920225882,0.6523186844
H,0,-7.8380193413,-2.0352965785,1.0412170063
C,0,0.9841085332,0.8645278032,0.5836853342
C,0,1.7097145467,2.0604637015,0.6290940586
C,0,0.1493748095,0.5490763024,1.660500762
C,0,1.6055608945,2.9188397305,1.7220768476
H,0,2.3671584334,2.3288505863,-0.1936894501
C,0,0.0450144596,1.4044239735,2.757089006
H,0,-0.4304885728,-0.3686315815,1.6338716892
C,0,0.7707538707,2.5942263754,2.7909338146
H,0,2.1796143028,3.8400941235,1.7366773295
H,0,-0.6083440881,1.1404875839,3.5830575229
H,0,0.6904113274,3.2612168335,3.6435114846
C,0,2.3809525281,-0.186734442,-1.2959097807
C,0,2.5102888163,-0.5475331777,-2.6429954917
C,0,3.5421613716,-0.115534851,-0.5182601032
C,0,3.7587662365,-0.8210954579,-3.1967351531
H,0,1.6359744192,-0.6318788096,-3.2805271162
C,0,4.7931762005,-0.3966123864,-1.0666339262
H,0,3.4778772881,0.1596730935,0.5293675149
C,0,4.9073094956,-0.7493401327,-2.409345792
H,0,3.8307873383,-1.0975923314,-4.2439599286
H,0,5.6775844573,-0.3394444144,-0.439746234
H,0,5.8803763419,-0.9658445802,-2.8388684226
C,0,-4.3213829505,-1.041037516,0.2375105537
C,0,-3.3859384176,0.0854786856,-0.0601019925
H,0,-3.6975878687,1.0823891139,0.2222828149
C,0,-2.18678662,-0.1320637135,-0.7326677131
H,0,-1.8935721372,-1.1389414669,-1.0161965979
N,0,-1.3307291902,0.8169736384,-1.0727102966
C,0,-1.5706691181,2.2417633546,-0.8199735988
C,0,-0.0334512675,0.5519101672,-1.7019307342
C,0,-0.4747404432,2.9816156435,-1.603832882
C,0,0.3218593352,1.8942168207,-2.3558482969
H,0,-0.1845665161,-0.2362529915,-2.4433700413
C,0,0.9917130673,-0.0231531633,-0.6632654574
O,0,-4.7076776244,-0.7250861825,-1.059513038
O,0,-6.2214986014,-1.7664348895,-1.5018619301
H,0,-6.4927136928,-1.186530247,-2.225110398
H,0,-7.0861503103,-1.4196327737,-0.1910735589
O,0,0.4590297048,-1.3026753214,-0.3544101978

Si,0,1.1829773548,-2.6907075637,0.2866012108
C,0,2.0477530352,-2.3562831151,1.9175110768
H,0,1.3551920333,-1.953017378,2.6623319061
H,0,2.4453828574,-3.3033936861,2.3005771676
H,0,2.8854578171,-1.6609668528,1.8172800374
C,0,2.3689639211,-3.4840604746,-0.9295671623
H,0,3.2953497356,-2.913046723,-1.04712088
H,0,2.6277205823,-4.4864050232,-0.5692769465
H,0,1.9032025449,-3.5879716008,-1.914975127
H,0,-5.0814736282,-0.7573270341,0.9743533257
C,0,-3.7827928618,-2.4386299013,0.4752200839
H,0,-3.1064260094,-2.3879734634,1.3370976759
H,0,-3.1890813886,-2.7499127181,-0.3907286793
H,0,1.3974163499,2.0813712138,-2.3388202114
H,0,0.0174364106,1.8592898421,-3.4049124107
H,0,0.1662767022,3.5375495979,-0.919124523
H,0,-0.9121422541,3.6964627851,-2.3024469236
H,0,-1.5143950755,2.4379632945,0.2581018799
H,0,-2.577764396,2.4914715703,-1.1675115495
C,0,-4.8873041803,-3.460891173,0.7432533227
H,0,-5.5661427737,-3.5204296708,-0.1096197289
H,0,-4.4560280755,-4.4492500697,0.926620486
H,0,-5.4683615445,-3.1761394996,1.6266843537

TS-10a anti-anti-up

M06-2X/6-31+G**, E = -1580.19377625 a.u.

Thermal correction to Gibbs Free Energy = 0.485400 a.u.

1 imaginary frequency = -647.15 cm⁻¹

SP at B2PLYP/6-311+G**, E = -1579.6689081960 a.u.

SP at mPW2PLYP/6-311+G**, E = -1579.6941647504 a.u.

O,1
C,0,-1.4011799144,-1.0503793788,-3.3375945289
C,0,-0.2115290844,-0.1769299806,-3.5339337726
H,0,-0.3685488153,0.8473463828,-3.8502540966
C,0,1.0423115944,-0.665368633,-3.1699553671
H,0,1.1055226982,-1.6690870325,-2.7568694502
N,0,2.1849448868,-0.0081086273,-3.2215451366
C,0,2.3651846343,1.3228605367,-3.8057457668
C,0,3.4319168077,-0.5034575425,-2.6119592188
C,0,3.8293186845,1.2888430325,-4.242528219
C,0,4.5216966625,0.4292047643,-3.1702814095
H,0,3.5651955752,-1.5393403833,-2.9351086211
C,0,3.2973232477,-0.5346511976,-1.0471720312
H,0,-1.1899585966,-2.1259396272,-3.3646717605
O,0,-1.2613607404,-0.5206141351,-2.060944711
O,0,-2.7291124501,-1.1837590123,-1.0604742047
H,0,-2.2293129502,-1.3339493415,-0.2471583123
H,0,-3.2184935259,0.3757021912,-1.1276837786
C,0,-2.6755577451,-0.676769057,-4.0528239093
H,0,-2.6463401213,-1.0306933469,-5.086647875
H,0,-3.5182013187,-1.1390062443,-3.5342982998
H,0,-2.8135626457,0.4078861461,-4.0458846686
O,0,2.3380639597,-1.5523323414,-0.8314092516
O,0,-3.4386519858,1.3464958197,-1.2300270243
H,0,-2.6971257101,1.6886507666,-1.7404166987
C,0,2.7499153279,0.8178208398,-0.5737453801
C,0,3.5807059137,1.9258139455,-0.3624156382
C,0,1.3662108371,0.9969218124,-0.4683866468
C,0,3.0430523968,3.17757278,-0.063851072
H,0,4.6600509468,1.8178017753,-0.4118437585
C,0,0.8263189014,2.2470953976,-0.171250142
H,0,0.6963637827,1.600896869,-0.6411777217
C,0,1.662215428,3.3448572843,0.0283484238
H,0,3.7082821628,4.0196781491,0.1001474365
H,0,-0.2516533453,2.3582787938,-0.0990090119
H,0,1.2429667877,4.3193226761,0.2588825085
C,0,4.6170242413,-0.9461196199,-0.3832004079
C,0,4.9323961591,-0.5334238061,0.9163325479
C,0,5.4575184117,-1.878514629,-1.0030889814

C,0,6.0547277561,-1.0337327595,1.5756311778
H,0,4.2959190284,0.1808225863,1.4283111496
C,0,6.5829247943,-2.3764048119,-0.350031655
H,0,5.2364908009,-2.2439405507,-2.0006190799
C,0,6.8853143008,-1.9574174273,0.9447723164
H,0,6.275079758,-0.7012045883,2.5852697707
H,0,7.2184640676,-3.098881732,-0.8525693155
H,0,7.7588562305,-2.3486500521,1.4567311607
Si,0,1.8579069283,-2.4409524575,0.5208034984
C,0,3.1687869119,-3.6984462164,0.9825996709
H,0,4.0713793375,-3.2254968925,1.3841670829
H,0,2.772421758,-4.3816731287,1.742151439
H,0,3.455774756,-4.2924230884,0.1085572739
C,0,1.4543769641,-1.3455134145,1.9888965325
H,0,2.2968670411,-0.7100962432,2.277065623
H,0,0.5962278698,-0.6987198224,1.7819403804
H,0,1.2042257167,-1.9800654487,2.846807163
C,0,0.3152444076,-3.2715297105,-0.1332354482
H,0,0.5675143328,-4.0077958051,-0.9039969916
H,0,-0.2331736078,-3.7869938136,0.6617552122
H,0,-0.3488981284,-2.5239042585,-0.5846751589
H,0,5.3548835097,-0.1444429882,-3.5802677611
H,0,4.9245508425,1.060828698,-2.3767423415
H,0,4.2588089207,2.2890831139,-4.3182457304
H,0,3.902354573,0.8081623475,-5.2220320525
H,0,2.1762820214,2.0886048605,-3.0412421352
H,0,1.6683220095,1.4620097594,-4.6341278252

TS-10b anti-anti-up

M06-2X/6-31+G**, E = -1619.49524007 a.u.

Thermal correction to Gibbs Free Energy = 0.512863 a.u.

1 imaginary frequency = -651.73 cm⁻¹

SP at B2PLYP/6-311+G**, E = -1618.9496529355 a.u.

SP at mPW2PLYP/6-311+G**, E = -1618.9761434404 a.u.

O,1
C,0,3.9485742358,1.8152174188,3.1266635341
H,0,4.4325523999,2.7617662963,3.3898042414
H,0,4.7274193508,1.0489595017,3.0405049401
H,0,3.2806265523,1.5345081317,3.9479245373
O,0,4.8757044037,3.7701756648,-4.8827605418
H,0,5.576812425,3.1126586109,-4.933311305
C,0,0.8446482317,3.11507667,3.617444369
C,0,0.4228118624,1.8415715022,4.0162180781
C,0,1.4937888548,3.9212964487,4.5602366308
C,0,0.6398460584,1.3880431643,5.3169058982
H,0,-0.0749725279,1.1886167125,3.3070261747
C,0,1.7069012715,3.4747590327,5.8623966655
H,0,1.8588606923,4.9057074397,4.2861303823
C,0,1.2829359604,2.2030533115,6.2460137033
H,0,0.3075041967,0.3941043406,5.5999289067
H,0,2.2123052101,4.1198231077,6.5743570023
H,0,1.4531806997,1.8507724429,7.258505744
C,0,-0.3688786102,2.894232853,1.3560011792
C,0,-0.1678479582,2.5861003458,0.0060353484
C,0,-1.6461898338,2.7013721426,1.8987833936
C,0,-1.2148099424,2.1115126526,-0.7825445781
H,0,0.8084948165,2.7372026105,-0.4443003774
C,0,-2.6948360434,2.2261343456,1.1117808565
H,0,-1.8319387667,2.9048466361,2.9489149039
C,0,-2.4851245368,1.9344682089,-0.235143736
H,0,-1.0324806008,1.8863934039,-1.82924252
H,0,-3.6747718096,2.0826633499,1.5563838254
H,0,-3.3016816354,1.5677899145,-0.8493409378
C,0,2.3672963907,5.2599778107,-2.5951995279
C,0,1.2223873012,5.5005199343,-1.6573092278
H,0,0.2400923713,5.6362720348,-2.0947799148
C,0,1.3847465003,5.3767637614,-0.2814771868
H,0,2.3551712107,5.097580881,0.1170965104
N,0,0.4339570096,5.5089330001,0.6280828392

C,0,-0.9352791913,5.9520213515,0.3622319397
C,0,0.6112597875,5.1172024559,2.0353995972
C,0,-1.3389261468,6.5750401856,1.6986920481
C,0,-0.609234897,5.7223292032,2.7530208936
C,0,0.7634814353,3.5570236872,2.1509093599
O,0,1.9838113315,3.9491029033,-2.3007256987
O,0,3.055606164,2.7774717664,-3.3001603322
H,0,2.3219639579,2.4298111155,-3.8233872791
H,0,4.1741167834,3.378897937,-4.2758824943
O,0,2.008035876,3.3095525162,1.5248871519
Si,0,3.0396781927,1.9710994187,1.4925007658
C,0,2.135942018,0.3731528508,1.1025604981
H,0,1.3212150874,0.1707263945,1.8039616577
H,0,2.8486606659,-0.4570798154,1.1680909041
H,0,1.7212168938,0.386702386,0.0902970225
C,0,4.2128108703,2.4251499584,0.1114873098
H,0,3.6696473699,2.6171536376,-0.8235029548
H,0,4.9320299869,1.6186717982,-0.0687534388
H,0,4.7801711683,3.325330162,0.3738164212
C,0,3.7784538709,5.6034171636,-2.1569212745
H,0,3.9255189605,6.6871132945,-2.1752112977
H,0,3.9927270049,5.2272547706,-1.1550396112
H,0,4.4804961223,5.1377219133,-2.8546504096
C,0,2.0806997996,5.6664373235,-4.0288707168
H,0,2.1675460509,6.7514057299,-4.1378597921
H,0,2.8070081214,5.1856127769,-4.6898281996
H,0,1.0729419424,5.3571921206,-4.3192856831
H,0,1.5544393277,5.5493635209,2.3798515846
H,0,-0.3000612104,6.3155879601,3.6154988782
H,0,-1.2619972191,4.9314041889,3.1253923426
H,0,-0.9853173334,7.6090990094,1.7351096744
H,0,-2.4209898043,6.5779130388,1.8402241769
H,0,-0.9407171152,6.6638010538,-0.4654834167
H,0,-1.560173612,5.08749154,0.0991704672

TS-10c anti-anti-up

M06-2X/6-31+G**, E = -1619.48972692 a.u.

Thermal correction to Gibbs Free Energy = 0.511977 a.u.

1 imaginary frequency = -643.49 cm⁻¹

SP at B2PLYP/6-311+G**, E = -1618.9468728675 a.u.

SP at mPW2PLYP/6-311+G**, E = -1618.9730271476 a.u.

0,1
C,0,-1.4049270571,-1.0575116898,-3.3296921702
C,0,-0.2146644497,-0.185000545,-3.5288024327
H,0,-0.3735178844,0.8396879331,-3.8442004333
C,0,1.0401871386,-0.6720306483,-3.1661972884
H,0,1.1045604795,-1.6754493445,-2.7525895672
N,0,2.1821327415,-0.0138660327,-3.2198134072
C,0,2.3604269596,1.3166135366,-3.8057435299
C,0,3.4301593889,-0.5074393206,-2.6110201914
C,0,3.8241991868,1.2837026525,-4.2439403564
C,0,4.5187245254,0.4248469397,-3.1723535464
H,0,3.5635854728,-1.5438379332,-2.932437728
C,0,3.2971862318,-0.5358735407,-1.0460290091
H,0,-1.1961463499,-2.1350830042,-3.3628542927
O,0,-1.264827587,-0.5298118821,-2.0548152667
O,0,-2.7359814769,-1.189775847,-1.0533269905
H,0,-2.2333371339,-1.3354801589,-0.2410220479
H,0,-3.2228642919,0.3709505594,-1.1234026818
C,0,-2.6723065007,-0.68377383,-4.0640756774
H,0,-3.5058698612,-1.145964764,-3.5263337299
H,0,-2.8076262318,0.401912801,-3.9978800796
O,0,2.3381692027,-1.5531405649,-0.8275187615
O,0,-3.4405738775,1.3423460925,-1.2256247693
H,0,-2.6998496851,1.6821049307,-1.7388298401
C,0,2.7502038606,0.8174158025,-0.5744448792
C,0,3.5811546691,1.9258707912,-0.3662644061
C,0,1.3666243895,0.9965420082,-0.4676026283
C,0,3.0437203649,3.178154652,-0.0694768733

H,0,4.6604487178,1.8178196261,-0.4167903277
C,0,0.8269269735,2.2472538977,-0.1723802229
H,0,0.6967742004,0.1591806057,-0.6377983998
C,0,1.6629698388,3.3454802808,0.0240354794
H,0,3.7090530377,4.0206512585,0.0920711219
H,0,-0.2509695492,2.3584563345,-0.0990647372
H,0,1.2438895973,4.320364715,0.2530960359
C,0,4.6175828142,-0.9458862575,-0.3826030241
C,0,4.9335143752,-0.5313990946,0.916221389
C,0,5.4583089916,-1.8784016165,-1.001967649
C,0,6.056550876,-1.0302126057,1.5754233984
H,0,4.2969171099,0.1831531184,1.4276439722
C,0,6.5844459815,-2.3747923805,-0.3490083405
H,0,5.2369558321,-2.2450140192,-1.9989888827
C,0,6.8873323129,-1.9541225927,0.9451288315
H,0,6.277335287,-0.6963205137,2.5845165673
H,0,7.2201919532,-3.0973936324,-0.8511061248
H,0,7.7614502102,-2.34417226,1.4570079424
Si,0,1.8595609111,-2.4404845195,0.5260043124
C,0,3.1712779299,-3.6971836828,0.9876078905
H,0,4.0740133736,-3.2236518894,1.3881628972
H,0,2.7758076612,-4.3801357529,1.7478705252
H,0,3.4577842715,-4.291539532,0.113663192
C,0,1.4573805705,-1.3435205095,1.9933326929
H,0,2.3004261525,-0.7084312863,2.2805928403
H,0,0.599560967,-0.6963360709,1.7862283094
H,0,1.2071947433,-1.9771522297,2.8519155873
C,0,0.3163796702,-3.2722177485,-0.1253172647
H,0,0.5679041564,-4.0083985789,-0.8964100472
H,0,-0.2301439958,-3.7880779244,0.6707229998
H,0,-0.3493218658,-2.525327548,-0.575653321
H,0,5.3509531963,-0.1491714113,-3.5837824781
H,0,4.9235077041,1.0569889288,-2.3802166857
H,0,4.2527119961,2.2843099093,-4.3203108654
H,0,3.8966689087,0.802941622,-5.2234381294
H,0,2.1712996865,2.0830971364,-3.0420520945
H,0,1.6626558781,1.453944424,-4.6336937772
C,0,-2.6308121064,-1.1420276306,-5.5196389095
H,0,-3.5582987771,-0.8844414941,-6.0364086702
H,0,-1.8017443702,-0.6692099815,-6.0563887713
H,0,-2.5000835464,-2.2269750172,-5.5864155174

TS-10a syn-anti-down

M06-2X/6-31+G**, E = -1580.19077555 a.u.

Thermal correction to Gibbs Free Energy = 0.486109 a.u.

1 imaginary frequency = -649.61 cm⁻¹

SP at B2PLYP/6-311+G**, E = -1579.6654069660 a.u.

SP at mPW2PLYP/6-311+G**, E = -1579.6905208407 a.u.

0,1
C,0,1.8424009892,-2.4997094872,1.7060106629
H,0,1.380822388,-3.2367717468,1.0406696454
H,0,2.5449311419,-3.0261761795,2.3605251137
H,0,1.053074673,-2.0633043512,2.3277316946
O,0,-5.0098898788,-0.9565859809,0.4135889379
H,0,-5.8817600368,-0.9464037747,0.8208215449
C,0,1.2033101801,1.9558170067,0.0143160072
C,0,1.4471765702,3.2583030861,-0.4388076096
C,0,0.6699604558,1.7882199819,1.2969710584
C,0,1.1631059309,4.3611921654,0.3662255937
H,0,1.8742932741,3.4253118765,-1.4227744723
C,0,0.3861234913,2.8881244783,2.104344482
H,0,0.4611301803,0.7846617599,1.654811694
C,0,0.6279228624,4.1808534635,1.6405179648
H,0,1.3630479985,5.3609604346,-0.0065734054
H,0,-0.0312328224,2.7336216807,3.0946716561
H,0,0.4037749441,5.0387918887,2.2665439775
C,0,2.5739252489,0.780130973,-1.8221708422
C,0,2.6107165813,-0.0176089173,-2.9733254712
C,0,3.7277305457,1.4908004765,-1.4753088933

C,0,3.7573793724,-0.0899803171,-3.7603681768
H,0,1.7476334522,-0.6086855517,-3.2630476343
C,0,4.8803026028,1.4171257408,-2.2575929497
H,0,3.7367156106,2.1075597688,-0.5832918921
C,0,4.8991943416,0.6280652823,-3.405412559
H,0,3.7594834585,-0.7146566095,-4.6480648886
H,0,5.7626037132,1.9777982566,-1.9650046631
H,0,5.794530029,0.5711943517,-4.0163382598
C,0,-2.2397691394,-2.5027926277,0.7253644
C,0,-1.3217466321,-1.5904847388,-0.0159414079
H,0,-0.3993394459,-1.9746887706,-0.4296644361
C,0,-1.7515246828,-0.2784588676,-0.1936882602
H,0,-2.7178278239,-0.019384663,0.2428792172
N,0,-1.1669622652,0.6921683592,-0.8764253899
C,0,-1.8158433632,1.9882836793,-1.1141245536
C,0,0.0330136426,0.5529661655,-1.714760895
C,0,-1.5681983328,2.205042983,-2.6048282025
C,0,-0.170774202,1.6006585332,-2.8344462079
H,0,-1.326849804,2.7587343893,-0.5058036048
H,0,-1.6162609471,3.2594561084,-2.8832934649
H,0,-2.8697425141,1.9284967575,-0.8386164241
H,0,-2.3211576699,1.6595985768,-3.1802948033
H,0,0.5988516283,2.3724746936,-2.7757552569
H,0,-0.0825665699,1.1370753356,-3.8186745608
H,0,0.034809157,-0.4699714108,-2.1026247625
C,0,1.355751857,0.728015069,-0.8897597193
O,0,-2.8591003558,-2.5209893157,-0.5144196836
O,0,-4.4442853267,-3.5058734283,-0.2647510416
H,0,-4.5798754395,-3.7197378146,-1.1964787659
H,0,-4.8559615023,-1.8947566041,0.1219275643
O,0,1.4281957828,-0.4475332438,-0.1023445385
Si,0,2.7150510876,-1.1705781079,0.7197240053
C,0,3.5867168554,0.0265635582,1.8719341906
H,0,2.8995414991,0.4302628371,2.6217079294
H,0,4.3860813923,-0.5105182363,2.3954882537
H,0,4.0430370023,0.8667967905,1.3404521735
C,0,3.9399934452,-1.9491941337,-0.4673771964
H,0,4.5281077229,-1.2041507938,-1.0128097026
H,0,4.631070358,-2.5870404803,0.0957445184
H,0,3.4196676666,-2.5764108113,-1.1989516389
C,0,-1.6832069284,-3.8277800467,1.1865463639
H,0,-1.026875543,-4.2530700816,0.4213727866
H,0,-1.1179186281,-3.7029936934,2.114067943
H,0,-2.5132118621,-4.5160014786,1.3604404497
H,0,-2.8614201987,-2.0068782437,1.4804034061

TS-10b *syn-anti-down*

M06-2X/6-31+G**, E = -1619.49165516 a.u.
Thermal correction to Gibbs Free Energy = 0.512416 a.u.
1 imaginary frequency = -640.33 cm⁻¹
SP at B2PLYP/6-311+G**, E = -1618.9473621504 a.u.
SP at mPW2PLYP/6-311+G**, E = -1618.9734815385 a.u.

O,1
C,0,1.7829757095,-2.4449732492,1.7548533699
H,0,1.3397515913,-3.2005227676,1.0981613979
H,0,2.4700895039,-2.9518247446,2.4405370565
H,0,0.9770308173,-1.9944216004,2.3449084686
O,0,-5.5789718506,-1.2233038807,-0.3722308854
H,0,-6.5217260205,-1.4103132615,-0.3229962895
C,0,1.2204685317,1.9879973431,-0.0046012616
C,0,1.4920692016,3.2811245768,-0.4685007986
C,0,0.6729810501,1.8432402205,1.2750409266
C,0,1.222492761,4.3970957972,0.3232988135
H,0,1.9292040861,3.4308507407,-1.4507568751
C,0,0.4029510881,2.956248417,2.0689102163
H,0,0.4427528605,0.8471999788,1.6409950264
C,0,0.6732682584,4.2395693174,1.5946114945
H,0,1.4443401756,5.3891829563,-0.0575393285
H,0,-0.0252492463,2.8193759464,3.0572118418

H,0,0.4600541187,5.1076959963,2.2103400299
C,0,2.5834860068,0.7700750734,-1.819045967
C,0,2.6153443386,-0.0419201927,-2.9604282015
C,0,3.7460424458,1.4669082964,-1.4732782895
C,0,3.7657969866,-0.141706002,-3.738742005
H,0,1.744473599,-0.6220580078,-3.2490975335
C,0,4.9022023931,1.3660729446,-2.2469378547
H,0,3.7593969342,2.0939205989,-0.5885499999
C,0,4.9163477901,0.5627765761,-3.3849016965
H,0,3.7638917903,-0.7766060236,-4.6191585538
H,0,5.791101529,1.9166917804,-1.9552169993
H,0,5.8146599408,0.4846076046,-3.9891233219
C,0,-2.2730181154,-2.4811142531,0.6871197577
C,0,-1.3792911927,-1.5089294331,-0.0280697719
H,0,-0.4549839763,-1.881099904,-0.4490766251
C,0,-1.781241854,-0.1912769809,-0.2136843351
H,0,-2.733064679,0.1182846471,0.2116221448
N,0,-1.1649309238,0.759641755,-0.8997720787
C,0,-1.7828221587,2.0678941242,-1.1564104248
C,0,0.0382680482,0.5870314703,-1.7275476039
C,0,-1.5227791827,2.2606490934,-2.6248058066
C,0,-0.136423469,1.6260081638,-2.8602463187
H,0,-1.2796982936,2.8346181464,-0.5551319141
H,0,-1.5481660729,3.3121677292,-2.9400734972
H,0,-2.8393644156,2.0364966526,-0.8866171434
H,0,-2.2830508635,1.7226310951,-3.2208204369
H,0,0.647485658,2.3835369261,-2.8037223279
H,0,-0.0497555387,1.1501766344,-3.8387424831
H,0,0.0239366255,-0.4396898666,-2.1046526548
C,0,1.3580971986,0.7480812315,-0.8945817702
O,0,-2.8792517879,-2.4570638868,-0.5646906095
O,0,-4.3724229394,-3.6002368502,-0.4542329272
H,0,-4.2753351335,-3.9595040492,-1.3452625621
H,0,-5.1327781786,-2.1140702682,-0.4256176085
O,0,1.4062650614,-0.4200880987,-0.0939275044
Si,0,2.6774735928,-1.1422076567,0.7536112208
C,0,3.5529840368,0.0636040651,1.8937141855
H,0,2.8667064265,0.4802552818,2.6372044159
H,0,4.3472525105,-0.4732173676,2.425298067
H,0,4.0165048033,0.8948384403,1.3546638862
C,0,3.9017842769,-1.9556315393,-0.4098958092
H,0,4.5046959464,-1.2281584416,-0.9628278096
H,0,4.5791807907,-2.5944994813,0.168405162
H,0,3.3776253437,-2.5864619988,-1.1356356967
C,0,-1.6086192215,-3.8074948457,1.0058947631
H,0,-0.9614203344,-4.122121296,0.182366518
H,0,-1.0139017704,-3.7306970161,1.9203760149
H,0,-2.3899916808,-4.5584206178,1.1460933697
C,0,-3.1634665747,-1.9901024733,1.8143857822
H,0,-3.7548874039,-1.1240446503,1.5136530265
H,0,-3.8639442428,-2.7893063889,2.0725466757
H,0,-2.5605927058,-1.7460075271,2.6938884881

TS-10c *syn-anti-down*

M06-2X/6-31+G**, E = -1619.48445969 a.u.
Thermal correction to Gibbs Free Energy = 0.513301 a.u.
1 imaginary frequency = -639.52 cm⁻¹
SP at B2PLYP/6-311+G**, E = -1618.9409002494 a.u.
SP at mPW2PLYP/6-311+G**, E = -1618.9669926736 a.u.

O,1
C,0,1.8584198594,-2.527869314,1.6879188085
H,0,1.3828397865,-3.2530457127,1.0192645006
H,0,2.5718126473,-3.0659033024,2.320924631
H,0,1.0824399839,-2.0994052247,2.3315847833
O,0,-5.0149970179,-0.9151719075,0.3619147239
H,0,-5.8943482982,-0.8936426022,0.7523619779
C,0,1.1929179794,1.9329783229,0.0275656737
C,0,1.4385683257,3.2407044591,-0.4091886886
C,0,0.6464420227,1.7507484483,1.3027386118

C,0,1.1446770733,4.334349954,0.4051475435
H,0,1.8732299474,3.4193626246,-1.3877832209
C,0,0.352177555,2.8412286388,2.118980975
H,0,0.4347123179,0.7429689273,1.6467348174
C,0,0.5968311923,4.1393526859,1.6717726606
H,0,1.3464406904,5.3384574279,0.0452022052
H,0,-0.0755158756,2.6754745654,3.1030757786
H,0,0.3649221047,4.9901732324,2.3046438173
C,0,2.5735522165,0.7769706976,-1.8163929876
C,0,2.6159686158,-0.0182725695,-2.9691834629
C,0,3.7232927138,1.4927872692,-1.4668837891
C,0,3.7634389054,-0.0829491269,-3.7554977201
H,0,1.756372006,-0.6137800686,3.2601753532
C,0,4.8769375024,1.4268941977,-2.2486103249
H,0,3.7291732596,2.1071305155,-0.5732284187
C,0,4.9010813003,0.6406490607,-3.3981350136
H,0,3.7696309104,-0.706099161,-4.6442506363
H,0,5.756071855,1.9914295608,-1.9538993453
H,0,5.7972633171,0.5898375101,-4.008340462
C,0,-2.2877222061,-2.5214359082,0.6578374594
C,0,-1.3531609557,-1.6039267351,-0.0571508423
H,0,-0.4239712789,-1.9877604177,-0.4567375941
C,0,-1.7739288114,-0.289638751,-0.2304200149
H,0,-2.7473551978,-0.0309246947,0.1902704453
N,0,-1.1728333472,0.6866667047,-0.8921181982
C,0,-1.8154834969,1.9862140973,-1.1270880034
C,0,0.033341197,0.548549779,-1.7212437533
C,0,-1.5559971351,2.2106807885,-2.6146209236
C,0,-0.1584000129,1.6040825427,-2.8361743554
H,0,-1.3293473767,2.7518653324,-0.5104579766
H,0,-1.5993352458,3.2665845616,-2.8882657619
H,0,-2.8716843323,1.9280744391,-0.8599556621
H,0,-2.3057508782,1.6698633593,-3.1986689184
H,0,0.6124802598,2.3737452228,-2.7657376375
H,0,-0.0625687593,1.1466759739,-3.8225886741
H,0,0.0344882515,-0.4719844261,-2.1155582545
C,0,1.352372163,0.7149032561,-0.8882345254
O,0,-2.8909901929,-2.5189604217,-0.5953530651
O,0,-4.5267522477,-3.4313158155,-0.4757456765
H,0,-4.6550426319,-3.4885694987,-1.4315256047
H,0,-4.8857855591,-1.8447883417,0.0305610607
O,0,1.4245690192,-0.4695663652,-0.1129806037
Si,0,2.7167583,-1.1850957079,0.7083304104
C,0,3.5738556864,0.014710635,1.8688759129
H,0,2.8799900255,0.4092682241,2.6173359492
H,0,4.3753607931,-0.5180718132,2.3935778968
H,0,4.0254071549,0.8611052228,1.3432398527
C,0,3.9534297709,-1.947535122,-0.4774217488
H,0,4.5376473243,-1.1950434441,-1.0166277456
H,0,4.6471889876,-2.5812203898,0.0871424428
H,0,3.4427774124,-2.5768229888,-1.2139680142
C,0,-1.6998185202,-3.833227124,1.1385857734
H,0,-1.1589508122,-4.2936154709,0.3025250796
H,0,-0.9596475153,-3.5961011067,1.9121580007
H,0,-2.9209842439,-2.0337811883,1.4105172238
C,0,-2.7490543615,-4.7927104039,1.6977224014
H,0,-3.4897889744,-5.0333618729,0.9340809138
H,0,-2.2776985172,-5.7131281374,2.0538798186
H,0,-3.2748722463,-4.334987059,2.5427737565

TS-10a *syn-syn-up*

M06-2X/6-31+G**, E = -1580.18770279 a.u.

Thermal correction to Gibbs Free Energy = 0.485703 a.u.

1 imaginary frequency = -655.16 cm⁻¹

SP at B2PLYP/6-311+G**, E = -1579.6623111103 a.u.

SP at mPW2PLYP/6-311+G**, E = -1579.6874328765 a.u.

O,1

C,0,0.9877860934,-5.0490198412,4.0283329725

H,0,0.601347634,-5.8103576337,3.3413156807

H,0,1.0003244366,-5.4816896488,5.0343879023
H,0,0.2919988128,-4.2029296096,4.0151423947
O,0,-3.4460779605,-4.8504749007,3.8337881039
C,0,3.3407837607,-1.5208014717,1.7561371891
C,0,4.3551585243,-0.6369304675,1.3683028033
C,0,2.3060751583,-1.0347341484,2.5636954238
C,0,4.3413947714,0.6945530768,1.7846537515
H,0,5.1742965536,-0.9805292794,0.7442686646
C,0,2.2897598737,0.2953325752,2.9792591495
H,0,1.4957707009,-1.7007388601,2.8491826853
C,0,3.3077010049,1.1666262512,2.5907629558
H,0,5.1421732008,1.3594184887,1.4761074893
H,0,1.4751266086,0.6507177287,3.6029912165
H,0,3.2957041798,2.2027667781,2.914297587
C,0,4.5806978037,-3.6673679941,1.0341956784
C,0,4.6695945311,-4.7786545444,0.1857154887
C,0,5.6872256027,-3.356544453,1.8313866596
C,0,5.8321051244,-5.5422739878,0.1206222179
H,0,3.821082499,-5.0760561173,-0.4229411297
C,0,6.8528074718,-4.1214888133,1.7722910276
H,0,5.6467226231,-2.5173151317,2.5172633396
C,0,6.9313628451,-5.215943171,0.9149251303
H,0,5.8739645812,-6.3993618555,-0.5442142044
H,0,7.6965699587,-3.8600057288,2.4032365714
H,0,7.836843467,-5.8127046241,0.8694586819
C,0,-1.7012257365,-3.4688009022,1.6163313403
C,0,-0.3231231933,-3.3752188319,1.0519554444
H,0,0.3801647209,-4.1548499219,1.3038803151
C,0,0.0951524183,-2.2322636746,0.3822771832
H,0,-0.6222087481,-1.4275660086,0.2391594554
N,0,1.2953679001,-1.9740887264,-0.1150095944
C,0,1.5765627378,-0.7450316301,-0.8689161738
C,0,2.454969293,-2.8849273565,-0.1608615579
C,0,2.4428692513,-1.2596147302,-2.0134095393
C,0,3.2948781823,-2.3487240618,-1.3439241112
H,0,2.069636395,-3.8919122341,-0.3493157691
C,0,3.2356884377,-2.9464125581,1.2049575463
O,0,-1.0806144819,-2.7130264287,2.605779513
O,0,-2.3400013779,-2.4925423133,3.9892308397
H,0,-1.6755866606,-2.4737217965,4.69010908
H,0,-3.0332619411,-3.9390119469,3.9398725893
O,0,2.4165966706,-3.7376089308,2.0446287797
Si,0,2.7052690136,-4.5115766865,3.5181288804
C,0,3.4497290985,-3.3450764896,4.7859618458
H,0,2.7572135241,-2.5363849449,5.0384141378
H,0,3.6681060189,-3.907019166,5.7012381018
H,0,4.3847429881,-2.8948804652,4.4387120389
C,0,3.7999998048,-6.0180074887,3.2912980315
H,0,4.8360379295,-5.7588528551,3.0511438126
H,0,3.7977680492,-6.6057167965,4.2165142026
H,0,3.4122865072,-6.6524473087,2.4872085317
H,0,4.231960947,-1.9250049706,-0.9761201432
H,0,3.5573159278,-3.1536368028,-2.0326770246
H,0,3.0505609624,-0.4718744618,-2.4622454362
H,0,1.8036461155,-1.6907332872,-2.7892900548
H,0,2.1286089802,-0.0457301676,-0.2283479446
H,0,0.6415496667,-0.2807957137,-1.1852465144
C,0,-2.8965995676,-2.8180227814,0.962027027
H,0,-3.1937689273,-3.3810803046,0.0732628513
H,0,-3.723961376,-2.8235317122,1.6758271178
H,0,-2.6936737461,-1.781393412,0.6830951655
H,0,-1.9221967661,-4.4868922435,1.9529096922
H,0,-4.1789538795,-4.8880535057,4.4563709092

TS-10c syn-syn-up

M06-2X/6-31+G**, E = -1619.48384445 a.u.
Thermal correction to Gibbs Free Energy = 0.512070 a.u.
1 imaginary frequency = -655.63 cm⁻¹
SP at B2PLYP/6-311+G**, E = -1618.9402641891 a.u.
SP at mPW2PLYP/6-311+G**, E = -1618.9662922319 a.u.

O,1

C,0,1.0237483343,-5.0020272908,4.087788709
H,0,0.6261782621,-5.7706373164,3.4153615373
H,0,1.048404403,-5.4217012293,5.0991036529
H,0,0.3303717209,-4.1542554586,4.0716427378
O,0,-3.6330334334,-4.9034058396,3.6473520986
C,0,3.3762294443,-1.5034249645,1.7523945267
C,0,4.3930397427,-0.6347867095,1.3370327211
C,0,2.3624819377,-0.997609137,2.5739505028
C,0,4.4016557572,0.7008968905,1.7394935187
H,0,5.1968237838,-0.9940839115,0.7018986369
C,0,2.3688625002,0.3365087764,2.97676462
H,0,1.5506287944,-1.6517924312,2.8808321309
C,0,3.3886273797,1.192463521,2.5601331411
H,0,5.2037495753,1.3537438095,1.4094945495
H,0,1.5708356269,0.7073376041,3.6127661766
H,0,3.3941574997,2.2317769131,2.87349225
C,0,4.5814963422,-3.6687760488,1.0326263518
C,0,4.6501159183,-4.7857075095,0.1895717438
C,0,5.7015662534,-3.3619769325,1.8125030256
C,0,5.8054793359,-5.5592504301,0.1139105695
H,0,3.7918398111,-5.0796327807,-0.4069539083
C,0,6.8598578187,-4.1366496179,1.7426879231
H,0,5.6776320776,-2.5175642997,2.4927582407
C,0,6.9179151982,-5.2372303898,0.8914003202
H,0,5.8315191067,-6.4207217811,-0.5460267318
H,0,7.7141917301,-3.8778182738,2.3603475794
H,0,7.8178067316,-5.8417254170,0.8377053472
C,0,-1.7140519836,-3.499116883,1.621682503
C,0,-0.3235861498,-3.3814145277,1.0904943004
H,0,0.3830449705,-4.1584937685,1.3413851911
C,0,0.0892427849,-2.2314348795,0.4296279979
H,0,-0.6333553492,-1.4305200871,0.2904108019
N,0,1.2866176994,-1.9656676087,-0.0704779156
C,0,1.55757003,-0.73804186,-0.8307508396
C,0,2.4443020413,-2.8778183352,-0.1345434158
C,0,2.4023600791,-1.2566759796,-1.9898789712
C,0,3.262840441,-2.3482433402,-1.3349576453
H,0,2.0537501537,-3.8847270872,-0.3118607218
C,0,3.2463861223,-2.9333141257,1.2176729227
O,0,-1.1267089651,-2.7646762428,2.6419194519
O,0,-2.4348401199,-2.6075947178,3.9930763645
H,0,-1.7961126312,-2.65053769,4.7162987916
H,0,-3.1878374476,-4.0204448053,3.831711145
O,0,2.4307187704,-3.7055206668,2.0782158665
Si,0,2.7367425693,-4.4780357552,3.5490676354
C,0,3.5068242655,-3.3125064323,4.80236883
H,0,2.8257132712,-2.4947590237,5.056718554
H,0,3.7273409225,-3.8716109532,5.7188957819
H,0,4.4436118269,-2.8747008502,4.444528003
C,0,3.8160221449,-5.993872043,3.3123238607
H,0,4.8513785451,-5.7444509411,3.0595752736
H,0,3.8191930352,-6.5792826915,4.2390080299
H,0,3.4130572345,-6.6266657777,2.5144557804
H,0,4.2090021309,-1.9281887712,-0.9870475213
H,0,3.507091436,-3.1558392819,-2.0272649545
H,0,3.0042044889,-0.4711463424,-2.4503016627
H,0,1.74795407,-1.6864307664,-2.7537770116
H,0,2.1222761733,-0.0392035007,-0.2011159659
H,0,0.6182937389,-0.2718096243,-1.1311320585
C,0,-2.8983580913,-2.8484553336,0.94098831
H,0,-3.7146345421,-2.8489511589,1.6705967155
H,0,-2.6758222259,-1.7993300589,0.7192333927
H,0,-1.9384670032,-4.528926369,1.9232715098

H,0,-4.3853667286,-4.9569569578,4.2451849446
C,0,-3.3047959097,-3.6043389217,-0.3214066796
H,0,-2.4989008215,-3.5935336768,-1.0629431695
H,0,-3.5356673706,-4.6493745657,-0.0903048478
H,0,-4.1918070969,-3.1579223055,-0.7774837386

TS-10a syn-anti-up

M06-2X/6-31+G**, E = -1580.19056399 a.u.
Thermal correction to Gibbs Free Energy = 0.486757 a.u.
1 imaginary frequency = -655.12 cm⁻¹
SP at B2PLYP/6-311+G**, E = -1579.6644584596 a.u.
SP at mPW2PLYP/6-311+G**, E = -1579.6897212709 a.u.

O,1

C,0,1.5908601749,-3.1237189806,1.703497474
H,0,1.284861484,-3.7756926594,0.8776269333
H,0,2.1719843092,-3.7276906776,2.4082030521
H,0,0.6848848032,-2.7681081065,2.2064821691
O,0,-4.1374688792,-0.337424522,2.5241676906
H,0,-4.988491399,-0.2975005052,2.9716663082
C,0,1.3615501863,1.5854912613,0.7391880559
C,0,1.7452185348,2.9170232311,0.5385636193
C,0,0.6833575605,1.2583953629,1.9191402664
C,0,1.4652913314,3.8936888841,1.4945386143
H,0,2.2748667663,3.2055882794,-0.3640979875
C,0,0.3991415773,2.2328255326,2.8734471164
H,0,0.3552193111,0.234605335,2.0768482022
C,0,0.7885198976,3.5559916421,2.6648834442
H,0,1.7775947223,4.9185896285,1.3195502344
H,0,-0.1355599871,1.9568638991,3.7771415908
H,0,0.5682339296,4.3160314529,3.4080006159
C,0,2.7916029355,0.6074250778,-1.1780579084
C,0,2.8593886161,-0.042381654,-2.4171854498
C,0,3.9610767788,1.1828997538,-0.6708959676
C,0,4.0509226902,-0.100292638,-3.1350507355
H,0,1.9822061837,-0.5312046606,-2.8295054187
C,0,5.1587201811,1.1239608146,-1.38519212
H,0,3.951827162,1.6745163323,0.2958718012
C,0,5.2081620345,0.4848199439,-2.6212252596
H,0,4.0763544787,-0.6112709263,-4.0925241263
H,0,6.0532026181,1.5752603531,-0.9671599037
H,0,6.1391536177,0.4377153955,-3.1772634953
C,0,-2.4342494502,-2.4270661477,0.8474391313
C,0,-1.4177041082,-1.5618505855,0.1831338291
H,0,-0.4538459912,-1.9714778623,-0.0851781846
C,0,-1.7230376864,-0.2097943374,0.0604229615
H,0,-2.6661863802,0.11738671,0.5015470021
N,0,-1.0122097347,0.7486302419,-0.5104781569
C,0,-1.5173132305,2.1215670037,-0.6454720403
C,0,0.2382679458,0.5812901558,-1.2713963381
C,0,-1.1289776398,2.466460931,-2.0795774832
C,0,0.2365270379,1.7806306043,-2.2488806318
H,0,0.1725335693,-0.379403063,-1.7917606337
C,0,1.5056406894,0.511613225,-0.3442527772
H,0,-3.4708964267,-2.0876844084,0.7389991506
O,0,-1.8290584812,-1.8750073099,1.9660112318
O,0,-2.8300587008,-2.5049511162,3.4309669336
H,0,-2.1580468161,-2.309453658,4.0963255617
H,0,-3.6566060749,-1.1126562264,2.9221067396
C,0,-2.2715232209,-3.9203240042,0.7002352949
H,0,-1.2161968132,-4.1955741947,0.7818891668
H,0,-2.825763113,-4.4154211684,1.5004426207
H,0,-2.6576091857,-4.253596763,-0.2668866339
O,0,1.4466406052,-0.7795125584,0.2356236871
Si,0,2.6072723423,-1.6931207248,1.0565795779
C,0,3.3911258349,-0.7270678677,2.4604103518
H,0,2.6508946671,-0.4507663812,3.2174186006
H,0,4.155438854,-1.3508114413,2.9379992366
H,0,3.8762421031,0.1894211075,2.1105839119
C,0,3.9302895006,-2.3380615452,-0.1076022758

H,0,4.5968113992,-1.5501888959,-0.4724483983
H,0,4.5361569568,-3.0835370469,0.4207381845
H,0,3.4739749662,-2.8273966838,-0.9746183457
H,0,1.0427877484,2.4724069742,-1.9951719587
H,0,0.4100758489,1.4494980575,-3.2744545155
H,0,-1.0780276604,3.5434264016,-2.249627081
H,0,-1.8632602564,2.0398808253,-2.7688925676
H,0,-1.0074598658,2.7690153723,0.0786736842
H,0,-2.5901518725,2.1419373006,-0.450352542

TS-10b *syn-anti-up*

M06-2X/6-31+G**, E = -1619.49137046 a.u.

Thermal correction to Gibbs Free Energy = 0.511206 a.u.

1 imaginary frequency = -648.87 cm⁻¹

SP at B2PLYP/6-311+G**, E = -1618.9466760979 a.u.

SP at mPW2PLYP/6-311+G**, E = -1618.9729372253 a.u.

0,1
C,0,1.4653692457,-3.0585121928,1.7691795896
H,0,1.2064066088,-3.751771307,0.9613058336
H,0,2.004018973,-3.6250446457,2.5360001752
H,0,0.53247914,-2.6765360944,2.1986826225
O,0,-3.7971563796,-0.3471323827,3.6694050396
H,0,-4.2922905795,-0.4005884048,4.4927869959
C,0,1.3489639699,1.6281142188,0.7128443453
C,0,1.7681817536,2.947198969,0.5019879438
C,0,0.6394274891,1.3340393331,1.8831755479
C,0,1.4931926987,3.943378253,1.4393516337
H,0,2.3209954237,3.2115395313,-0.3940898353
C,0,0.3593412028,2.3279186009,2.8183358421
H,0,0.2830242885,0.3209020456,2.0483115234
C,0,0.7851945081,3.6383026519,2.6001265968
H,0,1.8340385708,4.9578915443,1.2572344208
H,0,-0.2003471318,2.0764295099,3.7139283473
H,0,0.5686796525,4.413675684,3.3283456749
C,0,2.787142676,0.5890820772,-1.1676438894
C,0,2.8582581621,-0.0844149638,-2.3940386808
C,0,3.9618432592,1.1480743392,-0.6541498363
C,0,4.0577005294,-0.1805169787,-3.0941861469
H,0,1.9764613169,-0.5618594299,-2.8098722381
C,0,5.1673887752,1.0511792719,-1.3508424058
H,0,3.9508715671,1.6560599155,0.3040512065
C,0,5.2200766773,0.3892786768,-2.5746567422
H,0,4.0850241783,-0.7094020882,-4.0418059121
H,0,6.0657076564,1.4905211224,-0.9283346846
H,0,6.1575907407,0.3123785949,-3.1162733859
C,0,-2.5064152908,-2.3759770466,0.7720349685
C,0,-1.5096100739,-1.4534764142,0.1315371067
H,0,-0.5454435902,-1.8622634394,-0.140189891
C,0,-1.7735936923,-0.0954795534,0.004442667
H,0,-2.7062825177,0.2861464218,0.4123550868
N,0,-1.0213480653,0.8343742177,-0.5651237081
C,0,-1.4845582886,2.2197592903,-0.7281598022
C,0,0.2365035264,0.6218819502,-1.3020995232
C,0,-1.0610109167,2.5342268705,-2.1594992635
C,0,0.2847278019,1.804937992,-2.2975573439
H,0,0.1545214864,-0.3443893924,-1.8093968011
C,0,1.4865548978,0.5352947324,-0.3525198618
O,0,-1.8644593436,-1.8620589689,1.8937551594
O,0,-2.6470528067,-2.7074401161,3.3834359986
H,0,-1.8152962565,-2.8135922406,3.8624997418
H,0,-3.3397218658,-1.2315762525,3.5758878479
C,0,-2.2152937417,-3.8442519085,0.5200282021
H,0,-1.1438797298,-4.0405973789,0.6053618685
H,0,-2.7429006766,-4.4427613337,1.266462408
H,0,-2.5554557559,-4.1325942789,-0.478782363
O,0,1.3883030327,-0.7456478273,0.2448477283
Si,0,2.5169175646,-1.6601246322,1.1093169661
C,0,3.2924250641,-0.6788680301,2.5072248456
H,0,2.5468873171,-0.3889085323,3.2538697623

H,0,4.0476230123,-1.3020535057,2.9999069542
H,0,3.7870111104,0.2302442115,2.15192455
C,0,3.8473796432,-2.3518973256,-0.0188163515
H,0,4.5329579737,-1.5840378822,-0.3909599331
H,0,4.4317520986,-3.0969365655,0.533729868
H,0,3.393369109,-2.8510588989,-0.8814746793
H,0,1.1090352309,2.4750442362,-2.0437512767
H,0,0.462218495,1.451726052,-3.3150593147
H,0,-0.9740357563,3.6069773018,-2.3411870709
H,0,-1.7965362603,2.1220907256,-2.8561837891
H,0,-0.9704127463,2.8623715708,-0.002912107
H,0,-2.5599943982,2.2740915687,-0.5547760697
C,0,-3.9880449715,-2.0544547681,0.713468774
H,0,-4.3801460752,-2.2427760029,-0.2899875836
H,0,-4.5064693261,-2.7016640981,1.4265089335
H,0,-4.1926931909,-1.0229496,1.0040027143

TS-10c *syn-anti-up*

M06-2X/6-31+G**, E = -1619.48648516 a.u.

Thermal correction to Gibbs Free Energy = 0.512998 a.u.

1 imaginary frequency = -651.49 cm⁻¹

SP at B2PLYP/6-311+G**, E = -1618.9424740684 a.u.

SP at mPW2PLYP/6-311+G**, E = -1618.9686201549 a.u.

0,1
C,0,1.5857406219,-3.1168375857,1.7187157112
H,0,1.2727270866,-3.7704361239,0.8967247031
H,0,2.1681503959,-3.7207154427,2.4224652259
H,0,0.6833893009,-2.7567998651,2.2250819861
O,0,-4.1531003258,-0.3465242413,2.534923489
H,0,-5.0055419794,-0.3109694349,2.9800630651
C,0,1.3649002479,1.5881849654,0.7394323969
C,0,1.7514146645,2.9182815228,0.5348952864
C,0,0.688458596,1.2654751734,1.921599478
C,0,1.475802799,3.8978531529,1.4892071286
H,0,2.2798826145,3.2034719145,-0.3695285012
C,0,0.4086066994,2.2427754547,2.8742638903
H,0,0.3582906867,0.2428110848,2.082344442
C,0,0.8006971872,3.5645178947,2.6617430265
H,0,1.790217352,4.9215887521,1.3112015488
H,0,-0.1247572917,1.9701798136,3.7797598326
H,0,0.5838374827,4.3268100234,3.4035493587
C,0,2.7876675779,0.6021894473,-1.1794878064
C,0,2.8500359112,-0.0508405321,-2.4172128323
C,0,3.9601253268,1.1759577982,-0.677295356
C,0,4.0392098592,-0.1136267809,-3.1385611176
H,0,1.9703744899,-0.5384408585,-2.8256710888
C,0,5.1554407593,1.112050584,-1.3950824984
H,0,3.9551952684,1.6701007075,0.2882246022
C,0,5.199507991,0.4696917691,-2.62964641
H,0,4.0603591746,-0.6270998267,-4.0947984749
H,0,6.0523822833,1.562011718,-0.9809001838
H,0,6.1287304475,0.4188337072,-3.1883091087
C,0,-2.4404449877,-2.425941908,0.8502564458
C,0,-1.421762597,-1.5580175484,0.1922390389
H,0,-0.4574528655,-1.9687951921,-0.0742310239
C,0,-1.725935026,-0.2059082388,0.0694448188
H,0,-2.6693499768,0.1217283844,0.5095995095
N,0,-1.0140146341,0.7517553006,-0.5014734514
C,0,-1.5181458984,2.1248339161,-0.6384958319
C,0,0.2342195431,0.5813452134,-1.2653590288
C,0,-1.1332958494,2.4656698663,-2.075155542
C,0,0.2314894751,1.7787737384,-2.2451357726
H,0,0.1654492937,-0.3802027258,-1.7837829517
C,0,1.5039582656,0.5113728264,-0.3417261646
H,0,-3.4793052418,-2.09029416,0.7342150687
O,0,-1.8420511839,-1.8800838965,1.9725342163
O,0,-2.8472866043,-2.5205199199,3.4314731951
H,0,-2.1774290099,-2.3243536765,4.0988263586
H,0,-3.6733885029,-1.1251878758,2.9274198958

C,0,-2.2769320449,-3.9191638714,0.6728821461
H,0,-1.2192142914,-4.1704966693,0.81378771
H,0,-2.8364393585,-4.4055543813,1.4779964489
O,0,1.4438742372,-0.7781845001,0.2415739354
Si,0,2.6041873333,-1.6919013656,1.0628360235
C,0,3.3949487024,-0.7232357497,2.4610002025
H,0,2.6575178709,-0.4412404593,3.2186504623
H,0,4.1578519573,-1.3482430959,2.9392132701
H,0,3.8829256895,0.1899958569,2.1067830569
C,0,3.9214913001,-2.3448065224,-0.1034567745
H,0,4.5880472915,-1.5599402691,-0.4747186953
H,0,4.5280848,-3.0890591427,0.4257539742
H,0,3.4605089792,-2.8372469064,-0.9662391346
H,0,1.0384772958,2.4706673183,-1.994053884
H,0,0.4030412245,1.4455841762,-3.2703753241
H,0,-1.0823324596,3.542126689,-2.2477221042
H,0,-1.8694550706,2.0373939396,-2.7607884913
H,0,-1.0055437868,2.7735337354,0.08260171
H,0,-2.5904085639,2.1467864339,-0.4403923951
C,0,-2.7705420389,-4.3793383358,-0.6967307169
H,0,-2.2040697385,-3.896716808,-1.5000802676
H,0,-2.6622734358,-5.4609540059,-0.8096365825
H,0,-3.827938222,-4.1320547846,-0.8364537494

TS-10a *syn-syn-down*

M06-2X/6-31+G**, E = -1580.18777637 a.u.

Thermal correction to Gibbs Free Energy = 0.484468 a.u.

1 imaginary frequency = -656.48 cm⁻¹

SP at B2PLYP/6-311+G**, E = -1579.6636622485 a.u.

SP at mPW2PLYP/6-311+G**, E = -1579.6884751731 a.u.

0,1
C,0,-2.8814984425,-7.3786560399,4.5800528896
H,0,-2.9383783503,-7.503582712,3.4935742987
H,0,-3.397700774,-8.2248648407,5.0452643533
H,0,-3.4185596182,-6.4608374614,4.8440185446
O,0,-6.2148234676,-5.681025209,0.5353748159
C,0,0.4921117457,-4.1921923566,5.8349842626
C,0,1.6078597085,-3.5938176127,6.4333897296
C,0,-0.7791644364,-3.8532931795,6.3109076799
C,0,1.4560914961,-2.6788800981,7.4751647086
H,0,2.6097933911,-3.8460772909,6.0998106745
C,0,-0.9340111561,-2.9401247623,7.3522913042
H,0,-1.6536596689,-4.3000427568,5.8467174018
C,0,0.1839721003,-2.3447915128,7.9361216622
H,0,2.3360999336,-2.2303891172,7.9255232008
H,0,-1.9305727662,-2.6903640137,7.7034698972
H,0,0.0650910645,-1.6308318457,8.744955176
C,0,1.8176617064,-6.0226555316,4.6008656785
C,0,2.3106654597,-6.5458837655,3.988031249
C,0,2.3540929079,-6.5054094473,5.79973921
C,0,3.3141138353,-7.5118419306,3.9940648298
H,0,1.9067271608,-6.2170347997,2.4465966875
C,0,3.3550729678,-7.4764436211,5.7998489281
H,0,1.9872311647,-6.1285805995,6.7485629552
C,0,3.8402379218,-7.9833847398,4.5962878665
H,0,3.6790778741,-7.901001028,2.4487163655
H,0,3.7513166006,-7.8369981578,6.744015165
H,0,4.6193177643,-8.7393582598,4.5939660564
C,0,-3.7747096074,-4.4230687596,2.1912105241
C,0,-2.3341147025,-4.4448296816,2.5866915328
H,0,-1.7952908653,-5.3750984614,2.482038435
C,0,-1.7032807129,-3.2877000276,3.0247662816
H,0,-2.2852664455,-2.3704797689,3.0718833167
N,0,-0.4359945127,-3.1365122514,3.3801073129
C,0,0.1465007365,-1.8222043342,3.6804568436
C,0,0.6149295078,-4.1644526615,3.3204477566
C,0,1.4837989212,-1.8887733259,2.9466909778
C,0,1.9164742368,-3.3556234886,3.119363373
H,0,0.2842658654,-1.7210073733,4.7640256632

H,0,2.2149447152,-1.187655534,3.352927569
H,0,-0.5189207995,-1.0330016053,3.3278573595
H,0,1.3293264453,-1.656377055,1.8893599374
H,0,2.5672260251,-3.4626476632,3.989287448
H,0,2.4730519311,-3.7235999381,2.2555017685
H,0,0.3915333065,-4.8067339672,2.4634280746
C,0,0.603542645,-5.0836123449,4.5933527283
O,0,-3.2082699326,-3.9443322344,1.0197873724
O,0,-4.6237674554,-3.7492453267,-0.2071510707
H,0,-4.0993405216,-4.0039127929,-0.9771517693
H,0,-5.6179957769,-4.938800572,0.2117580518
O,0,-0.5735996659,-5.8544501081,4.4438317311
Si,0,-1.1019783412,-7.2901519734,5.154591387
C,0,-1.0310522289,-7.2182736691,7.0278101377
H,0,-1.6598992476,-6.4111997826,7.4160741448
H,0,-1.4035350581,-8.1662150333,7.4328974723
H,0,-0.0154458136,-7.0697174094,7.4054873034
C,0,-0.1373424428,-8.7578237997,4.5015918154
H,0,0.8872864613,-8.7932584131,4.885229234
H,0,-0.6447029668,-9.6854372824,4.7899745377
H,0,-0.0904436278,-8.7225499811,3.4080006273
C,0,-4.7704645108,-3.5040968993,2.8601468811
H,0,-4.999142961,-3.8694742063,3.8654636105
H,0,-4.4011047216,-2.4780573084,2.9238760139
H,0,-5.6889134754,-3.5016229309,2.2687449871
H,0,-4.1720099031,-5.4374728726,2.0792432589
H,0,-7.0930166235,-5.4863784726,0.1935039041

TS-10c *syn-syn-down*

M06-2X/6-31+G**, E = -1619.48493202 a.u.

Thermal correction to Gibbs Free Energy = 0.512844 a.u.

1 imaginary frequency = -653.96 cm⁻¹

SP at B2PLYP/6-311+G**, E = -1618.9412987937 a.u.

SP at mPW2PLYP/6-311+G**, E = -1618.9672669116 a.u.

0,1
C,0,-2.8601470916,-7.4067975631,4.5340378157
H,0,-2.9091445223,-7.5332188005,3.4472377024
H,0,-3.3802312067,-8.2519530861,4.9968594167
H,0,-3.3988193697,-6.487946195,4.7915555809
O,0,-6.3005264808,-5.627777024,0.7449430003
C,0,0.4737534951,-4.206392673,5.8277816936
C,0,1.5758531721,-3.6006871786,6.4435938958
C,0,-0.8069262408,-3.8797893138,6.2868462539
C,0,1.40136869,-2.6914191036,7.4869062335
H,0,2.5845600503,-3.8422692883,6.1228170043
C,0,-0.9846617472,-2.9717755376,7.3288393094
H,0,-1.6702226261,-4.3338235464,5.8086458382
C,0,0.120116509,-2.3697171078,7.93100027
H,0,2.2708779349,-2.2371248876,7.9515883708
H,0,-1.9884357204,-2.731721943,7.6663261663
H,0,-0.0159862653,-1.6599277592,8.7407814666
C,0,1.8299764093,-6.0214276503,4.6019112983
C,0,2.3343406431,-6.5406271971,3.4027536475
C,0,2.3608214621,-6.5020379023,5.8040536095
C,0,3.3438389651,-7.5001190706,3.4038504171
H,0,1.9340734448,-6.2136139166,2.4483445364
C,0,3.368128148,-7.4666835441,5.8099243132
H,0,1.984958882,-6.1289609445,6.7508064125
C,0,3.8647921225,-7.9693314068,4.6093080115
H,0,3.7173467975,-7.8863607444,2.4606445054
H,0,3.7601502243,-7.8257679542,6.756491688
H,0,4.6486820364,-8.7203072303,4.6117917295
C,0,-3.7718013308,-4.4156995232,2.2049336866
C,0,-2.3286918343,-4.4420350312,2.5931282657
H,0,-1.7988393133,-5.3790823745,2.5079906102
C,0,-1.6899069043,-3.2837925706,3.0158527259
H,0,-2.2676108206,-2.3632692685,3.0563720771
N,0,-0.422255227,-3.1361031186,3.3711621356
C,0,0.1609273201,-1.8228719127,3.6744750577

C,0,0.6272412717,-4.1664217023,3.3159380215
C,0,1.501718747,-1.8919292047,2.9480678548
C,0,1.9315705586,-3.3581959218,3.1289326901
H,0,0.2928611666,-1.722271424,4.7589538983
H,0,2.2313522757,-1.1900968426,3.355752205
H,0,-0.5014624014,-1.0325533707,3.3186594481
H,0,1.352824621,-1.6631626681,1.8891223396
H,0,2.5701980062,-3.4626662385,4.0082104651
H,0,2.4997924006,-3.7287758309,2.2738468793
H,0,0.4087031694,-4.8046363556,2.4544104292
C,0,0.6085640748,-5.0920663273,4.584670212
O,0,-3.2083597266,-3.9958295945,1.0124794958
O,0,-4.6347986931,-3.8529148824,-0.212918037
H,0,-4.1309012519,-4.2022356073,-0.9588614212
H,0,-5.6803294975,-4.9506749466,0.3358040481
O,0,-0.5588143049,-5.8738125221,4.4189566904
Si,0,-1.0856111241,-7.3135728629,5.1227311231
C,0,-1.0289543212,-7.2459257535,6.9965110359
H,0,-1.6656404762,-6.4439539506,7.3825385512
H,0,-1.3982784936,-8.1973218576,7.3963451481
H,0,-0.0168215185,-7.0921195754,7.381427084
C,0,-0.1075605668,-8.774331394,4.4741215631
H,0,0.9144839325,-8.8043893143,4.8651347695
H,0,-0.6113468943,-9.7054873546,4.7573487111
H,0,-0.0530153336,-8.7371043381,3.3809499408
C,0,-4.748989678,-3.4563985404,2.8509419943
H,0,-4.3475516632,-2.4378085767,2.8311933192
H,0,-5.6443821352,-3.4560822329,2.2215056962
H,0,-4.1879411967,-5.4286596999,2.1435854232
H,0,-7.1752398377,-5.4378162431,0.3915037016
C,0,-5.0943207432,-3.8853104702,4.2745279601
H,0,-5.8355843282,-3.2156993726,4.7175245448
H,0,-5.5080842603,-4.8993221031,4.2842472676
H,0,-4.2050393509,-3.8786704415,4.915430015

Cartesian coordinates and computed total energies for the structures presents in Scheme 9 and Scheme S4.

TS-11 (S)

M06-2X/6-31+G**, E = -1580.19514378 a.u.
Thermal correction to Gibbs Free Energy = 0.488500 a.u.
1 imaginary frequency = -787.38 cm⁻¹
SP at B2PLYP/6-311+G**, E = -1579.6467307944 a.u.
SP at mPW2PLYP/6-311+G**, E = -1579.6749828861 a.u.

O,1
H,0,7.1466533981,-3.6186473371,-0.3341561609
C,0,6.1961508171,-3.094704759,-0.3441073376
C,0,5.9644702096,-2.0388932251,0.5392407125
C,0,4.7434173453,-1.3724606691,0.5240420563
C,0,3.7364161648,-1.729868051,-0.3827944374
C,0,3.9718438414,-2.8003692861,-1.2481271258
C,0,5.1925894515,-3.4779441124,-1.2287642241
H,0,5.3549963782,-4.3038886963,-1.914078417
H,0,6.7323937641,-1.7380273205,1.245153107
H,0,3.218451995,-3.1214030901,-1.9580984095
H,0,4.5703471079,-0.5648964518,1.2297954906
C,0,2.4466021783,-0.8939868494,-0.411769091
C,0,1.9493288267,-0.7168873639,1.0296750164
C,0,1.3182350897,-1.776426538,1.692551254
H,0,1.1533028233,-2.7232663243,1.1849228962
C,0,0.8915523459,-1.6367409489,3.0108591276
C,0,1.104158626,-0.4389391392,3.6949272401
C,0,1.7519540693,0.6118887873,3.0500665004
C,0,2.1683831742,0.4742773422,1.7252150578
H,0,2.6712730698,1.3009294767,1.2346818271
H,0,0.3880206712,-2.4636322573,3.5013435505
H,0,0.7669130866,-0.3284946561,4.7206672401
H,0,1.9269197123,1.5485277264,3.5707701126

C,0,1.3468844293,-1.550674805,-1.2844395409
C,0,1.5730222874,-1.4400890976,-2.8160160184
H,0,1.5581786663,-2.4384718173,-3.2632161662
H,0,1.2604033499,-2.602924902,-0.9959843966
C,0,0.3841726549,-0.6210012776,-3.3363113217
H,0,0.1297359207,-0.8496189722,-4.3725488229
H,0,0.5910682434,0.4524610384,-3.2528516896
C,0,-0.7141279433,-0.9938838,-2.3521792338
H,0,-1.0778343029,-2.0141362404,-2.5185228088
H,0,-1.5618891548,-0.3054883458,-2.3294152098
H,0,2.533849996,-0.9826952598,-3.0573293286
N,0,0.0146624553,-0.91578496,-1.0629132191
H,0,-0.5287857363,-1.3812945743,-0.3165512146
O,0,-2.0661160293,-1.7389424213,0.6158138615
C,0,-2.8631065775,-0.7759627919,0.6880343817
C,0,-2.5551239858,0.5827918572,0.9404485372
C,0,-1.2721017579,1.0240300636,1.2659373378
H,0,-0.5404488507,0.2504322443,1.4990910149
H,0,-3.3724032677,1.297329055,0.8936931155
C,0,-1.0420928432,2.3481530237,1.9226066151
H,0,-0.0346146697,2.7140381081,1.7145289454
H,0,-1.145395396,2.2227227654,3.0067039619
H,0,-1.7754573639,3.0850036292,1.5837167538
O,0,-0.4757851149,1.4425594599,-0.459564144
O,0,0.6724465674,2.2969515468,-0.5143664806
O,0,2.693959314,0.3954937493,-0.9628930737
H,0,1.4154995625,1.6664300676,-0.597269846
H,0,-0.0866884555,0.2903743842,-0.7576038323
H,0,-3.9394335419,-0.9946674697,0.5514900366
Si,0,4.0013481265,1.1722236724,-1.7278090978
C,0,5.2174476651,0.0451313255,-2.5978437202
H,0,5.8173199677,-0.5538055031,-1.907092655
H,0,4.7384086896,-0.6313393752,-3.311919859
H,0,5.8960271798,0.6949452028,-3.1642242886
C,0,4.8767483244,2.2083597122,-0.4367883448
H,0,4.1832869655,2.9141876648,0.0336815288
H,0,5.325346077,1.5902931509,0.347243344
H,0,5.6771880188,2.7899413536,-0.9069264977
C,0,3.1592459093,2.268838505,-2.9873312632
H,0,3.8828985311,2.9665369979,-3.4220242117
H,0,2.7358934119,1.6717311113,-3.8023305042
H,0,2.3497395345,2.8507676671,-2.5350866305

TS-11 (R)

M06-2X/6-31+G**, E = -1580.19073850 a.u.
Thermal correction to Gibbs Free Energy = 0.486311 a.u.
1 imaginary frequency = -757.92 cm⁻¹
SP at B2PLYP/6-311+G**, E = -1579.6423866855 a.u.
SP at mPW2PLYP/6-311+G**, E = -1579.6707741157 a.u.

O,1
H,0,6.6075406602,-3.6412517932,-0.0735931351
C,0,5.6632472284,-3.1061352885,-0.0725405193
C,0,5.5076153717,-1.9536940485,0.7017690138
C,0,4.2962240083,-1.2728348476,0.6996338307
C,0,3.2203965789,-1.7180799572,-0.0804696375
C,0,3.3783206051,-2.8796498812,-0.8350422612
C,0,4.594649863,-3.5687382939,-0.833264175
H,0,4.6985824359,-4.4689295514,-1.431049701
H,0,6.3304131494,-1.5887727319,1.308760764
H,0,2.5657148934,-3.2687980581,-1.4380896935
H,0,4.1804138842,-0.3802005774,1.3103969931
C,0,1.9258112372,-0.8946762856,-0.0407454808
C,0,1.4528100052,-0.8673920106,1.4239376837
C,0,0.9147845262,-2.0195165954,2.0102014726
H,0,0.7840833473,-2.9259740461,1.4248899938
C,0,0.560133578,-2.0345833433,3.3559024896
C,0,0.74533146,-0.8982243355,4.1440382667
C,0,1.287419496,0.2490543517,3.5717891277
C,0,1.6403310036,0.2627166034,2.2214457296

H,0,2.0885891328,1.1556526565,1.7982471149
H,0,0.1393274395,-2.9370336851,3.7882355829
H,0,0.4685736004,-0.9094102053,5.1937139576
H,0,1.4408482847,1.1404842639,4.1724593485
C,0,0.8148561185,-1.4726980577,-0.945582902
C,0,1.0676451242,-1.4126150437,-2.4739198711
H,0,1.1739786224,-2.4232843088,-2.8742862061
H,0,0.6268105085,-2.51031166,-0.651525564
C,0,-0.1763404267,-0.7279801436,-3.0697870871
H,0,-0.4627288186,-1.1378425677,-4.039537822
H,0,-0.0058665987,0.3470308889,-3.1816574513
C,0,-1.2385730847,-0.947558454,-2.0003267305
H,0,-1.6317855234,-1.9697413734,-2.0136731821
H,0,-2.0707493967,-0.2419095148,-2.0455197651
H,0,1.9845653161,-0.8719271927,-2.7156118032
N,0,-0.4592359191,-0.725598581,-0.7578813967
H,0,-0.9953946668,-1.0353342999,0.0676327178
O,0,-2.3243984728,-1.0274127745,1.3409681619
C,0,-2.0755343675,-0.0659824489,2.1035278822
C,0,-1.978328731,1.3014305963,1.7447750346
C,0,-2.2878318302,1.7655611185,0.4720822758
H,0,-2.7771575217,1.0569799146,-0.197246505
H,0,-1.6742648569,2.0037136961,2.5161390685
C,0,-2.5856140557,3.2175781911,0.2416747026
H,0,-1.8448729823,3.8385753549,0.7518751059
H,0,-3.5726017718,3.4471640714,0.6586043372
H,0,-2.5880259014,3.4638240547,-0.8205430357
O,0,-0.6910343387,1.7528341723,-0.7060278798
O,0,0.2893649796,2.4815581407,0.0289081037
O,0,2.1676225893,0.4409365197,-0.445676745
H,0,0.9889336417,1.8145583401,0.147097233
H,0,-0.4049314355,0.4911224329,-0.6721252237
H,0,-1.9225998352,-0.2869619016,3.1762250427
Si,0,3.2495881029,1.2733474538,-1.4591098065
C,0,4.5896539464,0.2325418174,-2.2579504641
H,0,5.3325971146,-0.1182593157,-1.537352461
H,0,4.2027372189,-0.6367464915,-2.7979059664
H,0,5.0953003053,0.8788428225,-2.9859912583
C,0,4.0110947425,2.5637098777,-0.3366454223
H,0,3.2360442536,3.1881213212,0.1212273319
H,0,4.5901996538,2.0911289369,0.4638859714
H,0,4.6815909874,3.2202469232,-0.9009591635
C,0,2.2105039398,2.0843548001,-2.7894886251
H,0,2.7425618918,2.9537397013,-3.1914129711
H,0,2.0137153926,1.4005835844,-3.6220714573
H,0,1.2535788392,2.4218969877,-2.3769130738

8 (S)

M06-2X/6-31+G**, E = -1580.23218607 a.u.

Thermal correction to Gibbs Free Energy = 0.492809 a.u.

SP at B2PLYP/6-311+G**, E = -1579.6736723588 a.u.

SP at mPW2PLYP/6-311+G**, E = -15797036090638 a.u.

0,1

H,0,7.0836311451,-3.427836325,-0.4358443536
C,0,6.1156012749,-2.9410135225,-0.3720950036
C,0,5.9542970116,-1.7919158323,0.4045469936
C,0,4.7123717893,-1.1720749438,0.4807684551
C,0,3.608469793,-1.6743393675,-0.2202951453
C,0,3.7757816793,-2.8335729704,-0.9786509887
C,0,5.0217825284,-3.4609927615,-1.0566905011
H,0,5.1294178862,-4.3591001404,-1.6570167866
H,0,6.796564802,-1.3787140745,0.9509991354
H,0,2.9453130385,-3.2684196628,-1.5226005879
H,0,4.5996064271,-0.2800628383,1.0917792157
C,0,2.2676089533,-0.9380491689,-0.0922356956
C,0,1.8601310968,-0.9568231818,1.39221182
C,0,1.1828873108,-2.0484816569,1.944661384
H,0,0.9176690215,-2.9024016102,1.3287178163
C,0,0.8135434813,-2.0516085451,3.2879728505

C,0,1.1340763274,-0.970510784,4.1094631832
C,0,1.8358480337,0.1077596979,3.5757905902
C,0,2.1936159021,0.1136848153,2.2281201088
H,0,2.7234533954,0.9699796778,1.8221586681
H,0,0.2663691388,-2.8988473866,3.6895916094
H,0,0.8394518309,-0.97077878609,5.1542194489
H,0,2.0961006308,0.955903128,4.2017931986
C,0,1.1571204606,-1.5537758346,-0.9731000696
C,0,1.3751457378,-1.4374599616,-2.5120157272
H,0,1.5124113485,-2.4292946319,-2.9506979732
H,0,1.0499098512,-2.6118178261,-0.7113187893
C,0,0.0882565327,-0.7844381572,-3.0494233129
H,0,-0.2209369489,-1.1907797894,-4.0152406639
H,0,0.2218780115,0.2962944565,-3.1610115632
C,0,-0.9215826765,-1.0467436904,-1.9320278504
H,0,-1.3099198642,-2.0711917976,-1.9808496729
H,0,-1.7688857252,-0.356754341,-1.9167882426
H,0,2.264520542,-0.8527304244,-2.7595536241
N,0,-0.1389000512,-0.9060184261,-0.6918130048
H,0,-1.1761480951,-1.4115484708,0.4850541161
O,0,-2.028989092,-1.703772091,0.9600257509
C,0,-2.8641965959,-0.6629531203,1.1231304473
C,0,-2.5412509989,0.6186444048,1.3677430719
C,0,-1.1616650801,1.1337582267,1.6406661805
H,0,-0.4727064463,0.2976284278,1.823773273
H,0,-3.3595054537,1.3292140335,1.4517670965
C,0,-1.1430043096,2.0938526412,2.8197647899
H,0,-0.1385163527,2.4870118932,-2.9853034253
H,0,-1.4650071551,1.562685937,3.7199240802
H,0,-1.8298336213,2.9271424347,2.6385635277
O,0,-0.7405880088,1.8034682308,0.4232348343
O,0,0.5519392662,2.3837983318,0.6237001106
O,0,2.3943323601,0.4332956173,-0.4637641896
H,0,1.1559771384,1.6730669387,0.3255119025
H,0,0.0115190441,0.0950998019,-2.9530465874
H,0,-3.9136041454,-0.9505119395,1.0635156292
Si,0,3.409422731,1.3918134714,-1.4333663746
C,0,4.7831891885,0.4805739182,-2.3261071799
H,0,5.6225843895,0.2602347248,-1.6619417639
H,0,4.4575515944,-0.4607829428,-2.7778641167
H,0,5.1417419745,1.135129758,-3.1293453701
C,0,4.1203228601,2.6623251985,-0.2537584065
H,0,3.3232118005,3.1985328508,0.2734638294
H,0,4.7716253845,2.1933260495,0.4915753387
H,0,4.7144523636,3.4007918757,-0.8025453783
C,0,2.2864452472,2.2286856384,-2.6767195781
H,0,2.778212748,3.1253134842,-3.0696359055
H,0,2.0616285729,1.5732715368,-3.5242375515
H,0,1.3429939751,2.5347778772,-2.2120859231

8 (R)

M06-2X/6-31+G**, E = -1580.22777777 a.u.

Thermal correction to Gibbs Free Energy = 0.490956 a.u.

SP at B2PLYP/6-311+G**, E = -1579.6689518350 a.u.

SP at mPW2PLYP/6-311+G**, E = -1579.6989783262 a.u.

0,1

H,0,6.5642937964,-3.7531854694,0.1263776598
C,0,5.6278905263,-3.2065619463,0.0766780017
C,0,5.5408369807,-1.9098082837,0.5873592736
C,0,4.3391539349,-1.2145472108,0.519320072
C,0,3.2055531507,-1.7865887798,-0.0699364673
C,0,3.2945409437,-3.092693236,-0.5544779287
C,0,4.4998379785,-3.7959630847,-0.4866644644
H,0,4.5502700313,-4.807940859,-0.8763630124
H,0,6.409268207,-1.4416700216,1.040647087
H,0,2.4302542645,-3.5850814886,-0.9867430351
H,0,4.2771080728,-0.2092011415,0.928838451
C,0,1.8967606019,-0.9838929185,-0.0552721213
C,0,1.4119056842,-1.0009869602,1.407547545
C,0,0.7713645974,-2.1214077801,1.9451010427

H,0,0.5362421437,-2.9767884165,1.31905717
C,0,0.4305866682,-2.1683029427,3.2949708585
C,0,0.7366541811,-1.099153184,4.1371490868
C,0,1.3871365755,0.0155004973,3.6141939724
C,0,1.7214407446,0.0617646811,2.2612286298
H,0,2.251921581,0.9264660071,1.87315547
H,0,-0.0742933006,-3.0453521976,3.6885084483
H,0,0.4724096713,-1.1377362131,5.1894200123
H,0,1.6380937103,0.8545469815,4.2561240262
C,0,0.8299914104,-1.5555470516,-1.0179098114
C,0,1.237295233,-1.6420366741,-2.5142103446
H,0,1.5514860576,-2.6528728499,-2.7813068491
H,0,0.543146281,-2.5561643783,-0.6764736187
C,0,-0.0206018727,-1.2097894547,-3.3017763963
H,0,-0.296695509,-1.9281761578,-4.0769342652
H,0,0.1406125367,-0.2432490372,-3.787026907
C,0,-1.1064839204,-1.0701900698,-2.2250226346
H,0,-1.627179319,-2.0218744454,-2.0664271416
H,0,-1.8544765174,-0.305257265,-2.4475449808
H,0,2.0801137655,-0.9814275906,-2.7315082029
N,0,-0.3876058176,-0.7288732984,-0.9871541969
H,0,-1.446943496,-0.8334517769,0.1972254495
O,0,-2.1333016451,-0.8893617372,0.9616949703
C,0,-1.8567500123,0.0651996412,1.8730960329
C,0,-1.6522544586,1.3685925355,1.626543044
C,0,-1.839715427,2.043232419,0.300130742
H,0,-2.4684045297,1.4163872774,3.3469009509
H,0,-1.4038483179,2.000496985,2.4753898748
C,0,-2.4475755766,3.4303338228,0.4537888152
H,0,-1.7901732628,4.0613712971,1.0592096761
H,0,-3.4172707675,3.3621432956,0.9543570791
H,0,-2.5860810587,3.8983721058,-0.5239945531
O,0,-0.6349115565,2.1367692827,-0.4994175796
O,0,0.4153489721,2.6830050988,0.2911508669
O,0,2.1208766151,0.3757545462,-0.3941662861
H,0,0.9272387253,1.8765177079,0.494050836
H,0,-0.1110284438,0.2555661197,-1.0282290484
H,0,-1.8110200186,-0.3039533298,2.8982998948
Si,0,3.079474848,1.2835588515,-1.4577739651
C,0,4.5002953689,0.3551673084,-2.2642988061
H,0,5.3511018499,0.2617248175,-1.5842946176
H,0,4.2380733495,-0.6487413722,-2.6101401448
H,0,4.8209178671,0.9403539916,-3.1346540538
C,0,3.766536114,2.6652963304,-0.3963975295
H,0,2.9632971985,3.2826417805,0.0180825193
H,0,4.3669575785,2.2719766019,0.4309645728
H,0,4.4115615686,3.3130960202,-1.0000854036
C,0,1.9413798375,1.9834362215,-2.7715319155
H,0,2.3975398582,2.8770195006,-3.2119925332
H,0,1.7618839982,1.2697717121,-3.5818752802
H,0,0.9794217347,2.2712021845,-2.3333821345

TS-12 (SR) with H₂O

M06-2X/6-31+G**, E = -1656.60717204 a.u.

Thermal correction to Gibbs Free Energy = 0.508304 a.u.

1 imaginary frequency = -648.01 cm⁻¹

SP at B2PLYP/6-311+G**, E = -1656.0738487271 a.u.

SP at mPW2PLYP/6-311+G**, E = -1656.0999104261 a.u.

0,1
C,0,2.3868861373,-0.5060732555,0.0366854695
C,0,3.5045763494,-1.5321317544,-0.1976050674
C,0,4.7661432137,-1.295084983,0.3653099211
H,0,4.9639552434,-0.346794546,0.8560123515
C,0,5.7735277473,-2.2537045407,0.306905265
C,0,5.5424771136,-3.4720468373,-0.3323060113
C,0,4.3005935625,-3.713111396,-0.9136782642
C,0,3.2898843035,-2.7527322388,-0.8444804286
H,0,2.3365702842,-2.9857618297,-1.3053145064
H,0,6.7388835858,-2.0476305729,0.7589180618

H,0,6.3252225001,-4.2224172433,-0.3822907455
H,0,4.1090879776,-4.6530254994,-1.4216486267
C,0,1.1977229386,-0.7264856897,-0.9392566535
C,0,1.3955690603,-0.3454386488,-2.4090688164
H,0,0.7869495699,-1.0116168384,-3.0280108873
H,0,0.882941395,-1.7647463599,-0.8192611292
C,0,0.8894265263,1.102629063,-2.5337388148
H,0,0.4893785987,1.3026685854,-3.5294401395
H,0,1.6941508648,1.8154798376,-2.3447306464
C,0,-0.1992863904,1.2377363967,-1.4620242852
H,0,-1.2057119877,1.1208426351,-1.8696068675
H,0,-0.1523053233,2.1724586074,-0.9031396163
H,0,2.4360315042,-0.4599617629,-2.7242282791
N,0,0.02034958,0.0942219342,-0.5119544499
H,0,-0.8372844149,-0.5216404055,-0.5690999485
O,0,-2.0818606312,-1.4407843248,-1.0804019715
C,0,-3.2348888855,-1.2074501612,-0.6283282488
C,0,-3.5307820974,-0.7167546404,0.6533532398
C,0,-2.4478435951,-0.4981162826,1.6386882278
H,0,-1.5759959433,-1.1508704806,1.4816367016
H,0,-4.5500333187,-0.4645498116,0.9204047892
C,0,-2.8557042347,-0.4048460754,3.0919457889
H,0,-2.0354747143,-0.017980473,3.7037645499
H,0,-3.1159054464,-1.3976572177,3.4694171759
H,0,-3.7215611093,0.2550292386,3.197599947
O,0,-2.2805032722,0.7356151672,0.9975057877
O,0,-0.8363163512,1.5880058452,1.6556672367
O,0,1.7860967797,-0.715869911,1.3054123918
H,0,0.0819994157,0.4248015349,0.4667592297
H,0,-4.0945025528,-1.4170905665,-1.2856545896
H,0,-1.4697311273,2.9643004236,0.8201277143
H,0,-1.0893740104,1.6853392109,2.5841725492
O,0,-1.873686926,3.6953358722,0.2964438972
H,0,-2.6596247351,3.3007314748,-0.0966787483
Si,0,2.3410061767,-1.2873122283,2.7946212322
C,0,3.7890103244,-0.2778858975,3.4425955314
H,0,4.7520783157,-0.7393643864,3.2070066733
H,0,3.7802369295,0.7364063555,3.0289854199
H,0,3.7138813389,-0.1961827029,4.5325323796
C,0,0.8382230725,-1.0311678058,3.8775846177
H,0,-0.015195125,-1.602410579,3.4971977911
H,0,1.0350597778,-1.3526724548,4.905588005
H,0,0.5594553994,0.0282314137,3.8947505081
C,0,2.7731928612,-3.1082498963,2.6915786465
H,0,1.9525149437,-3.6717646942,2.2349915645
H,0,3.6803978486,-3.2859380176,2.1049350677
H,0,2.9355823618,-3.5043819666,3.7004809002
C,0,2.8951877391,0.9366936063,-0.0689446848
C,0,2.3038718257,1.9374502568,0.7067686625
C,0,3.8735184379,1.2982837057,-1.0039779917
C,0,2.6663580754,3.2745457047,0.5363266278
C,0,4.2419164909,2.6311415158,-1.1680704621
C,0,3.6338464615,3.6267211305,-0.4017250183
H,0,1.5425652117,1.6784401906,1.4383496257
H,0,4.3539325461,0.535926476,-1.6107394721
H,0,2.1861135233,4.0390422238,1.1396382714
H,0,5.0033457675,2.8915768663,-1.8969057234
H,0,3.9166615119,4.6664257036,-0.5335457258

TS-12 (SR) with H₂O₂

M06-2X/6-31+G**, E = -1731.71056115 a.u.

Thermal correction to Gibbs Free Energy = 0.514062 a.u.

1 imaginary frequency = -668.65 cm⁻¹

SP at B2PLYP/6-311+G**, E = -1731.1639063538 a.u.

SP at mPW2PLYP/6-311+G**, E = -1731.1899304711 a.u.

0,1
H,0,6.4034462285,-4.5094382817,0.526562098
C,0,5.5806779778,-3.8056384697,0.4511978878
C,0,5.4790710289,-2.7427290289,1.3507058047
C,0,4.4207520421,-1.8460253081,1.2499147621

C,0,3.4620744836,-1.9718764586,0.2367354784
C,0,3.5549982614,-3.0555129356,-0.6391992213
C,0,4.6080127657,-3.9668095293,-0.5316672999
H,0,4.6653078656,-4.800516343,-1.2243027327
H,0,6.2190998098,-2.6117612205,2.1350623114
H,0,2.8184034859,-3.2117184925,-1.4198237599
H,0,4.3329090907,-1.0341988281,1.9676521664
C,0,2.3898050329,-0.8819285433,0.1350777286
C,0,1.7305895682,-0.7014404285,1.5115992961
C,0,1.0286671054,-1.76353633,2.0936770604
H,0,0.9524118551,-2.7164150418,1.574585663
C,0,0.4329728172,-1.6166644089,3.343870966
C,0,0.5501147598,-0.4108197907,4.0388077163
C,0,1.2527681926,0.6460727601,3.466793614
C,0,1.8293403859,0.5064160732,2.202177503
H,0,2.350329967,1.3395653709,1.7442549485
H,0,-0.1152690039,-2.4462242283,3.7792699076
H,0,0.0933313418,-0.2986861289,5.0172780889
H,0,1.3465400644,1.5890000666,3.9974208946
C,0,1.3058753522,-1.2178530317,-0.9141120199
C,0,1.7779718684,-1.1339593225,-2.3866112632
H,0,1.4532995554,-2.0289731728,-2.9257826267
H,0,0.8574413123,-2.1892631205,-0.6888015694
C,0,1.0920311396,0.1106930524,-2.9634695927
H,0,0.9395476998,0.0511703118,-4.0425640203
H,0,1.6684889964,1.0137248369,-2.7409838726
C,0,-0.2187595316,0.1581793967,-2.1967790096
H,0,-0.9190212506,-0.6127119222,2.5317079437
H,0,-0.7170343508,1.1273717673,-2.1755966729
H,0,2.8652962123,-1.0760102356,-2.4540226897
N,0,0.205178177,-0.2010330857,-0.8108461306
H,0,-0.6333744265,-0.5824656732,-0.2852883356
O,0,-2.030703505,-1.3338761963,0.0659230254
C,0,-3.0288148297,-0.6407648887,0.4061225597
C,0,-2.9886382557,0.5837762911,1.0877623867
C,0,-1.6923006706,1.1441934853,1.5289411297
H,0,-0.9285330924,0.3735528888,1.7003140045
H,0,-3.9006259544,1.1411627534,1.2653974592
C,0,-1.7309556871,-2.1739773408,2.635248882
H,0,-0.7622008632,2.6731982453,2.7357503194
H,0,-1.9493016202,1.6831819876,3.5880592029
H,0,-2.5026890508,2.9224737257,2.4324324366
O,0,-1.5904289127,1.6858542392,0.234700394
O,0,-0.0004866706,2.4335778241,0.0113845204
O,0,2.9301313966,0.3564350741,-0.2752479494
H,0,0.5249800761,0.6643385495,-0.3396372918
H,0,-4.0295562481,-1.0358525581,0.1645399654
H,0,0.3304029755,3.0411921414,-1.4301821979
H,0,-0.0235550895,3.13097325,0.6807529416
O,0,0.5240093111,3.4064804957,-2.3475770357
Si,0,4.450552477,0.9920041322,-0.6307419774
C,0,5.4476335427,-0.1030430089,-1.7819147461
H,0,5.6365410398,-1.0909891619,-1.3485294233
H,0,4.9627084069,-0.2332202933,-2.7545412249
H,0,6.4168295079,0.3785212546,-1.9577510315
C,0,4.0122125508,2.6145536132,-1.450126967
H,0,3.3953308391,3.2247263914,-0.7816776837
H,0,4.9171057932,3.1813364616,-1.6930468215
H,0,3.4483695338,2.4579103097,-2.3747329668
C,0,5.4527176699,1.3341612442,0.9242157441
H,0,4.8147541621,1.6349961284,1.7618591634
H,0,6.0443620295,0.4685365571,1.2346680814
H,0,6.1457763723,2.1583056244,0.7200616959
O,0,-0.7557437137,3.2995046221,-2.9735805914
H,0,-1.119471947,4.1899529654,-2.8647344585

TS-12 (SS) with H₂O

M06-2X/6-31+G**, E = -1656.60267727 a.u.

Thermal correction to Gibbs Free Energy = 0.510957 a.u.

1 imaginary frequency = -646.74 cm⁻¹

SP at B2PLYP/6-311+G**, E = -1656.0671681446 a.u.

SP at mPW2PLYP/6-311+G**, E = -1656.0936169864 a.u.

0,1
C,0,-0.2568287244,1.605458792,1.2258620651
C,0,-1.2723218878,0.9752154438,2.1690804142
H,0,-2.1235894257,1.6295099601,2.3617316119
H,0,-0.0133555824,2.6360413387,1.4995894224
C,0,-0.4506732189,0.6657198254,3.4330436338
H,0,-0.5445483944,1.4692531575,4.1674888544
H,0,-0.7802636836,-0.2513818289,3.9221207557
C,0,1.0188446459,0.5839359927,2.9569532861
H,0,1.5815899965,1.4490303537,3.3142205939
H,0,-1.6438309265,0.0477683533,1.718213551
N,0,0.950285635,0.7641874936,1.4724407342
H,0,1.8218581525,1.1876391125,1.0586073238
O,0,3.1307116416,2.0040664419,0.3508780434
C,0,3.8469769289,1.3835391046,-0.4805707067
C,0,3.4303249413,0.5979098432,-1.5694502787
O,0,2.0092949753,0.4735173438,-2.0015310846
H,0,1.9222721067,-0.0855822741,-2.9412173321
H,0,4.1760119605,-0.0042289243,-2.0753485137
C,0,1.1294291175,1.7057810482,-2.0192195579
H,0,1.3005603871,2.322962468,-1.1360744667
H,0,1.3697775352,2.2945500946,-2.9093930511
H,0,0.076580048,1.4140501819,-2.0724348321
O,0,1.8635205798,-0.3763510999,-0.8982007061
O,0,0.1720669714,-0.8465193064,-0.6497677267
H,0,0.7858796421,-0.1223364327,0.9548580702
H,0,4.9430512026,1.4519623678,-0.3556925469
H,0,-1.3133585625,-0.1424595855,-1.195430686
H,0,0.3099329612,-1.8041779546,-0.659796412
O,0,-2.1199388989,0.370596869,-1.4300050355
H,0,-2.8422047424,-0.0322245642,-0.9367842987
H,0,-0.5305673619,1.5474659263,0.1729588618
C,0,1.8503198321,-0.6668417413,3.3499754224
C,0,1.7817031737,-0.8797211462,4.8703860733
C,0,1.8527897505,-2.1565004903,5.436002014
C,0,1.785536966,0.2265951281,5.7303959811
C,0,1.9289510567,-2.3247943501,6.8191939931
C,0,1.8501906192,0.0625034614,7.1111775817
C,0,1.9262302518,-1.2163190662,7.662658904
H,0,1.8533317618,-3.0339340645,4.7977720393
H,0,1.7594985291,1.2364606199,5.3333130142
H,0,1.9902091766,-3.3262966234,7.2334545694
H,0,1.8522728817,0.9364819589,7.7548288857
H,0,1.9840373216,-1.3463845658,8.7387037715
C,0,1.3903443392,-1.8890155677,2.540617473
C,0,0.1969039958,-2.5673203012,2.8292712683
C,0,2.1395898518,-2.3063655911,1.438583247
C,0,-0.2260576958,-3.6352428942,2.041234542
C,0,1.7295233683,-3.3893800962,0.6596155897
C,0,0.5438193083,-4.0565480855,0.955071893
H,0,-0.3979256825,-2.2876024819,3.6933744886
H,0,3.039455741,-1.7661576179,1.1667815873
H,0,-1.1509488537,-4.1479598257,2.2860269922
H,0,2.3345593635,-3.695520676,-0.1886712133
H,0,0.2202088564,-4.89680883,0.3487701055
Si,0,4.6748128632,-0.8948078696,3.4969513788
C,0,4.7999517671,-2.7673500122,3.4375819226
H,0,5.7642643997,-3.0633921941,3.867092184
H,0,4.0130023851,-3.2571362783,4.017418126
H,0,4.7550024308,-3.1461021107,2.4124218485
C,0,5.0773915169,-0.3041298757,5.2307988326
H,0,6.1411072008,-0.4807407695,5.4277823407
H,0,4.8837948213,0.767666275,5.3415110064
H,0,4.4974960183,-0.8369856941,5.9921465068
C,0,5.841196486,-0.1408029009,2.2443952934
H,0,5.7342192163,0.9481240415,2.2162827445
H,0,6.8812566391,-0.3809903255,2.4886036114
H,0,5.6276415519,-0.5292160139,1.24260766

O,0,3.1730714712,-0.3186667002,2.9770196064

TS-12 (SS) with H₂O₂

M06-2X/6-31+G**, E = -1731.70299768 a.u.

Thermal correction to Gibbs Free Energy = 0.513368 a.u.

1 imaginary frequency = -649.01 cm⁻¹

SP at B2PLYP/6-311+G**, E = -1731.1554277614 a.u.

SP at mPW2PLYP/6-311+G**, E = -1731.1815608287 a.u.

O,1

C,0,-0.2987826217,1.4322414167,1.0804493013
C,0,-1.2656072652,0.6967657601,1.9940530209
H,0,-2.2149024056,1.2218404607,2.1094779757
H,0,-0.2136803199,2.4924259829,1.3370692193
C,0,-0.4768853928,0.5838531455,3.3049111332
H,0,-0.6632883741,1.4606087341,3.9314993687
H,0,-0.7532130903,-0.3011383874,3.879911175
C,0,1.016965399,0.5503615059,2.8905315473
H,0,1.5767713357,1.3809412162,3.3301352097
H,0,-1.4668799132,-0.2969034682,1.5781550303
N,0,0.9982629091,0.7753429567,1.4057973706
H,0,1.8314308656,1.337665191,1.053862059
O,0,3.0437181205,2.3039580726,0.6099862907
C,0,3.9009221343,1.8797210158,-0.2181854124
C,0,3.6777721623,1.2214063881,-1.4345183707
C,0,2.3206107922,0.945874701,-1.9858297313
H,0,2.3781043201,0.4842864179,-2.9794504563
H,0,4.5317454885,0.7709592321,-1.9270408071
C,0,1.2768028658,2.0432533392,-1.9607894612
H,0,1.2878798012,2.5770453383,-1.0091894302
H,0,1.5032505533,2.7544035368,-2.7608761426
H,0,0.2835529507,1.6255264548,-2.1491492862
O,0,2.2160694584,-0.0367294284,-0.9871309446
O,0,0.6477343462,-0.7873345174,-0.9279632822
H,0,1.011610409,-0.1272900755,0.8979074335
H,0,4.9638714092,2.0433801049,0.0323580288
H,0,-0.7532988366,-0.307589543,-1.5039806018
H,0,0.9166563566,-1.680577309,-1.1794152009
O,0,-1.6526930595,0.0407151628,-1.7857758818
H,0,-0.5028861385,1.3223770384,0.0162433922
C,0,1.7539535394,-0.7798616634,3.1683303016
C,0,3.1722165938,-0.6878682281,2.5854076826
C,0,4.1204773494,0.1360901075,3.2048196012
C,0,3.5290904837,-1.3937451708,1.4395277443
C,0,5.4066585805,0.2443820516,2.6881802867
C,0,4.8229334639,-1.2891800898,0.9233488429
C,0,5.7640092722,-0.4760467803,1.5452289475
H,0,3.8553971923,0.6864195179,4.1050790481
H,0,2.791031652,-2.0177167238,0.9461706615
H,0,6.1324277452,0.8865331704,3.1777874137
H,0,5.0854524088,-1.8385097372,0.0243231233
H,0,6.7681601217,-0.3925196469,1.1405407937
C,0,1.8563107613,-1.1045758043,4.6613031421
C,0,1.3191441225,-0.311975292,5.6762414597
C,0,2.5469623655,-2.2699623069,5.0164493816
C,0,1.4293215797,-0.7009151923,7.0139617934
C,0,2.6451019028,-2.669059453,6.3445343048
C,0,2.0764459558,-1.8859558181,7.3513114524
H,0,0.8085060169,0.617531926,5.4500970762
H,0,3.0197611216,-2.8630612596,4.237934361
H,0,1.0024404683,-0.0722863962,7.7890608883
H,0,3.1754300249,-3.5825514613,6.5955014525
H,0,2.1521129526,-2.1909941807,8.3901971608
Si,0,0.1911114917,-3.1865020127,2.7788401705
C,0,-0.9643894351,-3.0279081184,4.2473282934
H,0,-1.4072220575,-4.0105812819,4.4474713778
H,0,-0.4398923087,-2.7033988869,5.1524580476
H,0,-1.7843999245,-2.3309690602,4.0461883899
C,0,1.3585846871,-4.6393235717,3.0224753891
H,0,0.8611314424,-5.5533610345,2.6789675363

H,0,2.270798066,-4.5120770898,2.4289411412
H,0,1.6424247948,-4.7849105326,4.0682435792
C,0,-0.7711215523,-3.4627975165,1.1977691702
H,0,-0.0864566906,-3.637259593,0.3610190233
H,0,-1.4162854557,-4.3426206617,1.2949592009
H,0,-1.3987738443,-2.6022766978,0.9471768167
O,0,1.0246783196,-1.7588638199,2.4547596209
O,0,-1.4619265089,0.2257696409,-3.1896386329
H,0,-1.9416269691,-0.5280161152,-3.5616816411

TS-12 (RS) with H₂O

M06-2X/6-31+G**, E = -1656.60834995 a.u.

Thermal correction to Gibbs Free Energy = 0.511893 a.u.

1 imaginary frequency = -646.12 cm⁻¹

SP at B2PLYP/6-311+G**, E = -1656.0730639781 a.u.

SP at mPW2PLYP/6-311+G**, E = -1656.0996274854 a.u.

O,1

C,0,0.2790345713,1.5917864668,0.8715287227
C,0,-0.8942546278,1.2668591192,1.78877036
H,0,-1.5105248589,2.1413494499,2.0013519094
H,0,0.8005315011,2.508294273,1.1610906936
C,0,-0.2284908899,0.6807234728,3.0521072543
H,0,-0.1725412504,1.4299719478,3.8441559189
H,0,-0.791190548,-0.1653310067,3.4465389136
C,0,1.2030931659,0.2834715609,2.6160239593
H,0,1.912967051,1.0340601295,2.9744166737
H,0,-1.5178513817,0.5102804058,1.3009239575
N,0,1.188644835,0.4413374712,1.1305119262
H,0,2.1422260473,0.5673110863,0.693068852
O,0,3.5660047956,0.8345012573,-0.1289685603
C,0,3.9127788055,0.1106691506,-1.1010390727
C,0,3.0894908104,-0.3545911018,-2.137229739
C,0,1.6633412752,0.0414540089,-2.2134611105
H,0,1.4705883297,1.0241423498,-1.7607308978
H,0,3.4846211853,-1.0469324055,-2.8715413853
C,0,0.9653990615,-0.1406602189,-3.5417117973
H,0,-0.1164119373,-0.0550289843,-3.4140927252
H,0,1.2964044376,0.6289225584,-4.2447095366
H,0,1.2015912173,-1.1253643549,-3.9559456649
O,0,1.4402687706,-0.9922119159,-1.2953337919
O,0,-0.2561373761,-0.9499816225,-0.7513698471
H,0,0.7492258775,-0.3730886659,0.6502074418
H,0,4.9750209803,-0.1849490303,-1.1662104715
H,0,-1.3031506575,0.2141327099,-1.4692512583
H,0,-0.4110491547,-1.9048044659,-0.7562282614
O,0,-1.7810065829,0.997299901,-1.828520695
H,0,-2.6148036609,1.0445087067,-1.3493397507
H,0,0.0157970199,1.6233559199,-0.1858960327
C,0,1.7742264123,-1.1037935687,3.013085029
C,0,1.7616079221,-1.3095257051,4.5318803567
C,0,1.9583985562,-2.6020234658,5.0341376011
C,0,1.6917798857,-0.2467039422,5.4364159675
C,0,2.0796870338,-2.8270575107,6.4015361671
C,0,1.8115809347,-0.4686591165,6.8098378288
C,0,2.0066619144,-1.7583679647,7.2964988185
H,0,2.0287141787,-3.4375681019,4.3432430644
H,0,1.5538238365,0.772807376,5.0917752731
H,0,2.2360061099,-3.8363257835,6.7695397215
H,0,1.7545772736,0.3715243552,7.4946735694
H,0,2.1019070028,-1.9313562841,8.3638479596
C,0,1.0131991406,-2.2229919632,2.2883707991
C,0,1.5599841627,-2.8096078044,1.1456133191
C,0,-0.2434899313,-2.6560486439,2.7323187928
C,0,0.8631485945,-3.8012943391,0.4527031191
C,0,-0.9458452985,-3.6351880309,2.0341332433
C,0,-0.3942926261,-4.2121381485,0.8882430644
H,0,2.5289870822,-2.4781976363,0.7903155785
H,0,-0.6665076436,-2.2570998563,3.6497473777
H,0,1.3061361408,-4.2432119714,-0.4348412523

H,0,-1.9165969792,-3.9599367737,2.3953173562
H,0,-0.9371604825,-4.9824770517,0.3493059887
Si,0,4.5547788683,-0.5252670859,3.15422831
C,0,5.7957826725,-0.8716526723,1.8016893229
H,0,5.6379149417,-0.1737400528,0.9754808975
H,0,6.816334366,-0.7457717609,2.1780686452
H,0,5.6924815008,-1.8932710442,1.4224727338
C,0,5.0662704367,-1.4044459699,4.7316691019
H,0,5.0297857184,-2.4913607484,4.6043127581
H,0,6.0998571693,-1.1258252267,4.9681561253
H,0,4.4373026231,-1.1394394696,5.5873560654
C,0,4.4507504706,1.3247479583,3.4642209229
H,0,3.7765984532,1.5836682014,4.2873640981
H,0,5.449037794,1.6902604844,3.7318302874
H,0,4.1334878046,1.8522465264,2.557989389
O,0,3.1082948656,-1.1377032704,2.5325977679

TS-12 (RS) with H₂O₂

M06-2X/6-31+G**, E = -1731.70645920 a.u.

Thermal correction to Gibbs Free Energy = 0.513792 a.u.

1 imaginary frequency = -655.61 cm⁻¹

SP at B2PLYP/6-311+G**, E = -1731.1613367810 a.u.

SP at mPW2PLYP/6-311+G**, E = -1731.1872792150 a.u.

0,1
C,0,0.2323588967,1.5598962733,0.836670752
C,0,-0.9259844729,1.1856696904,1.7523736634
H,0,-1.6071886255,2.0191052009,1.9275833024
H,0,0.7088485304,2.5012914107,1.1245702691
C,0,-0.2223421485,0.7035165396,3.0357325061
H,0,-0.1593501205,1.5142437846,3.7650275932
H,0,-0.7586060766,-0.1166469794,3.5124641966
C,0,1.2087029487,0.3025211876,2.5958003741
H,0,1.9227682596,1.0494014805,2.9517820622
H,0,-1.4872351731,0.367404035,1.2886272152
N,0,1.1931193995,0.4543397142,1.1077517996
H,0,2.144197617,0.6159454516,0.6694024361
O,0,3.5504462555,0.8966966537,-0.1356257386
C,0,3.9257644392,0.1754506234,-1.1003317352
C,0,3.1275725887,-0.3206305748,-2.1404304811
C,0,1.6912281726,0.0297964908,-2.2348061317
H,0,1.4637622127,1.0110551854,-1.7946049267
H,0,3.5507326514,-1.0062114696,-2.8653126373
C,0,1.0133846069,-0.1879662658,-3.5682603908
H,0,-0.0713470218,-0.2033216261,-3.4351705353
H,0,1.275375594,0.6165718842,-4.2606104262
H,0,1.3266269016,-1.1442353344,-3.9971640847
O,0,1.4721362143,-1.0001944833,-1.3098872247
O,0,-0.2200894433,-0.980761343,-0.8012329182
H,0,0.7973524184,-0.3839488816,0.6382650364
H,0,4.9965208893,-0.0882697679,-1.1546804617
H,0,-1.2340964115,0.0854269017,-1.4025348608
H,0,-0.3905069944,-1.9330357198,-0.8203272741
O,0,-1.8058767717,0.8672479643,-1.6702489631
H,0,-0.0161519306,1.5808544051,-0.224437722
C,0,1.7743688029,-1.0870455161,2.9928168075
C,0,1.7537772103,-1.2938526442,4.5111240357
C,0,1.9452246688,-2.5870089253,5.0133399154
C,0,1.6775349971,-0.2314137422,5.4156050167
C,0,2.0573888753,-2.8130359234,6.3813906279
C,0,1.7884776061,-0.4544237482,6.7895083794
C,0,1.9799560865,-1.7447055186,7.2763573766
H,0,2.0181885616,-3.4221000906,4.3220915464
H,0,1.5392265694,0.7880246806,5.0703996567
H,0,2.2096025795,-3.8227221962,6.7499164937
H,0,1.7266057566,0.3850455118,7.4747826329
H,0,2.0680117665,-1.9184528683,8.3441923705
C,0,1.0122771279,-2.2039486336,2.2652925864
C,0,1.5716671616,-2.8100684818,1.1389386057
C,0,-0.2582414047,-2.6151296976,2.6905876779

C,0,0.8738675294,-3.7995528459,0.4434562539
C,0,-0.9615347204,-3.5909427203,1.9890144191
C,0,-0.3972178357,-4.1875865914,0.8594201558
H,0,2.5518219638,-2.4959332132,0.7991147511
H,0,-0.6924163248,-2.202385796,3.5963976137
H,0,1.32740026,-4.2578762095,-0.4303624651
H,0,-1.9437656154,-3.8974315891,2.3346088531
H,0,-0.9413529879,-4.9554359352,0.3182524012
Si,0,4.5536614231,-0.5142763844,3.1481726685
C,0,5.8002656829,-0.8535713759,1.7985562473
H,0,6.8192793136,-0.7419298796,2.1834413264
H,0,5.6908324169,-1.8686808622,1.4040504988
H,0,5.6564042893,-0.1429995934,0.9806010734
C,0,5.0570674687,-1.4019262387,4.7233483431
H,0,5.0166094668,-2.4881803419,4.5917448327
H,0,6.0908798261,-1.1282264604,4.9643968465
H,0,4.4262107829,-1.1376028252,5.5778805596
C,0,4.4500614748,1.3343578237,3.4654594184
H,0,3.7727358672,1.5914053002,4.2865627126
H,0,5.4477947549,1.697199076,3.7387194854
H,0,4.1377723915,1.8653842227,2.5595697669
O,0,3.1097362412,-1.1234635955,2.5165033896
O,0,-2.5547133138,0.3249646086,-2.7599477437
H,0,-2.2112631269,0.8285317892,-3.5121578315

TS-12 (RR) with H₂O

M06-2X/6-31+G**, E = -1656.60340013 a.u.

Thermal correction to Gibbs Free Energy = 0.513260 a.u.

1 imaginary frequency = -651.31 cm⁻¹

SP at B2PLYP/6-311+G**, E = -1656.0667018143 a.u.

SP at mPW2PLYP/6-311+G**, E = -1656.0931949053 a.u.

0,1
H,0,4.0274420532,4.2413759806,-0.2761958187
C,0,3.7343875649,3.2007260615,-0.1767854282
C,0,4.2935389929,2.231303557,-1.0128822588
C,0,3.9225948801,0.8965875693,-0.8837357555
C,0,2.9837089195,0.5003982105,0.0816593614
C,0,2.4302599452,1.4805825237,0.9075222184
C,0,2.8024485999,2.8208342454,0.7831845117
H,0,2.343778871,3.5533893054,1.4401884111
H,0,5.0257135569,2.5132016941,-1.7635170152
H,0,1.6908883591,1.2080115246,1.6552214974
H,0,4.3878777843,0.1586099582,-1.5302536043
C,0,2.496811634,-0.9521724521,0.1837051806
C,0,3.6412331527,-1.9753579578,0.0640199815
C,0,4.9421665915,-1.650344094,0.4647401349
H,0,5.1773085259,-0.637579344,0.733180255
C,0,5.9537838076,-2.6098749919,0.4763765541
C,0,5.6844799079,-3.9177735501,0.0799907797
C,0,4.394459785,-4.255210786,-0.3259749798
C,0,3.3848727066,-3.2953029995,-0.3285301592
H,0,2.3894920765,-3.6048224633,-0.6283162334
H,0,6.9526145363,-2.3296719137,0.7960614143
H,0,6.4705353076,-4.6663941763,0.08735187
H,0,4.1670206897,-5.2708629297,-0.6342839732
C,0,1.4259396339,-1.2325590161,-0.9052395764
C,0,1.8848034105,-1.1468619404,-2.3757873601
H,0,1.5206625348,-2.0263139484,-2.9149195194
H,0,1.000205036,-2.2113683606,-0.6804702713
C,0,1.2219666795,0.1198149283,-2.9278850762
H,0,1.0880508315,0.0915307437,-4.0105753765
H,0,1.8098849846,1.0079940525,-2.6721139377
C,0,-0.1053318707,0.1471878344,-2.1866780668
H,0,-0.8072678575,-0.5946162998,-2.5769620065
H,0,-0.5937706973,1.1182747041,-2.128854663
H,0,2.9715526259,-1.1393003323,-2.4683963922
N,0,0.2657362744,-0.2786158595,-0.7996297565
H,0,-0.5665702004,-0.7557203446,-0.3682184592
O,0,-1.9038892376,-1.7595063724,-0.1992384202

C,0,-3.0423350128,-1.2236726543,-0.1339425053
C,0,-3.3847108234,0.0006572691,0.4666567628
C,0,-2.4233446861,0.8331074896,1.2424489026
H,0,-2.9270311758,1.6729119614,1.737590344
H,0,-4.378659595,0.3943121652,0.2912066957
C,0,-1.4225259722,0.1770801965,-2.1704224327
H,0,-0.6159201625,0.8814033995,2.3952453532
H,0,-0.991969909,-0.7313206014,1.74621668
H,0,-1.9234432289,-0.0826034676,3.1082294854
O,0,-1.9371889757,1.2077397083,-0.0122100029
O,0,-0.4830516346,2.2382682162,0.1984664976
O,0,1.792823714,-1.1494788808,1.4031269617
H,0,0.4470419649,0.5813862593,-0.2512894487
H,0,-3.8842079113,-1.7645353479,-0.6014649484
H,0,-0.0702456345,2.927919162,1.7190875337
H,0,-0.7320951795,2.9301178098,-0.4287501584
O,0,0.2259914428,3.2888687978,2.5904515499
H,0,-0.5763543583,3.4105335208,3.109081197
Si,0,2.3795666084,-1.5194032829,2.949090776
C,0,3.6650308776,-0.2870526255,3.5426274707
H,0,4.5555769795,-0.2511009482,2.9101981068
H,0,3.2468345595,0.7223507596,3.6041365042
H,0,3.982780185,-0.5839577959,4.5492455809
C,0,0.8729963923,-1.3980156551,4.0496394748
H,0,0.062516548,-2.0421489676,3.6947772567
H,0,1.1414501648,-1.7138173863,5.0638623255
H,0,0.4993047089,-0.3711402067,4.1016209133
C,0,3.059358425,-3.2660425903,3.031234475
H,0,2.3605918071,-3.9755941768,2.5759061206
H,0,4.0273245823,-3.3702473835,2.5318960622
H,0,3.1856178292,-3.5427192279,4.0844297853

TS-12 (RR) with H₂O₂

M06-2X/6-31+G**, E = -1731.70884216 a.u.

Thermal correction to Gibbs Free Energy = 0.517794 a.u.

1 imaginary frequency = -697.11 cm⁻¹

SP at B2PLYP/6-311+G**, E = -1731.1582702626 a.u.

SP at mPW2PLYP/6-311+G**, E = -1731.1844821510 a.u.

0,1

H,0,6.4730556941,-4.5277964034,0.1943960188
C,0,5.6777410151,-3.7898955116,0.1611471367
C,0,5.6843620304,-2.7077587029,1.0429536816
C,0,4.6586104372,-1.7702975191,0.9985709968
C,0,3.6254236782,-1.8714593735,0.0582998593
C,0,3.6118405477,-2.9731010392,-0.8005279956
C,0,4.6317309344,-3.9260964114,-0.7474581157
H,0,4.6046667395,-4.7743525622,-1.4240518555
H,0,6.4807954255,-2.6001435218,1.7727205833
H,0,2.817108423,-3.1115303875,-1.5250154072
H,0,4.6544858518,-0.9463073267,1.7073786973
C,0,2.5862377863,-0.7418530555,0.025835572
C,0,2.1141878539,-0.4883834179,1.4643495346
C,0,1.4823101362,-1.5256822219,2.1627314396
H,0,1.3211779226,-2.4874985329,1.681540792
C,0,1.0705861482,-1.3450038236,3.4784543327
C,0,1.2877613376,-0.1220803283,4.1175047767
C,0,1.9124514069,0.912442783,3.4273875066
C,0,2.3233832684,0.7312234592,2.10445044
H,0,2.7954412359,1.5461507772,1.5678154297
H,0,0.5792427136,-2.1576927627,4.0041845887
H,0,0.9660269291,0.0212180655,5.1444518834
H,0,2.0791762225,1.8696859702,3.9117689896
C,0,1.3682071617,-1.1004329178,-0.8558082352
C,0,1.6277211897,-1.0800716331,-2.3794320829
H,0,1.221663528,-1.990642529,-2.8299131692
H,0,0.9707683937,-2.0655789412,-0.5317712472
C,0,0.8851394786,0.1502243931,-2.9089744051
H,0,0.57162125,0.0374743127,-3.9483843481
H,0,1.5119664077,1.0432674824,-2.8335843484

C,0,-0.3021883743,0.2768729238,-1.9666814472
H,0,-1.0931365579,-0.4408223758,-2.2030081911
H,0,-0.7288917394,1.2760624214,-1.8908267935
H,0,2.6952743864,-1.0401176846,-2.6008134321
N,0,0.2604636628,-0.1032406495,-0.6350639884
H,0,-0.4953373636,-0.5615964966,-0.6362295409
O,0,-1.491042526,-1.6154575299,0.5697991947
C,0,-2.7254143637,-1.3580337098,0.6294330006
C,0,-3.3543332804,-0.1397703864,0.9192832463
C,0,-2.6806578865,1.1210822415,1.3464216216
H,0,-3.412643932,1.8463760815,1.7207455507
H,0,-4.4269635409,-0.0940565708,0.7723402875
C,0,-1.4501302867,1.0833539055,2.2274810761
H,0,-0.9468796717,2.0546265512,2.1964561696
H,0,-0.7440507286,0.3069349443,1.9261242217
H,0,-1.7502852646,0.8839660776,3.2607185138
O,0,-2.4450606606,1.3137682987,-0.0133905469
O,0,-1.6961536829,2.9358626273,-0.1841804841
O,0,3.1364501208,0.4558192017,-0.5226453102
H,0,0.575937274,0.7535711008,-2.1395960928
H,0,-3.4187976714,-2.1949183219,0.4358857451
H,0,-0.2689090104,2.7487282189,0.007421775
H,0,-2.028343873,3.1419105069,-1.0675652654
O,0,0.7093815344,2.5270661296,0.2849422976
Si,0,4.7025248981,0.8868471058,-1.0477226244
C,0,5.5146860709,-0.3910937457,-2.1513785372
H,0,5.798581554,-1.299043748,-1.6115104428
H,0,4.8884667406,-0.67180882864,-3.0038408171
H,0,6.4288892037,0.0633565042,-2.5523007775
C,0,4.3740880834,2.4466344056,-2.0319444375
H,0,4.0289722515,3.2697331105,-1.3984442495
H,0,5.3079633982,2.7644875786,-2.5082320481
H,0,3.6360730101,2.2865438362,-2.8253542502
C,0,5.8242276954,1.303716132,0.3971475209
H,0,5.2672897732,1.7720688283,1.2152015369
H,0,6.3478587065,0.4284837257,0.7898038515
H,0,6.5781445752,2.0213456169,0.0540623544
O,0,1.4434936646,2.8082786243,-0.9184625481
H,0,2.1186736635,2.1051284862,-0.8760611886

Cartesian coordinates and computed total energies for the structures presents in Scheme S3.

TS-14 anti-down

M06-2X/6-31+G**, E = -1580.14805678 a.u.

Thermal correction to Gibbs Free Energy = 0.484884 a.u.

1 imaginary frequency = -744.31 cm⁻¹

SP at B2PLYP/6-311+G**, E = -1579.6211989751 a.u.

SP at mPW2PLYP/6-311+G**, E = -1579.6464567405 a.u.

0,1

C,0,-1.4057712608,-1.5479252172,-3.4363577614
C,0,-0.4326824087,-0.7229808392,-2.911923404
H,0,-0.7193717952,0.1404444134,-2.3172265204
C,0,1.0418804319,-1.0435239933,-2.9506080768
H,0,1.2682689928,-1.7398139354,-2.1356242891
N,0,1.8283489701,0.1305289198,-2.7347277934
C,0,1.7320895937,1.1852086739,-3.7548641003
C,0,3.2262337939,-0.0740335249,-2.332069723
C,0,2.9717014128,2.0365679972,-3.5063579997
C,0,4.0213264446,0.9909244568,-3.1061551541
H,0,0.7967306154,1.7427242562,-3.6389092396
H,0,2.7905723017,2.7357278623,-2.6848395089
H,0,1.7483206593,0.7630281462,-4.7709661357
H,0,3.2639505218,2.6091749581,-4.3894383915
H,0,4.8465731593,1.4069704942,-2.5224302162
H,0,4.4506323952,0.5352531427,-4.0047455416
H,0,3.5462637816,-1.0845293785,-2.614502718
C,0,3.37385464,-0.0124375851,-0.77567023

H,0,-1.0888065125,-2.4633562466,-3.9309276278
O,0,-0.9223314432,-0.1885528268,-4.716805448
O,0,-0.7591095989,0.6302484768,-6.4241968091
H,0,-0.693733112,1.5250446951,-6.067088404
H,0,-0.1623111796,-0.6530004992,-5.12124358
C,0,-2.8659956515,-1.3465929455,-3.2086582813
H,0,-3.0703956573,-0.3485056453,-2.81526847
H,0,-3.418457535,-1.4864408856,-4.1406863075
H,0,-3.2302220842,-2.0887917303,-2.4904103687
O,0,2.493365148,-1.0329998361,-0.3190286056
Si,0,2.4075839867,-1.9624345413,1.078595661
C,0,2.4134965908,-0.9265407827,2.6495942429
H,0,2.0031577678,0.072727301,2.4697735034
H,0,1.7897850088,-1.416353686,3.4057040213
H,0,3.4187918247,-0.8175283443,3.0660085168
C,0,3.7731252805,-3.2467043938,1.1317122423
H,0,4.7603613458,-2.7901228172,1.2581344364
H,0,3.6016512733,-3.9297966855,1.9716377504
H,0,3.7844656694,-3.8395257922,0.2109720429
C,0,0.7417211927,-2.7951739131,0.8663080418
H,0,0.7175354667,-3.3888685475,-0.0535976356
H,0,0.5243465278,-3.4619709089,1.7070693834
H,0,-0.0558686715,-2.046279279,0.8096140039
O,0,1.2626595081,-1.7021598653,-4.2102774414
H,0,2.1524084631,-2.0753032373,-4.2341148011
C,0,2.8897775408,1.350639099,-0.2812796086
C,0,3.7483455004,2.4519358676,-0.1881146486
C,0,1.5290299193,1.5427712,-0.0223839631
C,0,3.2598057572,3.7134778776,0.1500579387
H,0,4.8108646244,2.3311506751,-0.3795820476
C,0,1.0373996929,2.8015557262,0.3200630196
H,0,0.8571558633,0.6942274962,-0.0978683734
C,0,1.9006531787,3.8939213112,0.4033283275
H,0,3.9443020961,4.5536492374,2.2165505485
H,0,-0.022744294,2.9297954649,0.5177610766
H,0,1.5189804043,4.875255373,0.668027637
C,0,4.8022266931,-0.3418212538,-0.3147817043
C,0,5.6679704994,-1.1262272984,-1.0860803307
C,0,5.2246259429,0.0300722601,0.9688964222
C,0,6.9064839448,-1.5327346767,-0.5894742686
H,0,5.3941394975,-1.4387045587,-2.0874472278
C,0,6.4579938156,-0.3782535497,1.4717801535
H,0,4.5820032646,0.6490076025,1.5877658771
C,0,7.305427891,-1.1664660629,0.6939597679
H,0,7.5567576042,-2.1414649263,-1.2101170651
H,0,6.7550013929,-0.0789796973,2.4723359979
H,0,8.2665753133,-1.4884420783,1.0822482081

TS-14 *syn-up*

M06-2X/6-31+G**, E = -1580.15224101 a.u.

Thermal correction to Gibbs Free Energy = 0.490543 a.u.

1 imaginary frequency = -739.86 cm⁻¹

SP at B2PLYP/6-311+G**, E = -1579.6234145947 a.u.

SP at mPW2PLYP/6-311+G**, E = -1579.6491958570 a.u.

0,1

C,0,1.3898024051,-3.1700198531,-4.6080208339
C,0,1.7728062017,-1.8960064376,-4.2454975968
H,0,2.4955584807,-1.3639267251,-4.8620614536
C,0,1.0924616272,-1.1223952147,-3.1179679386
H,0,0.1310786003,-0.7599033279,-3.509240278
N,0,1.8123414167,0.0499803416,-2.6723107324
C,0,1.7018609836,1.1741881587,-3.6174254672
C,0,3.2106568576,-0.1285685833,-2.2419034892
C,0,2.9646224187,1.9997747621,-3.3938944646
C,0,4.0053418712,0.9359846526,-3.0171335437
H,0,0.7809533636,1.7371544559,-3.4310944278
H,0,2.8136890633,2.7081847055,-2.5763775078
H,0,1.6707368992,0.8155162765,-4.6595606934
H,0,3.2456410041,2.5633995209,-4.2864410756

H,0,4.8486883985,1.3341569745,-2.4468746672
H,0,4.4141547464,0.479692885,-3.9253691275
H,0,3.5436185432,-1.1344087023,-2.5095585604
C,0,3.3510915729,-0.0349447908,-0.6792541229
H,0,0.5843296245,-3.6393722916,-4.045816843
O,0,2.8672014894,-3.2501375357,-3.3760068924
O,0,4.0324538863,-3.9868142192,-2.0739548773
H,0,4.1805520614,-4.8107752271,-2.5555877912
H,0,2.3191869896,-3.201356608,-2.5644113592
C,0,1.8779781151,-3.8695818258,-5.8324902786
H,0,2.7645242642,-3.3789679563,-6.2399494444
H,0,2.1151136212,-4.9120767351,-5.6075845125
H,0,1.0917868749,-3.8643724017,-6.5949100708
O,0,2.4831869282,-1.062535382,-0.1810621265
Si,0,2.457225643,-1.8489018364,1.3262234954
C,0,2.3625639325,-0.6077225604,2.726557883
H,0,1.4716802885,0.0213349576,2.6359828745
H,0,2.3090227719,-1.1459744844,3.6797700801
H,0,3.2392572986,0.0449651996,2.7582491163
C,0,3.9041488979,-3.0162224207,1.520453022
H,0,4.8315710656,-2.4925773332,1.7734122752
H,0,3.6834043301,-3.7375666665,2.3156285176
H,0,4.061739942,-3.5600879338,0.5815246774
C,0,0.8613529961,-2.8214731069,1.2067737866
H,0,0.9137977277,-3.5623982456,0.401734288
H,0,0.6734505336,-3.355282789,2.1442275586
H,0,0.0078856988,-2.1627650096,1.0139148381
O,0,0.8327165073,-2.0191187104,-2.0561635925
H,0,1.2864790445,-1.6509114323,-1.2633407199
C,0,2.8454466181,1.3285286815,-0.2079901986
C,0,3.6663602736,2.4636964339,-0.1778568828
C,0,1.4864629665,1.4894967072,0.0818780467
C,0,3.1483727814,3.7164652512,0.1460858713
H,0,4.7218353416,2.3808793482,-0.41822762
C,0,0.9640228915,2.7410915437,0.405184843
H,0,0.8323766895,0.625170022,0.0433081116
C,0,1.7931784122,3.8613916967,0.4395689651
H,0,3.8067869001,4.5795281757,0.1646041163
H,0,-0.0945872139,2.8397840509,0.6263597347
H,0,1.3883179368,4.8366210614,0.6921642273
C,0,4.7883758296,-0.3703106035,-0.2420561997
C,0,5.482682524,-1.4067843492,-0.8831371909
C,0,5.3839400617,0.2200710084,0.8801551671
C,0,6.7430226375,-1.804530662,-0.4417903222
H,0,5.0291481455,-1.9801932149,-1.6860387185
C,0,6.642803372,-0.1822025046,1.3273486467
H,0,4.8656449183,0.9990487461,1.4277673703
C,0,7.3347968067,-1.190996042,0.6607597046
H,0,7.2502751694,-2.6174658838,-0.9528380397
H,0,7.0764181451,0.2936638888,2.2016880518
H,0,8.3143799653,-1.5063961498,1.006670572

TS-14 *anti-up*

M06-2X/6-31+G**, E = -1580.14556024 a.u.

Thermal correction to Gibbs Free Energy = 0.484276 a.u.

1 imaginary frequency = -741.18 cm⁻¹

SP at B2PLYP/6-311+G**, E = -1579.6194238277 a.u.

SP at mPW2PLYP/6-311+G**, E = -1579.6446232910 a.u.

0,1

C,0,-0.816691438,-1.790162045,-3.840323626
C,0,0.3825843725,-1.1125193643,-3.9255936796
H,0,0.785397526,-0.8639650975,-4.9056290442
C,0,1.2728254132,-0.8470988569,-2.7288941342
H,0,1.8755164923,-1.7446286002,-2.5481214115
N,0,2.191613343,0.2496125784,-2.8623109351
C,0,1.6679382067,1.5141500145,-3.3980472603
C,0,3.5147932247,-0.0418004844,-3.4340041513
C,0,2.9332089291,2.302643854,-3.709103212
C,0,3.861945441,1.2117339017,-4.2586329458

H,0,1.0162822732,2.0005260775,-2.665482251
H,0,3.3443513674,2.7353484523,-2.7920929729
H,0,1.0804937781,1.3606429665,-4.315898794
H,0,2.7558247764,3.10704728,-4.4262349519
H,0,4.9212039978,1.4729872708,-4.2024066068
H,0,3.6276244957,1.02402158,-5.3120542774
H,0,3.4488829375,-0.9275974701,-4.0780192755
C,0,4.5487507228,-0.4088325302,-2.3188311744
O,0,-1.1621920894,0.0811810066,-3.7418081716
O,0,-2.1466598296,1.6547851707,-3.3296617684
C,0,-1.589615148,-2.2500641851,-5.0317034218
H,0,-1.2561555112,-1.7400104067,-5.938073725
H,0,-1.452888604,-3.3283503827,-5.1641848489
H,0,-2.6564221359,-2.0647627833,-4.8869994575
C,0,4.671020353,0.7440690866,-1.3220079652
C,0,3.8391824269,0.7863208013,-0.1999578658
C,0,5.5446283635,1.8157239531,-1.5419716787
C,0,3.8700423051,1.8716612075,0.6755830804
C,0,5.5764211494,2.9044377184,-0.6726094479
C,0,4.7348620306,2.9389171074,0.4390494456
H,0,3.1734664366,-0.0491623533,-0.0089128723
H,0,6.216004685,1.8031496018,-2.3956637538
H,0,3.216648807,1.8818580381,1.5427670567
H,0,6.2631474114,3.7234429415,-0.8634488387
H,0,4.7594689384,3.7856374509,1.1179133597
C,0,5.9100530582,-0.8141723145,-2.907055394
C,0,7.0495049935,-0.7977432107,-2.0913288479
C,0,6.0420384557,-1.320299399,-4.2050529445
C,0,8.2734177495,-1.2834771589,-2.5455709681
C,0,7.2673845951,-1.8016366856,-4.6678371847
C,0,8.3870005677,-1.791978633,-3.839026402
H,0,6.9801044238,-0.3969445601,-1.0848634286
H,0,5.1941517384,-1.3508093715,-4.8801974127
H,0,9.1373922774,-1.262720488,-1.8884307689
H,0,7.3419775059,-2.1877672412,-5.6797310365
H,0,9.3384817784,-2.1708816294,-4.1986807275
O,0,3.9605960394,-1.5328268451,-1.675454803
Si,0,4.5528890947,-2.8631143207,-0.8357354586
C,0,5.5614161643,-2.3785033666,0.6732391909
H,0,5.0766861265,-1.5692429141,1.2291930164
H,0,5.6395904189,-3.2462065466,1.3386005232
H,0,6.5768302684,-2.0630384731,0.4186611309
C,0,5.5348639573,-4.0070571439,-1.9521912832
H,0,6.4894194765,-3.5682936945,-2.2599985224
H,0,5.7421481565,-4.9448154965,-1.4241215485
H,0,4.9625355828,-4.2464708575,-2.854835583
C,0,2.9687133886,-3.700665215,-0.2903543114
H,0,2.3656225493,-3.9942838605,-1.1560256629
H,0,3.1853713209,-4.6014764196,0.2932265242
H,0,2.3674379286,-3.0284179589,0.3310057838
H,0,-1.1397546974,-2.1417231772,-2.8630651275
O,0,0.3983289028,-0.6298803387,-1.6245034022
H,0,-0.9961202397,0.1962986675,-2.78380339
H,0,-2.9480873215,1.367505846,-3.7842861383
H,0,0.9363178714,-0.2397541032,-0.9215726357
C,0,2.1080300482,1.6512123116,-2.7764936511
C,0,3.5509494542,-0.1393804337,-3.3943428931
C,0,2.9439206997,2.1945336324,-3.952555445
C,0,3.9142858904,1.0490163115,-4.3150865887
H,0,2.4903031651,2.038719559,-1.8271586692
H,0,3.4748559767,3.1066538532,-3.6663255039
H,0,1.0502800284,1.9279207136,-2.8359749895
H,0,2.3071671471,2.4442887015,-4.8069504379
H,0,4.960592211,1.3433508226,-4.2077588817
H,0,3.7794211259,0.7416159899,-5.356054764
H,0,3.4457631899,-1.0551738579,-3.9758916771
C,0,4.6073738149,-0.4875922888,-2.2980962692
O,0,2.1210930073,-2.780680485,-4.5666763017
O,0,3.5124319665,-2.8928577114,-5.8446863776
H,0,3.9006899612,-3.682886072,-5.4481320401
C,0,0.2067806967,-4.322561492,-3.3039392468
H,0,1.006890777,-4.619128348,-2.6230608766
H,0,-0.7543496696,-4.4680861262,-2.7988451079
H,0,0.2200668882,-4.97411675,-4.1810767946
C,0,4.6262208765,0.6202205869,-1.24526883391
C,0,3.8515240217,0.4922193781,-0.0890086042
C,0,5.2928103615,1.8323473262,-1.4672329404
C,0,3.7432769935,1.5429539846,0.8213371071
C,0,5.1812345324,2.8877771566,-0.5633486473
C,0,4.403204105,2.7484456298,0.5855208369
H,0,3.3107201607,-0.4321534646,0.0814861795
H,0,5.9115036345,1.9597813952,-1.24526883391
H,0,3.1337962798,1.4215727249,1.7121494207
H,0,5.7061796128,3.818140735,-0.7580948565
H,0,4.3157704119,3.5689417649,1.2910814423
C,0,5.9785502357,-0.7592849155,-2.9369441673
C,0,7.1713226516,-0.4893549982,-2.2573460946
C,0,6.0528957271,-1.4142894822,-4.1749134258
C,0,8.4059782832,-0.859098795,-2.7928513405
C,0,7.2857388485,-1.7757308886,-1.72140719519
C,0,8.468466476,-1.5033221607,-4.0263741153
H,0,7.144939737,0.013082634,-1.2956083354
H,0,5.1531360882,-1.6788468313,-4.7274097598
H,0,9.3161004586,-0.6412802954,-2.2421298217
H,0,7.3183763898,-2.2832280469,-5.6739668544
H,0,9.427147146,-1.7918731095,-4.4467234395
O,0,4.1200329803,-1.6958456928,-1.7214845863
Si,0,4.9088377005,-2.9047705182,-0.8580606989
C,0,5.8051695861,-2.2321191573,0.6482542073
H,0,5.1058689057,-1.7661910409,1.3494129126
H,0,6.3073033257,-3.0583538976,1.1646950797
H,0,6.5647377012,-1.4907717269,0.3834785897
C,0,6.0836990175,-3.9103605272,-1.9192842774
H,0,6.9964810771,-3.3622781736,-2.1728888097
H,0,6.3663200889,-4.8190826004,-1.3750360291
H,0,5.5953873502,-4.209519382,-2.8530829787
C,0,3.4821778851,-3.9942382302,-0.3175065645
H,0,3.0101206142,-4.4650765672,-1.1862320635
H,0,3.8302380509,-4.7913924645,0.3478028549
H,0,2.7226362548,-3.4119247729,0.214995336
H,0,-0.33198388,-2.5166055602,-4.4749122054
O,0,0.9767718357,-0.3734532144,-4.7847206074
H,0,1.8719178549,-2.0766266584,-5.1982496435
H,0,0.6937826654,0.5222853434,-5.0069555957

TS-14 syn-down

M06-2X/6-31+G**, E = -1580.14924870 a.u.

Thermal correction to Gibbs Free Energy = 0.489258 a.u.

1 imaginary frequency = -729.06 cm⁻¹

SP at B2PLYP/6-311+G**, E = -1579.6200732291 a.u.

SP at mPW2PLYP/6-311+G**, E = -1579.6457834108 a.u.

0,1

C,0,0.3453592069,-2.8954097724,-3.7117490067
C,0,1.1885276661,-1.9970928617,-3.0914271155
H,0,1.817829757,-2.3014339458,-2.2581628712
C,0,1.1287107619,-0.508632557,-3.3610276304
H,0,0.2244418986,-0.1171101582,-2.8765615141
N,0,2.246649395,0.1849647677,-2.7926450428