

Directed Electrostatic Activation in Enantioselective Organocatalytic Cyclopropanation Reactions. A Computational Study

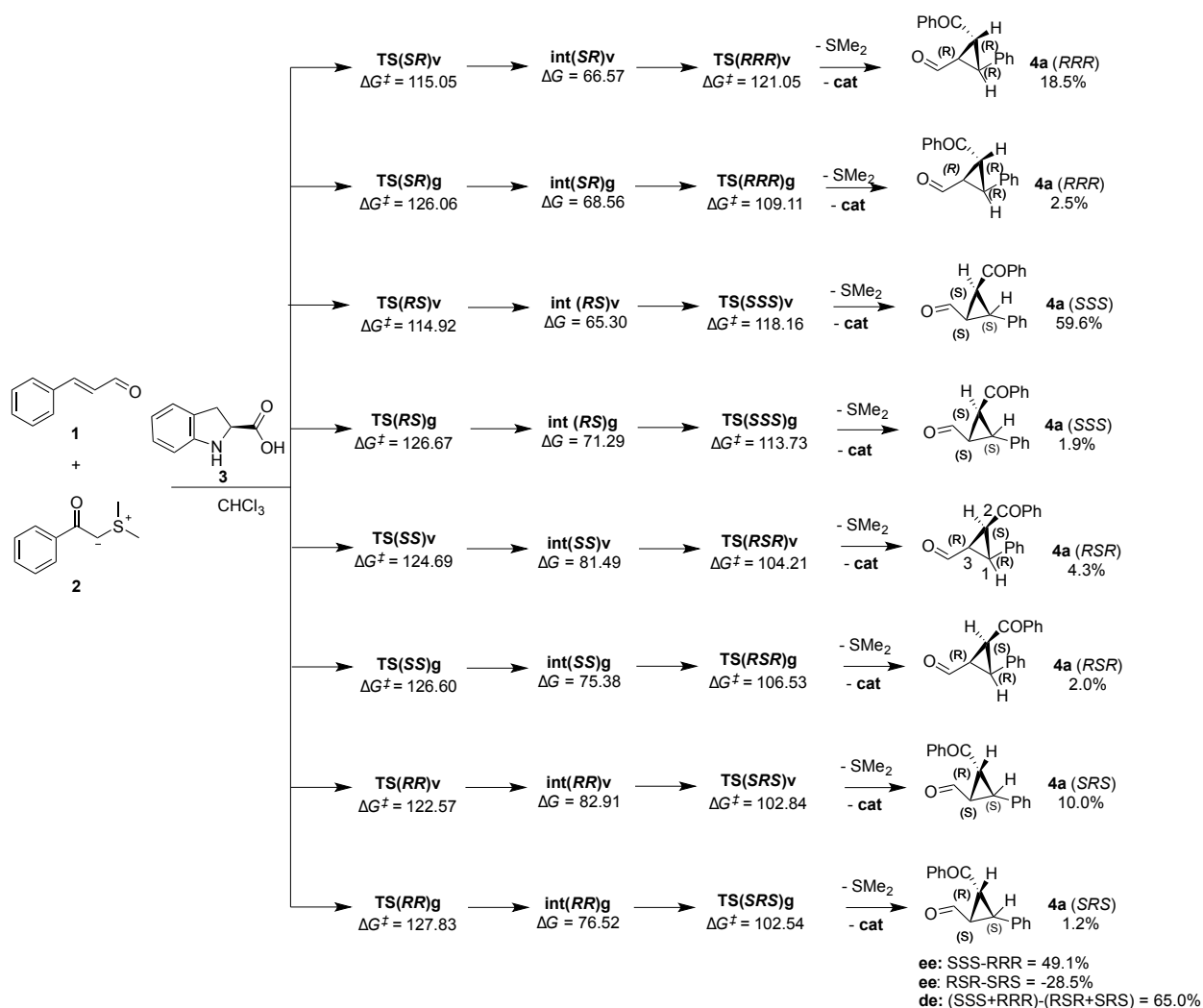
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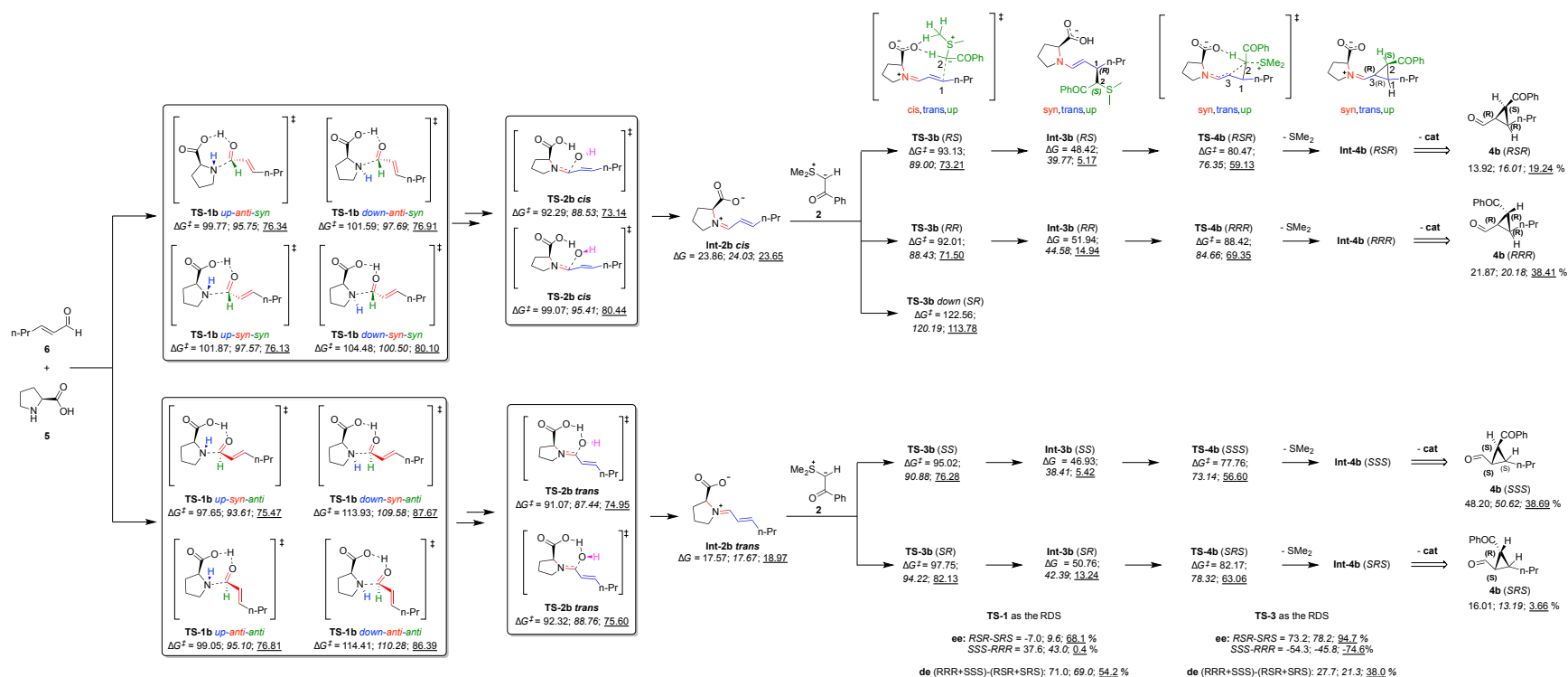
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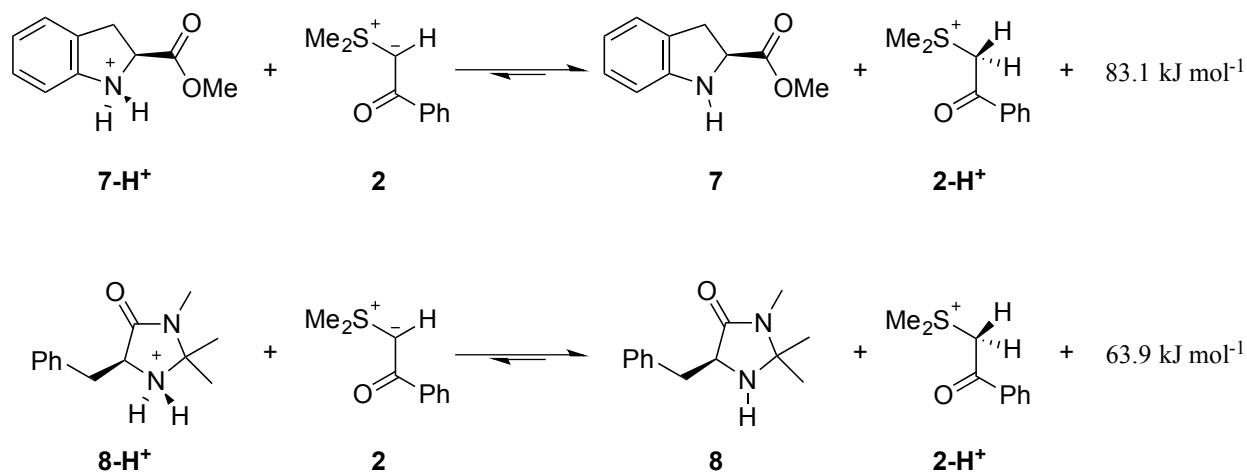
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Scheme S1. All possible calculated transition state structures and intermediates formed during the cyclopropanation reaction between cinnamaldehyde (**1**) and ylide **2**, under general acid/base catalysis by amine **3**. The energies, in kJ mol^{-1} , are relative to the reagents and were calculated in CHCl_3 with B2PLYP/6-311+G**//PBE1PBE/6-31G**.



Scheme S3. All possible calculated TS structures and intermediates for the cyclopropanation reaction between aldehyde **6** and ylide **2**, catalysed by proline (**5**), via iminium intermediate **Int-2b**. The energies, in kJ mol^{-1} , are relative to the reagents and were calculated in CHCl_3 with B2PLYP/6-311+G**//PBE1PBE/6-31G** (plain text), mPW2PLYP/6-311+G**//PBE1PBE/6-31G** (italic) and M06-2X/6-311+G**//PBE1PBE/6-31G** (underscore).



Scheme S4. Theoretical study of the acidity of amines **7** and **8** in comparison with ylide **2** calculated in CHCl_3 with M06-2X/6-311+G**.

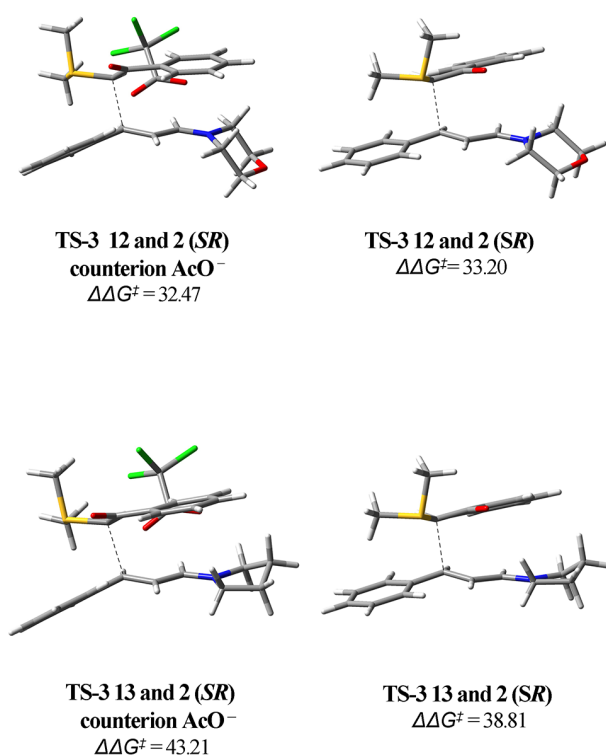
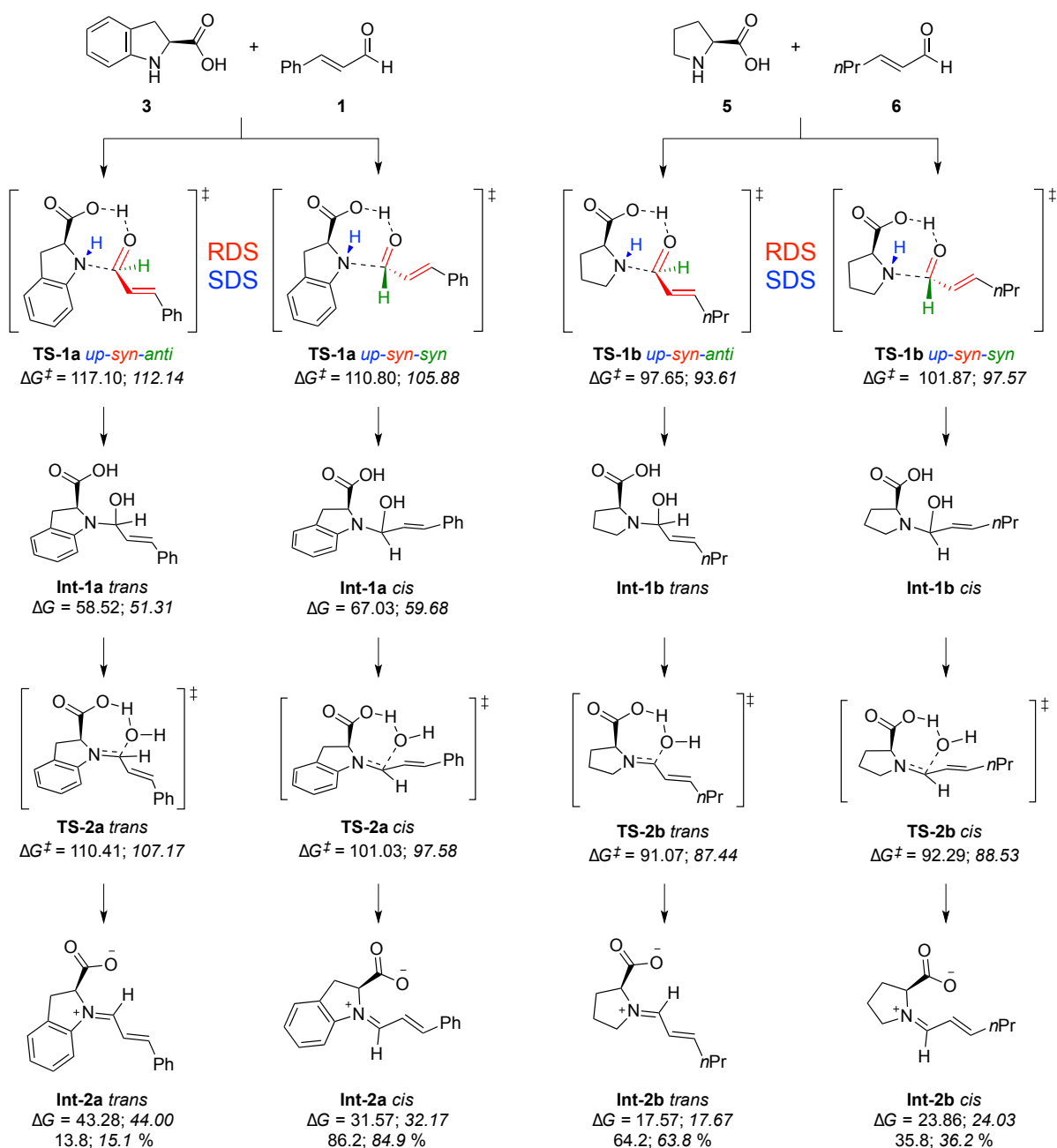
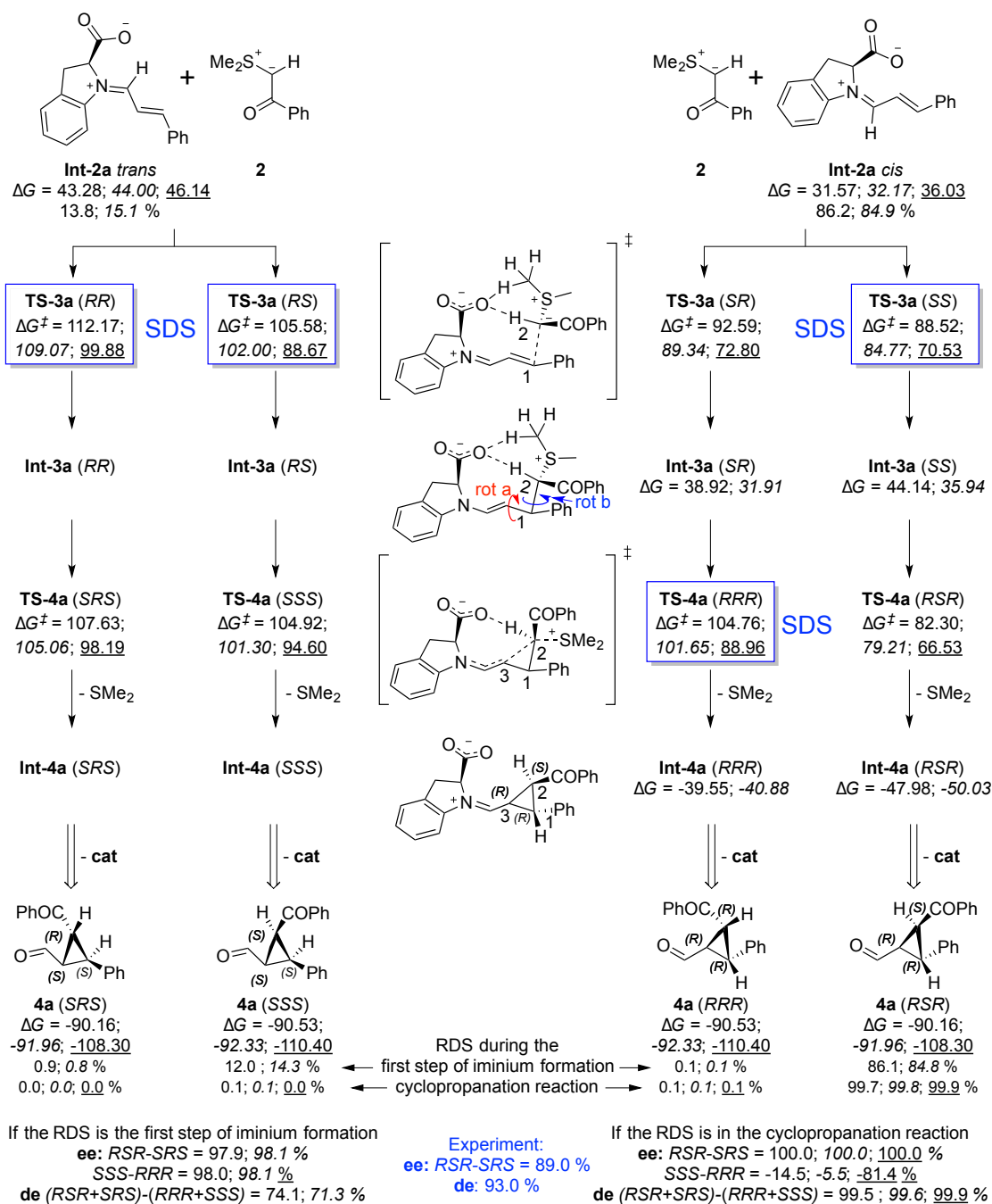


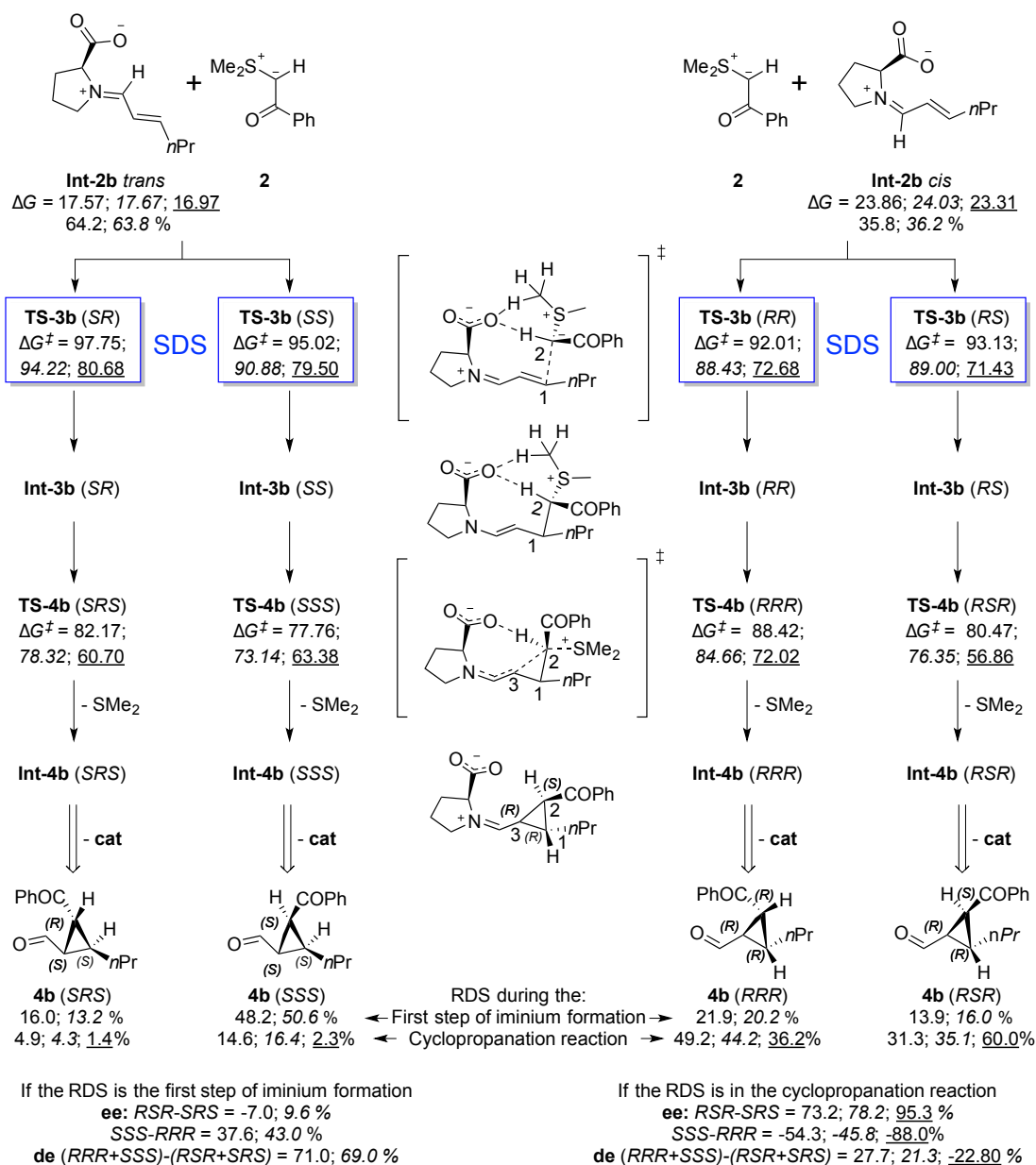
Figure S1. Lowest energy structures for the first step of the cyclopropanation reaction between iminium ions **12** and **13** and ylide **2** with or without trichloroacetate counterion. Gibbs energy values ($\Delta\Delta G_{act}$), in kJ mol^{-1} , are relative to the corresponding iminium ions and **2** and were calculated in CHCl_3 with M06-2X/6-311+G** at 20 °C.



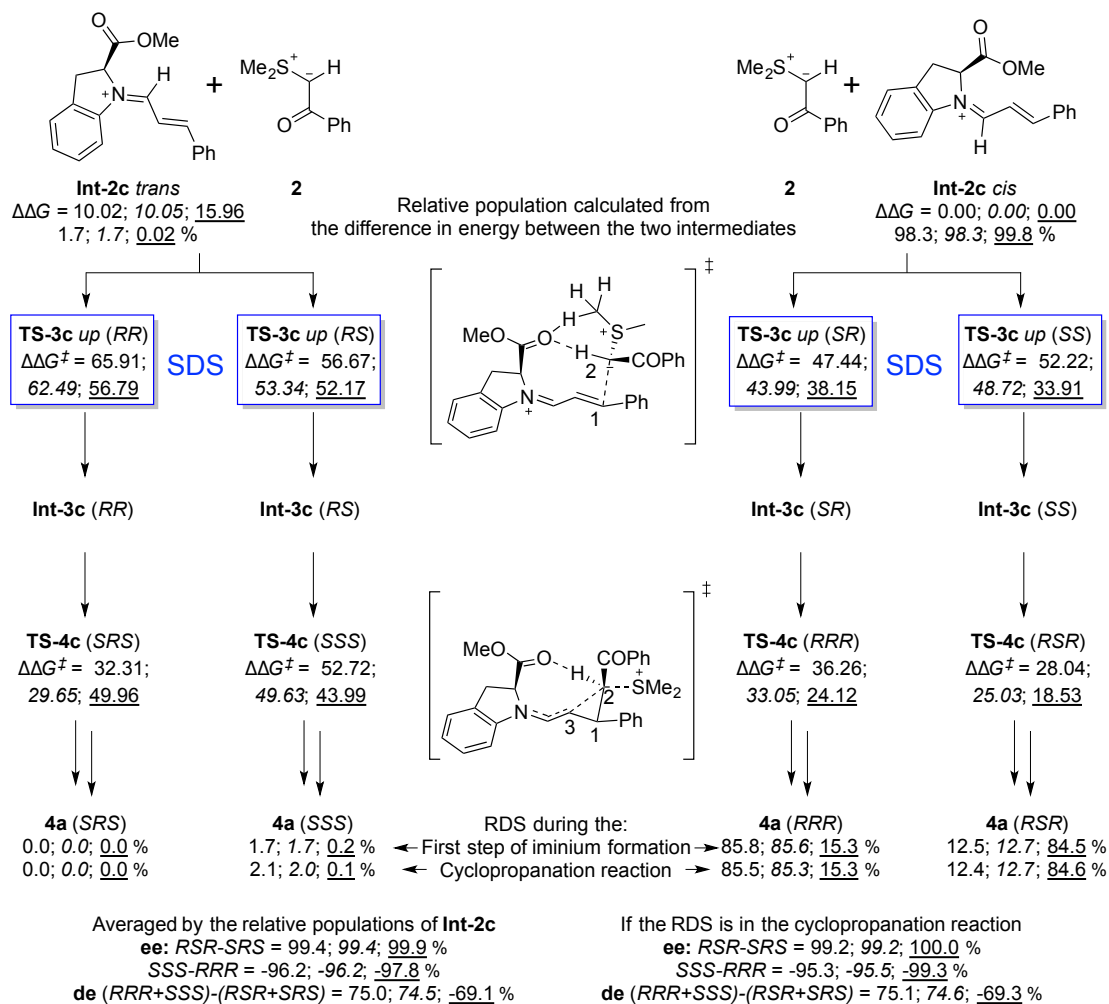
Scheme S5. Expanded version of Scheme 4, with the energies calculated in B2PLYP/6-311+G**//PBE1PBE/6-31G** (plain text) and mPW2PLYP/6-311+G**//PBE1PBE/ 6-31G** (italic).



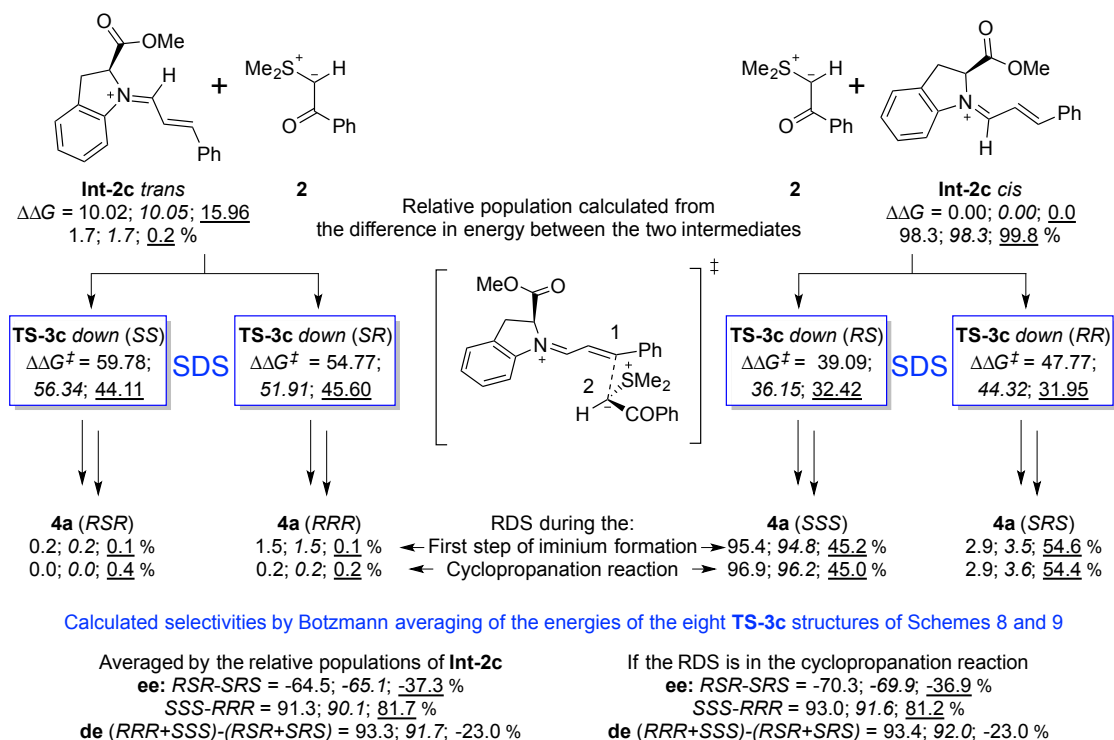
Scheme S6. Expanded version of Scheme 5, with the energies calculated in B2PLYP/6-311+G**//PBE1PBE/6-31G** (plain text), mPW2PLYP/6-311+G**//PBE1PBE/ 6-31G** (italic), and M06-2X/6-311+G** (underline). With M06-2X/6-311+G**, the selectivities were calculated by using only the TS structures shown in the scheme.



Scheme S7. Expanded version of Scheme 6, with the energies calculated in B2PLYP/6-311+G**//PBE1PBE/6-31G** (plain text), mPW2PLYP/6-311+G**//PBE1PBE/ 6-31G** (italic), and M06-2X/6-311+G** (underscore). The selectivities were calculated by using only the TS structures shown in the scheme.



Scheme S8. Expanded version of Scheme 8, with the energies calculated in B2PLYP/6-311+G**//PBE1PBE/6-31G** (plain text), mPW2PLYP/6-311+G**//PBE1PBE/ 6-31G** (italic), and M06-2X/6-311+G** (underscore).



Scheme S9. Expanded version of Scheme 9, with the energies calculated in B2PLYP/6-311+G**//PBE1PBE/6-31G** (plain text), mPW2PLYP/6-311+G**//PBE1PBE/ 6-31G** (italic), and M06-2X/6-311+G** (underscore).

Analysis of the distortion energy as described in the literature.[25]

Following an approach similar to that described by Lopez and Houk,[25] we calculated the electronic energies of the four TS structures **TS-3a** shown in Scheme 5, as well as the electronic energies of the ylide **2** and the two isomers of intermediate **Int-2a** (Scheme 5). The TS optimized structures were broken in the respective reagents (ylide and **Int-2a**), and single-point electronic energies have been calculated. The distortion energies have been calculated as the difference between the sum of the electronic energies of the optimized structures of ylide **2** and intermediate **Int-2a**, either in *cis* or *trans* conformations, and the sum of the electronic energies of their respective distorted structures, as obtained from the transition states.

The difference of electronic energy between **TS-3a** (SS) and **TS-3a** (SR) is 6.60 kJ mol⁻¹ (a value similar to the difference in free energy - 4.07 kJ mol⁻¹, Scheme 5), and the difference of strain energy calculated between the structures resulting from **TS-3a** (SS) and **TS-3a** (SR) is 5.30 kJ mol⁻¹ (Figure S2). These results clearly indicate that the difference in activation energy between

TS-3a (*SS*) and **TS-3a** (*SR*) mainly results from the increment of energy that is needed to distort the ylide and the iminium intermediate from their relaxed conformations to the conformations they have to adopt in the transition state. A similar conclusion is obtained from the comparison between **TS-3a** (*RS*) and **TS-3a** (*RR*), as their difference in electronic energy is 10.92 kJ mol⁻¹, and their difference in strain energy is 7.25 kJ mol⁻¹.

A similar study applied to structures **TS-4a** is not possible, due to the C-S bond cleavage that occurs during this type of TS.

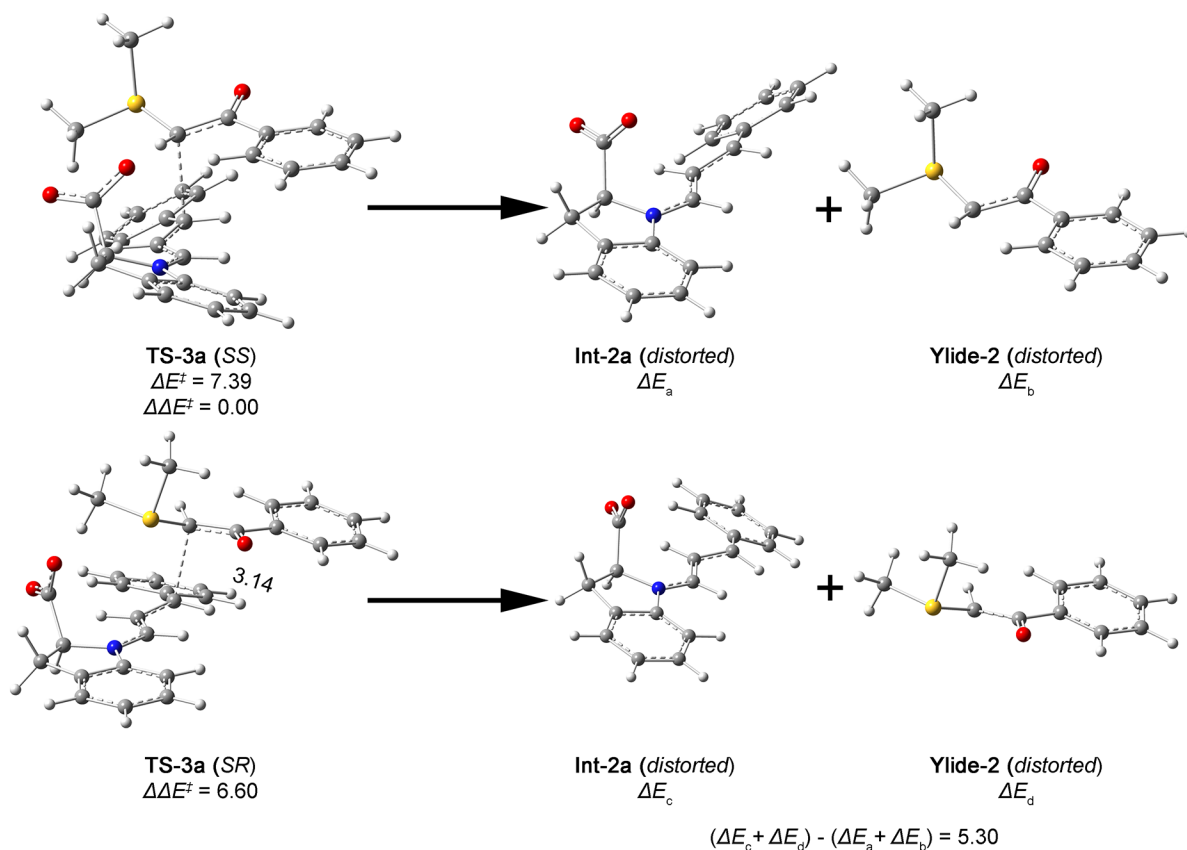


Figure S2. Comparison between the difference in activation energy between **TS-3a** (*SR*) and **TS-3a** (*SS*) and the difference in strain energy between the distorted fragments obtained from the respective transition structures. Electronic energies, in kJ mol⁻¹, were calculated with B2PLYP/6-311+G**. The activation energy of **TS-3a** (*SS*) is relative to the energy of the pre-complex in Figure 7.

1, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -422.494097837 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.109929 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -422.6695955 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -422.672296 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -422.9082197 a.u.

O; 1
O,0,-4.3577836759,0.3795781735,0.0041460817
C,0,-3.3413415902,-0.2923643388,0.0036926813
C,0,-1.9898801546,0.2519369441,0.0023452495
C,0,-0.9308337549,-0.5821036979,0.0019578711
H,0,-3.3939876897,-1.4035103749,0.0043022922
H,0,-1.8955685577,1.3346520435,0.0016921405
H,0,-1.1432682026,-1.6527177406,0.0027104607
C,0,0.4843293193,-0.236578338,0.000647158
C,0,1.4299559698,-1.2736515738,0.0003672334
C,0,0.944512942,1.0909479434,-0.0003480021
C,0,2.7922105344,-0.9978020072,-0.0008526795
C,0,2.3042264981,1.365315989,-0.0015671005
C,0,3.2326557097,0.3230276542,-0.0018219895
H,0,1.0853424436,-2.3047605174,0.0011175154
H,0,0.2345142403,1.9122164384,-0.0001563225
H,0,3.5095636316,-1.8128587965,-0.0010464117
H,0,2.6455530896,2.3961354421,-0.0023219261
H,0,4.2961452473,0.5427567571,-0.0027742519

2, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -860.975584836 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.156679 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -861.1753804 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -861.1930703 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -861.5713388 a.u.

O; 1
C,0,1.1334981511,-2.517515437,-7.3496880918
C,0,2.1715870837,-3.4001287578,-7.6331730097
C,0,1.3426430638,-1.1349073426,-7.3966697512
H,0,1.9927629309,-4.471259296,-7.5999799231
C,0,3.4341233977,-2.9135707158,-7.9661925141
C,0,2.6097795923,-0.6584788377,-7.7460799554
H,0,4.2437024393,-3.6039063431,-8.1859637338
H,0,2.7499431701,0.4167507603,-7.7955467944
C,0,3.6500482826,-1.5379231321,-8.0236808549
H,0,4.6307758295,-1.151725541,-8.2877045816
H,0,0.150097904,-2.9136007684,-7.1150561319
C,0,0.2716847205,-0.1139883001,-7.1088598108
O,0,0.465160985,1.0682942545,-7.4775847081
C,0,-0.8842457388,-0.5456700391,-6.4280542734
H,0,-1.0450543177,-1.5372488608,-6.0315398229
C,0,-1.434308288,1.9689668927,-5.2034632709
H,0,-0.5757341337,2.316977965,-5.7780654801
H,0,-2.2048433159,2.7370970646,-5.1112389131
H,0,-1.132071798,1.6198995528,-4.2156904911
C,0,-2.6148607421,1.3587206969,-7.6186604031
H,0,-3.10699445,0.6069986,-8.2361968862
H,0,-3.3087068745,2.1692611199,-7.3873498819
H,0,-1.7045267668,1.7252497912,-8.0937246198
S,0,-2.1447771246,0.5425016739,-6.0707040969

1, optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -422.908498497 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.109448 a.u.

O; 1
O,0,-4.3436156595,0.3893085713,0.0040432718
C,0,-3.3405440037,-0.2894205907,0.0036887468
C,0,-1.9797124876,0.2511633392,0.0023248083
C,0,-0.9344216175,-0.589773185,0.001986855
H,0,-3.4097339099,-1.3940882001,0.0043949585
H,0,-1.881369176,1.3312936564,0.0016223196
H,0,-1.1488446563,-1.6578361526,0.002786675
C,0,0.4886693931,-0.2417743134,0.0006515584
C,0,1.4326418243,-1.2749082611,0.0003493741
C,0,0.9402825092,1.0851075471,-0.00032316
C,0,2.7944422534,-0.9946785507,-0.0008775004
C,0,2.2986315232,1.3644618507,-0.0015507296
C,0,3.229751726,0.3260899216,-0.0018251415
H,0,1.0914305611,-2.3048345246,0.0010787332
H,0,0.2300542379,1.9031359562,-0.0001115551
H,0,3.5124893116,-1.8057642022,-0.0010912531
H,0,2.6360402401,2.3939898645,-0.0022863305
H,0,4.2901529307,0.5487472732,-0.0027706305

2, optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -861.571694505 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.155253 a.u.
Thermal correction to Gibbs Free Energy at 20 °C = 0.156134 a.u.

O; 1
C,0,1.1045778168,-2.4968497409,-7.4353587384
C,0,2.1334450392,-3.3913415959,-7.7131557473
C,0,1.3498760952,-1.1221785802,-7.4073998749
H,0,1.928695058,-4.4552296323,-7.7423346137
C,0,3.420376872,-2.9221468731,-7.9613568451
C,0,2.6397949195,-0.659655929,-7.6726175655
H,0,4.2215563265,-3.6199949769,-8.1753079056
H,0,2.8155418829,0.4092150106,-7.6661740127
C,0,3.6711336447,-1.5524049647,-7.9410970603
H,0,4.6702268395,-1.1805648828,-8.1372231521
H,0,0.1029115049,-2.8743059831,-7.2666739782
C,0,0.2743769037,-0.0991508179,-7.1229515912
O,0,0.4391296667,1.0672440548,-7.5382930599
C,0,-0.8433940706,-0.528140463,-6.3884352535
H,0,-0.964978326,-1.5067395915,-5.9558208678
C,0,-1.401181975,2.0207509355,-5.2374830261
H,0,-0.5975017086,2.3896130304,-5.8697095945
H,0,-2.1953740298,2.7557978707,-5.112465714
H,0,-1.0272704236,1.6982691441,-4.2681461807
C,0,-2.6535031443,1.2921681618,-7.5925570848
H,0,-3.1239011711,0.4966973163,-8.1662837469
H,0,-3.3765811107,2.0743633568,-7.3650800181
H,0,-1.7752652866,1.6832491403,-8.1006529258
S,0,-2.1230103233,0.5521310101,-6.0242884427

3, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -552.995053030 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.134586 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -553.2297452 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -553.2338914 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -553.5343609 a.u.

O; 1
N,0,-4.3754072153,0.480052427,0.2665404011
C,0,-4.8735097878,0.0197587938,-0.9706014801
C,0,-6.2611924959,0.1607894723,-1.0346299131
C,0,-6.7578215955,0.7730657144,0.2466555474
C,0,-5.4450991256,1.2359969042,0.9367949901
C,0,-5.4673983549,0.9235500427,2.4279642721
O,0,-6.1093536566,1.5651534812,3.2259461296
O,0,-4.749781149,-0.145445128,2.7661631394
C,0,-6.9519611776,-0.2723521505,-2.1558479678
C,0,-6.2390420349,-0.8337793509,-3.2187572291
C,0,-4.8531938822,-0.9619408976,-3.1449605996
C,0,-4.1494248923,-0.5398034963,-2.0156380617
H,0,-7.2813126459,0.0281241871,0.8585917959
H,0,-7.4458502255,1.6086327871,0.0998257502
H,0,-5.3170527212,2.3178034703,0.8219414039
H,0,-4.3295256485,-0.4419073367,1.9253347891
H,0,-8.0319494479,-0.1669006517,-2.213216314
H,0,-6.7667057933,-1.1674186335,-4.106905825
H,0,-4.3076389941,-1.3961935322,-3.9777544839
H,0,-3.0698479379,-0.64323764,-1.9589424232
H,0,-3.4966982177,0.9813765374,0.203197079

5, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -400.737093118 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.114738 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -400.9106066 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -400.9137054 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -401.1240122 a.u.

O; 1
N,0,-0.105433473,0.31132302,0.1784242724
C,0,-1.3999953753,-0.1499028134,0.7125316485
C,0,-2.3817587654,1.0108127553,0.4939903348
C,0,-1.7481913768,1.7704895279,-0.6708860773
C,0,-0.2615401992,1.6794054343,-0.3479361723
C,0,-1.829635942,-1.4028803608,-0.0639911866
O,0,-2.8685751655,-1.9897317195,0.1454069144
H,0,-1.338360382,-0.4363444467,1.7672922683
H,0,-2.4089471239,1.6435751283,1.3869776689
H,0,-3.3946947915,0.65258674,0.2994578175
H,0,-1.9608835546,1.2640658596,-1.6194946225
H,0,-2.0953075519,2.8028503412,-0.7547081456
H,0,0.0080673888,2.4303510425,0.4071731445
H,0,0.3804704026,1.8304990172,-1.220683281
O,0,-0.9483042482,-1.7649888652,-0.9849906789
H,0,-0.2437671792,-1.0563518917,-0.8822426772
H,0,0.636578627,0.2474619811,0.8646177321

3, optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -553.534853049 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.133966 a.u.

O; 1
N,0,-4.3680371908,0.4552802103,0.2672080841
C,0,-4.8701846218,0.0085801352,-0.9789157837
C,0,-6.2562472334,0.1450043228,-1.035680057
C,0,-6.7501783235,0.7321817208,0.2629787454
C,0,-5.4335921339,1.2324012164,0.9229963192
C,0,-5.4661707422,0.9769079979,2.4225390207
O,0,-6.0724111912,1.6756655727,3.1887659531
O,0,-4.8161634288,-0.1159887,2.8205135458
C,0,-6.9509085666,-0.2699580297,-2.1591581441
C,0,-6.2408422924,-0.8121819876,-3.2330661943
C,0,-4.8555726555,-0.9387945844,-3.1659201027
C,0,-4.1490451106,-0.5324841043,-2.0330434945
H,0,-7.2224118297,-0.0412964986,0.8773431228
H,0,-7.4667461212,1.5426393107,0.1388930831
H,0,-5.3142336089,2.30732102,0.7667762757
H,0,-4.3806058646,-0.4919405368,2.0313121474
H,0,-8.0292585953,-0.1671551581,-2.2087440204
H,0,-6.7695180527,-1.1315073295,-4.1227461268
H,0,-4.3141660086,-1.3588135788,-4.0054126866
H,0,-3.0714186054,-0.6345366564,-1.9801905912
H,0,-3.4820528227,0.9440006574,0.2052529041

5, optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -401.124515639 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.114174 a.u.

O; 1
N,0,0.7233594354,-1.0196056247,0.5972237508
C,0,-0.1290561328,0.1711431526,0.7706729232
C,0,0.6789753383,1.3520221726,0.2051256128
C,0,1.5965427642,0.6646949554,-0.8091716459
C,0,1.9787507241,-0.6207153656,-0.0794814095
C,0,-1.4367245009,-0.0203541862,-0.0094006021
O,0,-2.3029921976,0.8146509295,-0.0558236223
H,0,-0.4118766642,0.3322238188,1.8127766906
H,0,1.273333308,1.7993624479,1.0047760116
H,0,0.0354069677,2.12081847,-0.2202124961
H,0,1.0442980674,0.4286639769,-1.7237446165
H,0,2.4649395249,1.2646431701,-1.0791838624
H,0,2.771359224,-0.4194587405,0.6489754717
H,0,2.3162436078,-1.4111455272,-0.750372775
O,0,-1.5279395352,-1.1875704043,-0.6338048075
H,0,-0.6780411555,-1.6447274593,-0.414552476
H,0,0.8975392246,-1.4935127859,1.4741968525

6, optimization in solv. CHCl₃

PBE1PBE/6-31G(d,p), E= -309.505929756 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.114539 a.u.

SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -309.6302621 a.u.SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -309.6327093 a.u.SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -309.8029473 a.u.

0; 1

C,0,0.9960571957,-0.1275726382,0.5587636754

C,0,2.3405311329,0.3274489481,0.2154962735

C,0,3.3015431131,-0.5572309964,-0.0903713448

H,0,3.0450509666,-1.6194539508,-0.0678133334

H,0,0.8633560229,-1.2321170566,0.5424315543

H,0,2.5234792712,1.4000663911,0.2174202106

C,0,4.709462078,-0.2311689759,-0.44940639

C,0,5.7254854699,-0.8923640024,0.4904349727

H,0,4.8554558833,0.855104206,-0.4584140644

H,0,4.9001728158,-0.5879193627,-1.4724761584

C,0,7.1636421529,-0.5975219621,0.0860112263

H,0,5.5561418041,-1.9765736025,0.4997825196

H,0,5.5453545972,-0.5432900883,1.5142474624

H,0,7.8723705274,-1.0736351886,0.7699618543

H,0,7.3736377253,-0.9662658563,-0.9238579281

H,0,7.3639080529,0.4792432403,0.0944004728

O,0,0.0682768607,0.6066795053,0.8455520871

H₂O, optimization in solv. CHCl₃

PBE1PBE/6-31G(d,p), E= -76.3421211035 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.004016 a.u.

SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -76.3985472 a.u.SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -76.3976810 a.u.SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -76.4265413 a.u.

0; 1

O,0,-4.689648098,-0.135240123,1.0404876372

H,0,-4.689648098,0.619872086,1.6363209624

H,0,-4.689648098,-0.890352332,1.6363209624

SMe₂, optimization in solv. CHCl₃

PBE1PBE/6-31G(d,p), E= -477.763373938 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.049508 a.u.

SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -477.8064097 a.u.SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -477.8204752 a.u.SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -477.9804372 a.u.

0; 1

S,0,5.0495781178,-3.2654538171,2.7171498049

C,0,6.439164891,-2.3837411141,3.4671458049

H,0,6.1308262166,-1.3994997116,3.8294258837

H,0,6.872205512,-2.9594006516,4.2894535323

H,0,7.1971214511,-2.2519828226,2.6922012258

C,0,3.9452842431,-3.3699393648,4.145525988

H,0,3.0438536088,-3.8941901807,3.8213442745

H,0,4.4075830542,-3.9343560981,4.9596533478

H,0,3.6655389053,-2.3744832393,4.500472138

6, optimization in solv. CHCl₃

M06-2X/6-311+G(d,p), E= -309.803182362 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.114380 a.u.

0; 1

C,0,-2.6201463169,0.327491473,-0.0153615001

C,0,-1.3358621175,-0.3785140746,0.0250852291

C,0,-0.2382805993,0.2492779338,0.459124649

H,0,-0.3309525044,1.2895846333,0.774638944

H,0,-2.5896667005,1.3776612484,0.3336501405

H,0,-1.3202871624,-1.4121814406,-0.3080558938

C,0,1.1309312785,-0.3409386211,0.52825179

C,0,2.1281021373,0.4292063999,-0.3490888837

H,0,1.1023508132,-1.3926873929,0.2299259044

H,0,1.4787755523,-0.3036533352,1.567667641

C,0,3.5377934459,-0.1456114163,-0.2450377269

H,0,2.1314059772,1.4821784916,-0.0498905309

H,0,1.7857287822,0.3979549192,-1.3876226666

H,0,4.2363552179,0.4066915733,-0.8759602824

H,0,3.9018545522,-0.0980875148,0.7843879112

H,0,3.5551394687,-1.1923879576,-0.5588047835

O,0,-3.6595728245,-0.1629139193,-0.3957149414

H₂O, optimization in solv. CHCl₃

M06-2X/6-311+G(d,p), E= -76.4265806813 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.003898 a.u.

0; 1

O,0,-4.689648,-0.13524,1.0467368636

H,0,-4.689648,0.6255447944,1.6331965682

H,0,-4.689648,-0.8960247944,1.6331965682

SMe₂, optimization in solv. CHCl₃

M06-2X/6-311+G(d,p), E= -477.980534457 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.049166 a.u.

0; 1

S,0,5.0457752086,-3.2662804936,2.7014126186

C,0,6.4326585959,-2.3886988462,3.4706234269

H,0,6.1105692739,-1.4155701074,3.8420728463

H,0,6.8527259733,-2.9777318109,4.2864004474

H,0,7.1940219941,-2.2447868307,2.7054010817

C,0,3.9516889041,-3.3640388057,4.1432723889

H,0,3.0532426344,-3.8980189498,3.836984136

H,0,4.4347040071,-3.9122855506,4.9525996136

H,0,3.6757674086,-2.3656346052,4.4836074406

TS-1a up-syn-syn, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -975.478233444 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.266791 a.u.
1 imaginary frequency = 158.7500 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -975.8794034 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -975.8881345 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -976.4342304 a.u.
0; 1
C,0,2.8382790575,-3.0054495267,-2.4802962993
C,0,2.10064183,-1.9058583414,-2.2730460121
H,0,4.8728257615,-3.6568132864,-2.1893768587
C,0,4.0031898053,-3.3148998868,-1.5921561608
N,0,3.6228272493,-4.8278537723,-0.8745215907
C,0,2.5293356881,-4.6343089019,0.1456651225
C,0,1.5851283627,-5.8313946686,0.0116135432
C,0,3.1388136132,-4.4223561453,1.5371805769
O,0,4.1326131198,-3.5757777944,1.5640011968
O,0,2.7039663194,-5.0125568317,2.5071218914
O,0,4.2487890794,-2.5026475114,-0.6069058396
H,0,4.5027522334,-5.0547979829,-0.4051235915
H,0,4.2341819931,-3.0562012267,0.6120504464
H,0,2.0284325502,-3.7026604826,-0.1442531855
H,0,0.5392328183,-5.5145596022,-0.0020324611
H,0,1.7127074898,-6.5020014081,0.8686441892
C,0,0.9626725038,-1.4303242818,-3.0609588683
C,0,0.4251520172,-2.1448294128,-4.1436830219
C,0,0.376238317,-0.2031711711,-2.7193290663
C,0,-0.6547749005,-1.6441877547,-4.8578542956
H,0,0.8530305138,-3.1019174244,-4.4274489175
C,0,-0.7058150694,0.2992292986,-3.4344023769
H,0,0.780506168,0.3601725348,-1.8820316674
C,0,-1.2249250019,-0.419705415,-4.5073821917
H,0,-1.0571746056,-2.2111458879,-5.6924138364
H,0,-1.1436069473,1.2524828796,-3.1529381826
H,0,-2.0701131689,-0.0314540885,-5.0680704894
H,0,2.6581238623,-3.678266311,-3.315521685
H,0,2.3986959839,-1.2840557753,-1.4290696766
C,0,3.2000668148,-5.9163093751,-1.7300768077
C,0,3.866461632,-6.3656299833,-2.8600995276
C,0,2.0147351416,-6.4771027223,-1.2722834903
C,0,3.2838800353,-7.4162964682,-3.5672229849
H,0,4.8010163598,-5.920867766,-3.1864844216
C,0,1.4454480735,-7.5255107445,-1.9859296888
C,0,2.0843735579,-7.9851513068,-3.1368945718
H,0,3.7712013549,-7.7925042344,-4.4609810524
H,0,0.5202382995,-7.9832541803,-1.6490500415
H,0,1.6464000872,-8.8012500402,-3.7032801049

TS-1a down-syn-syn, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -975.475383397 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.265270 a.u.
1 imaginary frequency = 434.3248 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -975.8774904 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -975.8859365 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -976.4308994 a.u.
0; 1
C,0,5.5391623251,-3.7243400197,-0.6152379361
C,0,5.9516019215,-2.456693753,-0.4630018811
H,0,5.2008895028,-5.5527541029,0.4989198232
C,0,4.9597235139,-4.4770371461,0.5189261933
N,0,3.1944250976,-4.7002576443,0.081186992
C,0,2.5415656265,-5.8659921534,0.7845663264
C,0,2.6251671702,-7.0018082223,-0.2482859746
C,0,2.9867248588,-6.3113689519,2.1937608585
O,0,3.8132767026,-5.6176713806,2.8983150473
O,0,2.4467100623,-7.3422921753,2.5720458065
O,0,4.8989644584,-3.8948139451,1.6732942286
H,0,2.8578932264,-3.8069929069,0.4408389929
H,0,4.3534508797,-4.7338273711,2.3722894528
H,0,1.4865796528,-5.5868951031,0.8931978883
H,0,1.8008705744,-7.7038652574,-0.1184716255
H,0,3.5567720569,-7.570095298,-0.1373765292
C,0,6.5537998771,-1.5944538302,-1.4780759622
C,0,6.6153803184,-1.9406543362,-2.8378781515
C,0,7.0849758404,-0.3586907135,-1.0805478745
C,0,7.1987234278,-1.0830971536,-3.760318059
H,0,6.1931041816,-2.8818321974,-3.1779759823
C,0,7.6710987619,0.4995600688,-2.0043629666
H,0,7.0384957447,-0.0759615602,-0.0318938112
C,0,7.7309203335,0.1391757136,-3.3477457671
H,0,7.2363375982,-1.3651159937,-4.808514271
H,0,8.0798024117,1.4503606004,-1.6752912313
H,0,8.1855109222,0.8076756124,-4.0728899824
H,0,5.6447302853,-4.2593145548,-1.5542828361
H,0,5.8427453078,-2.0244952525,0.5308961394
C,0,2.8789942151,-4.9067817047,-1.3080546631
C,0,2.8866976048,-3.9505333,-2.313308246
C,0,2.5878462025,-6.2472301295,-1.5446081601
C,0,2.5989307401,-4.3818760937,-3.6079603392
H,0,3.1059305342,-2.9088060142,-2.1038170194
C,0,2.310583483,-6.6656447985,-2.8395892149
C,0,2.3201035866,-5.7239739131,-3.8691808699
H,0,2.5869524877,-3.6603596888,-4.4189052136
H,0,2.0770533888,-7.7060402412,-3.0453679301
H,0,2.0960741166,-6.0366740881,-4.8844422512

TS-1a up-anti-syn, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -975.474484891 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.264432 a.u.
1 imaginary frequency = 418.3075 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -975.8768323 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -975.8854046 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -976.4311668 a.u.
0; 1
C,0,2.5140546678,-3.2753402461,-2.485121731
C,0,2.5391228191,-3.4211465829,-3.8171219799
H,0,4.6226735405,-3.6542198623,-2.261148423
C,0,3.7353833311,-3.411487964,-1.6463969516
N,0,3.6215380908,-4.9146593544,-0.8077080411
C,0,2.7368060872,-4.7552686413,0.4054097155
C,0,1.9030312171,-6.0327832443,0.5124072243
C,0,3.6133888703,-4.4155188522,1.6220778698
O,0,4.5018047384,-3.4945040317,1.3846065332
O,0,3.4568012627,-4.9916813058,2.6833207876
O,0,3.8742546401,-2.5079397145,-0.7110059921
H,0,4.5884455028,-5.0446354452,-0.5007978315
H,0,4.2909363702,-2.9763805202,0.3946180833
H,0,2.1141455643,-3.8770278877,0.2070165914
H,0,0.8476696005,-5.8089145241,0.6878025736
H,0,2.255597905,-6.631201474,1.3598964491
C,0,1.4308999346,-3.2443332515,-4.7573016198
C,0,0.136854764,-2.8758961774,-4.3565660797
C,0,1.6688548648,-3.4539516436,-6.1231271846
C,0,-0.8779202624,-2.7253952162,-5.2915355883
H,0,0,-0.0786404212,-2.7027084548,-3.306493915
C,0,0.652260431,-3.3042090559,-7.0602404673
H,0,2.6664970856,-3.7375760294,-6.4494508852
C,0,-0.6258129419,-2.9392183054,-6.6471589318
H,0,-1.8726792591,-2.4385833139,-4.9631238236
H,0,0.8591590637,-3.4713890321,-8.1131993888
H,0,-1.422647108,-2.8198470431,-7.37527817
H,0,1.6129977629,-2.9723193613,-1.9558984678
H,0,3.4900322806,-3.6901288787,-4.2792537286
C,0,3.1525058053,-6.089545392,-1.5095465952
C,0,3.638380636,-6.5599744812,-2.7195942875
C,0,2.1424777721,-6.7240448706,-0.7979305022
C,0,3.0507335452,-7.7118813596,-3.2384571457
H,0,4.4432537875,-6.0572415178,-3.2455014892
C,0,1.5635554008,-7.8721872307,-1.3272917344
C,0,2.0202027939,-8.3558912568,-2.5523375763
H,0,3.3990697322,-8.1085401232,-4.1866871756
H,0,0.7735387343,-8.3887754112,-0.7904815506
H,0,1.5731923905,-9.2501829424,-2.9754985706

TS-1a down-anti-syn, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -975.474462250 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.264986 a.u.
1 imaginary frequency = 422.2041 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -975.8791111 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -975.8874028 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -976.4311944 a.u.
0; 1
C,0,5.5434258884,-3.7592522383,-0.6077925579
C,0,6.1033812476,-4.3305127062,-1.6862946542
H,0,5.1604523159,-5.6296842374,0.4212883452
C,0,4.9552851898,-4.5502831597,0.4797406151
N,0,3.146318675,-4.7193823632,0.1050505623
C,0,2.4983503566,-5.8927232261,0.804716087
C,0,2.5305648548,-7.003562955,-0.2568836802
C,0,2.9840322958,-6.376049852,2.1901237539
O,0,3.8465461062,-5.7136441204,2.8708212546
O,0,2.431117034,-7.4068770513,2.5593234414
O,0,4.9405993082,-3.9921322631,1.6537689381
H,0,2.8360439349,-3.8318987433,0.4995109841
H,0,4.4269160551,-4.7867723161,2.3244748544
H,0,1.4519548522,-5.5997443889,0.9533350408
H,0,1.6989975407,-7.6952058279,-0.1177397529
H,0,3.4548080231,-7.5908611398,-0.1885379311
C,0,6.7530384724,-3.6586912293,-2.809647828
C,0,7.2534376461,-4.4406205548,-3.8607429678
C,0,6.9001186899,-2.2641167118,-2.8854829138
C,0,7.8791197188,-3.8531487012,-4.9547350906
H,0,7.1472543312,-5.5214861003,-3.8139789479
C,0,7.5256050542,-1.6780783533,-3.9767056146
H,0,6.5281088491,-1.6330446792,-2.0839789823
C,0,8.0172639167,-2.4693717088,-5.0158406942
H,0,8.2600069208,-4.4761006204,-5.7584570546
H,0,7.6334103028,-0.598263575,-4.0188026884
H,0,8.5070537103,-2.0065373754,-5.8674086026
H,0,5.5268046319,-2.6823053903,-0.4589687274
H,0,6.0838156394,-5.4189960746,-1.7505240656
C,0,2.7881560604,-4.8882468148,-1.274641681
C,0,2.7865190093,-3.9120756889,-2.2604069595
C,0,2.4669407333,-6.2185436211,-1.5336865233
C,0,2.4478812222,-4.3069931281,-3.5541561853
H,0,3.0316487223,-2.878869127,-2.0377314892
C,0,2.142208988,-6.6020518342,-2.8280458559
C,0,2.1354469369,-5.6369228402,-3.8360999544
H,0,2.4282622842,-3.5676682614,-4.348595512
H,0,1.8835279406,-7.6332888744,-3.0496012747
H,0,1.8741215513,-5.9221865971,-4.8505905674

TS-1a up-syn-anti, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -975.476483241 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.266073 a.u.
1 imaginary frequency = 475.9551 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -975.8762995 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -975.8850347 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -976.4313601 a.u.
0; 1
C,0,-1.2781678692,2.1671557197,-0.1782367794
C,0,-1.0605117498,3.4882900744,-0.1941610065
C,0,-2.6228730292,1.6076973591,0.187143792
N,0,-2.2832863418,0.6040106921,1.5176003279
C,0,-3.3984408374,0.6477150476,2.5382056495
C,0,-3.3838944426,-0.7144516415,3.2240279175
C,0,-3.2363262306,1.8737905633,3.4565665617
O,0,-3.1141971462,2.9989477604,2.8268526373
O,0,-3.2299755651,1.7273102417,4.6682532402
H,0,-0.5009745341,1.4582369484,-0.4587380265
H,0,-1.9014545351,4.1216047511,0.0851188588
O,0,-3.561341301,2.4517007782,0.5430340681
H,0,-2.9561820053,0.8409308183,-0.5324410984
H,0,-1.4355934449,1.0110150524,1.9231734788
H,0,-3.3224955714,2.8449251628,1.6908797944
H,0,-4.3083902007,0.7878485784,1.9454843388
H,0,-4.3940809422,-1.0433434796,3.4785152918
H,0,-2.812261793,-0.6572472323,4.1573921651
C,0,0.1753287885,4.1868809746,-0.5502005883
C,0,1.3235191352,3.5309528866,-1.0219402698
C,0,0.2161336108,5.5820307228,-0.4156302576
C,0,2.4689681813,4.2473901485,-1.340537866
C,0,1.3640931147,6.3003928062,-0.7325674809
C,0,2.4953656487,5.6350061139,-1.196129952
H,0,1.3207989298,2.4521018918,-1.1475894373
H,0,-0.6662785994,6.1037009968,-0.0539150089
H,0,3.3471432032,3.7229439952,-1.705978495
H,0,1.3739118181,7.380336456,-0.6183906251
H,0,3.3932853454,6.1920620878,-1.4467786262
C,0,-2.0728250197,-0.8130782673,1.249459026
C,0,-2.7134724165,-1.5905562457,2.2080564551
C,0,-1.3444789446,-1.3539794037,0.2021110475
C,0,-2.632705088,-2.9748566382,2.1208243645
C,0,-1.2733622377,-2.7448046367,0.1248545101
C,0,-1.9107183152,-3.544751693,1.0725620833
H,0,-0.8509008436,-0.7355351182,-0.5391912221
H,0,-3.1258279093,-3.6024654047,2.8569403858
H,0,-0.7186518281,-3.2045940172,-0.686656635
H,0,-1.8459323312,-4.6253762353,0.991188281

TS-1a down-syn-anti, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -975.474526539 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.266201 a.u.
1 imaginary frequency = 501.5413 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -975.8772749 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -975.8856893 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -976.4315718a.u.
0; 1
C,0,5.5054371543,-3.7718588887,-0.6660419587
C,0,6.2418256432,-4.2304937716,-1.6883732212
O,0,5.1993556953,-5.9625631793,0.241805989
C,0,4.9319061945,-4.697320493,0.3354851308
N,0,3.1415439076,-4.5474026137,0.1340534502
C,0,2.4104906046,-5.5701867006,0.9795246904
C,0,2.2034450063,-6.7653433173,0.0337821451
C,0,3.0405435011,-5.9573580419,2.3413205222
O,0,4.2074179827,-6.5161696463,2.3309918272
O,0,2.3543020055,-5.7851672708,3.3384712352
H,0,4.9264819866,-4.2693792319,1.3522214217
H,0,2.8993753022,-3.6033007499,0.4332848248
H,0,4.7513794161,-6.3763929527,1.2958256849
H,0,1.4422164148,-5.1238784395,1.2161802669
H,0,1.2683345979,-7.2819491703,0.2647532508
H,0,3.0206092897,-7.4872933208,0.1232302285
C,0,6.9062223266,-3.450263649,-2.7303314548
C,0,7.5589580004,-4.136002171,-3.76513186
C,0,6.9220335815,-2.0461494534,-2.7486739133
C,0,8.1990140076,-3.4474334346,-4.7897825907
H,0,7.5578624719,-5.22300976,-3.7610496966
C,0,7.5624208466,-1.3583856214,-3.7701504246
H,0,6.4380030814,-1.4866780038,-1.953449233
C,0,8.2022954011,-2.0554118357,-4.795903316
H,0,8.69697004,-3.998383762,-5.5821799022
H,0,7.5673777577,-0.2722748615,-3.7669953559
H,0,8.7033895668,-1.5134851015,-5.5925322958
H,0,5.3259793702,-2.7102752116,-0.5080139614
H,0,6.3631657942,-5.3110150756,-1.7485961207
C,0,2.7132899261,-4.8201438622,-1.2149889744
C,0,2.806558424,-3.9637017348,-2.301761117
C,0,2.2012634349,-6.1085053541,-1.3153354242
C,0,2.3632495518,-4.4411749201,-3.5345769152
H,0,3.19857791,-2.9573998651,-2.2018187598
C,0,1.7705354592,-6.5771240398,-2.5496537235
C,0,1.8567076723,-5.7347989502,-3.6582615826
H,0,2.4133258125,-3.7946080943,-4.4049362232
H,0,1.3622212652,-7.5785454202,-2.6476141125
H,0,1.5159465957,-6.0864680301,-4.6273125306

TS-1a up-anti-anti, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -975.475893461 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.266233 a.u.
1 imaginary frequency = 472.0725 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -975.8765746 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -975.8851705 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -976.4309699 a.u.
0; 1
C,0,-1.9646285428,2.0253621312,-0.3122577685
C,0,-1.4200086885,1.7159783484,-1.4968202025
C,0,-3.173118199,1.3326269335,0.2310906256
N,0,-2.6031339763,0.5178063499,1.6219061778
C,0,-3.6406436919,0.5407824278,2.7203113792
C,0,-3.4516060126,-0.7536452416,3.5047236376
C,0,-3.5228119244,1.8518273877,3.5164967727
O,0,-3.5426326697,2.9213724736,2.7798213038
O,0,-3.4119389476,1.8259931005,4.730524319
H,0,-1.6138826651,2.8710842765,0.279047258
H,0,-1.8510964302,0.880400198,-2.0510226861
O,0,-4.1571929145,2.1113761972,0.6119183852
H,0,-3.4741163107,0.4707162122,-0.3864305303
H,0,-1.7848325228,1.0589796188,1.9121694494
H,0,-3.8437603054,2.6502671476,1.7006943749
H,0,-4.6005352944,0.5554473737,2.1935411041
H,0,-4.4086481766,-1.160750033,3.8391270759
H,0,-2.844409087,-0.5644581637,4.3972886762
C,0,-0.2988278516,2.382718849,-2.1636025147
C,0,0.3342222174,3.5211898773,-1.6406201524
C,0,0.1686778779,1.8607409938,-3.377972012
C,0,1.3992475317,4.1088615104,-2.3091839991
C,0,1.2366735932,2.4486928915,-4.0475338257
C,0,1.8566232026,3.5751232394,-3.5144531833
H,0,-0.0108136694,3.9561962566,-0.7073675448
H,0,-0.3153734319,0.9824399366,-3.7982402387
H,0,1.8755508059,4.9905142363,-1.8904044965
H,0,1.5829446599,2.0272952003,-4.9866811676
H,0,2.6896328192,4.0384164923,-4.0347786835
C,0,-2.2303501059,-0.8817816469,1.473701366
C,0,-2.7383080088,-1.6373785858,2.5244691982
C,0,-1.4625524938,-1.4208465733,0.4540760625
C,0,-2.4966825517,-3.0056039985,2.5503597969
C,0,-1.2288476949,-2.7952067151,0.4921069786
C,0,-1.7448338536,-3.5781444475,1.5247045379
H,0,-1.0548052422,-0.8025596077,-0.3374496881
H,0,-2.8841362693,-3.6180467629,3.3589255383
H,0,-0.63878021,-3.256656558,-0.2932453511
H,0,-1.5540208761,-4.6468741301,1.5326321389

TS-1a down-anti-anti, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -975.474616499 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.266364 a.u.
1 imaginary frequency = 507.6504 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -975.8787857 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -975.8872862 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -976.4332785 a.u.
0; 1
C,0,5.5135183139,-5.8438920569,0.5613774091
C,0,6.0950701199,-6.2860809731,-0.564617455
H,0,5.1614631458,-3.8610215352,-0.2199327921
C,0,4.9145339008,-4.490243464,0.6491275392
N,0,3.1713818922,-4.7254096363,0.2034775816
C,0,2.4149204099,-5.8023153574,0.9405491989
C,0,2.4662968135,-7.0133752775,-0.007911161
C,0,2.7743779287,-6.1638633738,2.3952825882
O,0,3.6354063462,-5.4797833231,3.072872547
O,0,2.1467259387,-7.1156799262,2.837933055
O,0,4.8618243997,-3.8829510723,1.7927995794
H,0,2.8320885931,-3.7994726161,0.4633673259
H,0,4.2524530699,-4.6772747168,2.5168346164
H,0,1.3775263499,-5.4500121257,0.9830354162
H,0,1.5647159272,-7.6197985697,0.0904396279
H,0,3.3240139273,-7.6570128949,0.2181988434
C,0,6.7268345561,-7.5869733438,-0.7852187782
C,0,7.3560544545,-7.8281022643,-2.0150561724
C,0,6.7257296031,-8.6107886001,0.1759017452
C,0,7.9710025493,-9.0470674885,-2.2783774122
H,0,7.3608241065,-7.0453126791,-2.7694999218
C,0,7.3394368706,-9.8277532329,-0.087178963
H,0,6.2406360907,-8.4567246752,1.135236356
C,0,7.9651087396,-10.0512357157,-1.3141843154
H,0,8.4541510782,-9.2129058679,-3.2367561253
H,0,7.3289885233,-10.608688809,0.6674407737
H,0,8.4432128748,-11.0052215947,-1.515913068
H,0,5.4840282451,-6.4384127029,1.4709486345
H,0,6.1143386682,-5.6149319876,-1.4242661409
C,0,2.9849296765,-5.0297759055,-1.1869671263
C,0,3.2025600374,-4.1695245831,-2.2535017341
C,0,2.6173415406,-6.3618879955,-1.3507993058
C,0,3.0323978654,-4.6881179225,-3.5367547877
H,0,3.4798201704,-3.1306777113,-2.100769691
C,0,2.4580960013,-6.8676008901,-2.6346675654
C,0,2.6678053801,-6.0219993521,-3.7244112876
H,0,3.1819767311,-4.043087737,-4.3968298606
H,0,2.1677241366,-7.9025916246,-2.7882618851
H,0,2.5389150235,-6.4044943977,-4.7322572888

Int-1a cis, optimization in solv. CHCl₃

PBE1PBE/6-31G(d,p), E= -975.500330548 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.269357 a.u.

SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -975.898651 a.u.SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -975.9082984 a.u.SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -976.4567772 a.u.

0; 1
C,0,-2.0753569524,-0.5788303752,-0.9093708788
C,0,-1.1596284123,-0.0423971257,-1.7254090064
C,0,-3.3534791651,0.1152883941,-0.5270795004
N,0,-3.8052036213,-0.2417373659,0.7767438873
C,0,-5.2202034585,-0.3293011059,1.1294996049
C,0,-5.2105324569,-1.0785621458,2.4748925916
C,0,-5.9658736926,1.0147371078,1.2817809479
O,0,-5.4616678635,2.0965986313,0.7070990486
O,0,-7.0180900219,1.0596704984,1.8806227887
O,0,-3.2668900704,1.5398133706,-0.7205935317
H,0,-4.149596498,-0.1828472259,-1.2217517056
H,0,-4.6162068849,1.9298945338,0.223325362
H,0,-5.7658511711,-0.8841744482,0.3568823067
H,0,-5.3311841933,-2.1569507323,2.3165835728
H,0,-6.0286763515,-0.735956233,3.1106756602
H,0,-2.4688074902,1.8525473168,-0.2716901198
C,0,0.0883535667,-0.6633397801,-2.1785703806
C,0,0.8351184541,-0.0169134441,-3.1735140841
C,0,0.5765073672,-1.8736382447,-1.661627417
C,0,2.0221065961,-0.5636965303,-3.6493867315
H,0,0.4732793474,0.9244062385,-3.5798937182
C,0,1.7621743365,-2.4190793616,-2.135336103
H,0,0.0318069716,-2.3880979284,-0.8754056572
C,0,2.4895633127,-1.7685853451,-3.1324363599
H,0,2.5825550765,-0.0472089661,-4.4231121182
H,0,2.125308459,-3.3554011463,-1.7215611235
H,0,3.4173014091,-2.1981043851,-3.4987049595
H,0,-1.9704825946,-1.5864157226,-0.514790784
H,0,-1.3497967381,0.9557407869,-2.1186395974
C,0,-3.0375659365,-0.3041093848,1.9443213183
C,0,-1.6969056108,0.0146274991,2.1460814338
C,0,-3.8335043141,-0.7723602074,3.0014912158
C,0,-1.1675281936,-0.1522796946,3.4292789284
H,0,-1.0686167955,0.3766816522,1.3395628577
C,0,-3.2966288064,-0.9280414815,4.2664361064
C,0,-1.9504268611,-0.6127919113,4.4830539193
H,0,-0.1238009295,0.0948958884,3.6014200389
H,0,-3.9150676598,-1.2912859484,5.0829720719
H,0,-1.5191542542,-0.7247321437,5.4729209763

Int-1a trans, optimization in solv. CHCl₃

PBE1PBE/6-31G(d,p), E= -975.500506017 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.268420 a.u.

SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -975.900958 a.u.SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -975.9105504 a.u.SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -976.4577092 a.u.

0; 1
C,0,-3.6867974605,1.0149195431,-1.4501406004
C,0,-2.971525358,0.596084433,-2.5020524107
C,0,-3.09520915,1.1488559292,-0.0820300985
N,0,-3.6841366034,0.2861076737,0.8782710425
C,0,-5.0676387812,-0.174877154,0.888879148
C,0,-5.0620581899,-1.3118365598,1.9346698206
C,0,-6.1238445188,0.8863170541,1.2560366889
O,0,-5.7870341894,2.1671783824,1.2080058795
O,0,-7.2528290942,0.545411501,1.534326371
O,0,-3.2644354379,2.5067935517,0.4005622279
H,0,-4.8358611791,2.3209932709,0.9804183569
H,0,-5.3559548517,-0.5484270458,-0.0996770408
H,0,-4.944513723,-2.2847760799,1.4431918862
H,0,-6.00460912,-1.3277987187,2.485436313
H,0,-2.019746584,0.9313211142,-0.1151752721
H,0,-3.0738427812,3.1217570769,-0.3202275436
H,0,-4.7273634579,1.3183260265,-1.5538640373
H,0,-1.9283336267,0.3275670519,-2.3311319179
C,0,-3.4255256374,0.4472645676,-3.8867001225
C,0,-4.7408708112,0.7164167747,-4.2967043261
C,0,-2.5036587896,0.0147875114,-4.8502802749
C,0,-5.1142938013,0.5589038705,-5.6242551296
H,0,-5.4802900727,1.0491747551,-3.5742604739
C,0,-2.8775781674,-0.1437015794,-6.1804472889
H,0,-1.4816143721,-0.1992149211,-4.5474938375
C,0,-4.1851605766,0.1284072976,-6.5720589886
H,0,-6.1365541324,0.7710694031,-5.9233931449
H,0,-2.1473121093,-0.4802440397,-6.910364598
H,0,-4.4821346126,0.0055656719,-7.609342263
C,0,-3.0703178621,-0.0485280145,2.084381894
C,0,-1.866461433,0.4139587291,2.6052175709
C,0,-3.8512599517,-0.9885884527,2.7705341925
C,0,-1.4452816358,-0.1059654617,3.8321652162
H,0,-1.2842742833,1.1755084418,2.0963061199
C,0,-3.4245834991,-1.4883538456,3.987888468
C,0,-2.2091629301,-1.0435708683,4.5216616714
H,0,-0.5099793572,0.2445674774,4.2594627625
H,0,-4.0256080813,-2.2185496258,4.5234500823
H,0,-1.8666320109,-1.4244855267,5.4787809662

TS-2a cis, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -975.475044369 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.265857 a.u.
1 imaginary frequency = 394.4958 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -975.8822038 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -975.8903612 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -976.4317664 a.u.

O; 1
C,0,-3.712180586,0.5721757153,-1.4715328502
C,0,-2.9521678861,0.5165363673,-2.5816236069
C,0,-3.0944447766,0.5899679906,-0.1544197631
N,0,-3.6828669054,-0.0014800211,0.8862298511
C,0,-5.1216295075,-0.3091608446,1.0011853887
C,0,-5.1991111496,-1.2220593021,2.2371385331
C,0,-6.0303835675,0.9484946142,1.1396861515
O,0,-5.553659235,2.0806726083,0.7946330364
O,0,-7.1786876957,0.7240583141,1.5212990188
O,0,-3.1958815022,2.4436706337,0.3114841036
H,0,-4.2489875222,2.3335187398,0.5565845187
H,0,-5.4480452543,-0.8344345347,0.0990987939
H,0,-5.2380055637,-2.2803265046,1.9535967434
H,0,-6.1061627685,-0.992240817,2.8001494506
H,0,-2.0091019014,0.5824050923,-0.12675346
H,0,-3.153273855,2.9606857333,-0.5036458533
H,0,-4.7947347173,0.6260125966,-1.5195887842
H,0,-1.8695751332,0.4822426957,-2.4555520105
C,0,-3.4106754026,0.4841087173,-3.9657983385
C,0,-4.7678461658,0.5295730238,-4.3259789967
C,0,-2.4491783072,0.4052721946,-4.9846500529
C,0,-5.1431675058,0.4975586494,-5.661039678
H,0,-5.5354924237,0.5911107423,-3.5606900495
C,0,-2.8264201814,0.3730520071,-6.3219371804
H,0,-1.3958110108,0.3694329702,-4.7184567691
C,0,-4.1752218961,0.4190558288,-6.6635627089
H,0,-6.1959345307,0.5340299403,-5.9242978928
H,0,-2.0681847091,0.3123013748,-7.0966510257
H,0,-4.474775679,0.3941212411,-7.7070170819
C,0,-3.0654286674,-0.1970294635,2.1394077229
C,0,-1.8096393347,0.227022199,2.5544701996
C,0,-3.9247203108,-0.9153416149,2.9720878679
C,0,-1.410913975,-0.1148904637,3.8464541764
H,0,-1.1682845835,0.8285842282,1.9190696944
C,0,-3.5159828877,-1.2438788489,4.2556421521
C,0,-2.2500443615,-0.8433632811,4.6885687754
H,0,-0.4369341839,0.2065678174,4.2025254748
H,0,-4.1735086106,-1.8014364153,4.9164099282
H,0,-1.9208945507,-1.090290989,5.6931946415

TS-2a cis 2, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -975.473280834 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.266026 a.u.
1 imaginary frequency = 398.0101 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -975.8803622 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -975.8884919 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -976.4299906 a.u.

O; 1
C,0,-3.7202434498,0.5166414453,-1.4783862095
C,0,-2.9541466631,0.4994462684,-2.5840600968
C,0,-3.1071848623,0.5458956025,-0.1599959569
N,0,-3.6835639246,-0.0724407805,0.8756244319
C,0,-5.1235355028,-0.3803652682,0.9975064982
C,0,-5.2007075421,-1.2692955982,2.2503859892
C,0,-6.0447267831,0.8721503474,1.1098875617
O,0,-5.593682625,1.9979369419,0.7141430753
O,0,-7.1821692482,0.6455667076,1.5214988532
O,0,-3.2530428728,2.4158085555,0.2060088886
H,0,-4.3006751131,2.2820717784,0.4605608296
H,0,-5.4461886307,-0.924262499,0.1050115402
H,0,-5.2474841113,-2.332373797,1.9873292784
H,0,-6.1040352362,-1.0230622506,2.8123614535
H,0,-2.0215542104,0.5516629792,-0.1400467816
H,0,-2.7964979712,2.5756406733,1.0433022412
H,0,-4.8033889803,0.5289238481,-1.5311206565
H,0,-1.8717467798,0.5104967203,-2.4540752451
C,0,-3.4060749923,0.4529192523,-3.9700733125
C,0,-4.7619974869,0.4834662615,-4.3361115736
C,0,-2.4400028112,0.3759264831,-4.984628188
C,0,-5.1317681732,0.4362510778,-5.67229782
H,0,-5.5327582172,0.5498321088,-3.5744232442
C,0,-2.8115385999,0.327807249,-6.3230799571
H,0,-1.3873641172,0.3539378466,-4.7140524054
C,0,-4.1593319313,0.357404929,-6.6703982451
H,0,-6.1837490902,0.4628477171,-5.9399797389
H,0,-2.0495754874,0.2683862128,-7.0942873177
H,0,-4.4544808085,0.3211038019,-7.7148070359
C,0,-3.0566577844,-0.2703144182,2.1236339637
C,0,-1.7855875009,0.1267198882,2.5222452667
C,0,-3.9213263518,-0.9609524728,2.9745127163
C,0,-1.386198042,-0.1966220168,3.8195480941
H,0,-1.1140371689,0.672351264,1.866226545
C,0,-3.5109236888,-1.2730678239,4.2613038485
C,0,-2.2361895793,-0.8866917688,4.68173751
H,0,-0.3999855001,0.1037169288,4.1597863803
H,0,-4.1740300355,-1.8087822457,4.9343824658
H,0,-1.9062271256,-1.1209889483,5.6890023536

TS-2a trans, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -975.470448361 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.265272 a.u.
1 imaginary frequency = 347.4771 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -975.8780436 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -975.8861247 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -976.4268843 a.u.

O, 1
C,0,-1.802163636,-0.5096009481,-0.6623095827
C,0,-1.2487797332,-0.2881440745,-1.8689853181
C,0,-3.1443977552,-0.0350603805,-0.3453103588
N,0,-3.6957530022,-0.2591959795,0.8462423651
C,0,-5.1566224643,-0.2204796825,1.0675671714
C,0,-5.336442083,-1.0294115724,2.358262845
C,0,-5.7368249849,1.2226753972,1.1989229348
O,0,-5.088963382,2.181327514,0.6672560186
O,0,-6.8225912737,1.3028223872,1.7743193279
O,0,-3.0156223311,1.8910160321,-0.5767066882
H,0,-3.8640022458,-0.0255932076,-1.1579833051
H,0,-3.9222626793,2.0617661563,-0.012874537
H,0,-5.6505103348,-0.6893658738,0.2109412509
H,0,-5.5485069701,-2.0847897642,2.1489373363
H,0,-6.1689675602,-0.6152663629,2.9299022005
H,0,-2.280841186,2.1817232698,-0.0219999043
C,0,0.0433799515,-0.7641462749,-2.347497369
C,0,0.4516188198,-0.3971635408,-3.6390233342
C,0,0.8987211338,-1.5717320068,-1.5788622051
C,0,1.6739292939,-0.8188418127,-4.1490275012
H,0,-0.201971449,0.2264292275,-4.2435722853
C,0,2.1179261548,-1.9926665831,-2.0890061303
H,0,0.6107983982,-1.875570724,-0.5769051681
C,0,2.5108833049,-1.6176832654,-3.374882789
H,0,1.9726654542,-0.5238964531,-5.1503329031
H,0,2.7680057482,-2.6168137934,-1.4832429501
H,0,3.4666559694,-1.9491742409,-3.7695761528
H,0,-1.2990408317,-1.1014645421,0.0951532484
H,0,-1.8062972431,0.3306128095,-2.5714785825
C,0,-3.0592374086,-0.4131822493,2.0995580406
C,0,-1.7479649926,-0.1251507777,2.4644844072
C,0,-3.9994238472,-0.8741310746,3.0272195005
C,0,-1.3772042924,-0.3614931114,3.7887707316
H,0,-1.0346700567,0.2947113724,1.7643108842
C,0,-3.6162954781,-1.1009775379,4.3394506689
C,0,-2.2948421049,-0.8503563019,4.7157611981
H,0,-0.3601653723,-0.1427672608,4.0991253609
H,0,-4.3387063701,-1.4574936561,5.0678706114
H,0,-1.9851789911,-1.0188519999,5.7425001727

TS-2a trans 2, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -975.469599458 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.264926 a.u.
1 imaginary frequency = 346.9249 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -975.8783881 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -975.8864648 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -976.426419 a.u.

O, 1
C,0,-1.6649157744,-0.3149866704,-0.6104116013
C,0,-1.2504531197,-0.325658726,-1.8916889574
C,0,-3.0054339473,0.13711472,-0.2817447303
N,0,-3.6219183325,-0.1931206425,0.8526758156
C,0,-5.0939440758,-0.2090453118,0.977164788
C,0,-5.3308963894,-1.0873929838,2.2142011967
C,0,-5.7377252367,1.2042215109,1.1198870854
O,0,-5.0762890986,2.2104471217,0.7057295859
O,0,-6.8829414503,1.2137515238,1.5732471966
O,0,-2.7645109163,2.0519308962,-0.0625005269
H,0,-3.6875968415,0.2340260522,-1.1222776762
H,0,-3.775295095,2.1726332336,0.2882944014
H,0,-5.5139472853,-0.6563203079,0.0708855217
H,0,-5.5093721268,-2.1335711554,1.9381302472
H,0,-6.2051216745,-0.7208926487,2.7556223097
H,0,-2.7045028782,2.4766842552,-0.9275921125
C,0,0.031123377,-0.796123992,-2.4032186057
C,0,0.2519928863,-0.7537796533,-3.7883558738
C,0,1.053965007,-1.2906118114,-1.5764929917
C,0,1.4524518508,-1.1921412289,-4.3345358229
H,0,-0.5309321695,-0.3718475933,-4.4385741194
C,0,2.2513353277,-1.7289350684,-2.1227256075
H,0,0.9157666745,-1.3320520767,-0.5003848046
C,0,2.4555170117,-1.6819777155,-3.5026695607
H,0,1.6047140681,-1.1514222635,-5.4087672591
H,0,3.0324811215,-2.1087167307,-1.4711230359
H,0,3.3949337466,-2.0257406534,-3.9251176357
H,0,-1.0384422496,-0.6897108011,0.1899633414
H,0,-1.9356792948,0.0519809708,-2.6516360879
C,0,-3.0616866686,-0.3993506044,2.1323338019
C,0,-1.7917490803,-0.0756399621,2.5972900056
C,0,-4.040396222,-0.9421203341,2.9710449645
C,0,-1.4932227499,-0.3782380095,3.9260374739
H,0,-1.0692699879,0.4392854988,1.9751942039
C,0,-3.7298983019,-1.2322669799,4.2903452837
C,0,-2.4439562468,-0.9601187382,4.7621982213
H,0,-0.5094785293,-0.1340592857,4.3149893088
H,0,-4.4820918444,-1.652616161,4.9516065382
H,0,-2.1911134845,-1.1792136727,5.7949997185

Int-2a cis, optimization in solv. CHCl₃

PBE1PBE/6-31G(d,p), E= -899.125246044 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.242470 a.u.

SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -899.4907419 a.u.SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -899.4982250 a.u.SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -900.0042866 a.u.

0; 1

C,0,-3.4850483481,-0.8967438564,-1.0393350226

C,0,-3.482499937,-1.9020976714,-2.0095631407

C,0,-2.3532755264,-2.1359627153,-2.7921409563

C,0,-1.2211252366,-1.3569480706,-2.5907590891

C,0,0.1177923658,-1.3892202771,-3.2602258365

C,0,-2.3610960838,-0.1046522575,-0.8281402543

C,0,-1.2438718209,-0.3619745925,-1.6150126249

N,0,0.0119770424,0.2950897047,-1.5908164802

C,0,0.7997162505,-0.1162361223,-2.7574868191

C,0,0.8559650395,1.0519433133,-3.8537213458

C,0,0.374958759,1.184918419,-0.705489725

C,0,1.6294920549,1.8427704272,-0.6499318213

C,0,1.9015804273,2.6566002175,0.4035776464

O,0,0.8211890847,2.2031330977,-3.3865842543

O,0,0.9869396252,0.6320673831,-5.0133095051

H,0,-4.3770803416,-0.7214173658,-0.4466340325

H,0,-4.3742348019,-2.5029257122,-2.1589408054

H,0,-2.3571298433,-2.9138210802,-3.5495964678

H,0,-2.3812844948,0.6866829485,-0.0861942481

H,0,1.8323750303,-0.2858438514,-2.4417127469

H,0,-0.3465483815,1.3910319225,0.0806828372

H,0,2.3248834689,1.7108605613,-1.4686186914

H,0,1.1342139394,2.7670644429,1.1699183315

C,0,3.1161319048,3.4113959739,0.636141293

C,0,3.2339693275,4.1342750459,1.8360142453

C,0,4.1804356755,3.4550122207,-0.2832429622

C,0,4.3778690349,4.8698463497,2.1153198014

C,0,5.3200217812,4.192787742,-0.0029947908

C,0,5.4241620208,4.9004564554,1.1961713174

H,0,2.4153507678,4.1113182417,2.5507657969

H,0,4.1112786078,2.9191482932,-1.2245306291

H,0,4.4533370335,5.4212858958,3.0474019839

H,0,6.1322525762,4.2219395688,-0.722759748

H,0,6.319069091,5.4773420275,1.4094025843

H,0,0.0645074103,-1.3449865517,-4.35125601

H,0,0.6717554969,-2.2927981281,-2.9804278299

Int-2a cis, optimization in solv. CHCl₃

M06-2X/6-311+G(d,p), E= -900.005483835 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.241294 a.u.

Thermal correction to Gibbs Free Energy at 20 °C = 0.242389 a.u.

0; 1

C,0,-4.2599191975,-2.3879528784,1.0908286831

C,0,-5.2420625242,-1.6468842451,0.4308058051

C,0,-4.8949166162,-0.6252255127,-0.4491892286

C,0,-3.5512795606,-0.3545013148,-0.6666975005

C,0,-2.8960085502,0.6597562754,-1.5624205807

C,0,-2.9099162501,-2.125072805,0.8862950737

C,0,-2.5915122044,-1.107268939,-0.0017932213

N,0,-1.2945299627,-0.6473104019,-0.3755792829

C,0,-1.4223294475,0.6177546178,-1.1296077606

C,0,-0.9962627362,1.8573582309,-0.2308963037

C,0,-0.1732952833,-1.1966399034,-0.0276918747

C,0,1.1212438716,-0.7145282309,-0.382728998

C,0,2.2060606609,-1.4330128044,-0.0196725318

O,0,-0.3483689189,1.5922550858,0.7908282748

O,0,-1.3479615254,2.9419310521,-0.7155560942

H,0,-4.5492883655,-3.1714359353,1.7798200438

H,0,-6.2870989012,-1.8660106854,0.6131033254

H,0,-5.6596441261,-0.0476158714,-0.9547978548

H,0,-2.1542495425,-2.6892646062,1.4178794303

H,0,-0.7423125009,0.5882898371,-1.9809799493

H,0,-0.2422970014,-2.1082658418,0.5585148961

H,0,1.2045356249,0.2278285703,-0.9054134113

H,0,2.0451474086,-2.3614027801,0.5250808663

C,0,3.5993610516,-1.0959813567,-0.27994674

C,0,4.5907130618,-1.9990642091,0.12664299

C,0,3.9847906275,0.0952466784,-0.9140000341

C,0,5.9337612847,-1.7266896851,-0.0989976598

C,0,5.3253013192,0.3658402494,-1.1366118053

C,0,6.3024746003,-0.5438857974,-0.7319254405

H,0,4.2996219065,-2.9177249643,0.6244551423

H,0,3.2401443456,0.8171820395,-1.2264591611

H,0,6.6900603757,-2.4328530732,0.2211133014

H,0,5.6133352168,1.2893208043,-1.6237573482

H,0,7.3493054712,-0.3264705247,-0.9076840879

H,0,-3.2920019705,1.6661102533,-1.4328033294

H,0,-3.0168651715,0.3761307419,-2.6107639635

Int-2a cis oxa, optimization in solv. CHCl₃

PBE1PBE/6-31G(d,p), E= -899.144540503 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.244626 a.u.

SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -899.4976326 a.u.SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -899.5064137 a.u.SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -900.0198336 a.u.

O; 1
C,0,-2.7592945427,-1.6778931254,-1.0781701046
C,0,-2.4917797781,-2.6476613693,-2.043071853
C,0,-1.4856405511,-2.4399879999,-2.9893263458
C,0,-0.7654478793,-1.2550349779,-2.9610349822
C,0,0.3721054466,-0.7811353881,-3.8238631918
C,0,-2.0342688883,-0.4867066729,-1.0339789822
C,0,-1.0445779784,-0.2886492509,-1.9906820131
N,0,-0.181257657,0.8277281664,-2.1047698934
C,0,0.5163301166,0.6849539336,-3.3911830078
C,0,-0.2222964785,1.6673838502,-4.2909693517
C,0,-0.7845524129,2.1481739887,-2.1157942601
C,0,0.0653563221,3.1881366092,-1.4680311679
C,0,-0.4060429391,3.9963903799,-0.5116563346
O,0,-0.1790588245,1.7459640195,-5.4913166987
O,0,-0.9663175813,2.4832464239,-3.5239271919
H,0,-3.5403071952,-1.8504469991,-0.3434114213
H,0,-3.065906771,-3.5689271862,-2.0579036539
H,0,-1.2761285171,-3.1934709817,-3.7437494654
H,0,-2.2357822419,0.2563158759,-0.2679941016
H,0,1.5632460918,1.0015850778,-3.3280134004
H,0,-1.7809617927,2.1196560383,-1.6682895038
H,0,1.0948485169,3.248551958,-1.815533472
H,0,-1.4508755724,3.8821955899,-0.2197516632
C,0,0.3226168844,5.042012184,0.2113947424
C,0,-0.3717453593,5.8164029924,1.1512559663
C,0,1.6863406851,5.3060401597,0.0096605355
C,0,0.2688376143,6.8236545008,1.8650966792
C,0,2.3262818149,6.3112100742,0.7218063572
C,0,1.6211748533,7.0749848569,1.6524592909
H,0,-1.4283695022,5.6231575993,1.3195273609
H,0,2.254153716,4.7196373656,-0.7066385448
H,0,-0.2890570747,7.4119585719,2.5877178873
H,0,3.3822678842,6.5006971372,0.5524863068
H,0,2.1255667407,7.8599493246,2.208137907
H,0,0.1786067819,-0.8533699591,-4.8986663653
H,0,1.2914822534,-1.3378924783,-3.6141097965

Int-2a cis syn, optimization in solv. CHCl₃

PBE1PBE/6-31G(d,p), E= -899.118103430 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.243450 a.u.

SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -899.4827712 a.u.SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -899.4903376 a.u.SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -899.9965853 a.u.

O; 1
C,0,-3.2964700945,-0.9438391519,-1.1189672784
C,0,-3.5210755187,-1.9209875838,-0.1466010556
C,0,-2.5095500057,-2.3004488309,0.7352510225
C,0,-1.2679640662,-1.6873884172,0.6365042622
C,0,-0.0104555172,-1.8704682484,1.4315569001
C,0,-2.0577061124,-0.3182241679,-1.2300287779
C,0,-1.0711995328,-0.7058524314,-0.3325619351
N,0,0.2565067362,-0.2065184435,-0.221866083
C,0,1.0370982597,-1.1590848338,0.5749611345
C,0,1.840785677,-2.1707043708,-0.368348541
C,0,0.6261068045,0.9543010983,-0.6973712221
C,0,1.8743862561,1.632629129,-0.5829157703
C,0,3.1079143174,1.0695289403,-0.480817508
O,0,2.2945712154,-1.6491451119,-1.4064586802
O,0,1.9471365244,-3.3181111504,0.0840414222
H,0,-4.0904468171,-0.6766804296,-1.8088352575
H,0,-4.4933336235,-2.4002221669,-0.086271035
H,0,-2.6870268263,-3.0677671142,1.4825620695
H,0,-1.8783311508,0.4178950433,-2.0069904779
H,0,1.7825609351,-0.5995953474,1.1499617311
H,0,-0.1816135385,1.5143990553,-1.1616985976
H,0,1.7743049514,2.712214492,-0.6676499789
H,0,3.169198666,-0.0121827635,-0.6101237856
C,0,4.361475745,1.7850440389,-0.340270875
C,0,5.5538801205,1.0521663894,-0.4727915183
C,0,4.4440831306,3.1638529943,-0.0721911966
C,0,6.789103884,1.6761423196,-0.3567511874
C,0,5.6781743642,3.7838873171,0.0458546424
C,0,6.8535721162,3.043377687,-0.0986377159
H,0,5.4973451421,-0.0138541383,-0.6753604797
H,0,3.5388821974,3.7493493119,0.0576010463
H,0,7.7008777569,1.0972007432,-0.4659467349
H,0,5.7299031584,4.8479130355,0.2556410889
H,0,7.817715081,3.5342315879,-0.004701924
H,0,0.2887272399,-2.9152424103,1.540763207
H,0,-0.1092674761,-1.4188930709,2.4261030891

Int-2a trans, optimization in solv. CHCl₃

PBE1PBE/6-31G(d,p), E= -899.121726716 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.242186 a.u.

SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -899.4859955 a.u.SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -899.4934329 a.u.SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -899.9982094 a.u.

O; 1
C,0,-3.1540130563,-1.8785000064,-0.5238606609
C,0,-2.5898300392,-3.0186431296,-1.0960277405
C,0,-1.4203813788,-2.9242256605,-1.8475767184
C,0,-0.8363024973,-1.6799898531,-2.0394833037
C,0,0.4472926724,-1.3279300881,-2.7233616999
C,0,-2.5847809841,-0.6222503123,-0.7123313694
C,0,-1.4405608233,-0.5374835966,-1.5043696272
N,0,-0.6577148254,0.5946531959,-1.8348640456
C,0,0.4575566458,0.1962888072,-2.7066730483
C,0,0.2577956626,0.852039694,-4.1462283971
C,0,-0.8925133455,1.8812091671,-1.6924309832
C,0,-2.0869564104,2.5059507572,-1.2401059558
C,0,-2.080476766,3.8427025678,-1.0001451305
O,0,-0.3669165369,1.9318573322,-4.1493895079
O,0,0.8006563852,0.2181559981,-5.0629566218
H,0,-4.0471176274,-1.9655831574,0.0867474364
H,0,-3.054095697,-3.9869912827,-0.9373172211
H,0,-0.9605011316,-3.8132429576,-2.2687514098
H,0,-3.0172269409,0.2378510489,-0.2196426718
H,0,1.388061793,0.6160709014,-2.3126275427
H,0,-0.0517742911,2.5195122691,-1.9331335763
H,0,-3.0004826144,1.9313518984,-1.1614984307
H,0,-1.1339434679,4.3687809738,-1.1223974508
C,0,-3.1978226266,4.6717502819,-0.5945263456
C,0,-2.9688415372,6.0437185842,-0.3928264747
C,0,-4.497089071,4.1696855919,-0.3956630333
C,0,-4.0002377414,6.8885877005,-0.0048166384
C,0,-5.5249667331,5.015126472,-0.0089587123
C,0,-5.2806488755,6.3758312888,0.1882490108
H,0,-1.9693204766,6.4420278846,-0.545902131
H,0,-4.7056840371,3.1153684931,-0.5479331874
H,0,-3.8066336175,7.946030519,0.1457481949
H,0,-6.5237341381,4.6162428705,0.1392261749
H,0,-6.0900737148,7.0333986594,0.4907427189
H,0,0.5029689962,-1.6629443501,-3.763517009
H,0,1.2999122232,-1.7597915214,-2.1881892209

Int-2a trans oxa, optimization in solv. CHCl₃

PBE1PBE/6-31G(d,p), E= -899.142244156 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.245425 a.u.

SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -899.4952771 a.u.SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -899.5041564 a.u.SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -900.0184153 a.u.

O; 1
C,0,-2.7272944732,2.7496377242,0.6398815037
C,0,-3.5512189732,1.8113913169,1.2590396081
C,0,-3.2349373682,0.4536625609,1.1922362438
C,0,-2.1120837321,0.0532119629,0.4831033421
C,0,-1.5130037288,-1.3169513932,0.3259845521
C,0,-1.5887533778,2.3593420327,-0.0651499742
C,0,-1.3060637678,0.9981598826,-0.1623275071
N,0,-0.1814154259,0.3845768548,-0.7694832361
C,0,-0.4075683104,-1.0686549553,-0.7055591095
C,0,-0.81517659,-1.4199846784,-2.1298421985
C,0,0.188317829,0.64032712,-2.1531729931
C,0,-0.1846782829,1.9571266905,-2.730429309
C,0,0.7355373776,2.8385293353,-3.1408821754
O,0,-1.3501912186,-2.4262105234,-2.5188101896
O,0,-0.4790987492,-0.4008919445,-2.9361427878
H,0,-2.9653835282,3.8069826503,0.712521231
H,0,-4.430949166,2.1375432569,1.8052512352
H,0,-3.8604374558,-0.2829347157,1.6893308115
H,0,-0.9406099742,3.1000008706,-0.519756606
H,0,0.5191560202,-1.6084833571,-0.4770272706
H,0,1.2641419526,0.4598145764,-2.2624745322
H,0,-1.2505893671,2.1459263258,-2.8247783236
H,0,1.7861227338,2.5632892414,-3.0429655019
C,0,0.4923160097,4.161526056,-3.7201189164
C,0,-0.783276695,4.7440742592,-3.7828351131
C,0,1.5801437856,4.8837465738,-4.2304608619
C,0,-0.9604621859,5.9999220902,-4.3474028784
C,0,1.402553756,6.1413727022,-4.7970579217
C,0,0.1305643145,6.7034004141,-4.8585075535
H,0,-1.6428660403,4.2166041613,-3.3799192985
H,0,2.5749767959,4.4477225578,-4.1832586026
H,0,-1.9543391391,6.4361067065,-4.3863538647
H,0,2.2584709879,6.6828163151,-5.1890295549
H,0,-0.0120765392,7.6862206658,-5.2978775128
H,0,-1.0910563087,-1.6737390572,1.2713384502
H,0,-2.215444341,-2.0768286654,-0.0308630364

Int-2a *trans* syn, optimization in solv. CHCl₃
 PBE1PBE/6-31G(d,p), E= -899.111693201 a.u.
 Thermal correction to Gibbs Free Energy at 25 °C = 0.242887 a.u.
 SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -899.4767294 a.u.
 SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -899.4841248 a.u.
 SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -899.990679 a.u.
 0; 1
 C,0,2.1412975736,-3.422581573,-1.0219993802
 C,0,1.4282652847,-4.3143114091,-0.217380898
 C,0,0.3335026647,-3.8770792301,0.5226902974
 C,0,-0.0545527566,-2.5459513021,0.4341609439
 C,0,-1.1332237543,-1.8164268954,1.1690431466
 C,0,1.762252968,-2.0890143311,-1.1270394841
 C,0,0.644330755,-1.6753572542,-0.4053423715
 N,0,0.0912786397,-0.3698238126,-0.271947688
 C,0,-0.8116175123,-0.3526583021,0.8931926178
 C,0,-0.1306000704,0.4120003771,2.1225860847
 C,0,0.3792968214,0.7631540419,-0.8568947297
 C,0,1.1216260997,1.0264485538,-2.0556484576
 C,0,1.1209253896,0.248448121,-3.1638701599
 O,0,0.6025803381,1.3646640491,1.7962026784
 O,0,-0.4832087337,-0.0116227916,3.2325224256
 H,0,3.0102506977,-3.7684640337,-1.5726645851
 H,0,1.7414844022,-5.3519970003,-0.157167577
 H,0,-0.2033553854,-4.5598031313,1.1742168112
 H,0,2.3393435152,-1.4052521539,-1.7351948515
 H,0,-1.6958717832,0.2323067405,0.6303878883
 H,0,-0.0400224304,1.6200465974,-0.3385680445
 H,0,1.5549566126,2.0225076323,-2.0882295101
 H,0,0.5772876632,-0.6941653334,-3.1308946918
 C,0,1.7329262107,0.5553970605,-4.4454771662
 C,0,1.4923773167,-0.3165354734,-5.5205645204
 C,0,2.5593595348,1.6732774235,-4.6579055286
 C,0,2.0507051234,-0.0789000999,-6.7700196435
 C,0,3.1176204043,1.9067824428,-5.905211824
 C,0,2.8643310389,1.0340746743,-6.9654799066
 H,0,0.8577424894,-1.1855086884,-5.3669938276
 H,0,2.7746534717,2.3575279833,-3.8430446493
 H,0,1.852524773,-0.7618928255,-7.5902340769
 H,0,3.7563191646,2.7717794557,-6.0552522522
 H,0,3.3042221057,1.2226237865,-7.9401509774
 H,0,-1.1078208688,-1.9835459998,2.2492922418
 H,0,-2.1262517632,-2.096235299,0.7986556658

TS-Int-2a rot-C3-C4 *cis*, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -899.106653054 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.241811 a.u.
1 imaginary frequency = 186.6564 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -899.4725154 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -899.4800262 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -899.9885424 a.u.
0; 1
C,0,-3.6584680573,-0.77748608,-1.372621573
C,0,-3.3401759571,-1.9882789346,-1.9944610276
C,0,-2.0424749227,-2.2536233629,-2.4254424182
C,0,-1.058671046,-1.2918624398,-2.2283144014
C,0,0.4016788101,-1.3053770075,-2.5627421364
C,0,-2.6866278684,0.1960911107,-1.1687094288
C,0,-1.4011263403,-0.091800636,-1.6102293153
N,0,-0.2398731426,0.7255739185,-1.5143534678
C,0,0.8250711337,0.1413304784,-2.3277689233
C,0,0.9571495381,0.9950684792,-3.6879295383
C,0,-0.1715372994,1.8988817167,-0.9773950447
C,0,1.0695844852,2.6679017858,-0.8331190371
C,0,1.8775557691,2.5079321534,0.2247697492
O,0,0.5569493723,2.1686162969,-3.6125037165
O,0,1.4924120215,0.3514007921,-4.6002987217
H,0,-4.6764170666,-0.5892635126,-1.0473919505
H,0,-4.117870809,-2.730651508,-2.1447798403
H,0,-1.8018857808,-3.1953159448,-2.9090127342
H,0,-2.9419824495,1.1361579428,-0.6911530722
H,0,1.7790975378,0.2544762393,-1.8106988709
H,0,-1.0978329836,2.2947584666,-0.5641665825
H,0,1.2647412429,3.3822489856,-1.6279708538
H,0,1.6035749534,1.7741009858,0.9826656388
C,0,3.1216270608,3.2360865178,0.487824333
C,0,3.7615294017,3.0439265843,1.7199524526
C,0,3.7015881378,4.1170616112,-0.4376658951
C,0,4.9382714196,3.7185927502,2.0273292527
C,0,4.8764358378,4.7896446097,-0.130749459
C,0,5.4987493857,4.5952260789,1.1028295681
H,0,3.3257369669,2.3596094084,2.4437664265
H,0,3.2395493945,4.2703514175,-1.4083402789
H,0,5.4177072875,3.5579580863,2.9884262308
H,0,5.3136924738,5.4658818867,-0.8593432611
H,0,6.4188694066,5.1220109598,1.337702078
H,0,0.611409071,-1.5665040151,-3.603316309
H,0,0.941906016,-2.0089778213,-1.9189208727

TS-Int-2a rot-C3-C4 *trans*, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -899.106657646 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.241946 a.u.
1 imaginary frequency = 150.4714 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -899.4716156 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -899.4790764 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -899.9865573 a.u.
0; 1
C,0,3.4240716572,-2.1442347119,-0.4040998835
C,0,3.2520421645,-2.976525068,0.7038022435
C,0,2.1432265625,-2.8341634356,1.5341417799
C,0,1.2032244096,-1.8538478557,1.2425639923
C,0,-0.0583755621,-1.4953713052,1.9629733507
C,0,2.4952737887,-1.1550231033,-0.71018401
C,0,1.3913582615,-1.0312287179,0.1300739498
N,0,0.3125156541,-0.1040883627,0.0613438103
C,0,-0.4963576795,-0.2043936942,1.2848962325
C,0,-0.2634088568,1.1122744582,2.1660245288
C,0,0.0890510639,0.8735259398,-0.7591280973
C,0,0.9085000966,1.239832207,-1.916420398
C,0,0.7369473796,0.6993254607,-3.1315178125
O,0,-0.0153270726,2.1417851832,1.5091787698
O,0,-0.4213773756,0.9278150803,3.3804124551
H,0,4.2958494701,-2.2643528715,-1.0391976226
H,0,3.992696062,-3.740024797,0.9210563742
H,0,2.0132026343,-3.4764480479,2.3997359039
H,0,2.6356840192,-0.5131787721,-1.5690906791
H,0,-1.5532432916,-0.1981319023,1.0080964795
H,0,-0.7953327834,1.4597503261,-0.5309769299
H,0,1.6147940171,2.0503053975,-1.73675136
H,0,-0.0082804267,-0.0877129616,-3.2423565765
C,0,1.4638655318,1.0401719983,-4.3560652562
C,0,1.1593048965,0.3342045889,-5.5283469504
C,0,2.453555834,2.0338536887,-4.411183054
C,0,1.8208634821,0.6082375727,-6.7204439317
C,0,3.1135317447,2.3070083644,-5.6012174648
C,0,2.8007554213,1.595774037,-6.7602910286
H,0,0.3948824706,-0.4382618002,-5.4999276648
H,0,2.710654524,2.6010404548,-3.5214209
H,0,1.5704505504,0.0500503789,-7.6175631517
H,0,3.8762237471,3.0795651359,-5.6270978013
H,0,3.319804429,1.8132009795,-7.6889776688
H,0,0.0911823048,-1.2959747113,3.0280847665
H,0,-0.8054777609,-2.2909927122,1.8681484558

TS-1b up-syn-syn, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -710.236213209 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.252354 a.u.
1 imaginary frequency = 175.7515 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -710.5251468 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -710.5323305 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -710.9210384 a.u.

O; 1
C,0,-1.2355361246,0.0346009993,1.0407667681
C,0,-2.0389103599,-0.2749832558,0.0184256137
C,0,-0.0339941989,-0.7830977835,1.3619167077
N,0,1.3812283833,0.3442588887,0.8809510356
C,0,1.702499199,0.1153823898,-0.5601535079
C,0,2.1018645998,1.4788964608,-1.1354685505
C,0,2.7799455056,-0.9718020988,-0.6769905818
O,0,2.5257168843,-2.0655722681,0.0064388828
O,0,3.7877188315,-0.816916798,-1.3367511427
H,0,-1.4622174518,0.8761141896,1.6941589179
H,0,-1.7747162013,-1.1557509727,-0.5685563907
H,0,2.136438589,-0.0282878287,1.4547688183
H,0,1.5382919166,-2.0647468306,0.3651345759
H,0,0.7911229528,-0.2850249919,-1.023395201
H,0,1.2941796615,1.8748909839,-1.7574592486
H,0,2.9951505109,1.3728207188,-1.7535185486
C,0,2.318301947,2.3678198781,0.0924758437
H,0,2.1605914636,3.4297769886,-0.1107669
H,0,3.3339061401,2.2443368461,0.4849645069
C,0,1.3049908544,1.8079551027,1.0815768154
H,0,1.4928174902,2.0506258453,2.1294295866
H,0,0.292184425,2.1277369706,0.8187567474
C,0,-3.2867832078,0.4510558149,-0.3602228814
C,0,-4.5286566973,-0.4461568117,-0.3107155234
H,0,-3.178485207,0.8348064948,-1.385570388
H,0,-3.4311499218,1.3235588441,0.28901924
C,0,-5.7922575057,0.28127948,-0.7501614332
H,0,-4.6519203141,-0.8283587937,0.7099322279
H,0,-4.363694277,-1.3238159389,-0.9484880983
H,0,-6.6661585338,-0.3753047471,-0.7020357221
H,0,-5.9919382889,1.148914702,-0.1117907796
H,0,-5.7022587797,0.6424144327,-1.7805966869
H,0,0.2285740941,-0.7546965919,2.4357682984
O,0,0.172289621,-1.8609743196,0.7051639981

TS-1b up-syn-syn, optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -710.921766008 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.250775 a.u.
1 imaginary frequency = 189.8183 i cm⁻¹

O; 1
C,0,-1.2191629604,-0.0424338689,1.0167984732
C,0,-1.9370767678,-0.4331285731,-0.0358229445
C,0,-0.0419069916,-0.82374268,1.4935597968
N,0,1.3922160612,0.3345447179,0.9280430853
C,0,1.6014264866,0.1100222205,-0.5353224703
C,0,1.8824098141,1.4894361242,-1.1458213374
C,0,2.7137694939,-0.9245059525,-0.7420482574
O,0,2.5277018215,-2.0651785015,-0.1061138413
O,0,3.6859316014,-0.7128725974,-1.4227386307
H,0,-1.4872023367,0.8496248006,1.5770693205
H,0,-1.6411386694,-1.3570989022,-0.5319276762
H,0,2.1698352862,-0.0580189761,1.4572643497
H,0,1.6158021373,-2.0997217396,0.3519889286
H,0,0.6798962533,-0.331764998,-0.9311367439
H,0,0.9721693594,1.8737271332,-1.6102186562
H,0,2.6630732528,1.4258202273,-1.9013983912
C,0,2.2664750622,2.3586299004,0.0565392911
H,0,2.1097485737,3.4229983076,-0.1164198918
H,0,3.3143191656,2.1992552499,0.3250187937
C,0,1.3563787238,1.8013294293,1.1470237128
H,0,1.6601008019,2.0293271202,2.1676796783
H,0,0.3297810504,2.1407383186,0.9929895561
C,0,-3.1472409616,0.2677735254,-0.5666098627
C,0,-4.3935822764,-0.6262001169,-0.5317578683
H,0,-2.9593795354,0.5602333342,-1.6072488257
H,0,-3.3309739629,1.1865425716,-0.0008224667
C,0,-5.6117522332,0.0681175742,-1.1337722509
H,0,-4.5975965845,-0.9114122038,0.5047116614
H,0,-4.1847636764,-1.5523975048,-1.0763807048
H,0,-6.4924909344,-0.5758356944,-1.1012067173
H,0,-5.8459660365,0.9861740158,-0.5885896378
H,0,-5.4289045865,0.3363146219,-2.1776636257
H,0,0.1878074843,-0.6727341972,2.558904857
O,0,0.2410317343,-1.9354839962,0.9565487962

TS-1b down-syn-syn, optimization in solv. CHCl₃
PBE1PBE/6-311G(d,p), E = -710.235083934 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.252051 a.u.
1 imaginary frequency = 159.9594 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -710.523849 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -710.5309110 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -710.9192233 a.u.
0; 1
C,0,1.4088121654,0.5496415435,-0.9438013074
C,0,2.4562084062,0.2042671883,-0.1900190224
H,0,-0.3201695322,-0.2294066254,-2.016754691
C,0,0.2037381496,-0.3117998684,-1.0471719553
N,0,-1.1041252648,0.8463220994,-0.204893591
C,0,-2.2475909363,0.1080679628,0.3877984636
C,0,-3.1926148868,1.229677131,0.8067959121
C,0,-2.9157278799,-0.8530092128,-0.6249154548
O,0,-2.1912507045,-1.8585118161,-1.0542175183
O,0,-4.0740190126,-0.6939780762,-0.9601137053
O,0,0.1402076036,-1.4076051863,-0.4102033389
H,0,-0.5606378056,1.2316530564,0.565496238
H,0,-1.1930800868,-1.7986770592,-0.7298703396
H,0,-1.8742938153,-0.4925329145,1.2221743354
H,0,-2.8541217688,1.6465238904,1.7608961416
H,0,-4.2143339841,0.8680941523,0.9257671705
H,0,1.4150993318,1.46601003,-1.5331928154
H,0,2.3876744426,-0.7386097917,0.3542277847
C,0,-3.0581954461,2.2653262085,-0.3246568255
H,0,-3.0929505255,3.2887876123,0.0556942098
H,0,-3.8675374103,2.1476996093,-1.0478384134
C,0,-1.6998378176,1.947532253,-0.9897780095
H,0,-1.0082957875,2.7916585763,-1.0118345282
H,0,-1.8311980726,1.5939721479,-2.0178491333
C,0,3.7246084862,0.9788273003,-0.0548527804
C,0,4.9542411909,0.178513619,-0.4989576441
H,0,3.8587758943,1.2611119032,1.000087046
H,0,3.6619972589,1.9134585881,-0.6259375779
C,0,6.2533484932,0.9490930042,-0.3059967833
H,0,4.836555053,-0.1000107138,-1.5532122333
H,0,4.9928722188,-0.7627147045,0.0640338795
H,0,7.1163958779,0.3615033619,-0.6330556511
H,0,6.249206548,1.8823583387,-0.8797260901
H,0,6.4060772269,1.208949992,0.7473035686

TS-1b down-syn-syn, optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -710.919678045 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.250484 a.u.
1 imaginary frequency = 153.3650 i cm⁻¹
0; 1
C,0,1.4365008961,0.4480154681,-0.7961787591
C,0,2.4568146205,0.076706641,-0.0252343362
H,0,-0.2638111028,-0.2994357882,-1.9425605188
C,0,0.2306830202,-0.4065454167,-0.9640148485
N,0,-1.1127684054,0.8117206916,-0.1491357242
C,0,-2.3037826031,0.0963387311,0.3728763983
C,0,-3.2388139057,1.2344424214,0.7798680765
C,0,-2.9369493325,-0.7937518265,-0.7217203405
O,0,-2.2464305659,-1.8482599025,-1.0985758922
O,0,-4.0275939456,-0.5461932976,-1.1775191918
O,0,0.1009206683,-1.4889506272,-0.3365123043
H,0,-0.5958637156,1.1688936699,0.6530712575
H,0,-1.2872805656,-1.850670343,-0.7194244348
H,0,-1.9963718103,-0.5475364617,1.1983368234
H,0,-2.9234330445,1.6124273121,1.7546554489
H,0,-4.2741036906,0.9072452446,0.8487924203
H,0,1.4600788168,1.3765402807,-1.3620371536
H,0,2.3758823514,-0.876959261,0.4946338098
C,0,-3.0205042187,2.2980026332,-0.3177937481
H,0,-3.0218564921,3.3062040475,0.0949592704
H,0,-3.8047412625,2.2364016406,-1.0708701026
C,0,-1.649394353,1.9403919818,-0.9442614981
H,0,-0.9337312363,2.7610910836,-0.9382456989
H,0,-1.7646465937,1.5938748523,-1.9746767571
C,0,3.7278539005,0.8450708316,0.1522009862
C,0,4.9526155335,0.0429746967,-0.3068215576
H,0,3.8517838416,1.0902905241,1.2141843682
H,0,3.6757481676,1.7912708746,-0.3953739591
C,0,6.2535763507,0.8092979091,-0.0863401835
H,0,4.8379305211,-0.2055490446,-1.3661426486
H,0,4.9823854386,-0.9066384678,0.2367046977
H,0,7.1170029993,0.2275329553,-0.4142972943
H,0,6.2504878467,1.7498836296,-0.6431215348
H,0,6.3901322611,1.047078846,0.9718155694

TS-1b *up-anti-syn*, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -710.235429757 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.251613 a.u.
1 imaginary frequency = 184.7212 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -710.5252035 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -710.5322824 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -710.9202181 a.u.
0; 1
C,0,-1.2475631163,-0.5333279069,-0.1908499133
C,0,-2.3354083126,-0.0806116685,0.4399342733
C,0,-0.092418054,-1.1359380181,0.5206904693
N,0,1.1613395088,0.2291571529,0.6470974684
C,0,2.0583189064,0.1985862499,-0.5494329398
C,0,2.3910335433,1.6585695359,-0.875012859
C,0,3.2700941235,-0.6950720385,-0.2504720798
O,0,2.9623588821,-1.8762579499,0.2361624709
O,0,4.4112444295,-0.3245084932,-0.4395695017
H,0,-1.1919462631,-0.5407978786,-1.2790992505
H,0,-2.3577724112,-0.1246988982,1.5317667798
H,0,1.6913672015,-0.0706367027,1.4641031073
H,0,1.9240572984,-2.0595894446,0.1634068563
H,0,1.4994790039,-0.2972438137,-1.3523370734
H,0,1.842741737,1.979387479,-1.765117381
H,0,3.4598991234,1.7585785048,-1.072381036
C,0,1.9280507342,2.4465775423,0.354430232
H,0,1.659647998,3.4808895151,0.1263698927
H,0,2.7117981749,2.4612386576,1.1199843762
C,0,0.7377785328,1.6310775388,0.8426382874
H,0,0.4626417421,1.7931025818,1.8868494627
H,0,-0.1465609734,1.7995274302,0.2202428641
C,0,-3.5656328382,0.4504764309,-0.2204124694
C,0,-4.8126854882,-0.3813834888,0.0994149265
H,0,-3.4174716398,0.4966104582,-1.3061643098
H,0,-3.7392404438,1.4819494723,0.1199530221
C,0,-6.0734152761,0.1916522284,-0.5339467556
H,0,-4.9375629206,-0.4402450888,1.1883616251
H,0,-4.653029772,-1.4096711715,-0.2467693079
H,0,-6.9505055026,-0.4169947926,-0.2946192053
H,0,-6.2661518736,1.2101004769,-0.1791061281
H,0,-5.9840622961,0.232509408,-1.6249655029
O,0,0.5306183153,-2.08796754,-0.0703768315
H,0,-0.2505320737,-1.1895437684,1.6148694311

TS-1b *up-anti-syn*, optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -710.921073559 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.251067 a.u.
1 imaginary frequency = 207.6457 i cm⁻¹
0; 1
C,0,-1.1861718081,-0.6920435203,-0.0889615112
C,0,-2.254697208,-0.1008866574,0.4445142176
C,0,-0.0932723811,-1.2605809259,0.7420880286
N,0,1.1797960757,0.1771499422,0.7695694613
C,0,1.8828871229,0.2114674967,-0.5512952266
C,0,2.0456757871,1.6940518781,-0.9123383513
C,0,3.1928414577,-0.5789229069,-0.452046925
O,0,3.0569710849,-1.8099719864,0.0036387536
O,0,4.2626392177,-0.1154734893,-0.7561983329
H,0,-1.097125494,-0.8360956845,-1.1637048917
H,0,-2.3119266137,-0.0130348716,1.5309312855
H,0,1.8146794409,-0.1577011209,1.4929405965
H,0,2.0785000305,-2.0649718078,0.1365758212
H,0,1.2564725804,-0.3208438689,-1.2741684589
H,0,1.2773659347,1.9804342251,-1.6327550375
H,0,3.023839696,1.8786918637,-1.352545117
C,0,1.825867326,2.4306676185,0.414099274
H,0,1.4973947878,3.4609352231,0.2801004431
H,0,2.7437309182,2.4339275135,1.0080290748
C,0,0.7683267938,1.5624780753,1.0902253709
H,0,0.6938007132,1.6838985563,2.170270568
H,0,-0.2157534583,1.7281766144,0.6438770423
C,0,-3.4237663745,0.4292151776,-0.3250097452
C,0,-4.7286079035,-0.2923262923,0.0353334301
H,0,-3.233358469,0.3386886154,-1.3986527673
H,0,-3.5431591677,1.4972440242,-0.1051446981
C,0,-5.9244780224,0.2805642109,-0.7197288528
H,0,-4.8966320779,-0.2143584098,1.1143268614
H,0,-4.6175623827,-1.3573532671,-0.1887356827
H,0,-6.8446271912,-0.2478784818,-0.4642501666
H,0,-6.0652729336,1.3380596942,-0.4815461368
H,0,-5.7776810894,0.1977042175,-1.7997001074
O,0,0.577000998,-2.2383471988,0.2911555979
H,0,-0.2831853905,-1.1870634568,1.8247471821

TS-1b down-anti-syn, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -710.234811564 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.251599 a.u.
1 imaginary frequency = 189.2518 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -710.5244958 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -710.5315274 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -710.9199884 a.u.
0; 1
C,0,-1.3934229495,-0.4692708423,-0.3333887106
C,0,-2.2212334313,0.0287113013,0.5900382548
H,0,0.1917058931,-0.9540569982,1.0733035975
C,0,-0.039086243,-0.9737331503,-0.008160496
N,0,1.0376513963,0.5719348302,-0.3360843965
C,0,2.4522922859,0.2694683686,-0.6730668973
C,0,3.102804807,1.6490634328,-0.6678829317
C,0,3.1099326724,-0.6793733042,0.3587242285
O,0,2.613508917,-1.8880556547,0.4478995468
O,0,4.0690265857,-0.3128066563,1.0118395159
O,0,0.4686921648,-1.8896219094,-0.7326985406
H,0,0.6079743626,0.9666750562,-1.1712272317
H,0,1.7292920649,-2.0036550202,-0.1276299596
H,0,2.4758009735,-0.2283594051,-1.6466641251
H,0,2.9015137719,2.1462039925,-1.6223759968
H,0,4.182280501,1.5787202512,-0.5315709274
H,0,-1.6995092429,-0.5671198891,-1.3744870354
H,0,-1.8747916145,0.0787242469,1.625211996
C,0,2.4044737733,2.3830375901,0.4927140019
H,0,2.2184961214,3.4327526554,0.2540575375
H,0,3.0204366795,2.347907652,1.3934703069
C,0,1.0885026448,1.6057453966,0.7182183795
H,0,0.1887403046,2.2204158918,0.6641996028
H,0,1.0879575515,1.0945523713,1.6867251508
C,0,-3.615528373,0.5023428425,0.3409215023
C,0,-4.6576545205,-0.2703210572,1.1568292969
H,0,-3.8499835637,0.4303362547,-0.7280497777
H,0,-3.68404392,1.5671116888,0.609160003
C,0,-6.0725219754,0.2465955001,0.933931783
H,0,-4.4018483224,-0.2052590131,2.222266598
H,0,-4.6009381284,-1.3331107758,0.8921815846
H,0,-6.7995926158,-0.3194993045,1.5237243841
H,0,-6.158385061,1.3006679502,1.2201885055
H,0,-6.3621314898,0.1648911569,-0.1193516217

TS-1b down-anti-syn, optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -710.920383216 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.251413 a.u.
1 imaginary frequency = 189.3245 i cm⁻¹
0; 1
C,0,-1.4053992037,-0.5072106909,-0.3517652824
C,0,-2.2040444719,0.0164226131,0.5772774553
H,0,0.1785646757,-1.0084668486,1.0551879355
C,0,-0.0598178707,-1.035842094,-0.0208066674
N,0,1.030331657,0.5550312917,-0.3438530026
C,0,2.4499780319,0.2750373345,-0.6764879339
C,0,3.0834439748,1.6656334076,-0.673496444
C,0,3.0937489574,-0.6476757267,0.3855604288
O,0,2.6350456072,-1.8762470301,0.4531709962
O,0,3.9962346897,-0.2566047484,1.0874741612
O,0,0.4651611641,-1.9312846982,-0.7411256003
H,0,0.5952164241,0.9527349216,-1.175348298
H,0,1.782135921,-2.0211319756,-0.1251896327
H,0,2.4950970782,-0.2360609063,-1.6394770449
H,0,2.867323238,2.151357971,-1.6273475707
H,0,4.1621696938,1.6209579897,-0.5411532513
H,0,-1.7180565185,-0.6035212,-1.3888555214
H,0,-1.842217792,0.0649827882,1.6056222972
C,0,2.3678987649,2.3932606719,0.4865815815
H,0,2.1450186926,3.4287923452,0.231387316
H,0,2.9862414333,2.3896456072,1.3831669704
C,0,1.0744377403,1.5758075648,0.7272706125
H,0,0.1606252295,2.1672597393,0.7034274244
H,0,1.1147280917,1.0470301184,1.6835904972
C,0,-3.5932543003,0.5188350221,0.3397758116
C,0,-4.6352763996,-0.2633005331,1.1495364205
H,0,-3.831893558,0.4635745025,-0.7266178207
H,0,-3.6458275488,1.575220656,0.6306580671
C,0,-6.0452910243,0.2823141681,0.942853446
H,0,-4.3712029795,-0.2212032267,2.211160861
H,0,-4.5934616269,-1.3168628101,0.8574201597
H,0,-6.7783753346,-0.2858172073,1.5181723377
H,0,-6.1073018176,1.3278504177,1.2559749689
H,0,-6.3315666187,0.2310955652,-0.1108166784

TS-1b *up-syn-anti*, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -710.236887922 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.251727 a.u.
1 imaginary frequency = 133.9396 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -710.5261254 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -710.5332107 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -710.9206645 a.u.
0; 1
C,0,1.3138252517,0.7705418266,0.4803542237
C,0,2.233082136,-0.1521967903,0.1853266468
C,0,0.1341327003,0.4631723918,1.3380522446
N,0,-1.2494128945,0.7963790944,0.0538568159
C,0,-2.3714155947,-0.1534370048,0.2839227828
C,0,-3.6579679251,0.5792224131,-0.1277270277
C,0,-2.0978469235,-1.4703470551,-0.4531352718
O,0,-0.962400725,-2.0540854597,-0.1310603395
O,0,-2.8642030813,-1.9284842111,-1.2752559823
H,0,1.4132256352,1.7961021979,0.1237008758
H,0,2.0909994318,-1.1514258626,0.5994723181
O,0,-0.0710624934,-0.7110865332,1.7787539742
H,0,-0.1689185666,1.3092379551,1.9829065711
H,0,-0.8025377483,0.6045014625,-0.8418795298
H,0,-0.5060944686,-1.5733219139,0.6632204218
H,0,-2.3528186592,-0.3871989906,1.3561137162
H,0,-4.311998707,0.7011686395,0.7394095
H,0,-4.1927329844,-0.0069702499,-0.8776336398
C,0,-3.1911648153,1.9414893265,-0.6623264643
H,0,-3.894952185,2.7495117741,-0.4487308939
H,0,-3.0466583858,1.9013193877,-1.7473465426
C,0,-1.8469427773,2.143799972,0.0265843321
H,0,-1.1741141819,2.843330856,-0.4741928164
H,0,-1.9790521856,2.469737731,1.0647927983
C,0,3.4565560901,0.0723738387,-0.6400695942
C,0,4.7507320421,-0.2290456335,0.1231295831
H,0,3.4762315466,1.1034331686,-1.0147247191
H,0,3.4143206556,-0.5830929903,-1.5226695256
C,0,5.9927365905,-0.0444538138,-0.7384140609
H,0,4.7121787627,-1.25739443,0.5044600455
H,0,4.8057384844,0.4223430646,1.0039715763
H,0,6.9045756592,-0.2614706977,-0.1739578982
H,0,5.9726153265,-0.7096692204,-1.608703201
H,0,6.0675869899,0.9835367569,-1.109778919

TS-1b *up-syn-anti*, optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -710.921087789 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.250847 a.u.
1 imaginary frequency = 153.4982 i cm⁻¹
0; 1
C,0,1.3266278096,0.740566388,0.5220414146
C,0,2.2361068338,-0.1735348907,0.1894005628
C,0,0.1548848757,0.4111698468,1.3869538003
N,0,-1.2406328919,0.7584916845,0.0533300478
C,0,-2.3949521099,-0.1505466254,0.3001415615
C,0,-3.6634193559,0.6252687192,-0.1033173479
C,0,-2.1607628329,-1.4714907104,-0.4409362019
O,0,-1.0450087043,-2.0971029287,-0.1153402078
O,0,-2.9218335233,-1.9002032343,-1.2715381036
H,0,1.4154677707,1.7723916678,0.1879204607
H,0,2.1054593037,-1.1841427332,0.5745343751
O,0,-0.0496157416,-0.7639840842,1.7945760853
H,0,-0.1838754558,1.245173011,2.0215471811
H,0,-0.7944349003,0.5322775369,-0.8355013629
H,0,-0.5646555328,-1.6432976634,0.6616383524
H,0,-2.386663237,-0.3828014876,1.3698729354
H,0,-4.2660717625,0.8270546103,0.7827914112
H,0,-4.2630633522,0.0440325397,-0.8016240264
C,0,-3.1434772767,1.9373500557,-0.7139971171
H,0,-3.8197599328,2.7766772676,-0.5544578981
H,0,-2.9841610055,1.8242739043,-1.7893321269
C,0,-1.7988298693,2.1248163359,-0.015783019
H,0,-1.1025075441,2.7870173815,-0.5293004665
H,0,-1.93585371,2.4804035131,1.0100353111
C,0,3.4516446836,0.0851440663,-0.643851373
C,0,4.748551136,-0.2174699835,0.117144729
H,0,3.4562864916,1.1241286649,-0.9883978371
H,0,3.4150473271,-0.5517453195,-1.5361185138
C,0,5.9856370213,0.0197991503,-0.7439919458
H,0,4.72745913,-1.2562673789,0.4616791746
H,0,4.7888471756,0.4090230987,1.0134179196
H,0,6.9015246628,-0.2000634162,-0.1924276805
H,0,5.9677609325,-0.6148502601,-1.633907417
H,0,6.0345155848,1.0599612739,-1.0767806775

TS-1b down-syn-anti, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -710.229773919 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.252105 a.u.
1 imaginary frequency = 180.2642 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -710.5203014 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -710.5275072 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -710.9163958 a.u.
0; 1
C,0,-0.6485358466,-0.8406554056,0.6271012968
C,0,-1.6731945891,0.0011973744,0.4607142669
H,0,0.6856175891,-1.5971938551,2.1627782138
C,0,0.362207344,-0.6459907015,1.7001330487
N,0,2.0180279318,-0.56109454,0.6860250377
C,0,2.1403471002,0.4277554121,-0.4168812716
C,0,1.8752915929,-0.4032620309,-1.6680761262
C,0,1.3473169711,1.7416974181,-0.3742988821
O,0,0.768499214,2.1592448598,0.7242505887
O,0,1.3697300115,2.4160210379,-1.3872382164
O,0,0.3820633137,0.3966702109,2.4206630155
H,0,2.5966368516,-0.2847243814,1.4747368125
H,0,0.6156356231,1.449093226,1.4671430514
H,0,3.188903106,0.7596516605,-0.4482313132
H,0,2.2302810439,0.1074358251,-2.5629456781
H,0,0.7998229153,-0.5764769794,-1.7767401184
H,0,-0.5677861282,-1.7415200533,0.0201732075
H,0,-1.7292744273,0.8657452165,1.1229645527
C,0,2.6209814446,-1.6983791246,-1.3593009742
H,0,3.6843818079,-1.5794564525,-1.5900636887
H,0,2.2511830297,-2.5537812063,-1.9288717302
C,0,2.4274012535,-1.8875958156,0.150711781
H,0,3.3330055681,-2.2362987529,0.652513711
H,0,1.6316560772,-2.6070083008,0.3723371412
C,0,-2.7675352926,-0.1506664459,-0.5423245863
C,0,-4.1558002633,-0.2258749133,0.1023340658
H,0,-2.5940899292,-1.0394735162,-1.1616889566
H,0,-2.7456996457,0.7158459574,-1.2195731357
C,0,-5.2726202023,-0.3245197547,-0.928128767
H,0,-4.308036838,0.6603818012,0.731359163
H,0,-4.1906842336,-1.090213259,0.7769193041
H,0,-6.2541149526,-0.3767939632,-0.44738384
H,0,-5.2725569917,0.5453045961,-1.5941046921
H,0,-5.1587794491,-1.218311144,-1.5513532817

TS-1b down-syn-anti, optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -710.917230835 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.250123 a.u.
1 imaginary frequency = 195.0933 i cm⁻¹
0; 1
C,0,-0.602320674,-0.8984368481,0.7472854254
C,0,-1.5886412317,-0.0287665646,0.5330759373
H,0,0.807232726,-1.6368468609,2.241632485
C,0,0.4214494782,-0.6994942339,1.8135432998
N,0,2.0206110134,-0.5438208372,0.6749200519
C,0,1.982594339,0.4174222868,-0.4605464833
C,0,1.7148530276,-0.4609733641,-1.6794326289
C,0,1.0625597526,1.6423815575,-0.3663492895
O,0,0.7157138813,2.1205058701,0.8093090671
O,0,0.7914339308,2.2198253215,-1.3927003107
O,0,0.4384430264,0.334363927,2.5338769934
H,0,2.6636080139,-0.2244598348,1.3946228235
H,0,0.6353836877,1.4292920792,1.568046909
H,0,2.9833486678,0.8570528961,-0.5652057646
H,0,1.9831404347,0.0487893399,-2.6018642836
H,0,0.6530515376,-0.7168532678,-1.7215790365
H,0,-0.5281059061,-1.8067121733,0.1542324009
H,0,-1.644754051,0.8540811335,1.1684407968
C,0,2.5775605535,-1.6874324829,-1.3821314318
H,0,3.6190909141,-1.4749474152,-1.6331376396
H,0,2.2692719125,-2.5748722254,-1.9332978808
C,0,2.4279477211,-1.8735874034,0.1335727116
H,0,3.3443233001,-2.2129356782,0.6152702279
H,0,1.6395445482,-2.5932228217,0.3698612093
C,0,-2.6413824367,-0.1711610634,-0.5191506361
C,0,-4.0599561074,-0.1157974124,0.0594852155
H,0,-2.4966114059,-1.105923893,-1.0703368489
H,0,-2.5247041038,0.6493751597,-1.2387833554
C,0,-5.1243214046,-0.2383443732,-1.0271448748
H,0,-4.1872270526,0.826655691,0.6012246525
H,0,-4.1789760509,-0.9185319845,0.7936089548
H,0,-6.1298766571,-0.1857979038,-0.6058197021
H,0,-5.0234827799,0.5653536321,-1.7611448131
H,0,-5.0305206047,-1.1894262527,-1.5577321821

TS-1b up-anti-anti, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -710.236346644 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.252007 a.u.
1 imaginary frequency = 150.4734 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -710.5258711 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -710.5329237 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -710.9204358 a.u.

O; 1
C,0,1.3527554418,-0.5797231768,0.2872168381
C,0,2.4316393364,0.206454605,0.3288963405
C,0,0.2017615651,-0.4249056145,1.2210844492
N,0,-0.9643812371,0.5569490186,0.159415592
C,0,-2.3542821336,0.041502962,0.2843434375
C,0,-3.2837117023,1.2337233253,0.0135293089
C,0,-2.5448008409,-1.1760149492,-0.6315161846
O,0,-1.7205242634,-2.1717622628,-0.3956010467
O,0,-3.3859832132,-1.2007849889,-1.5073392155
H,0,1.2863828677,-1.4086440324,-0.4182057635
H,0,2.4626504163,1.0052587847,1.0744551419
O,0,-0.4450770233,-1.4616191028,1.601638532
H,0,0.3664650216,0.3718382025,1.9700573941
H,0,-0.6255568861,0.429059538,-0.7938867657
H,0,-1.1384520034,-1.983972039,0.4578843985
H,0,-2.4348411227,-0.3237359286,1.3157733525
H,0,-3.939913827,1.3993652871,0.8713548806
H,0,-3.9101974771,1.0198680055,-0.8547671461
C,0,-2.3490398689,2.4349439546,-0.2155668741
H,0,-2.7363964505,3.3649410089,0.2070591195
H,0,-2.1868147734,2.59883348,-1.2860986428
C,0,-1.0436864012,2.0027385468,0.4426499289
H,0,-0.147669666,2.504325522,0.0712081396
H,0,-1.0883394982,2.1223429004,1.5308683758
C,0,3.6400466997,0.0732324205,-0.5397684927
C,0,4.9198839723,-0.189820912,0.2609105567
H,0,3.7734206457,1.0029840763,-1.1125373723
H,0,3.4875003578,-0.72859026,-1.2724220369
C,0,6.1561384399,-0.2687622932,-0.6247275417
H,0,4.8018634408,-1.1233246028,0.8242755433
H,0,5.0479969735,0.6046725301,1.0075709397
H,0,7.0572645088,-0.458278845,-0.0338559705
H,0,6.0645600769,-1.0751406743,-1.360459264
H,0,6.3082499543,0.6660387939,-1.175511902

TS-1b up-anti-anti, optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -710.921380814 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.250499 a.u.
1 imaginary frequency = 178.2128 i cm⁻¹

O; 1
C,0,1.4304383018,-0.7706578055,0.0880716855
C,0,2.3898300185,0.1204992387,0.3343913794
C,0,0.2175155512,-0.8809331468,0.9377385729
N,0,-1.0235105872,0.2417672131,-0.1175863616
C,0,-2.3866632613,0.1004404617,0.470481081
C,0,-3.032320527,1.4970581718,0.4292756432
C,0,-3.1543837492,-0.9937671044,-0.2762249489
O,0,-2.5468105325,-2.1682280589,-0.3124583376
O,0,-4.2203353795,-0.8088199834,-0.804522843
H,0,1.5138889963,-1.4914275867,-0.7225529045
H,0,2.2658372105,0.7991445413,1.1798754605
O,0,-0.3817642608,-1.9786348261,1.0619656974
H,0,0.1859842267,-0.1537984879,1.7692692596
H,0,-0.9889115567,-0.1568654436,-1.055056334
H,0,-1.7013684473,-2.1772171164,0.2337949292
H,0,-2.2610229882,-0.2547542209,1.4996668149
H,0,-3.0712601926,1.9113036736,1.4375676287
H,0,-4.0468118731,1.4404473985,0.0388568987
C,0,-2.0912834955,2.3279041662,-0.4547895923
H,0,-2.1117792049,3.3909539498,-0.2159415515
H,0,-2.3498931077,2.2057923061,-1.5098826036
C,0,-0.732487901,1.6869519089,-0.1830735653
H,0,0.0294740566,1.8779970356,-0.9370557864
H,0,-0.3449832164,1.9954232372,0.7941261324
C,0,3.6668011304,0.2498368146,-0.4354945177
C,0,4.8972210059,-0.0420601993,0.4329006689
H,0,3.7487194077,1.2715554505,-0.8259348102
H,0,3.6517722997,-0.4252606995,-1.2964826144
C,0,6.1991925694,0.1387064736,-0.341981059
H,0,4.8257425418,-1.0648155771,0.8146297009
H,0,4.8876696536,0.6192888182,1.3053996254
H,0,7.0665491545,-0.0825324802,0.2826318614
H,0,6.2309036385,-0.5264283301,-1.2088201718
H,0,6.2969625179,1.1651242074,-0.7048580383

TS-1b down-anti-anti, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -710.231095524 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.252078 a.u.
1 imaginary frequency = 209.5373 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -710.5200943 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -710.527214 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -710.9168565 a.u.
0; 1
C,0,-1.0418417591,-0.4541371604,-0.2963947955
C,0,-2.130840799,0.2752662012,-0.554504741
C,0,-0.0229624841,-0.7483703572,-1.3417026544
N,0,1.358678023,0.425316871,-0.9867603455
C,0,2.5499170784,-0.2053116797,-0.3471706273
C,0,3.47551897,0.985294159,-0.1256824998
C,0,2.1955010507,-0.9211891467,0.9791407076
O,0,1.4124153156,-1.9631546185,0.8834614798
O,0,2.6727180104,-0.5388133028,2.0322322209
H,0,1.651260447,0.6719091385,-1.9317201168
H,0,1.0213923545,-2.0694964583,-0.1186637005
H,0,2.9454731652,-0.9552201386,-1.0371272776
H,0,4.0219180438,1.1967920587,-1.0503417404
H,0,4.1968675529,0.7756835761,0.6644300434
H,0,-0.8998295689,-0.9258135573,0.6744040278
H,0,-2.2449697227,0.7061128006,-1.5527492052
C,0,2.5259091047,2.1467353627,0.2311088459
H,0,2.8249909134,3.0743795634,-0.2624427336
H,0,2.5206037989,2.3284957809,1.3076309083
C,0,1.1309269043,1.6807032338,-0.2334001931
H,0,0.6062326402,2.3942273989,-0.8711148787
H,0,0.4785885682,1.444776297,0.610519605
C,0,-3.2507159534,0.5322757861,0.4004846793
C,0,-4.5966085916,0.0109210127,-0.114748925
H,0,-3.3379416561,1.6161478438,0.5675562963
H,0,-3.0233293357,0.0805267155,1.3735120263
C,0,-5.7437605672,0.3101930346,0.8409733165
H,0,-4.5196650969,-1.0705398735,-0.2802904621
H,0,-4.8043531795,0.457473783,-1.095818703
H,0,-6.693381795,-0.0716124342,0.4541770368
H,0,-5.573026597,-0.1512615351,1.8196026693
H,0,-5.8564226651,1.3885227139,0.9985747796
O,0,0.5306195359,-1.9086425981,-1.3797201814
H,0,-0.2921327061,-0.2966184709,-2.3119438619

TS-1b down-anti-anti, optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -710.917303399 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.252472 a.u.
1 imaginary frequency = 209.5022 i cm⁻¹
0; 1
C,0,-1.0549688792,-0.5061465173,-0.3077680635
C,0,-2.1208054254,0.2503135119,-0.5622942299
C,0,-0.0429118983,-0.8012770754,-1.3614732966
N,0,1.3451891382,0.4175564771,-0.9718633815
C,0,2.5607833426,-0.1951983806,-0.3607768364
C,0,3.4704649287,1.012351288,-0.1422286474
C,0,2.2099718791,-0.9020461832,0.9701623287
O,0,1.4573237247,-1.9695024208,0.8790691369
O,0,2.6433775832,-0.4935456085,2.0231325216
H,0,1.6177640662,0.7042135562,-1.9120846548
H,0,1.0710794185,-2.098484104,-0.096094396
H,0,2.9612731031,-0.9403828573,-1.0486769961
H,0,3.9910930786,1.2349812521,-1.0755503131
H,0,4.2111106345,0.8197656294,0.6305346142
H,0,-0.9193828487,-0.9865287228,0.6583537571
H,0,-2.2232440995,0.6904455326,-1.5557996433
C,0,2.5005167044,2.1582987362,0.2316189677
H,0,2.7499113272,3.0746868292,-0.3026595513
H,0,2.5338878018,2.3700826464,1.2994033279
C,0,1.100469714,1.6385561291,-0.1638883728
H,0,0.5006831528,2.3422511299,-0.739031096
H,0,0.5244766904,1.3387648133,0.7125985987
C,0,-3.2345562596,0.5279077869,0.3983441969
C,0,-4.5863852813,0.030443067,-0.1289247223
H,0,-3.3012329463,1.6100058358,0.5661380936
H,0,-3.0172581695,0.0633771294,1.3647590755
C,0,-5.7293986307,0.3551301603,0.8283254684
H,0,-4.527683554,-1.0499752724,-0.2910173933
H,0,-4.7786704813,0.4843931952,-1.1066264789
H,0,-6.6840763701,-0.008304324,0.4435142443
H,0,-5.5623017393,-0.1074801434,1.804389524
H,0,-5.8152828598,1.4342907399,0.9800923008
O,0,0.5305106346,-1.9420583201,-1.3935673024
H,0,-0.2939804796,-0.3353125159,-2.3245997807

TS-2b *cis*, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -710.230224246 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.248878 a.u.
1 imaginary frequency = 448.2570 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -710.525319 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -710.5322972 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -710.9187039 a.u.
0; 1
C,0,-3.4937108497,-0.2496234316,-1.5031812929
C,0,-2.6094879891,-0.6237302885,-2.4358366473
C,0,-3.0611100581,0.1837721417,-0.1727508905
N,0,-3.7741143179,-0.1083038801,0.9086494936
C,0,-5.2127266904,-0.3929611179,0.9291482456
C,0,-5.4366291102,-0.8198637602,2.3794190002
C,0,-6.1337445709,0.7963696094,0.533820345
O,0,-5.6081209812,1.8366321331,0.0047938551
O,0,-7.3352855914,0.6221360588,0.7352365236
O,0,-3.2228875639,2.066389018,-0.3133091178
H,0,-4.3202952029,2.005574818,-0.1563779834
H,0,-5.4366053636,-1.20825729,0.2331911884
H,0,-5.1531363269,-1.8695308763,2.5123674981
H,0,-6.4857055698,-0.7000951554,2.6509097651
H,0,-1.9876365457,0.2320136037,-0.0095997829
H,0,-3.0815275493,2.3120955403,-1.236560505
H,0,-4.559249096,-0.2508970241,-1.7170363296
H,0,-1.5461824658,-0.6023455798,-2.1885863679
C,0,-2.9584381412,-1.1016632387,-3.8048569336
C,0,-2.4714369089,-2.5304741763,-4.0741530074
H,0,-2.4923855356,-0.4301198584,-4.5406871362
H,0,-4.0419315255,-1.0393274988,-3.9599586445
C,0,-2.7833680179,-2.9917930474,-5.4913010567
H,0,-2.9365938068,-3.2086065657,-3.3485534133
H,0,-1.3898092043,-2.5830336339,-3.8955607725
H,0,-2.4315057435,-4.0135938246,-5.6612438411
H,0,-3.8612237475,-2.9736333771,-5.684871366
H,0,-2.3022438702,-2.3446464374,-6.2326435642
C,0,-3.2482575988,0.1525324873,2.2571911995
H,0,-2.7440477015,1.1225723932,2.2841309399
H,0,-2.5218442018,-0.62662779,2.5175523643
C,0,-4.4855204749,0.0946528845,3.1510926074
H,0,-4.924855043,1.0928018191,3.2487884704
H,0,-4.2507477957,-0.2697562247,4.1535050865

TS-2b *cis*, optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -710.919552107 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.248019 a.u.
1 imaginary frequency = 482.7358 i cm⁻¹
0; 1
C,0,-3.4949943152,-0.2518848902,-1.511015878
C,0,-2.6152815888,-0.6175410961,-2.4440253709
C,0,-3.0499846196,0.1820267187,-0.1761163352
N,0,-3.7655395765,-0.1288963458,0.9012969227
C,0,-5.2074910445,-0.4112323209,0.90720794
C,0,-5.444380924,-0.817278917,2.3666261628
C,0,-6.1116550135,0.7880444785,0.5140896078
O,0,-5.5591008717,1.8943845936,0.183509501
O,0,-7.3182787762,0.5820822675,0.5555512059
O,0,-3.1997420703,2.0169486819,-0.2802499758
H,0,-4.2951671983,2.0209456933,-0.0565631512
H,0,-5.4350616626,-1.2291313619,0.2215283616
H,0,-5.1409594484,-1.8573235927,2.5093208258
H,0,-6.4923554011,-0.7135661835,2.6392883024
H,0,-1.9765724591,0.2063200921,-0.0165452972
H,0,-3.0559277726,2.3360707204,-1.1790812404
H,0,-4.5613662999,-0.2600883152,-1.7165174307
H,0,-1.5524771874,-0.5897733509,-2.2030104317
C,0,-2.9739632736,-1.1009678892,-3.8122900521
C,0,-2.4634985067,-2.5238783344,-4.0741743203
H,0,-2.5259938954,-0.4266878597,-4.5522506278
H,0,-4.0582342355,-1.0594852683,-3.9504045845
C,0,-2.7965692161,-2.9964922184,-5.486197651
H,0,-2.9045705048,-3.2023772984,-3.3378534076
H,0,-1.3803626051,-2.5510394429,-3.9178044748
H,0,-2.4245895845,-4.0072661537,-5.6623659007
H,0,-3.8770128165,-3.0014627335,-5.6499131733
H,0,-2.3479182822,-2.3362136513,-6.2327579155
C,0,-3.2499065489,0.1442734897,2.2584221694
H,0,-2.7357364366,1.1063299506,2.2747166149
H,0,-2.5459498007,-0.6438689906,2.5393426623
C,0,-4.5060039522,0.121264254,3.1315015289
H,0,-4.9416140434,1.1218716926,3.1841592678
H,0,-4.2941080682,-0.2154464184,4.1453021456

TS-2b cis 2, optimization in solv. CHCl₃
 PBE1PBE/6-31G(d,p), E= -710.227728561 a.u.
 Thermal correction to Gibbs Free Energy at 25 °C = 0.249033 a.u.
 1 imaginary frequency = 444.0395 i cm⁻¹
 SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -710.5228898 a.u.
 SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -710.5298309 a.u.
 SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -710.9160788 a.u.
 O; 1
 C,0,-3.4888265912,-0.2260946605,-1.5043705204
 C,0,-2.604579327,-0.621100315,-2.4260381181
 C,0,-3.0598428092,0.216984916,-0.1758493523
 N,0,-3.7737547176,-0.0823038862,0.9051824603
 C,0,-5.2143228575,-0.3583472652,0.9203976393
 C,0,-5.4362044343,-0.8442009751,2.3513850597
 C,0,-6.1226095541,0.8560709681,0.571915555
 O,0,-5.5947958649,1.8819974239,0.0181302652
 O,0,-7.3181720099,0.7131636528,0.8265970013
 O,0,-3.2320675705,2.0824795464,-0.4555409197
 H,0,-4.3142260713,2.0341438985,-0.2181800931
 H,0,-5.4449755171,-1.1426768678,0.1918678458
 H,0,-5.1609657047,-1.9006911689,2.4390836445
 H,0,-6.4828118898,-0.7258072526,2.6323886669
 H,0,-1.9850922221,0.258450268,-0.014513988
 H,0,-2.8051699886,2.5294089913,0.2867983865
 H,0,-4.5526235901,-0.2139620449,-1.7251010715
 H,0,-1.5421299099,-0.6038359954,-2.1754790128
 C,0,-2.9517667394,-1.110961596,-3.7914705538
 C,0,-2.4654358675,-2.5411190746,-4.0520459627
 H,0,-2.4852389468,-0.4434293689,-4.5306720145
 H,0,-4.0349740843,-1.0483228334,-3.9486493282
 C,0,-2.7755754584,-3.0107353042,-5.4669308344
 H,0,-2.9314730667,-3.2153708283,-3.3232328239
 H,0,-1.3839448349,-2.5932175521,-3.8719535464
 H,0,-2.4235831052,-4.0334498446,-5.6313964833
 H,0,-3.853224745,-2.9934152577,-5.6619221824
 H,0,-2.2938971833,-2.3673478124,-6.2112100651
 C,0,-3.2442903572,0.126916346,2.2603765814
 H,0,-2.7428125108,1.0973279137,2.3360409381
 H,0,-2.5107285293,-0.6559237447,2.4858332236
 C,0,-4.4764228484,0.0295443918,3.1584035103
 H,0,-4.9128262188,1.022714347,3.3069318474
 H,0,-4.2354221443,-0.382192075,4.1407384752

TS-2b *trans*, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -710.229178874 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.248953 a.u.
1 imaginary frequency = 369.6721 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -710.5258563 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -710.5327873 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -710.9180904 a.u.
0; 1
C,0,-1.9679956619,-0.4093607148,-0.95196505
C,0,-1.7681729173,-0.718776332,-2.2381033348
C,0,-3.2640800845,0.0689299089,-0.4750759248
N,0,-3.7167979736,-0.250918327,0.7267911322
C,0,-5.1161012118,-0.0830360734,1.1402636569
C,0,-5.1791399428,-0.9369328229,2.4035915725
C,0,-5.5707722464,1.3822324729,1.4123384859
O,0,-4.859030145,2.3414912827,0.962561517
O,0,-6.6345237373,1.4956221752,2.0233109841
O,0,-2.8503925988,1.94090497,-0.3295428496
H,0,-4.0385464559,0.1964984085,-1.2283503707
H,0,-3.7479517989,2.1569860937,0.2585471242
H,0,-5.768379656,-0.4690851269,0.3484788433
H,0,-5.2875053575,-1.9953567482,2.1428476598
H,0,-6.0226933106,-0.6336254006,3.0233628512
H,0,-2.9564064943,2.3568520861,-1.1941757381
H,0,-1.1668467693,-0.5180181924,-0.2258708863
H,0,-2.5911895437,-0.5881272646,-2.9437517899
C,0,-0.4862488511,-1.2255224936,-2.8084442382
C,0,0.0785520049,-0.3027700834,-3.8950874152
H,0,-0.6607134685,-2.2174722327,-3.2497906948
H,0,0.253214933,-1.3590341937,-2.0099036214
C,0,1.3595807866,-0.8493079661,-4.5106813966
H,0,0.2638664382,0.6874218306,-3.4616633957
H,0,-0.6782649348,-0.1604030136,-4.6770654558
H,0,1.7462828107,-0.1771375721,-5.282312482
H,0,2.1411850096,-0.9722524501,-3.7532612788
H,0,1.1894541608,-1.8274225009,-4.9736308122
C,0,-3.815971019,-0.677595968,3.0448239775
H,0,-3.5276857001,-1.435878112,3.7759557111
H,0,-3.8222134374,0.2932069106,3.5508673548
C,0,-2.8576593972,-0.6415053372,1.8537206038
H,0,-2.0437593709,0.0777755896,1.9851234698
H,0,-2.4227474193,-1.6273514623,1.6532032709

TS-2b *trans*, optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -710.918731116 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.249464 a.u.
1 imaginary frequency = 437.5794 i cm⁻¹
0; 1
C,0,-1.9661242849,-0.4058209661,-0.9647234445
C,0,-1.7819092308,-0.7357566798,-2.242529356
C,0,-3.2640996293,0.0969829969,-0.4904520666
N,0,-3.7258607724,-0.2504310391,0.7029169732
C,0,-5.1258167371,-0.0781215324,1.118235354
C,0,-5.1855590539,-0.9498516279,2.3742967794
C,0,-5.5450984165,1.3862900653,1.4315714921
O,0,-4.7520547947,2.3330144334,1.1035935912
O,0,-6.6366530902,1.5260687381,1.9705406124
O,0,-2.8413121027,1.8966309818,-0.2974338443
H,0,-4.0309228813,0.2286913329,-1.2496399493
H,0,-3.7064565485,2.1509017118,0.346052506
H,0,-5.7870950132,-0.4389008771,0.3267002166
H,0,-5.2588548774,-2.0020993453,2.0886318835
H,0,-6.0359465885,-0.6865295027,2.9983643457
H,0,-2.880293293,2.3861155001,-1.1273838142
H,0,-1.1662112439,-0.5046248079,-0.2380277987
H,0,-2.6071338811,-0.6091083786,-2.9434262192
C,0,-0.5003113238,-1.2516263562,-2.8145973856
C,0,0.0644107195,-0.3105390039,-3.8872754438
H,0,-0.6794851738,-2.2333923762,-3.2684147537
H,0,0.2352277783,-1.3913575481,-2.0169865932
C,0,1.3504394928,-0.8552502346,-4.5018820305
H,0,0.2486829721,0.6699052196,-3.4379024975
H,0,-0.688511207,-0.1625897394,-4.6680587715
H,0,1.7461521824,-0.1751609973,-5.2582012074
H,0,2.1189927055,-0.9921472634,-3.7369336431
H,0,1.1746072666,-1.8238584881,-4.9767923913
C,0,-3.8285187624,-0.6641335692,3.0258814157
H,0,-3.5382296574,-1.4099590726,3.7643971452
H,0,-3.8539705194,0.3123303961,3.5156924925
C,0,-2.8608122808,-0.628489557,1.8384332617
H,0,-2.0613320225,0.1036518576,1.9669947518
H,0,-2.4195917307,-1.6098012708,1.6454723892

TS-2b *trans* 2, optimization in solv. CHCl₃
 PBE1PBE/6-31G(d,p), E= -710.229180499 a.u.
 Thermal correction to Gibbs Free Energy at 25 °C = 0.248386 a.u.
 1 imaginary frequency = 418.0052 i cm⁻¹
 SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -710.5248146 a.u.
 SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -710.5317166 a.u.
 SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -710.9172738 a.u.
 O; 1
 C,0,-1.3670954768,-0.1502994605,0.361529975
 C,0,-2.4978521553,-0.6200184548,-0.1786300082
 C,0,-0.0593636879,-0.4340163971,-0.2307871307
 N,0,0.9555217948,0.40359845,-0.0592801727
 C,0,2.1998722295,0.3352943851,-0.8321033545
 C,0,2.7621841975,1.7399606658,-0.6462225492
 C,0,3.208873854,-0.7498806374,-0.3479395257
 O,0,2.7624215653,-1.7303344542,0.3402335956
 O,0,4.3787092666,-0.5889823194,-0.6958589489
 O,0,0.3887440408,-2.0826801325,0.6209415158
 H,0,-0.0664251228,-0.9517774925,-1.1860213243
 H,0,1.4830301779,-1.9343554883,0.5225521037
 H,0,1.9592873886,0.1111015112,-1.87774518
 H,0,2.2467898049,2.4461316051,-1.3059522417
 H,0,3.8299076859,1.7551588684,-0.8638331063
 H,0,0.1708998751,-1.9756412824,1.5552366065
 H,0,-1.4021367853,0.4632283432,1.2584384888
 H,0,-2.4306170973,-1.2365662432,-1.0767148742
 C,0,-3.8706146466,-0.3589263829,0.3410126762
 C,0,-4.7750863351,0.3230288827,-0.6920476067
 H,0,-3.8199702529,0.2463673894,1.2539880791
 H,0,-4.326282496,-1.3198837967,0.6217490062
 C,0,-6.1910257056,0.5339301059,-0.173189963
 H,0,-4.8005981626,-0.2847554995,-1.6054052796
 H,0,-4.332403308,1.2856770469,-0.9751804438
 H,0,-6.8190357796,1.0225313814,-0.92389868
 H,0,-6.6621783843,-0.4199874405,0.0874458046
 H,0,-6.1946099758,1.1617059961,0.7244057883
 C,0,2.4343839289,2.0256107667,0.8200951356
 H,0,2.4327931693,3.0898043949,1.0653691914
 H,0,3.1708510412,1.5345541381,1.4638659266
 C,0,1.0531649537,1.3938483495,1.0227225863
 H,0,0.9524591482,0.917111413,2.0033803118
 H,0,0.2499782496,2.1303067883,0.9122575979

Int-2b *cis*, optimization in solv. CHCl₃
PBE1PBE/6-311G(d,p), E= -633.880172752 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.226676 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -634.1346505 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -634.1409956 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -634.4928258 a.u.

O; 1
C,0,-0.9065370947,-0.9339662543,-0.5257306632
N,0,0.3164639013,-0.8742113242,-0.1027982931
C,0,0.8738931841,0.1419562276,0.777710109
C,0,2.2299003607,-0.424050347,1.1707669789
C,0,2.6601313203,-1.1653529444,-0.0943182763
C,0,1.3634562267,-1.8066021333,-0.5718491017
C,0,0.9729505117,1.5554933823,0.0201698036
O,0,0.10719109,1.7428630847,-0.8513616528
O,0,1.8786508445,2.2814648496,0.4583516466
H,0,0.2033115852,0.2997635522,1.6276632913
H,0,2.1448334601,-1.1149802155,2.0171198449
H,0,2.8936296647,0.3985196224,1.437637277
H,0,3.0260628427,-0.4511701471,-0.8384309099
H,0,3.4386882979,-1.9112735925,0.0771926664
H,0,1.1927757996,-2.7743163218,-0.0882395331
H,0,1.2893855149,-1.9330392816,-1.6540922421
C,0,-1.9937797481,-0.1101048427,-0.0961939739
C,0,-3.23938965,-0.36519486,-0.5429964153
H,0,-3.3865291476,-1.1990513072,-1.2322542369
H,0,-1.1196571588,-1.7260550594,-1.2417530186
H,0,-1.7948191004,0.7286399756,0.5606482619
C,0,-4.4558252763,0.4031162937,-0.169076175
C,0,-5.5391532168,-0.4779923328,0.4674710124
H,0,-4.8707319707,0.8589483857,-1.0804133601
H,0,-4.1914330359,1.2256046078,0.5050061582
C,0,-6.8009228053,0.3084732093,0.7957003737
H,0,-5.1369667424,-0.9379030875,1.3781034317
H,0,-5.781162427,-1.3027558779,-0.214792151
H,0,-7.5590668539,-0.3349068686,1.2517015603
H,0,-6.5883947738,1.1227489034,1.4965043187
H,0,-7.2360720027,0.7517330032,-0.1063664317

Int-2b *cis*, optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -634.494281541 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.226700 a.u.

O; 1
C,0,0.0892872688,-1.0879648807,-0.4267223141
N,0,1.2981249866,-0.952217348,-0.0116359825
C,0,1.8057887193,0.2006750467,0.7496440565
C,0,3.2145128539,-0.2422578217,1.1467718349
C,0,3.6530984217,-1.0819144144,-0.0568461102
C,0,2.3944858915,-1.8803494791,-0.383070125
C,0,1.8219924798,1.5089060078,-0.1461471507
O,0,1.3448820372,1.410683352,-1.2865970672
O,0,2.3172569663,2.4806715501,0.4443715015
H,0,1.1574178694,0.3874873904,1.6061772324
H,0,3.1859807475,-0.858012182,2.0495316908
H,0,3.8471209284,0.6232503322,1.3296877377
H,0,3.9111013578,-0.4327816574,-0.8959404742
H,0,4.4982285855,-1.7345856443,0.1554765453
H,0,2.3110736726,-2.7680225481,0.2485800975
H,0,2.2916207686,-2.1628672301,-1.4294906
C,0,-0.9979603879,-0.1973476902,-0.1244551869
C,0,-2.2267655021,-0.4831284402,-0.5826340342
H,0,-2.3675709627,-1.390949486,-1.1694537573
H,0,-0.1180112352,-1.9608532868,-1.0418078642
H,0,-0.808319147,0.7035996878,0.4464606457
C,0,-3.4389465395,0.3466894402,-0.340601225
C,0,-4.5457067421,-0.4482741595,0.3684654838
H,0,-3.8213936456,0.690953022,-1.3093138265
H,0,-3.1765672393,1.2345752034,0.2405851303
C,0,-5.7951439863,0.3999887716,0.5850591931
H,0,-4.1665653873,-0.8101072336,1.3286542251
H,0,-4.792749472,-1.332272059,-0.2277940715
H,0,-6.576146412,-0.170559223,1.0903704839
H,0,-5.567921544,1.2765954784,1.19663688
H,0,-6.1956683518,0.7517275015,-0.3689389491

Int-2b *trans*, optimization in solv. CHCl₃
PBE1PBE/6-311G(d,p), E= -633.882736300 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.226077 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -634.1364451 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -634.142821 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -634.4940104 a.u.

O; 1
C,0,0.9501572657,-0.3357406305,0.3359481842
N,0,-0.1148105274,0.4045174481,0.3327393558
C,0,-1.4278991876,-0.1198010873,0.6949294087
C,0,-2.3332649264,1.1005216951,0.6755457133
C,0,-1.7057480668,1.9739480844,-0.409357885
C,0,-0.2081238229,1.7742881037,-0.2012176006
C,0,-1.8539074226,-1.2796618904,-0.3259737104
O,0,-0.9090021635,-1.9833148842,-0.7295418375
O,0,-3.0760420967,-1.3501584417,-0.5258495275
H,0,-1.3661927627,-0.6009283987,1.6759488917
H,0,-2.3278593109,1.6162250498,1.6423453039
H,0,-3.3497988013,0.7849010218,0.4393395499
H,0,-1.996461855,1.6058120918,-1.3981579638
H,0,-1.9844612048,3.0273644546,-0.3407808334
H,0,0.1949425871,2.4636973913,0.5489906884
H,0,0.379740607,1.8654039499,-1.116614991
C,0,2.2435449853,0.0792436893,-0.1179378787
C,0,3.2839895105,-0.7765078441,-0.0675729478
H,0,3.1124944099,-1.7781066211,0.3301119805
H,0,0.8208623651,-1.3404865945,0.7222151061
H,0,2.3822808612,1.0847864709,-0.5054283798
C,0,4.6693765747,-0.4701591278,-0.5082438659
C,0,5.7015037523,-0.6763848612,0.6091499415
H,0,4.7289486747,0.5529900409,-0.8966762208
H,0,4.9216257619,-1.1441703967,-1.3403767698
C,0,7.1233042336,-0.4120582853,0.1328565116
H,0,5.6201856213,-1.7021406217,0.9896680569
H,0,5.4582105421,-0.0141949838,1.4485225177
H,0,7.8435429107,-0.5619933813,0.9422921782
H,0,7.3964410964,-1.0841583717,-0.6876328373
H,0,7.2354685793,0.6159269204,-0.227805179

Int-2b *trans*, optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -634.495095063 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.225098 a.u.

O; 1
C,0,-0.009170198,-0.2036198959,0.3428509632
N,0,-1.1146545817,0.4521593946,0.2879727792
C,0,-2.391710932,-0.1076455311,0.7592738488
C,0,-3.3437391269,1.0801429069,0.6872695973
C,0,-2.8343471472,1.8378870052,-0.5413465387
C,0,-1.3151668371,1.7460983848,-0.4045701941
C,0,-2.8164649521,-1.3386732602,-0.1537030607
O,0,-1.8844503534,-1.9283206951,-0.7243151342
O,0,-4.031267068,-1.5782624641,-0.1336359611
H,0,-2.2582258949,-0.5007725719,1.7685978494
H,0,-3.2593835892,1.7004017004,1.5836396043
H,0,-4.3688693747,0.7328589366,0.5856495028
H,0,-3.1551125853,1.3265744947,-1.4517096989
H,0,-3.1708715472,2.8723176072,-0.5862815189
H,0,-0.9131984796,2.5377959276,0.2326518937
H,0,-0.7863969383,1.7411499612,-1.3564359156
C,0,1.2458516455,0.2515941209,-0.1948284409
C,0,2.3337788098,-0.5274929477,-0.0846879436
H,0,2.2360480588,-1.4894388705,0.417672679
H,0,-0.0463918924,-1.1645045944,0.8451572701
H,0,1.3023525413,1.2161645931,-0.6867093538
C,0,3.6911986789,-0.1732733771,-0.5825980313
C,0,4.7158691201,-0.1120795063,0.5614417987
H,0,3.6627356822,0.7806620152,-1.1160366362
H,0,4.0108340603,-0.9421450018,-1.2962077702
C,0,6.1160971401,0.2045202158,0.045090912
H,0,4.7202483845,-1.0691051732,1.0919653651
H,0,4.3997372227,0.6479850971,1.2818040216
H,0,6.8347485199,0.2534901708,0.8647348548
H,0,6.4542660645,-0.5621787443,-0.6562338723
H,0,6.1315105694,1.1655041017,-0.4748168698

TS-3a (SS), optimization in solv. CHCl₃
PBE1PBE/6-311G(d,p), E = -1760.10090291 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.424177 a.u.
1 imaginary frequency = 186.1453 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6694577 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6962876 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.5868217 a.u.

0; 1
C,0,0.9911057575,4.6311984354,-1.0159095479
C,0,1.415970144,5.0641813487,-2.2721202078
C,0,1.9115290753,4.1508303186,-3.2045110623
C,0,1.9786962055,2.8077601941,-2.8657886657
C,0,2.4773128993,1.6324143547,-3.6561556549
C,0,1.0495146152,3.2843774395,-0.6623932494
C,0,1.5579921755,2.3925692614,-1.6021910686
N,0,1.7163747696,1.0040837152,-1.4829300552
C,0,2.2555192776,0.4195197645,-2.7250619851
C,0,3.5874099163,-0.3568921414,-2.4474832111
C,0,1.6019305187,0.3035333769,-0.3608120844
C,0,1.6962627126,-1.0782624572,-0.2826556384
C,0,1.933825629,-1.6910588593,0.9473178319
O,0,3.7392995723,-1.3914570689,-3.1268334941
O,0,4.3547819186,0.1509971526,-1.5964950248
H,0,0.5983514742,5.3492590716,-0.3024736196
H,0,1.3557571079,6.117545929,-2.5275618135
H,0,2.2407067265,4.4872739775,-4.1835427882
H,0,0.6972598739,2.9564354987,0.3100075735
H,0,1.5216426096,-0.2766104725,-3.1408164666
H,0,1.4442609242,0.8820399215,0.5459350729
H,0,1.75429318,-1.6571714855,-1.199269946
H,0,1.9261337559,-1.0438140761,1.8214669328
C,0,4.080327444,1.304225425,1.611129643
C,0,3.8271474536,2.6352123444,1.9390384673
C,0,4.2454851204,0.3540322789,2.6294823815
H,0,3.7070478309,3.367648959,1.1457465905
C,0,3.7336630373,3.0284093745,3.2721076738
C,0,4.1609872298,0.7607000454,3.9662166535
H,0,3.5371216326,4.0676913894,3.5204372262
H,0,4.3068432849,0.0102939557,4.7370779634
C,0,3.9016533287,2.0868212805,4.287388434
H,0,3.8333855459,2.3900789197,5.3283493113
H,0,4.1651865137,1.0236581834,0.5621884175
C,0,4.5277919772,-1.0925091294,2.3627130778
O,0,4.8784035106,-1.8424509237,3.297250409
C,0,4.3190576275,-1.580391883,1.037854545
H,0,4.3730272487,-0.9596847709,0.1430861095
S,0,4.9564244924,-3.1958075837,0.8293530764
C,0,4.6112259105,-3.5249440311,-0.9068971736
H,0,3.5722729986,-3.8509569546,-0.9633194447
H,0,4.756392337,-2.6387581293,-1.5354825452
H,0,5.2595798642,-4.3478816559,-1.21267907
C,0,6.7560986137,-2.9856125071,0.7931266251
H,0,7.0344315439,-2.6362234102,1.7879497399
H,0,7.2138166436,-3.9565880278,0.5917219148
H,0,7.0261391136,-2.2537706465,0.0307898411
C,0,1.7185032684,-3.111807924,1.2342389202
C,0,1.1920702764,-3.9951293348,0.2775162203
C,0,1.9906443191,-3.6016714523,2.5229011726
C,0,0.9560303831,-5.3268595144,0.5987261149
C,0,1.7530117903,-4.9326444966,2.8402103097
C,0,1.2356446081,-5.8000143594,1.879470292
H,0,0.9392259638,-3.6335726148,-0.7147340362
H,0,2.4151667524,-2.9335686369,3.2668766038

TS-3a (SS), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1761.59007027 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.423240 a.u.
Thermal correction to Gibbs Free Energy at 20 °C = 0.424792 a.u.
1 imaginary frequency = 249.6195 i cm⁻¹

0; 1
C,0,1.3803856965,4.6779457691,-0.7692169312
C,0,1.7558941369,5.1111809603,-2.0398481239
C,0,2.0783184342,4.1883830915,-3.0354878084
C,0,2.0280582595,2.8351633215,-2.7423039595
C,0,2.3069542744,1.6427677747,-3.6204715367
C,0,1.3249669957,3.3204675923,-0.4613812265
C,0,1.6684767539,2.4218890061,-1.4630358642
N,0,1.7080519871,1.0136324526,-1.3903201898
C,0,2.1172378411,0.4251351801,-2.6813506967
C,0,3.4488220352,-0.3857055268,-2.5524915082
C,0,1.6104420499,0.3002089111,-0.2826741986
C,0,1.6585895682,-1.0866253584,-0.2288570298
C,0,1.9194026132,-1.6907361403,0.997293163
O,0,3.561447064,-1.3191837816,-3.3651382425
O,0,4.2613136246,0.0064581734,-1.6889538636
H,0,1.1217574998,5.4038498201,-0.0076963128
H,0,1.7906912472,6.1718053168,-2.2565320962
H,0,2.3640952015,4.5241777549,-4.0257477815
H,0,1.0216907489,2.9939786179,0.5257132695
H,0,1.3311720903,-0.2424082277,-3.03629566
H,0,1.516412868,0.8634254424,0.6419947458
H,0,1.6772765901,-1.6602530818,-1.148173989
H,0,1.8830461653,-1.0467688494,1.8721642968
C,0,4.1094634016,1.3079682021,1.5891698563
C,0,3.7967008639,2.6374557687,1.8638768462
C,0,4.104859317,0.3617526907,2.6214818873
H,0,3.8201318532,3.3672569238,1.0627616143
C,0,3.4589428242,3.0270866643,3.1569068866
C,0,3.7778599377,0.7631152436,3.9189455877
H,0,3.2140464606,4.0623608469,3.3655783064
H,0,3.7894075598,0.0210712862,4.70860265
C,0,3.4467681161,2.086208686,4.1846195517
H,0,3.186094722,2.3866603044,5.1927731006
H,0,4.3664364446,1.0279478964,0.5712983297
C,0,4.430861417,-1.0889992624,2.3924340593
O,0,4.7342083529,-1.8240907269,3.3456931575
C,0,4.2696829959,-1.562880064,1.0649551079
H,0,4.3092287282,-0.9312021567,0.1864310343
S,0,4.8745610556,-3.1849813006,0.7870982422
C,0,4.6851444571,-3.260825443,-1.0076438415
H,0,3.6195961391,-3.3402138478,-1.213721432
H,0,5.0772581552,-2.3477567345,-1.4557871573
H,0,5.2011018897,-4.1532117745,-1.3577548763
C,0,6.6754785435,-3.0188651464,0.9283857302
H,0,6.8710575196,-2.7777051726,1.9717337017
H,0,7.1239700343,-3.9757533419,0.6638990293
H,0,7.0089703291,-2.2211196093,0.2672720253
C,0,1.7859477882,-3.1229716465,1.2881854748
C,0,1.4677369461,-4.0648106674,0.3016080791
C,0,1.9871183823,-3.5598666216,2.6047465823
C,0,1.3668513385,-5.4124644764,0.6245045748
C,0,1.8849744983,-4.9066129717,2.924694783
C,0,1.578589126,-5.8364590613,1.9342708159
H,0,1.2762697728,-3.747474861,-0.7173034577
H,0,2.242940971,-2.8364831191,3.371558405

H,0,0.5412671432,-5.9946881655,-0.1503959891
H,0,1.9719817231,-5.294853425,3.8401228053
H,0,1.0453157579,-6.8395824073,2.1291765186
H,0,1.9428738403,1.5175370368,-4.6035045438
H,0,3.5406229111,1.7475483546,-3.8925595863

H,0,1.1154198796,-6.1317347601,-0.1456925951
H,0,2.045683559,-5.2317918102,3.9454096048
H,0,1.4979155039,-6.888088361,2.1824860804
H,0,1.6208037609,1.6037743006,-4.4676256862
H,0,3.3240576102,1.6721709046,-4.0169585147

TS-3a (SR), optimization in solv. CHCl₃
PBE1PBE/6-311G(d,p), E = -1760.09860598 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.423217 a.u.
1 imaginary frequency = 260.2026 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6669454 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6935862 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.5848171 a.u.

0; 1
C,0,3.7674872965,4.3835541659,-2.9798024254
C,0,3.8754553372,4.4670006712,-4.3678510366
C,0,3.726006086,3.3245860731,-5.1562952126
C,0,3.4659541985,2.1078896245,-4.5438833053
C,0,3.3032673173,0.7389317416,-5.1364305621
C,0,3.5046582323,3.16834067,-2.3506368389
C,0,3.3583902909,2.0415014247,-3.1546230193
N,0,3.0735593086,0.7231941296,-2.762899689
C,0,2.9446096627,-0.1648655951,-3.9424038233
C,0,3.9045995715,-1.401508405,-3.8180399328
C,0,2.917404685,0.3097818594,-1.5068763436
C,0,2.5546334277,-0.9722143336,-1.1343534026
C,0,2.509897468,-1.3430647742,0.2210877225
O,0,3.3405043596,-2.5171554761,-3.7149888919
O,0,5.1227470494,-1.1285696313,-3.8190666428
H,0,3.8846140133,5.277459534,-2.3746843235
H,0,4.0769470864,5.4252370969,-4.8367067595
H,0,3.8134733141,3.3862715879,-6.2374230599
H,0,3.4160634726,3.1221606674,-1.270263249
H,0,1.9093708977,-0.5179341978,-3.9853593267
H,0,3.1060712997,1.0563402341,-0.7389442957
H,0,2.3860376281,-1.7120641484,-1.9107900859
H,0,2.4885597165,-0.5330263045,0.9459206781
C,0,4.1343856226,-2.2635221631,3.8188116945
C,0,3.7587859538,-2.4064875087,5.1509487851
C,0,4.3538958344,-0.9905368808,3.2788964594
H,0,3.59740569,-3.3988001101,5.5614687011
C,0,3.5930733229,-1.281736678,5.9558489042
C,0,4.1933729984,0.1327038765,4.0992441907
H,0,3.298473,-1.3959769,6.9950447557
H,0,4.3795405687,1.1110388485,3.6678395611
C,0,3.8105888487,-0.010054245,5.4266084036
H,0,3.6836972823,0.8688436271,6.0519147356
H,0,4.265536576,-3.1523761615,3.2104905844
C,0,4.7787465827,-0.7540910451,1.8661046467
O,0,5.1820597058,0.3733488168,1.520348644
C,0,4.633201154,-1.7980823211,0.8945612478
H,0,4.5665428862,-2.8501684916,1.1462447272
S,0,5.5254378848,-1.4275849427,-0.5746881635
C,0,7.2596080548,-1.3528976355,-0.0685220623
H,0,7.3379589158,-0.5148700702,0.6239005681
H,0,7.5596778101,-2.2886300397,0.4048363632
H,0,7.8509696525,-1.1588716682,-0.9653997768
C,0,5.4997173517,-2.9895213914,-1.4578852222
H,0,4.5022571358,-3.1268640766,-1.882240531
H,0,6.1704737809,-2.8617538652,-2.307840651
H,0,5.8030800168,-3.8036334514,-0.7973292982
C,0,1.8519338681,-2.5831647948,0.6585083476
C,0,1.7209492496,-3.6968448515,-0.1868923855
C,0,1.3167042441,-2.6554911562,1.9523806145
C,0,1.0731266784,-4.8432036816,0.2543618423
C,0,0.6636896693,-3.8028940213,2.3898213192
C,0,0.5415113682,-4.9012508308,1.542880954
H,0,2.1250713394,-3.6691815876,-1.1952284209
H,0,1.4109241334,-1.8003192092,2.6155073262

TS-3a (SR), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1761.58798469 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.422019 a.u.
1 imaginary frequency = 286.7632 i cm⁻¹

0; 1
C,0,4.2068080557,4.2250100015,-3.3284122773
C,0,4.1737742161,4.2286851026,-4.721644357
C,0,3.7724496522,3.0904024739,-5.4218731992
C,0,3.4059161665,1.9571625767,-4.7141662298
C,0,2.935884963,0.6147039129,-5.2121893671
C,0,3.8423331315,3.091926905,-2.6043326986
C,0,3.4442998995,1.9724721089,-3.323312063
N,0,3.0331380515,0.7168218928,-2.825924368
C,0,2.7867498417,-0.2356080836,-3.9296704529
C,0,3.8320691471,-1.3967476936,-3.8782618111
C,0,2.9560005685,0.3735258292,-1.5524015803
C,0,2.579775163,-0.8797241013,-1.0849537278
C,0,2.6046604984,-1.1269802035,0.2926908783
O,0,3.3626127423,-2.5485434267,-3.9613229081
O,0,5.0197633736,-1.0385212152,-3.7633325924
H,0,4.5236537571,5.1128685915,-2.7947509996
H,0,4.464086246,5.12028128,-5.2638553808
H,0,3.7505798347,3.0901186728,-6.505654925
H,0,3.8804099161,3.0998867283,-1.5223349016
H,0,1.7825029073,-0.6454753345,-3.8170919503
H,0,3.2118015564,1.1469602614,-0.8330674732
H,0,2.3287484292,-1.6664040612,-1.7864777232
H,0,2.6675255718,-0.2533586609,0.936417381
C,0,4.3771677354,-2.1263421707,3.7701662858
C,0,3.8387329668,-2.3193487653,5.0376287322
C,0,4.3960274772,-0.8512149786,3.2017870284
H,0,3.8327873291,-3.3107686426,5.474595454
C,0,3.2999632253,-1.2439022497,5.737722297
C,0,3.8780282989,0.2289493149,3.920164938
H,0,2.8692424287,-1.3973601072,6.720413819
H,0,3.9111168157,1.2151419357,3.4720485178
C,0,3.3214844853,0.0319799458,5.178056215
H,0,2.9062425963,0.8712615171,5.7233538639
H,0,4.7886081808,-2.9734173702,3.2342779851
C,0,4.9102703465,-0.5890528083,1.818729472
O,0,5.3091027404,0.5408751402,1.5016633112
C,0,4.7685423396,-1.6343110271,0.8589272167
H,0,4.6667945167,-2.6795884911,1.1144533812
S,0,5.5810143571,-1.2937900578,-0.6628804707
C,0,7.3430890376,-1.2752127589,-0.2445448076
H,0,7.4871041609,-0.4316851434,0.4274140985
H,0,7.614535911,-2.216170075,0.2296387122
H,0,7.8896231273,-1.1222043263,-1.1744349034
C,0,5.4435948776,-2.8899239432,-1.4828860412
H,0,4.4025164966,-3.0192770519,-1.775017915
H,0,6.0348181062,-2.8224243321,-2.3928236054
H,0,5.787450438,-3.671210488,-0.8063563328
C,0,1.9597343472,-2.3023315092,0.9029602676
C,0,1.8094759391,-3.5098125246,0.2085361768
C,0,1.4731805126,-2.2079665448,2.2110731924
C,0,1.1872610527,-4.5933501974,0.8119559137
C,0,0.8428974812,-3.2924773496,2.8115330739
C,0,0.700450435,-4.4873026116,2.1150592596
H,0,2.183042771,-3.6080702003,-0.805042197
H,0,1.5893780594,-1.2792045517,2.7605627899

H,0,0.9792832784,-5.6961389156,-0.4112525409
H,0,0.2495267364,-3.8374217221,3.3931402597
H,0,0.0329872901,-5.7987642042,1.8824321411
H,0,2.5358935224,0.7078884367,-5.915174781
H,0,4.2495668536,0.399341021,-5.5706002149

H,0,1.0780332749,-5.5227322056,0.2660254774
H,0,0.4672824682,-3.2018138156,3.8238829358
H,0,0.2124217698,-5.3346271059,2.5819608144
H,0,1.9858987326,0.7031181505,-5.7425369392
H,0,3.6641664721,0.1685168423,-5.891314223

TS-3a (RR), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1760.09312455 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.422991 a.u.
1 imaginary frequency = 206.5280 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.659264 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6858487 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.574249 a.u.
0; 1
C,0,0.5588156066,4.555425828,-1.9592859789
C,0,0.7441418368,4.7971207733,-3.318933087
C,0,1.3430671258,3.8300700605,-4.127811525
C,0,1.7690341715,2.6389776805,-3.5610734358
C,0,2.3585786587,1.4250291029,-4.2141161782
C,0,0.9868006471,3.3654558023,-1.3721266823
C,0,1.6172767173,2.4244758863,-2.1851899099
N,0,2.1078943449,1.1482926122,-1.8572043448
C,0,2.7577536018,0.538188701,-3.034438224
C,0,4.3215100317,0.4460216881,-2.8272980507
C,0,2.2819368744,0.5718962836,-0.6684253801
C,0,2.2136197765,1.1244461156,0.6025537694
C,0,2.5445437976,0.3181056487,1.6975309491
O,0,4.9968366906,0.524891656,-3.8628449519
O,0,4.7003986421,0.2517158078,-1.6429259852
H,0,0.0680218592,5.3004496199,-1.3403535737
H,0,0.4072073586,5.7335177387,-3.7528693728
H,0,1.465540073,4.0013440853,-5.1935701917
H,0,0.7941487106,3.1845426539,-0.3229961682
H,0,2.3986212351,-0.4912392421,-3.1425048571
H,0,2.5469053291,-0.4775788602,-0.7463091376
H,0,2.1132869514,2.1937912976,0.7291106642
H,0,2.4842378044,-0.7579728092,1.5602768372
C,0,4.6725789983,-2.9857598663,0.8732418074
C,0,4.3526237587,-4.3346010822,0.7448527087
C,0,4.9524308057,-2.4434506893,2.1337082281
H,0,4.1514737705,-4.7484421453,-0.2390067453
C,0,4.2989389144,-5.1534053538,1.8705639547
C,0,4.9147020129,-3.2791085731,3.25575983
H,0,4.0448244224,-6.2044236003,1.7671632725
H,0,5.1578104118,-2.8476416127,4.2219658523
C,0,4.5820754368,-4.6223267716,3.1282009319
H,0,4.5478274392,-5.2587152375,4.0079612389
H,0,4.7379637223,-2.3695574606,-0.019402943
C,0,5.3315792815,-1.002568066,2.3533676591
O,0,5.9532574847,-0.6966986926,3.3835264155
C,0,4.831354778,-0.0770917209,1.3840859579
H,0,4.549938157,-0.4111891046,0.3927457476
S,0,5.4594984123,1.5354013413,1.1716628633
C,0,7.0285093261,1.3280288326,0.2988037056
H,0,7.4791837937,2.313129044,0.1581188221
H,0,7.6855493718,0.6668241258,0.8656395004
H,0,6.7419498254,0.8922139752,-0.6626077099
C,0,5.993814417,2.144347088,2.7821267242
H,0,6.4127816304,3.1376597808,2.6103074927
H,0,5.1053846464,2.2173675653,3.4104804228
H,0,6.7064571017,1.4555573282,3.2291785464
C,0,2.4759242755,0.7607391216,3.092069502
C,0,2.3438726787,2.1119354568,3.4534259368
C,0,2.5237537218,-0.2008389307,4.113854645
C,0,2.2683685676,2.483562059,4.790196556
C,0,2.4415308593,0.1716418612,5.4494174053
C,0,2.3161639182,1.5158062444,5.7930625341
H,0,2.3004679972,2.8817012415,2.6889741633
H,0,2.628709003,-1.2499283126,3.8501710381

TS-3a (RR), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1761.57667404 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.421022 a.u.
1 imaginary frequency = 250.1578 i cm⁻¹
0; 1
C,0,0.5061367099,4.4384037018,-1.9919081515
C,0,0.7198811914,4.6826715928,-3.3454611741
C,0,1.3463554546,3.723589954,-4.1413248265
C,0,1.7730646115,2.5402591647,-3.5633272439
C,0,2.3681328435,1.319996407,-4.2131902089
C,0,0.9361979663,3.2545189402,-1.3944242211
C,0,1.5983299976,2.3270427691,-2.1933938204
N,0,2.100929803,1.0479668245,-1.8553239876
C,0,2.8074663721,0.4647490055,-3.0197084159
C,0,4.370988573,0.4784082254,-2.7848133418
C,0,2.2705861417,0.4943313257,-0.6641004293
C,0,2.1821247555,1.0749633212,0.5962347149
C,0,2.5186165499,0.2954335276,1.6998848585
O,0,5.0442674639,0.3969032711,-3.8194808395
O,0,4.7512139142,0.5187696241,-1.5939406016
H,0,-0.0085493755,5.1748063205,-1.3868232888
H,0,0.3812382608,5.6131503882,-3.7846462455
H,0,1.487434808,3.8932435249,-5.2026992757
H,0,0.7183256487,3.0726310159,-0.3531080022
H,0,2.5192921459,-0.5837880831,-3.1225363892
H,0,2.5745590203,-0.5476523529,-0.7160011285
H,0,2.0943120284,2.1451964846,0.6927635973
H,0,2.4666644629,-0.783919719,1.5989867309
C,0,4.6935570338,-2.9546633031,0.7657121436
C,0,4.3296660943,-4.2826562421,0.5650500213
C,0,4.8628757465,-2.4601313708,2.0622143663
H,0,4.2173153579,-4.6628461028,-0.4434432646
C,0,4.1195684328,-5.1236383443,1.6542577016
C,0,4.6676406211,-3.3155468954,3.1487573015
H,0,3.8320676362,-6.1562163232,1.4944325831
H,0,4.8227484893,-2.9242597164,4.1478222368
C,0,4.2891583127,-4.637570394,2.9484179656
H,0,4.1313973172,-5.2909764663,3.7984851752
H,0,4.8777935045,-2.3195692777,-0.0941680892
C,0,5.2615978514,-1.0325911398,2.3581806351
O,0,5.8002443623,-0.774653126,3.4417020784
C,0,4.838232504,-0.0758314644,1.3960121667
H,0,4.5985869618,-0.356215558,0.381804226
S,0,5.3786457125,1.5852069497,1.3602220787
C,0,6.9775886931,1.5409539993,0.5101780949
H,0,7.3773628271,2.5546604924,0.4920609976
H,0,7.6382912104,0.8566710179,1.0399268273
H,0,6.747115026,1.1905393012,-0.4958783475
C,0,5.886501474,2.0359076145,3.0391583075
H,0,6.0723840573,3.1089822149,3.0110478556
H,0,5.0613255219,1.8036587924,3.7088561351
H,0,6.7678312558,1.470963136,3.3238350489
C,0,2.5375372357,0.8009459954,3.0775155137
C,0,2.3537028483,2.1573844058,3.3839687681
C,0,2.7787403173,-0.0996779003,4.1237456959
C,0,2.419696105,2.5957934567,4.6999682731
C,0,2.8450744816,0.3403253862,5.4384818857
C,0,2.6705344266,1.6908738453,5.7297811954
H,0,2.1614114372,2.8783710876,2.5989577825
H,0,2.9254636087,-1.1501384425,3.8953742234

H,0,2.1658366981,3.532694615,5.0513062625
H,0,2.4781365296,-0.588239718,6.2241050462
H,0,2.2543765757,1.8092747868,6.8366768832
H,0,1.6228799603,0.9438453954,-4.8682900805
H,0,3.2532664512,1.6305919449,-4.8088023611

H,0,2.2755063008,3.6460822236,4.9233662051
H,0,3.0393208568,-0.3683846955,6.2343427192
H,0,2.7257010497,2.0376466001,6.7547622106
H,0,1.6114764661,0.8153437804,-4.8191164608
H,0,3.2247445147,1.5388852297,-4.8496395668

TS-3a (RS), optimization in solv. CHCl₃
PBE1PBE/6-311G(d,p), E = -1760.09522398 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.424641 a.u.
1 imaginary frequency = 210.7598 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.663424 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6901899 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.5795125 a.u.
0; 1

C,0,1.8695334111,4.3366884978,-2.9430571818
C,0,1.8777946086,4.0391197699,-4.304016164
C,0,1.8040594467,2.7122911215,-4.7309386012
C,0,1.740612607,1.6977457656,-3.7889536361
C,0,1.5911328715,0.2194329487,-3.9880530166
C,0,1.8116122863,3.3273789794,-1.9823565125
C,0,1.7714343841,2.0050045834,-2.4225372434
N,0,1.6991098572,0.8153753853,-1.6765347101
C,0,1.7448027735,-0.3553800962,-2.5773196115
C,0,3.0620037916,-1.2018407934,-2.3895908085
C,0,1.8426160013,0.6010550368,-0.3686549952
C,0,2.1947734932,1.4608725128,0.6594692823
C,0,2.4594830962,0.8867057045,1.9104001626
O,0,3.3578526497,-1.9051756454,-3.3659859462
O,0,3.6236878367,-1.1247524222,-1.2654856201
H,0,1.9039523209,5.3714660624,-2.6158434169
H,0,1.9276719383,4.8416662703,-5.0334504092
H,0,1.7872192083,2.4739510116,-5.7907122713
H,0,1.7706858718,3.5902660129,-0.9344031061
H,0,0.9190009536,-1.0268791587,-2.3175150524
H,0,1.690886437,-0.4396867744,-0.1061989548
H,0,2.4564886212,2.4928004465,0.4770097793
H,0,2.0620418248,-0.1136967602,2.0670948204
C,0,5.3079788469,2.1426863811,-0.1809020062
C,0,5.5659424662,3.2906354896,-0.9268049802
C,0,5.7128869853,2.0699281379,1.1586416688
H,0,5.2487406237,3.3386735896,-1.9643359005
C,0,6.2282007839,4.3698541094,-0.3472749736
C,0,6.388873273,3.1560215274,1.7284757027
H,0,6.4283580053,5.2626275118,-0.9331300815
H,0,6.702047303,3.0748599417,2.764459664
C,0,6.6420434864,4.2998118731,0.9835250762
H,0,7.1630866099,5.1386189701,1.4363820488
H,0,4.8106270044,1.301431342,-0.6556138015
C,0,5.4702553283,0.8749852807,2.0210584273
O,0,6.0414914594,0.7668476533,3.1231885782
C,0,4.531382401,-0.1068157216,1.571624862
H,0,4.3130928646,-0.3053019219,0.5250711848
S,0,4.6353149307,-1.5607595273,2.5477882611
C,0,3.5925171285,-2.6900304719,1.6029821542
H,0,3.7479066104,-2.5334384799,0.53019781
H,0,3.8466471419,-3.7061777116,1.9084170846
H,0,2.5539792344,-2.4889114624,1.8701873585
C,0,6.2710775855,-2.2664876268,2.2128531268
H,0,6.3566205368,-3.2106014383,2.7547334676
H,0,6.3925879356,-2.4097865472,1.1382894283
H,0,6.9871427609,-1.5396525729,2.5968389936
C,0,2.677182621,1.6413474835,3.1455714826
C,0,3.0231247431,3.0013605068,3.1512073821
C,0,2.5085970234,0.9890350675,4.3762741702
C,0,3.1821396536,3.6837655097,4.3507286861
C,0,2.6662408421,1.6724784088,5.5750493334
C,0,3.0021659542,3.0244725099,5.5655467719
H,0,3.1768960907,3.529041574,2.2156466663
H,0,2.240255427,-0.0645667052,4.3864155963

TS-3a (RS), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1761.58422431 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.424300 a.u.
1 imaginary frequency = 234.1758 i cm⁻¹

0; 1
C,0,-3.7327509725,-2.7333584552,-0.9607355112
C,0,-4.8478685895,-2.3777023829,-0.2059902041
C,0,-5.0855311523,-1.0398788398,0.1165866503
C,0,-4.1826887573,-0.0764568373,-0.3004130899
C,0,-4.1919302638,1.4146948866,-0.0915547396
C,0,-2.8160948904,-1.7733454133,-1.3851055166
C,0,-3.0436367444,-0.4546183894,-1.0112608331
N,0,-2.2677800152,0.6920106931,-1.3007052802
C,0,-3.0442098679,1.9215012075,-0.9966325251
C,0,-2.2340801385,3.0276383852,-0.2550492203
C,0,-0.9741141347,0.7560185556,-1.5750567583
C,0,-0.0207162098,-0.2525583465,-1.5355842888
C,0,1.3132468459,0.155453133,-1.5388197664
O,0,-2.7376766469,4.1561324,-0.3464605227
O,0,-1.2210199392,2.6645122888,0.3850089865
H,0,-3.5748949403,-3.7699335239,-1.2328258368
H,0,-5.5465672089,-3.1410230064,0.1142777432
H,0,-5.9667468855,-0.7574289731,0.6814325634
H,0,-1.9781888113,-2.0575576074,-2.0053875268
H,0,-3.4354433942,2.3282348092,-1.9306879282
H,0,-0.6238440349,1.763404352,-1.7713268142
H,0,-0.2819114196,-1.2600383291,-1.2514425716
H,0,1.5200270451,1.1453124156,-1.9350686578
C,0,-0.5780124604,-0.6841190537,1.551638371
C,0,-1.5492779342,-1.6470069494,1.816850951
C,0,0.7785860676,-1.0130986506,1.6548982783
H,0,-2.600064456,-1.3895438771,1.7356523965
C,0,-1.1768354588,-2.9385929668,2.1751166334
C,0,1.1439471306,-2.309928535,2.0283523743
H,0,-1.937705089,-3.6854687779,2.3721211098
H,0,2.1995254562,-2.5432990898,2.1032984779
C,0,0.1734199953,-3.2700451,2.2816051106
H,0,0.4656265136,-4.2752888753,2.5624963822
H,0,-0.8896121229,0.3197012338,1.2753777841
C,0,1.8801924563,-0.0370457764,1.3617765137
O,0,3.0458674413,-0.2844136958,1.7056556138
C,0,1.5369873079,1.1201085754,0.6055725294
H,0,0.5470247893,1.5602709657,0.5851423056
S,0,2.830080126,2.3032750097,0.5479828398
C,0,1.9612821122,3.6864925238,-0.2249341224
H,0,0.9571493809,3.7599314923,0.1966499293
H,0,2.5484720151,4.5842209676,-0.039800963
H,0,1.9164394217,3.4949788321,-1.2955579047
C,0,2.9664154055,2.9254587652,2.2486750341
H,0,3.7014221141,3.7292099147,2.2581821879
H,0,1.985099928,3.2693241093,2.5708986019
H,0,3.3075957305,2.0819412687,2.8455450354
C,0,2.4640662443,-0.7500790513,-1.5095014588
C,0,2.3396246261,-2.1038639098,-1.1721646989
C,0,3.7333130955,-0.2438351203,-1.8165358509
C,0,3.457509127,-2.9273029836,-1.1521186983
C,0,4.8493066349,-1.0687877796,-1.7988520031
C,0,4.7130864819,-2.4138369157,-1.465917432
H,0,1.3720959591,-2.518586616,-0.9155279952
H,0,3.8402517159,0.8039743798,-2.0789176442

H,0,3.4493096782,4.7362340095,4.3379218002
H,0,2.5254446363,1.1511868169,6.5170924687
H,0,3.1257479848,3.5622727882,6.5008164174
H,0,0.6140934345,-0.0136915359,-4.4257980434
H,0,2.3544200212,-0.2205577496,-4.635722995

H,0,3.3490155941,-3.9723328531,-0.887300493
H,0,5.8242610926,-0.6643997399,-2.0427266454
H,0,5.5834159993,-3.0590887064,-1.449039232
H,0,-5.143415139,1.8740088478,-0.3559024089
H,0,-3.981433176,1.6512921152,0.9561797388

TS-3a (RS) 2, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -1760.09703913 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.426824 a.u.
1 imaginary frequency = 210.7973 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6650683 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6918771 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.5820366 a.u.

0; 1
C,0,3.093694759,1.8180234914,-3.8598866974
C,0,2.0986343292,2.4083254273,-4.6381326956
C,0,0.802819552,2.5508535022,-4.1375484189
C,0,0.520302734,2.1044171078,-2.8560007138
C,0,-0.758388994,2.1503575385,-2.0721888882
C,0,2.8225448504,1.3601460755,-2.5713043722
C,0,1.5283206258,1.5225281112,-2.0868289802
N,0,1.0164356208,1.1608475693,-0.8277964068
C,0,-0.4425391857,1.3272052433,-0.8021651735
C,0,-1.213766785,-0.0248846258,-0.8111508622
C,0,1.7734795376,0.7888031385,0.2050381218
C,0,1.4315864855,0.3324608478,1.4702496257
C,0,0.189305941,-0.0816445869,1.9740049296
O,0,-2.3310876149,0.0401375763,-0.2428111893
O,0,-0.662497214,-0.9987340216,-1.3641187437
H,0,4.0947581926,1.6996650011,-4.2633981661
H,0,2.3305277962,2.7499337026,-5.6421214134
H,0,0.0246990731,3.0047027473,-4.744719834
H,0,3.5978921215,0.8744343676,-1.9880050911
H,0,-0.7069588246,1.8714850338,0.1084812759
H,0,2.8370334018,0.908864312,0.0190514564
H,0,2.2910692967,0.2289513379,2.1253680273
H,0,-0.7075164211,0.0890808511,1.3880300445
C,0,2.353031051,-2.277234898,-0.3671857494
C,0,3.5128316,-2.225358072,-1.1381013988
C,0,2.4075386613,-2.7645577932,0.9459260349
H,0,3.459758898,-1.8556545947,-2.1583721458
C,0,4.7307886123,-2.6473464901,-0.6102108785
C,0,3.6360076257,-3.1875357736,1.4674376359
H,0,5.6309391206,-2.6072301499,-1.2173710393
H,0,3.6539551585,-3.5665792177,2.4845215289
C,0,4.7909351435,-3.1269982416,0.6983186032
H,0,5.7384758188,-3.4577417799,1.11425039
H,0,1.415971909,-1.9302315709,-0.7976113914
C,0,1.205750557,-2.8871977098,1.8262168093
O,0,1.3103850565,-3.4117556444,2.9547858034
C,0,-0.0417077425,-2.3758152148,1.3603017609
H,0,-0.2787895016,-2.1655870963,0.3186491246
S,0,-1.3988016263,-2.951134078,2.3164347948
C,0,-2.7774650378,-2.6655553256,1.1927662139
H,0,-2.7171683109,-3.3728837629,0.3635003921
H,0,-3.6986240301,-2.8117507202,1.7586094587
H,0,-2.707166409,-1.641597274,0.7932661835
C,0,-1.3202133828,-4.7622383619,2.2913331416
H,0,-2.2162263126,-5.1354827084,2.7914583351
H,0,-1.2673839282,-5.1138629259,1.2598581293
H,0,-0.4227045909,-5.0336520266,2.8459328935
C,0,-0.0596159534,-0.20365433,3.4120647703
C,0,0.935429226,-0.5445518289,4.3419094516
C,0,-1.3555993502,0.0645216094,3.8832913962
C,0,0.6415911585,-0.5980821497,5.6983051384
C,0,-1.6439580029,0.0205744814,5.2418849504
C,0,-0.6445954363,-0.3108340845,6.1540307116
H,0,1.9363776556,-0.7901990682,4.003541586
H,0,-2.1324879025,0.329738031,3.1699500673

TS-3a (RR) 2, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -1760.09175693 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.425592 a.u.
1 imaginary frequency = 191.0416 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6610557 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6877309 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.5779569 a.u.

0; 1
C,0,1.8269607313,5.332292464,-1.5694573997
C,0,0.5209009756,5.8075465635,-1.6874223063
C,0,-0.5615329926,4.9877221726,-1.3642367537
C,0,-0.3219574377,3.6964378991,-0.9192485823
C,0,-1.2793112983,2.6245656588,-0.4891053601
C,0,2.0823777936,4.0353905665,-1.1284624782
C,0,0.9903684144,3.2379435471,-0.8016224623
N,0,0.9864982501,1.9119219871,-0.3265012183
C,0,-0.3814654755,1.3815841875,-0.3118268976
C,0,-0.6352064257,0.3396137634,-1.445175527
C,0,2.0713958329,1.2568952593,0.0755035414
C,0,2.2384657483,-0.0515536199,0.5212901061
C,0,1.35148095,-1.1396366262,0.5262170751
O,0,0.122210165,0.3842199846,-2.4390599827
O,0,-1.5916848107,-0.4261064178,-1.2063617215
H,0,2.6607669233,5.9748189023,-1.8351547946
H,0,0.3455552415,6.8185973255,-2.0415896632
H,0,-1.5791985698,5.3546557099,-1.4616392462
H,0,3.1027210338,3.6711669913,-1.0670205634
H,0,-0.5492015293,0.8951038764,0.6527082655
H,0,2.9611335154,1.880296742,0.1036485511
H,0,3.2274207864,-0.2226012627,0.9355288867
H,0,0.3269720099,-1.01266699,0.1940486739
C,0,-1.0000946017,-3.6275527473,-1.4285780196
C,0,-2.204627754,-4.3247477793,-1.3793008247
C,0,0.2080599403,-4.3127612315,-1.2450578557
H,0,-3.1377386461,-3.7856923839,-1.515980513
C,0,-2.2189042254,-5.6998261262,-1.1556098167
C,0,0.1855518067,-5.6927670112,-1.0125312123
H,0,-3.1629533684,-6.2369190108,-1.1234514793
H,0,1.1340699349,-6.1990572433,-0.8647879657
C,0,-1.0180658558,-6.3843969074,-0.9709184211
H,0,-1.0229110978,-7.4563573073,-0.7937789198
H,0,-1.0305488215,-2.5502407473,-1.5868930138
C,0,1.5473074246,-3.6494777457,-1.2873203204
O,0,2.5748297447,-4.301125081,-1.0018846933
C,0,1.6334460345,-2.2728430676,-1.637340314
H,0,0.8837806136,-1.6935426965,-2.1690784118
S,0,3.2873292775,-1.765172594,-1.9281843049
C,0,3.0502292977,-0.2573044584,-2.8905396967
H,0,3.9686265001,0.3271655574,-2.8291471486
H,0,2.830895085,-0.5240649168,-3.9257505573
H,0,2.1862845579,0.2772448974,-2.4808116286
C,0,3.9692846201,-2.852598146,-3.2076903871
H,0,4.9588718398,-2.4709701801,-3.467360071
H,0,4.0342061375,-3.8430348812,-2.7597871921
H,0,3.3076751369,-2.8570373077,-4.0750550794
C,0,1.5651918198,-2.2848090678,1.4091455502
C,0,2.8331153591,-2.6801363331,1.8665274056
C,0,0.4400008205,-2.9956252186,1.8584397845
C,0,2.964445223,-3.7345355652,2.7598434091
C,0,0.5732747501,-4.0428508106,2.7611181571
C,0,1.8361821417,-4.4144579499,3.216430519
H,0,3.7245898257,-2.1713781745,1.5133682573
H,0,-0.5446516883,-2.709847376,1.4995275309

H,0,1.4199628103,-0.8687481814,6.4055368
H,0,-2.6480783812,0.2457410754,5.5888720744
H,0,-0.8665853059,-0.3491518254,7.2164656922
H,0,-1.0266957063,3.1822511597,-1.8191290127
H,0,-1.601985429,1.7232087933,-2.6216790908

H,0,3.9521832896,-4.0303564678,3.1006198898
H,0,-0.3098698242,-4.5717627299,3.1064331197
H,0,1.9428558869,-5.2351874355,3.9196432142
H,0,-1.7728059306,2.8964980476,0.4508756317
H,0,-2.0669050863,2.4396415125,-1.2246427645

TS-3a (RR) 3, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1760.08935124 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.421833 a.u.
1 imaginary frequency = 222.4418 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.657238 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6834328 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.5705861 a.u.

0; 1
C,0,1.4296979958,5.1585574314,-2.7926365248
C,0,1.5750677896,5.1573747695,-4.1798181115
C,0,1.9899576695,4.0016930102,-4.8443492151
C,0,2.2422365008,2.8518605927,-4.111319175
C,0,2.7469442841,1.510227634,-4.5499547151
C,0,1.6843035314,4.0122577013,-2.0422428803
C,0,2.0765926393,2.8645031382,-2.7260172182
N,0,2.3555303394,1.5925298209,-2.1991045584
C,0,2.7078443707,0.6381481662,-3.2849686601
C,0,4.0689200342,-0.1276335923,-3.0515168225
C,0,2.1387793496,1.2335323522,-0.93030781
C,0,2.5068017598,0.0155331782,-0.3999492344
C,0,2.1606738075,-0.3906303594,0.8937817303
O,0,5.098744395,0.5266153381,-3.2718093036
O,0,3.9517446769,-1.3262537047,-2.6782490354
H,0,1.1197822131,6.0660397834,-2.2833240806
H,0,1.3745813659,6.0630942635,-4.7437892508
H,0,2.1184040641,4.0027871132,-5.9230768141
H,0,1.584857486,4.0349728079,-0.9619060871
H,0,1.9011940913,-0.1021033588,-3.3171088507
H,0,1.6566106663,1.9841733312,-0.3075696809
H,0,3.084126131,-0.6504886851,-1.033439823
H,0,1.5873341219,0.3006351728,1.5103254419
C,0,-1.2972245275,0.7019240993,1.637685776
C,0,-1.9917057884,1.7738697537,2.1889311389
C,0,-1.1153800075,-0.4771926077,2.3711610686
H,0,-2.1285045727,2.682755282,1.6105384491
C,0,-2.5120671462,1.6813290147,3.4781824466
C,0,-1.6409027012,-0.5583033625,3.6655113386
H,0,-3.0556832289,2.5186876807,3.9058378795
H,0,-1.4905480005,-1.4792984784,4.2195293752
C,0,-2.3343171527,0.5121717227,4.2160466397
H,0,-2.7384852944,0.4364488578,5.221262899
H,0,-0.9019813232,0.7933748614,0.6302922872
C,0,-0.3840844623,-1.6737993118,1.8492111767
O,0,-0.2386611578,-2.6785298418,2.5726033713
C,0,0.1985169151,-1.6231404014,0.5459669864
H,0,-0.1805634385,-0.9994998143,-0.2548348196
S,0,0.7934263681,-3.1975953154,0.045862596
C,0,1.1468605101,-2.9632094662,-1.7055975307
H,0,1.3017769369,-3.9593120703,-2.124121131
H,0,0.2974808868,-2.481022345,-2.1943289812
H,0,2.0621944607,-2.3760952396,-1.8428136198
C,0,-0.6625895181,-4.2697225683,-0.0591067927
H,0,-0.3277011729,-5.2531207642,-0.3957411511
H,0,-1.0585102271,-4.3292227433,0.9545577245
H,0,-1.3941953598,-3.8444832715,-0.7472525828
C,0,2.9356205775,-1.3901623158,1.6303749703
C,0,3.955190824,-2.1413625599,1.0165887976
C,0,2.6866766684,-1.5820539047,2.999031729
C,0,4.6901547881,-3.0583233868,1.7560177925
C,0,3.429845933,-2.4962236943,3.734889975
C,0,4.4309485948,-3.2396082131,3.1144219795
H,0,4.1913425265,-1.9955313959,-0.0344984719
H,0,1.9066856954,-1.0033910602,3.484886892

TS-3a (RS) 3, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1760.09024803 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.423758 a.u.
1 imaginary frequency = 272.8712 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6595069 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6860569 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.5752546 a.u.

0; 1
C,0,2.3476258027,3.6929331346,-3.4982168589
C,0,2.2482869598,3.1455448891,-4.7770249213
C,0,2.0800462927,1.7694441162,-4.9433018837
C,0,2.0024111445,0.9554708448,-3.823399146
C,0,1.8827447947,-0.5344285102,-3.7092647035
C,0,2.2744444477,2.8873456721,-2.3631005702
C,0,2.0906943758,1.5197876397,-2.5502080403
N,0,1.9555371143,0.5187774239,-1.5740646042
C,0,1.6986742372,-0.8028941643,-2.2077077384
C,0,2.6446706893,-1.9586977779,-1.6930996133
C,0,1.8395337616,0.7506730694,-0.2649460529
C,0,1.7359003482,-0.243009255,0.68577968
C,0,1.5227366044,0.0207783035,2.0434060191
O,0,3.8020269517,-1.9440864165,-2.1405734206
O,0,2.1092944709,-2.7748210639,-0.8963539918
H,0,2.4870916285,4.7631911099,-3.3787639064
H,0,2.3091854785,3.7922517878,-5.6469508777
H,0,2.0132171135,1.3392318614,-5.9386729772
H,0,2.3621421007,3.3289933613,-1.3757248902
H,0,0.6656134176,-1.0668444109,-1.9567803511
H,0,1.8465647007,1.7975960204,0.0292315021
H,0,1.8100594064,-1.2690336406,0.3407311502
H,0,1.575734452,1.0576622165,2.3726128738
C,0,-0.572248094,3.0675176735,3.0229518217
C,0,-0.3075110436,4.4189455164,3.2215591195
C,0,-0.781582603,2.5691550822,1.7310320448
H,0,-0.155675042,4.7959458595,4.2285120742
C,0,-0.2414024928,5.2866906698,2.1336894951
C,0,-0.7244466426,3.4529513831,0.6457093676
H,0,-0.0308881709,6.3403715606,2.2916388975
H,0,-0.8999238846,3.0550792828,-0.3487831024
C,0,-0.4510664191,4.8006400567,0.8440823209
H,0,-0.4036990672,5.4742582816,-0.0065343368
H,0,-0.6371266668,2.4136621622,3.8872346924
C,0,-1.0641458232,1.129785338,1.4254430113
O,0,-1.4930276494,0.8196418398,0.3033253609
C,0,-0.6828955628,0.144066057,2.3987264973
H,0,-0.5722277806,0.3985146186,3.4460762563
S,0,-1.3345432037,-1.4800761942,2.2828104238
C,0,-3.1274612838,-1.2628444074,2.1495812372
H,0,-3.3406445009,-0.5974467834,1.3123515034
H,0,-3.5756967099,-2.2476688935,2.0012121337
H,0,-3.4719874781,-0.8350237619,3.0915148226
C,0,-1.0003911712,-2.1453179674,0.6353641535
H,0,-1.5892306943,-3.0626599433,0.5727512594
H,0,-1.3111213409,-1.4084250725,-0.1031026852
H,0,0.0573983375,-2.3868119039,0.5234930345
C,0,1.8589758234,-0.9736686403,3.0801504143
C,0,2.1971685267,-2.298940253,2.7611754008
C,0,1.8760975689,-0.5811268862,4.4273739134
C,0,2.5197052086,-3.2014133947,3.7692978973
C,0,2.2040810515,-1.4838361997,5.4303415764
C,0,2.5207933191,-2.801574959,5.1037455501
H,0,2.243287942,-2.6244392135,1.7244942865
H,0,1.6380684199,0.4486476462,4.6851080667

H,0,5.478241419,-3.6273628601,1.2721293276
H,0,3.2273671945,-2.6285559986,4.7933180309
H,0,5.0136948289,-3.9538798432,3.6886762036
H,0,2.1541835274,1.0771873616,-5.360905387
H,0,3.7888451514,1.5845599058,-4.8807239436

H,0,2.7845340738,-4.2213876229,3.5072483119
H,0,2.2182824851,-1.1594456667,6.4666348437
H,0,2.7784395793,-3.5101333727,5.8853044422
H,0,1.0577411687,-0.9427186667,-4.2998924303
H,0,2.8137385279,-1.0171064365,-4.0279853538

TS-3a (SR) 2, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -1760.08790569 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.425320 a.u.
1 imaginary frequency = 171.7190 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6557762 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6824388 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.5725112 a.u.
0; 1
C,0,5.8316512792,4.0981670478,0.744050357
C,0,6.0630846838,5.3132005538,0.1005129155
C,0,4.9891835868,6.1227926122,-0.2702642667
C,0,3.6936958149,5.6985239028,-0.0119804884
C,0,2.396325657,6.4216154845,-0.2120248632
C,0,4.5368023246,3.6501472592,0.9976944046
C,0,3.4711309611,4.4518299716,0.5862194694
N,0,2.0901781684,4.2740986864,0.7980726246
C,0,1.3389317046,5.4121888479,0.2279248996
C,0,0.4595524412,4.8430093933,-0.9483320493
C,0,1.4079558764,3.2586670946,1.3471035131
C,0,1.7359137102,1.9048457948,1.3912161053
C,0,2.5575541391,1.2621711455,0.466828755
O,0,0.5632616984,5.395054074,-2.0581578201
O,0,-0.2442144786,3.8589046875,-0.61659795
H,0,6.6705117557,3.4840193562,1.0574848159
H,0,7.0803621331,5.6365753202,-0.0972854662
H,0,5.1619227841,7.086789419,-0.7405664479
H,0,4.3753502536,2.7167216608,1.5227668238
H,0,0.6530396954,5.8031958921,0.9878242886
H,0,0.4643485962,3.5663329944,1.7885666493
H,0,1.1253570158,1.3078373269,2.0601408357
H,0,3.1898909403,1.8819788713,-0.1589755324
C,0,-1.2016496903,0.7834138176,0.2276134634
C,0,-2.2134195414,0.5245378305,1.1499951504
C,0,-0.5291118902,-0.2810981899,-0.3869186107
H,0,-2.7389731659,1.3534801476,1.6158971881
C,0,-2.5589004006,-0.7863013831,1.4698677193
C,0,-0.8893536536,-1.5958966076,-0.0675668702
H,0,-3.3491743711,-0.9809327472,2.1897095801
H,0,-0.3586066174,-2.4033518085,-0.5620251013
C,0,-1.8935959231,-1.8488291902,0.8577568192
H,0,-2.1622152203,-2.8728524357,1.1019334729
H,0,-0.9559693894,1.8126761688,-0.0209069794
C,0,0.5592257796,-0.0892358916,-1.3928004373
O,0,0.9604957159,-1.0577373009,-2.0706519732
C,0,1.1542353149,1.2006278897,-1.5259104601
H,0,0.6610656931,2.1414400189,-1.2816606544
S,0,2.2285162179,1.2406871187,-2.9052555415
C,0,1.1850638665,1.0879059523,-4.3803732374
H,0,0.4208096981,1.8661855653,-4.3695196461
H,0,1.8239734147,1.1683231007,-5.2620659712
H,0,0.7392294567,0.0951809132,-4.3189350493
C,0,2.6768539053,2.9823551441,-3.0048458301
H,0,3.3592629896,3.2025457077,-2.1818795764
H,0,3.2041282607,3.123812522,-3.9499713746
H,0,1.7962887124,3.6303222722,-2.9449985108
C,0,2.990435142,-0.1286091407,0.5594776399
C,0,2.3682149421,-1.068108611,1.3979607347
C,0,4.1027789827,-0.5380277459,-0.1940402691
C,0,2.8550669402,-2.3652472934,1.4865865081
C,0,4.5899347436,-1.83513659,-0.1020591819
C,0,3.9677613086,-2.7531362428,0.7410740089
H,0,1.4953247124,-0.7877266465,1.9779404217
H,0,4.5932388332,0.1778808127,-0.8489851191

TS-3a (SS) 2, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -1760.08727220 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.424171 a.u.
1 imaginary frequency = 209.3239 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6563505 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6830975 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.5731623 a.u.
0; 1
C,0,5.6836335253,4.3174689425,0.0814087831
C,0,5.7197651045,5.5786516046,-0.5110381052
C,0,4.5498715507,6.3306531229,-0.6269693972
C,0,3.3514468166,5.8009069112,-0.1718791144
C,0,2.0008861635,6.4448707333,-0.0754794182
C,0,4.4865346622,3.7656302562,0.5328163494
C,0,3.3184606996,4.5101325424,0.3711020358
N,0,2.0143507404,4.2221335269,0.8102452592
C,0,1.1081703762,5.3412169599,0.4982479561
C,0,-0.0311141927,4.8791740484,-0.4817223602
C,0,1.4908702663,3.128760366,1.3757115141
C,0,1.9009354946,1.796841442,1.3395495767
C,0,2.6211664461,1.1777837417,0.3150563259
O,0,-0.5476708523,5.7853886462,-1.1503966324
O,0,-0.312509878,3.6537812558,-0.4332570445
H,0,6.601224269,3.7487680977,0.1977005201
H,0,6.6626165897,5.9843013851,-0.8646654739
H,0,4.5770918478,7.3309001722,-1.0504679037
H,0,4.4814573525,2.799335489,1.0214984768
H,0,0.6034251271,5.6525954197,1.4210558545
H,0,0.6033794061,3.3506312045,1.9632565557
H,0,1.4173385611,1.1710947902,2.0833320275
H,0,3.1765723009,1.8062108667,-0.3730785501
C,0,2.8643997041,3.0452130857,-2.9655067201
C,0,3.7727859226,3.9096509273,-3.5689104261
C,0,2.9298455423,1.668577147,-3.2113762254
H,0,3.7142673723,4.9747837227,-3.3677127907
C,0,4.757170957,3.4094612283,-4.4179076804
C,0,3.9175547011,1.1766845151,-4.0731606672
H,0,5.4665845854,4.0863430588,-4.8854581813
H,0,3.9447115014,0.1075786259,-4.2587572215
C,0,4.8278631458,2.0396225657,-4.6697029263
H,0,5.5925409979,1.6469912408,-5.3339454128
H,0,2.0949223395,3.4517858656,-2.3160393327
C,0,1.9855063713,0.6805532095,-2.6039792976
O,0,1.9926705396,-0.5048925495,-2.9960242618
C,0,1.1381448117,1.0967858681,-1.5361117865
H,0,0.7840008536,2.1095921432,-1.3538784956
S,0,-0.0245629481,-0.1569032015,-1.1465458978
C,0,-1.1239669506,0.6875085069,0.0061506766
H,0,-1.2744423595,1.7243601629,-0.3071979529
H,0,-2.0562423262,0.1211463456,0.0346484585
H,0,-0.6541419932,0.6634211836,0.9885717187
C,0,-1.1089915414,-0.2752341207,-2.5935931705
H,0,-0.4736971368,-0.6168217552,-3.4106674633
H,0,-1.8839976323,-1.0136360709,-2.3778245125
H,0,-1.5408199528,0.702781909,-2.8101445272
C,0,3.0786140986,-0.2126505108,0.3739139152
C,0,2.567328717,-1.1482914582,1.2891912889
C,0,4.0976297911,-0.6260192017,-0.4998406747
C,0,3.0660254879,-2.4430965304,1.3324924871
C,0,4.6016795468,-1.9197955686,-0.4492352423
C,0,4.0872755986,-2.8334760042,0.4667340512
H,0,1.7780266841,-0.8674698062,1.9795894526
H,0,4.499992082,0.082909061,-1.2181946253

H,0,2.3627501884,-3.0796311681,2.1396144324
H,0,5.4552577478,-2.1305369081,-0.6876691918
H,0,4.3455676343,-3.7685438806,0.8151256487
H,0,2.367673714,7.3450757926,0.3755324153
H,0,2.2014922076,6.6736626104,-1.2601611906

H,0,2.6593570336,-3.1516867165,2.0479454722
H,0,5.3949905631,-2.2154093724,-1.1290393882
H,0,4.4776496806,-3.8460416618,0.5062993202
H,0,2.0387523531,7.3290006373,0.5695358629
H,0,1.5902734819,6.763553993,-1.0384730584

TS-3a (SS) 3, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1760.08542318 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.423155 a.u.
1 imaginary frequency = 249.6512 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6557372 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.68221a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.5707977 a.u.
0; 1
C,0,1.6048252996,4.094257351,-3.1442126103
C,0,1.8759701869,3.737511987,-4.4634031222
C,0,2.1470403442,2.4075484441,-4.7948250492
C,0,2.1583880222,1.4495014224,-3.7937460594
C,0,2.3998887623,-0.0307823371,-3.8559249724
C,0,1.6158213527,3.1431727679,-2.1233795626
C,0,1.9150461313,1.8281725031,-2.4678319324
N,0,1.9682458189,0.6856021504,-1.6439314613
C,0,1.8581572535,-0.5268063969,-2.5160932337
C,0,2.5117646227,-1.8319655554,-1.9606398594
C,0,2.1041380744,0.5933923504,-0.3272803856
C,0,2.2925912964,1.5714746527,0.6375606941
C,0,2.369941046,1.1345401831,1.9692108753
O,0,3.2793969953,-2.4188028575,-2.7383753303
O,0,2.1419251166,-2.1846509364,-0.8062446304
H,0,1.3657240641,5.1253631008,-2.9020428596
H,0,1.8606005206,4.4953439714,-5.2408457719
H,0,2.337988254,2.1250991759,-5.826364513
H,0,1.3466827976,3.4240206663,-1.1128688693
H,0,0.7814308255,-0.7306425677,-2.6065968649
H,0,2.1117361303,-0.4563408975,-0.0244557111
H,0,2.3846322421,2.6218602054,0.3973039196
H,0,2.4577152936,0.0587534372,2.1087791208
C,0,0.4068768716,2.6143787383,5.2474979387
C,0,0.5204720346,3.4397620908,6.3608035289
C,0,-0.0298401872,3.1338796088,4.0237860569
H,0,0.8622836011,3.0265151455,7.3050713992
C,0,0.199887733,4.7920687526,6.2655096209
C,0,-0.3575107456,4.49254746,3.9407694529
H,0,0.2902222943,5.4346734278,7.1366101583
H,0,-0.7027969371,4.876652326,2.9863155106
C,0,-0.24064104,5.3174978071,5.0513435752
H,0,-0.4944539318,6.3707359748,4.9738260059
H,0,0.6686933373,1.5659067501,5.3419883491
C,0,-0.1999333314,2.3125617176,2.7892108072
O,0,-0.7062718108,2.8204325575,1.769687777
C,0,0.2442760036,0.9478406914,2.7551831368
H,0,0.376933322,0.3427731568,3.6462665605
S,0,-0.5323646097,0.1208724348,1.4095973891
C,0,-0.0792814634,-1.6111824311,1.636358482
H,0,0.0547985525,-1.8438350938,2.6936644995
H,0,-0.89905954,-2.2034711357,1.2257063141
H,0,0.8154018303,-1.8180111336,1.0415204092
C,0,-2.2901382705,0.0812625054,1.8374114197
H,0,-2.8148368077,-0.4578042917,1.046111926
H,0,-2.4320471664,-0.4009257894,2.8050777644
H,0,-2.614153138,1.1217629592,1.8614510377
C,0,2.9863519815,1.9183807938,3.0464459217
C,0,3.1101892688,3.313926124,2.9897380247
C,0,3.515609685,1.2426368156,4.1551865357
C,0,3.7491314353,4.0076531245,4.0092762825
C,0,4.1578065103,1.9367207525,5.1734937868
C,0,4.276100023,3.3229200319,5.1029694225
H,0,2.6956259639,3.8633478167,2.150351402
H,0,3.4307540896,0.1597614395,4.2076722925

TS-3a (SR) 3, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1760.08432107 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.422751 a.u.
1 imaginary frequency = 263.8473 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.653889 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6803509 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.567536 a.u.
0; 1
C,0,1.3263921768,4.4973662552,-2.5220406374
C,0,1.4646613077,4.3009728771,-3.8940203658
C,0,1.6631662346,3.0160953501,-4.4044206053
C,0,1.729544206,1.9419556092,-3.5315375226
C,0,1.9385033585,0.4823571122,-3.8022712119
C,0,1.3941438661,3.427240562,-1.629378443
C,0,1.6089311249,2.154190355,-2.1525082162
N,0,1.6941754724,0.9174808776,-1.4820969507
C,0,1.5473901171,-0.1870843305,-2.4868894359
C,0,2.319710577,-1.5100601777,-2.1573168841
C,0,1.8788474662,0.6505177542,-0.1933224074
C,0,2.0801592613,1.4784146894,0.8978575663
C,0,2.2748276813,0.8438393987,2.1409763363
O,0,3.0471551107,-1.9445517168,-3.0642478964
O,0,2.0699073312,-2.0233868444,-1.0333723165
H,0,1.1531142851,5.4966857981,-2.1341518493
H,0,1.4076246329,5.1489849898,-4.5696401407
H,0,1.759459902,2.8572383609,-5.4748299254
H,0,1.2421962538,3.6006382734,-0.5721345988
H,0,0.4789977061,-0.443480814,-2.4985051192
H,0,1.889327726,-0.4322430156,-0.0404882527
H,0,2.1039433552,2.5570368899,0.8333292885
H,0,2.5457125003,-0.2081106847,2.085303456
C,0,-0.8729390033,2.8048693655,2.0991342028
C,0,-1.3397094341,4.0761831254,1.7774940639
C,0,-0.660680509,2.4468807002,3.4364113407
H,0,-1.5020050405,4.342722286,0.7370702399
C,0,-1.6037564174,4.9998559562,2.7862531767
C,0,-0.9301748476,3.3826804305,4.4421238603
H,0,-1.9719314804,5.9899948074,2.5335449007
H,0,-0.7565865489,3.0887742703,5.4722031256
C,0,-1.3987751406,4.6495269784,4.1207314004
H,0,-1.6041593422,5.367681753,4.909178863
H,0,-0.6751346014,2.0991365251,1.2991130311
C,0,-0.1486712091,1.1098719438,3.8568074557
O,0,-0.0045045667,0.8394161353,5.0619354558
C,0,0.2374863051,0.1651040225,2.8461566473
H,0,-0.2388352165,0.129750024,1.872194499
S,0,0.5328518603,-1.4238489287,3.5426871123
C,0,-1.0144816991,-1.9712597902,4.3071515192
H,0,-1.8238854164,-1.9196553383,3.5774361402
H,0,-0.8672689416,-2.9925621142,4.6641650049
H,0,-1.1902030496,-1.2924823054,5.1412278952
C,0,0.5502059078,-2.4741304302,2.0771077118
H,0,1.3814051661,-2.1994028652,1.4243989359
H,0,0.6835718487,-3.5017830041,2.4179746103
H,0,-0.3917051085,-2.3722544449,1.5349974063
C,0,2.8148810866,1.5273367793,3.3212614878
C,0,2.6986766281,2.9131461389,3.5074959416
C,0,3.4939266929,0.7747482848,4.2904287737
C,0,3.2578361041,3.523804763,4.6226427381
C,0,4.0553806297,1.3871748906,5.4040732284
C,0,3.9397267658,2.7648208072,5.5724333118
H,0,2.1595632954,3.5161398237,2.7838779723
H,0,3.5916722259,-0.2997294411,4.1581653626

H,0,3.8350760482,5.0885486494,3.9516664159
H,0,4.5707003998,1.3955499979,6.0196786185
H,0,4.7782035353,3.8684714513,5.8964517135
H,0,1.9006994616,-0.5137834752,-4.6986549443
H,0,3.4662665462,-0.2752695711,-3.9264674024

H,0,3.1601679238,4.5974632175,4.7525065112
H,0,4.5849756188,0.7894036096,6.1396636579
H,0,4.377921279,3.2464629439,6.4415220392
H,0,1.3428569397,0.1115022591,-4.6395525293
H,0,2.9862426419,0.246382252,-4.0214229623

Int-3a (SS), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1760.13122641 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.429253 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6914364 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.7199619 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.6189941 a.u.

O; 1
C,0,0.2456066676,4.2098365853,-1.6002041589
C,0,0.9631443318,4.8137795068,-2.6290719393
C,0,1.9792222312,4.1068365735,-3.2849009648
C,0,2.2580976304,2.8074129085,-2.9013684209
C,0,3.3166844623,1.8444916396,-3.3699264297
C,0,0.5113754858,2.8962555907,-1.2052741602
C,0,1.5294745688,2.2115683361,-1.8639794657
N,0,1.9784092605,0.9143084891,-1.6486623164
C,0,2.93619823,0.5095831287,-2.6894955103
C,0,4.1711417328,-0.2474026364,-2.12045933
C,0,1.7271111337,0.173274024,-0.5309715551
C,0,2.0083257067,-1.1381536514,-0.3905987938
C,0,2.2831920219,-1.7086387424,0.9670098574
O,0,4.4882765249,-1.286218164,-2.7412823597
O,0,4.7390966605,0.2436803464,-1.108976948
H,0,-0.5477900707,4.76009247,-1.1019726028
H,0,0.7315811983,5.8316100056,-2.927701553
H,0,2.5447068892,4.5762288271,-4.0858768831
H,0,-0.076596727,2.423838471,-0.4244801626
H,0,2.4418019526,-0.1609013254,-3.402299326
H,0,1.3555242828,0.7498553215,0.316363892
H,0,2.3713537854,-1.6986834301,-1.2487785035
H,0,1.8508838848,-1.0220647551,1.7094654911
C,0,3.8383510685,1.3024354376,1.8986198858
C,0,3.6124030463,2.627280181,2.2616891416
C,0,3.9544890002,0.3249765431,2.8983365178
H,0,3.5312592364,3.3862300226,1.4895560747
C,0,3.4947001004,2.9798048481,3.6037653586
C,0,3.8550698485,0.6887030702,4.2491209402
H,0,3.3119402469,4.0149470456,3.8774532264
H,0,3.9613720513,-0.0820022915,5.0060795431
C,0,3.6179682512,2.009147635,4.5994665764
H,0,3.5297850483,2.2863098133,5.645463873
H,0,3.9637389445,1.0527921157,0.8450958622
C,0,4.2199306929,-1.0994675839,2.5905992355
O,0,4.7002348102,-1.8631034451,3.4175421475
C,0,3.846062601,-1.5923357516,1.1996192064
H,0,4.2348714991,-0.8986217244,0.4334095013
S,0,4.7978119696,-3.1378172144,0.9398045107
C,0,4.3908737268,-3.6266013414,-0.7457218779
H,0,4.5341243321,-2.7922063607,-1.4516839499
H,0,5.0604045976,-4.4588781431,-0.9750132202
H,0,3.3622301483,-3.9896581483,-0.7396341815
C,0,6.4256833835,-2.4055794767,0.6650931701
H,0,6.7821059917,-2.0325224256,1.6255456052
H,0,7.0852274893,-3.1990684185,0.3102306583
H,0,6.3309735967,-1.6023260681,-0.0720208926
C,0,1.7031072038,-3.0878229238,1.2439720659
C,0,0.7775236624,-3.6483539633,0.3592185523
C,0,2.0320099945,-3.7976735384,2.406354743
C,0,0.2067324509,-4.8924004512,0.6167421261
C,0,1.4614992911,-5.0414427253,2.6634601696
C,0,0.5490292367,-5.5948929615,1.7687107715
H,0,0.4973550679,-3.0930402345,-0.5316145959
H,0,2.7365670003,-3.3797141345,3.12048665
H,0,-0.5097709751,-5.3101593921,-0.0846855568

Int-3a (SR), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1760.12468015 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.426468 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.69064 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.7187109 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.6145335 a.u.

O; 1
C,0,2.8848669483,4.0658146218,-4.4160996861
C,0,3.0400628616,3.8135914968,-5.7766260266
C,0,3.3134790778,2.5138442133,-6.2178642464
C,0,3.4252508962,1.4902220285,-5.2935307915
C,0,3.7578868664,0.0359548132,-5.4797538905
C,0,2.9913109439,3.0429969609,-3.4714794845
C,0,3.2676595301,1.7554209192,-3.9275856608
N,0,3.4041376436,0.5789570957,-3.1968713598
C,0,3.5665336853,-0.5866226805,-4.0820233323
C,0,4.7903050395,-1.4460943962,-3.6380283285
C,0,3.3387026545,0.4825928202,-1.8413396398
C,0,3.2993935649,-0.6611198967,-1.1207614534
C,0,3.2927136648,-0.6290573206,0.3755853952
O,0,4.5281254134,-2.6179608715,-3.2531873907
O,0,5.8986279252,-0.8763175924,-3.6766487401
H,0,2.667107892,5.07464938,-4.0764547637
H,0,2.9468230754,4.6231152738,-6.4941104286
H,0,3.43820852,2.3087886055,-7.27812922
H,0,2.8475022668,3.2593176395,-2.4176818221
H,0,2.6601693752,-1.2030425062,-4.0246482601
H,0,3.3289011791,1.4411489872,-1.3262003754
H,0,3.3004795396,-1.623151187,-1.6268928451
H,0,3.3546712848,0.4141699701,0.7093445699
C,0,4.1038225833,-3.2999880979,3.2542867489
C,0,3.9730089665,-4.2029630261,4.302938548
C,0,4.5398089158,-1.9918230556,3.5043453376
H,0,3.6267252935,-5.2121306326,4.1041157954
C,0,4.2826450727,-3.8129103842,5.6035602685
C,0,4.8376905824,-1.6051622497,4.8203653609
H,0,4.1844139119,-4.5231495574,6.4191662995
H,0,5.1678912238,-0.5870219253,4.9984255007
C,0,4.7149444166,-2.5113963256,5.8618789023
H,0,4.9534714452,-2.2077064898,6.8764244813
H,0,3.8345833909,-3.6187177137,2.2531689989
C,0,4.7078442849,-0.9691112579,2.4485650633
O,0,4.9673942065,0.1960329431,2.7124027634
C,0,4.5504820713,-1.3349333779,0.9721527988
H,0,4.5067436669,-2.4103849472,0.7895661112
S,0,6.029245423,-0.7475417621,0.0241480306
C,0,7.3896358391,-0.7600332092,1.2170017806
H,0,7.2463171713,0.0715429211,1.9047465771
H,0,7.4441086871,-1.7104239181,1.7507305695
H,0,8.2954383117,-0.6057061718,0.627498693
C,0,6.4655721654,-2.2074012914,-0.9363808296
H,0,5.6617102351,-2.4419336726,-1.6548369803
H,0,7.3443252895,-1.9307414668,-1.5202399686
H,0,6.6814098492,-3.0316101198,-0.2529187569
C,0,2.0649737314,-1.2601937895,1.0139162178
C,0,1.5775828335,-2.4962042938,0.575934207
C,0,1.4176046777,-0.6191614372,2.0729191049
C,0,0.4697016687,-3.0764058278,1.1859384543
C,0,0.3067535878,-1.1975800338,2.6825552775
C,0,-0.1688968573,-2.4289365462,2.2419116431
H,0,2.055818164,-3.005725452,-0.256668156
H,0,1.7859312539,0.3426561812,2.4216979879
H,0,0.1001799379,-4.0341482623,0.830908283

H,0,1.7298554583,-5.5766305811,3.5697350679
H,0,0.1046905321,-6.5649850032,1.9709790472
H,0,3.3634836106,1.744684333,-4.4572631515
H,0,4.3036789411,2.1726387377,-3.0203896592

H,0,-0.1874876921,-0.6825687965,3.5012376416
H,0,-1.0357336493,-2.8808130655,2.7150079971
H,0,3.1347668749,-0.4524880472,-6.234282771
H,0,4.8072558511,-0.0754522443,-5.7759789489

Int-3a (RR), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1760.11746660 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.424093 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6841855 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.7122771 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.6075972 a.u.

0; 1
C,0,3.6934573311,0.8647333588,-5.1071776781
C,0,3.1811822025,0.1500914261,-6.1849123621
C,0,2.477831258,-1.037760601,-5.9583902184
C,0,2.2876973214,-1.4819406223,-4.662135039
C,0,1.5826274094,-2.7075511511,-4.1568899305
C,0,3.5115740359,0.4309377566,-3.7915385489
C,0,2.7914600921,-0.7451775313,-3.5762588503
N,0,2.4802670616,-1.4013588278,-2.3853717972
C,0,1.9762273335,-2.7595186928,-2.6757849406
C,0,3.014571149,-3.8864192486,-2.3412240615
C,0,2.7495246627,-1.052936834,-1.1015764181
C,0,3.2265424196,0.1007505946,-0.5741608833
C,0,3.4913911843,0.1711866441,0.8998698266
O,0,2.9065096801,-4.924206624,-3.0206285609
O,0,3.7973156196,-3.6604019002,-1.3837821892
H,0,4.2547442502,1.7782512582,-5.2834457172
H,0,3.3340662273,0.5078139039,-7.1986976917
H,0,2.0866071958,-1.6130768556,-6.7936367948
H,0,3.9581821992,0.9916783287,-2.9816979693
H,0,1.1041996917,-2.948999164,-2.0390006278
H,0,2.5423987756,-1.8760094793,-0.4239318864
H,0,3.4353337962,0.9809723126,-1.167060602
H,0,3.3472384106,-0.8340661714,1.3152053412
C,0,5.1958828401,2.6293281206,3.3390056404
C,0,5.3066033299,3.607069462,4.3203896777
C,0,5.4380684484,2.950019512,1.9967997902
H,0,5.1130127224,3.3531225637,5.3576624757
C,0,5.662847966,4.9080702065,3.9734209603
C,0,5.794548032,4.2640630587,1.6574841673
H,0,5.7504606338,5.6686403535,4.7435915056
H,0,5.9807863617,4.4966554134,0.6142623886
C,0,5.9061641237,5.2361724044,2.6393078064
H,0,6.1828980558,6.2504520539,2.3691093599
H,0,4.8997071607,1.6278879652,3.6303325121
C,0,5.3702423799,1.9678010275,0.8915390865
O,0,5.626743464,2.2820895134,-0.2624736732
C,0,4.9973755665,0.5092638871,1.1720932011
H,0,5.2872736343,0.198381933,2.1796743554
S,0,6.0078746867,-0.4695656377,-0.0107443736
C,0,5.6921447835,-2.1724471161,0.4812487479
H,0,4.8343751954,-2.5494124821,-0.0949366759
H,0,6.576644885,-2.7380121537,0.1795676618
H,0,5.5581593406,-2.24381658,1.5624364634
C,0,7.6540912845,-0.2131251759,0.692887343
H,0,8.3446644668,-0.8317522606,0.1176925404
H,0,7.9142097017,0.836938121,0.5554770775
H,0,7.6783717072,-0.4907587545,1.7478881604
C,0,2.5945675257,1.103261796,1.7006008861
C,0,2.1595732615,2.3273919112,1.1858875958
C,0,2.188888074,0.7330660612,2.9854509614
C,0,1.3507563308,3.1668037083,1.9461373113
C,0,1.3772413465,1.5698212936,3.747072551
C,0,0.9591782521,2.7926848344,3.2295481471
H,0,2.4452085508,2.6257266697,0.181313173
H,0,2.504425805,-0.2258235542,3.3920835953
H,0,1.0208482837,4.1147270935,1.5311225527

Int-3a (RS), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1760.12039638 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.429557 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.683621 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.7122431 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.6112782 a.u.

0; 1
C,0,2.8158502936,4.7427146285,-2.5648252731
C,0,3.149379466,4.4005702346,-3.8730424567
C,0,2.9777478735,3.08483818,-4.3193655448
C,0,2.4779578045,2.1316677612,-3.4481531909
C,0,2.2431734045,0.6583693197,-3.6441046827
C,0,2.3093452853,3.7923855829,-1.6757125562
C,0,2.151870939,2.4852018655,-2.1328830161
N,0,1.6354200868,1.3903619411,-1.4439511103
C,0,1.537774661,0.2064838895,-2.3508149556
C,0,2.2081726695,-1.0147928202,-1.6536946861
C,0,1.8234037863,1.1127655942,-0.1120433256
C,0,2.5701426718,1.7089219238,0.8348457759
C,0,2.9346569641,0.835777761,2.0118727374
O,0,1.4416869894,-1.9104534447,-1.2394445489
O,0,3.4585210084,-0.9439656616,-1.4901923718
H,0,2.9421257663,5.7675094352,-2.2269695757
H,0,3.5385525616,5.1556857899,-4.5493757617
H,0,3.2372990846,2.8134965238,-5.3395574357
H,0,2.0235008615,4.0733342483,-0.6678850597
H,0,0.4815951593,-0.0251085104,-2.5226545265
H,0,1.353393765,0.1653609436,0.1491403225
H,0,3.124346105,2.6222980543,0.6551269104
H,0,2.053671862,0.2234277121,2.2377917969
C,0,5.4977804722,1.4566685249,-0.5691492518
C,0,6.0800305948,2.3954993149,-1.4170326484
C,0,6.0123043613,1.2828204364,0.7235786997
H,0,5.6806871939,2.5306280851,-2.4177903936
C,0,7.1601720567,3.1594614417,-0.9842644557
C,0,7.1152061041,2.040667411,1.1471911251
H,0,7.6034717328,3.8956673057,-1.6487600028
H,0,7.5027340736,1.8817064618,2.1485669165
C,0,7.6805253851,2.9804523745,0.2996028795
H,0,8.5252267406,3.5752414767,0.6336985809
H,0,4.6777349158,0.8412550176,-0.9356542579
C,0,5.4645951016,0.2888008725,1.6718042329
O,0,6.123494295,-0.1476196098,2.6061319977
C,0,4.0292766051,-0.1840143796,1.4885148611
H,0,3.8063796009,-0.4192613431,0.4352769618
S,0,3.9437461533,-1.8221447948,2.3242254878
C,0,2.3390778363,-2.4459967518,1.7787098481
H,0,2.1927088373,-2.3249402285,0.6928105321
H,0,2.3254790435,-3.5024849965,2.0565367625
H,0,1.5593187762,-1.9344203711,2.3440769975
C,0,5.0062718295,-2.7653280194,1.2091781464
H,0,4.8690129791,-3.8218970873,1.4432062543
H,0,4.7068497028,-2.5419312046,0.1801324166
H,0,6.0359503288,-2.4700026706,1.4074998563
C,0,3.3194838303,1.5408975975,3.2957120341
C,0,4.0987365745,2.7025209456,3.2980507238
C,0,2.8901292248,1.0276572491,4.5231104507
C,0,4.4430211349,3.3257719607,4.4940383341
C,0,3.2340862329,1.6475106865,5.7213069473
C,0,4.0137774249,2.8002260172,5.710068371
H,0,4.4438785001,3.1301897378,2.3616230881
H,0,2.2644704537,0.138018416,4.5456830174
H,0,5.0470869829,4.2282747444,4.4736727024

H,0,1.0658058913,1.261900166,4.7410585333
H,0,0.3237204318,3.4470449477,3.8188972928
H,0,0.4977934966,-2.6173632226,-4.2928364976
H,0,1.9074566719,-3.6344810202,-4.6371027018

H,0,2.8852029412,1.2324756825,6.662413322
H,0,4.2810633539,3.2892318564,6.6421475856
H,0,1.6421707623,0.4387472202,-4.5311141834
H,0,3.1980910454,0.1280853195,-3.7394253131

Int-3a (SS) 2, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1760.10682454 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.424619 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6755686 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.7031568 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.595828 a.u.

0; 1
C,0,1.3346866028,4.2970867846,0.1407753966
C,0,1.6435672514,4.7635197748,-1.1333497557
C,0,2.0934189869,3.8681827127,-2.1098921216
C,0,2.2097942616,2.5236798872,-1.8042307807
C,0,2.6778085727,1.3780570041,-2.6532621682
C,0,1.4464057281,2.9436826241,0.4670929436
C,0,1.8723796165,2.0559617253,-0.5228713781
N,0,2.0931098217,0.6838058404,-0.4488067966
C,0,2.7859208107,0.2057203705,-1.6676224996
C,0,4.2570805376,-0.274446529,-1.4054637722
C,0,1.7932918554,-0.1880909639,0.5501554598
C,0,0.9769986598,-0.0328847,1.6202881995
C,0,0.8170959656,-1.1471333162,2.6206570286
O,0,4.4569547303,-0.8383823125,-0.3057392019
O,0,5.0470781093,-0.1026144283,-2.3571380806
H,0,1.007234514,4.9956500322,0.9061118061
H,0,1.5471633123,5.8198990295,-1.365742973
H,0,2.3571235884,4.225244485,-3.1023390243
H,0,1.2448121793,2.6141481029,1.4781268401
H,0,2.245089579,-0.6717917855,-2.0415152357
H,0,2.3280157242,-1.1257386799,0.4219159018
H,0,0.4061768161,0.8700280227,1.8045398217
H,0,1.503576643,-1.9525700507,2.3354992257
C,0,-2.515700841,-0.5242480361,0.3803728509
C,0,-3.3761976953,0.0023683694,-0.5754016323
C,0,-1.7108437134,-1.6292975628,0.0709730124
H,0,-3.9937415997,0.860307013,-0.329660335
C,0,-3.4397113992,-0.5640823073,-1.8462458047
C,0,-1.7816271005,-2.1909213481,-1.2133821348
H,0,-4.1106054144,-0.1472201646,-2.5913860961
H,0,-1.1486911652,-3.042097594,-1.4410964105
C,0,-2.6394807279,-1.6615874525,-2.1648255244
H,0,-2.6850788227,-2.099777016,-3.156844157
H,0,-2.4767472497,-0.0533221859,1.3564628638
C,0,-0.7745760054,-2.2613556189,1.0262031274
O,0,-0.118192627,-3.2478337872,0.7262879942
C,0,-0.6106751941,-1.7032608036,2.4468419761
H,0,-1.3498956891,-0.9367512222,2.6884812197
S,0,-0.9870657415,-2.9909546785,3.7284630076
C,0,-2.3551055716,-3.9222169923,3.0133246227
H,0,-2.0482144765,-4.398252232,2.0814546025
H,0,-2.6553294786,-4.6672749714,3.7516189318
H,0,-3.177354202,-3.2247414038,2.8454166701
C,0,0.3653089645,-4.1754153245,3.6219905804
H,0,1.237456595,-3.7110164486,4.0837194699
H,0,0.0617407909,-5.0435627705,4.2099122885
H,0,0.5468925765,-4.429485967,2.5778639599
C,0,1.1354343021,-0.7269884989,4.0440897156
C,0,0.2666380007,0.0737818686,4.7940658367
C,0,2.355608527,-1.1048330088,4.6138318619
C,0,0.606217934,0.4775462417,6.0822546349
C,0,2.6974193981,-0.7006108508,5.901279094
C,0,1.8216685015,0.089695394,6.6408975579
H,0,-0.6819958458,0.4002663565,4.3734299449
H,0,3.0531630146,-1.7048259046,4.0337789677
H,0,-0.0799830417,1.0998025411,6.6493164721

Int-3a (SR) 2, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1760.10233883 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.423900 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6710533 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.698826 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.5921585 a.u.

0; 1
C,0,-1.4501328525,3.0991087902,-0.3718632779
C,0,-1.2114044367,3.7055965829,-1.6006145283
C,0,-0.2259004417,3.1876330868,-2.4482719013
C,0,0.4838239487,2.0627095669,-2.0670426759
C,0,1.6310814669,1.3742082023,-2.7443684887
C,0,-0.7453167115,1.960949744,0.0272647349
C,0,0.210024716,1.4306882983,-0.8426165557
N,0,1.0440612235,0.3281354654,-0.6774953545
C,0,1.9327982281,0.158112383,-1.8641359451
C,0,3.4411386753,0.0024966515,-1.4638988779
C,0,1.016041713,-0.6452292611,0.2787279687
C,0,0.0987113805,-0.902650309,1.2386568586
C,0,0.3292223468,-2.0300856914,2.2048225313
O,0,4.2271577299,0.8843931095,-1.8613847574
O,0,3.6985760314,-1.0304788406,-0.794177717
H,0,-2.1977942394,3.5138503435,0.2988490845
H,0,-1.7767543598,4.5848407686,-1.8948312304
H,0,-0.0097493451,3.6703815935,-3.3982103221
H,0,-0.9255341412,1.5367833715,1.0058195479
H,0,1.6401057461,-0.7761870148,-2.3614773992
H,0,1.9080863088,-1.2699395283,0.1936096903
H,0,-0.8188144402,-0.3379533958,1.346647573
H,0,1.3610949079,-2.3757772208,2.0731730787
C,0,-1.7902510521,-2.747225933,-0.9166512909
C,0,-2.3839836008,-2.5739133086,-2.1612727447
C,0,-2.5843118074,-2.8254600945,0.2360648671
H,0,-1.7624497382,-2.5043334875,-3.0481450684
C,0,-3.7694737606,-2.4814356337,-2.2681067551
C,0,-3.9795183064,-2.7231376597,0.1177179682
H,0,-4.2289561567,-2.3469715395,-3.2428087224
H,0,-4.5814493875,-2.7801901096,1.0185857504
C,0,-4.5677404556,-2.5554500701,-1.1259957543
H,0,-5.6473543597,-2.4796602617,-1.2096620572
H,0,-0.7085779188,-2.7817974735,-0.8534459994
C,0,-2.042607781,-3.0166304311,1.602275635
O,0,-2.7714030202,-2.9990185505,2.5829329658
C,0,-0.5424349718,-3.2638484436,1.7879215151
H,0,-0.1064868487,-3.6473950696,0.8604831786
S,0,-0.2028182829,-4.6966882107,2.9056110543
C,0,-1.1700148075,-4.5789396613,4.4238352725
H,0,-2.2278447887,-4.479015666,4.1930948427
H,0,-0.9483288464,-5.4987376432,4.9700097998
H,0,-0.8076766804,-3.7162519912,4.98178218
C,0,-1.0443233566,-6.0461786485,2.0587082635
H,0,-0.574338666,-6.1752017819,1.0830658758
H,0,-0.8918668161,-6.9456458268,2.6570006142
H,0,-2.1087289597,-5.8289860483,1.9581315167
C,0,0.1770531073,-1.636762415,3.6619840009
C,0,-0.9598038183,-0.9786683114,4.1455781489
C,0,1.2077728061,-1.9388394045,4.5585380483
C,0,-1.0693517226,-0.6555651335,5.4941935628
C,0,1.0999679227,-1.6141358815,5.9096425308
C,0,-0.0433547753,-0.97658352,6.3819799254
H,0,-1.7712644618,-0.7236365001,3.4719327798
H,0,2.1087627105,-2.4265183872,4.1935381796
H,0,-1.959782512,-0.1481768081,5.8536735639

H,0,3.6512508639,-1.0017774137,6.324187033
H,0,2.0860187968,0.4058583254,7.6454920866
H,0,1.9671784827,1.1735565214,-3.4635053212
H,0,3.6614189875,1.5377413037,-3.1056748024

H,0,1.9132735351,-1.8535858571,6.5883218386
H,0,-0.1317683412,-0.7206469487,7.4335926611
H,0,1.4044833573,1.0892334802,-3.7768231902
H,0,2.5337074142,1.9976453882,-2.7619396767

Int-3a (RR) 2, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1760.11246832 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.426068 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6795512 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.7074618 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.6021491 a.u.

0; 1
C,0,2.2316887376,4.0372262623,0.6866146824
C,0,2.265072184,4.6056159603,-0.5842811547
C,0,2.3129942073,3.782200941,-1.7149757017
C,0,2.3111987789,2.4070608533,-1.5580266493
C,0,2.4208513144,1.3039147479,-2.5694227783
C,0,2.2341741199,2.6519542246,0.8616916668
C,0,2.2580585938,1.8460182717,-0.2756589939
N,0,2.2341831233,0.4561741864,-0.357855766
C,0,2.168223228,0.0128899698,-1.7708392481
C,0,3.1966845382,-1.116379322,-2.1489334867
C,0,1.87505535,-0.3589902376,0.6814648015
C,0,1.8092220553,-1.7012193641,0.5990713564
C,0,1.3480150045,-2.6112629365,1.6988424012
O,0,4.3746692624,-0.7514511581,-2.3123866492
O,0,2.7174508378,-2.2784154747,-2.2660919492
H,0,2.206946113,4.6785829022,1.5634202599
H,0,2.2635344783,5.685534033,-0.6974218085
H,0,2.3527853632,4.2182338233,-2.7101001446
H,0,2.2251625919,2.2297605522,1.8616602678
H,0,1.1569829104,-0.3825949668,-1.9327266599
H,0,1.6224949944,0.1613262053,1.6034376539
H,0,2.1231494963,-2.1798034917,-0.3267199707
H,0,0.8646292995,-2.0365957647,2.4984942157
C,0,-0.5475010886,-2.7250798644,-1.8464672474
C,0,-1.0462985118,-2.6121777658,-3.140627011
C,0,-1.4145868155,-2.5564096523,-0.756353688
H,0,-0.3658592714,-2.716769042,-3.9799182712
C,0,-2.3973720199,-2.3530322599,-3.3578847195
C,0,-2.7689336102,-2.2641820497,-0.981948374
H,0,-2.7787246386,-2.2779787553,-4.3721073142
H,0,-3.4209026277,-2.1176819661,-0.1264233364
C,0,-3.2602713781,-2.1761374502,-2.2755882305
H,0,-4.3117843252,-1.9649791916,-2.443952366
H,0,0.5276596209,-2.8547261708,-1.7259635964
C,0,-0.978527087,-2.647925582,0.6543990046
O,0,-1.6206743997,-2.1444306047,1.5644334189
C,0,0.2636873539,-3.474681841,1.0195015712
H,0,0.6935610813,-3.9721275834,0.1441003953
S,0,-0.2061608064,-4.9424177961,2.0480802259
C,0,-0.8918262392,-4.2856887082,3.5768881313
H,0,-1.5878542377,-3.4768571469,3.3550688651
H,0,-1.3789775822,-5.1230132285,4.0800259391
H,0,-0.0539569511,-3.9366353625,4.1804939455
C,0,-1.6812683424,-5.5623122926,1.21915062
H,0,-1.4035401353,-5.8204155932,0.1959539036
H,0,-1.990011526,-6.4633368158,1.7513964925
H,0,-2.4754013107,-4.8148553545,1.2314210304
C,0,2.4676257437,-3.4484146694,2.2945095134
C,0,3.3112455807,-4.2082278904,1.4749663898
C,0,2.6882848644,-3.4524979176,3.6742274586
C,0,4.3353962203,-4.96767295,2.0290858159
C,0,3.7173075119,-4.2110462419,4.2301325282
C,0,4.5392416756,-4.975307129,3.4086469577
H,0,3.1895680937,-4.1810110768,0.3947845331
H,0,2.0679947698,-2.8341339664,4.3201230509
H,0,4.9856927873,-5.546595456,1.3800063689

Int-3a (RS) 2, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1760.10427660 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.425105 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6726099 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.7003306 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.5941925 a.u.

0; 1
C,0,4.2071866387,3.4599335684,1.493163522
C,0,4.9973544951,3.978717064,0.4704196
C,0,5.1222128227,3.2838918585,-0.7384572803
C,0,4.4489890196,2.0864013751,-0.9113744757
C,0,4.3841117609,1.155212914,-2.0876237818
C,0,3.5280886224,2.2494519882,1.3385839909
C,0,3.6479287046,1.5807056797,0.1214995513
N,0,3.0498878278,0.3858201364,-0.2697965671
C,0,3.6071667326,-0.0655325196,-1.5625498956
C,0,4.4856891946,-1.366513827,-1.4621460441
C,0,1.9170993653,-0.1014100286,0.3149062642
C,0,1.3101847269,-1.2781173894,0.055268809
C,0,0.040428901,-1.6485284807,0.7578158534
O,0,3.978427514,-2.3020272806,-0.8028808387
O,0,5.5641242573,-1.3499258406,-2.0923033303
H,0,4.1269608652,3.9939792717,2.4361139512
H,0,5.5258815334,4.9163015849,0.6146830101
H,0,5.7427765063,3.6821238063,-1.5374269664
H,0,2.9464709957,1.8375740608,2.1576081241
H,0,2.7576019336,-0.3271900232,-2.2071179612
H,0,1.4824572087,0.5831572243,1.0448943279
H,0,1.8318521256,-1.9997062651,-0.5664719278
H,0,-0.1890341867,-0.8288122541,1.4511615074
C,0,0.1878639227,-1.6361921598,-2.9605965134
C,0,0.8870953575,-1.6662094964,-4.1615116104
C,0,-0.3917400401,-2.8092381158,-2.4585604125
H,0,1.333940188,-0.7559152207,-4.5483568758
C,0,1.0215789046,-2.8624788474,-4.8613517949
C,0,0.2613817985,-4.0082227507,-3.1775632799
H,0,1.5778737506,-2.8828892172,-5.7935562578
H,0,-0.7196046086,-4.9065973007,-2.7774667305
C,0,0.447754765,-4.0349452622,-4.3675812912
H,0,0.5586623332,-4.967118404,-4.9122339003
H,0,0.1082453946,-0.7012200126,-2.4174947051
C,0,-1.1887222374,-2.851738971,-1.2199041585
O,0,-1.8889083081,-3.8157889349,-0.9341981368
C,0,-1.1743350367,-1.6774820782,-0.2428142778
H,0,-1.2307690876,-0.7078496296,-0.7470921725
S,0,-2.7520973746,-1.8735090053,0.701423251
C,0,-2.8764689858,-0.2770840643,1.5308435241
H,0,-2.6753419255,0.5457884365,0.8429361471
H,0,-3.8904160499,-0.205829709,1.928068806
H,0,-2.1738884713,-0.2668256014,2.3635499084
C,0,-4.0191271331,-1.6753978828,-0.5674898582
H,0,-4.0159968564,-2.583940804,-1.1677503062
H,0,-4.9749645316,-1.5779214838,-0.0497779602
H,0,-3.8222607894,-0.7937839168,-1.1799066253
C,0,0.1411501487,-2.9254397768,1.5752368984
C,0,0.7214744726,-4.0868166311,1.0544419706
C,0,-0.3298886321,-2.9475150519,2.8910425151
C,0,0.8080587342,-5.2408275835,1.8252413295
C,0,-0.2445283628,-4.1024350634,3.6654124708
C,0,0.3214897666,-5.2549833208,3.1311026686
H,0,1.1322195028,-4.0888733595,0.0489963891
H,0,-0.746333465,-2.0434471122,3.331308997
H,0,1.267564814,-6.1309437005,1.4060663823

H,0,3.8792347301,-4.195554089,5.3040231636
H,0,5.3438305592,-5.5651093669,3.8375757737
H,0,1.7251354338,1.4117229115,-3.4069815761
H,0,3.4407367277,1.2519452344,-2.9689891395

H,0,-0.6105269459,-4.0949677501,4.6879611177
H,0,0.3958614252,-6.1567161548,3.7316121127
H,0,3.8897628851,1.6329387961,-2.9429218522
H,0,5.365151622,0.7973920402,-2.4166205184

TS-4a (RSR), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1760.10691081 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.424509 a.u.
1 imaginary frequency = 346.6484 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6721592 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6987381 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.5892733 a.u.
0; 1
C,0,0.3896518196,4.0995301772,0.5102624828
C,0,0.1730549416,4.6976097159,-0.7306146958
C,0,0.5129397708,4.0237992491,-1.9059989138
C,0,1.0601067321,2.7525580323,-1.8261683556
C,0,1.5202879779,1.8210172496,-2.9090689435
C,0,0.9414342209,2.823199483,0.6073338152
C,0,1.2619133113,2.1637628541,-0.5763136145
N,0,1.799877084,0.8791099225,-0.7370377292
C,0,2.1370512822,0.6290232339,-2.1600071848
C,0,3.7015187468,0.5260484381,-2.3466708591
C,0,1.906829844,-0.0314800114,0.2435837394
C,0,2.4226220974,-1.290834041,0.0818489747
C,0,2.5840093737,-2.2772216275,1.2060213673
O,0,4.1807037489,-0.6258592219,-2.1765837931
O,0,4.2944548381,1.5836037234,-2.6190743302
H,0,0.1338590413,4.6353755333,1.4195350031
H,0,-0.2532601559,5.694791862,-0.7823416032
H,0,0.3528522543,4.4910936058,-2.8737747894
H,0,1.1235617546,2.37984302,1.5810047891
H,0,1.6895919137,-0.3293266524,-2.4425486483
H,0,1.5379309038,0.2912163689,1.2140170005
H,0,2.8628502633,-1.5459465815,-0.880370559
H,0,2.0001938296,-1.9935044033,2.0857082758
C,0,5.6977224061,0.5069530948,0.4610122215
C,0,6.6368830162,1.4799499798,0.1321273833
C,0,5.2445054323,0.4034620241,1.7829372761
H,0,6.9456529886,1.5848117551,-0.9025682146
C,0,7.1468262574,2.3256105522,1.1132039038
C,0,5.7391874334,1.2789712029,2.7622953357
H,0,7.8853701765,3.0775927155,0.8503470267
H,0,5.3574904938,1.199647133,3.7757666451
C,0,6.6988051112,2.2232993428,2.4321319967
H,0,7.0912423002,2.8893655562,3.1946581017
H,0,5.2851059808,-0.1107544169,-0.336397724
C,0,4.1954953347,-0.5595011016,2.1845637106
O,0,3.5208578705,-0.3966691516,3.1970856343
C,0,3.9906240208,-1.8120127671,1.370476734
H,0,4.6589387635,-1.9793920617,0.5312819137
S,0,5.0952567319,-3.3131714645,2.6926114319
C,0,6.4797619221,-2.4126512263,3.4217441622
H,0,6.1328629023,-1.5114388444,3.9308150604
H,0,6.9896962973,-3.0713866636,4.128059081
H,0,7.1643609594,-2.1449312416,2.6156218923
C,0,3.9801787558,-3.4134253199,4.1034478131
H,0,3.1317608499,-4.0279579272,3.7987396755
H,0,4.500527559,-3.8982929066,4.9319407469
H,0,3.6446016089,-2.4110382184,4.3798637485
C,0,2.3467353291,-3.722987251,0.8515666052
C,0,3.0465048668,-4.3510548081,-0.1841645699
C,0,1.3889180941,-4.4555642104,1.5574727995
C,0,2.7972466354,-5.683371572,-0.4977803702
C,0,1.1373215915,-5.7891032379,1.2430235135
C,0,1.8431167663,-6.4069814929,0.215168829
H,0,3.7842155287,-3.7987693261,-0.7612832394
H,0,0.8275793657,-3.9736722412,2.3548625098

TS-4a (RSR), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1761.59173259 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.423377 a.u.
1 imaginary frequency = 469.7104 i cm⁻¹
0; 1
C,0,1.7388672496,4.2310779633,0.6653212516
C,0,1.4865627664,4.8885092114,-0.5359599844
C,0,1.3805393386,4.1681357189,-1.7292035599
C,0,1.5188670482,2.7919969264,-1.7001597224
C,0,1.4576991137,1.770310191,-2.807752946
C,0,1.885448749,2.8440766992,0.7089069304
C,0,1.7512907718,2.1494539453,-0.4853178691
N,0,1.8677834314,0.761955626,-0.7017078699
C,0,2.0172964446,0.4934480126,-2.155149869
C,0,3.5381479826,0.2482740235,-2.4637330407
C,0,1.885790132,-0.1610648077,0.2668757864
C,0,2.2142905473,-1.4790121116,0.0845595756
C,0,2.4316593636,-2.4541351785,1.2213697646
O,0,3.9223167386,-0.9379820318,-2.3393074478
O,0,4.211251555,1.2530379815,-2.7427689026
H,0,1.8411164396,4.8019428933,1.5805119538
H,0,1.3880452906,5.9671594637,-0.5475424007
H,0,1.2020844213,4.6815156206,-2.6672930993
H,0,2.1203681261,2.3442351483,1.6419257336
H,0,1.4463432584,-0.403469216,-2.3980912962
H,0,1.6439949287,0.2144736084,1.2580035382
H,0,2.5461374713,-1.800149521,-0.8955564928
H,0,1.8399906574,-2.2246986632,2.1067995026
C,0,5.1069919913,0.6912931573,0.3881714066
C,0,5.7746176153,1.8463255177,-0.0084981045
C,0,4.7615149741,0.5176118004,1.7310341346
H,0,5.9847804893,1.9898241567,-0.9607657278
C,0,6.1213797156,2.8064013854,0.9350499337
C,0,5.105877825,1.4923041068,2.6771659236
H,0,6.6402278499,3.7056194621,0.6236280086
H,0,4.8170677494,1.3487034375,3.7117152307
C,0,5.7964059752,2.6257256992,2.2811591453
H,0,6.0700888889,3.3772095094,3.0119539975
H,0,4.8288805444,-0.0376086878,-0.3663121395
C,0,3.9157185089,-0.6140955245,2.1805299034
O,0,3.2990691613,-0.5755886207,3.2282034923
C,0,3.7907166883,-1.858177878,1.321977981
H,0,4.4617031442,-1.985992669,0.4810884653
S,0,5.1167827627,-3.2487817001,2.6308228865
C,0,6.2686889792,-2.1279671475,3.4667183393
H,0,5.7146041891,-1.3760316157,4.0289572928
H,0,6.8965177341,-2.7146516581,4.136262442
H,0,6.8846529412,-1.6538038424,2.7037269227
C,0,3.9977019524,-3.6095762092,4.002600394
H,0,3.2541878542,-4.3160009008,3.6372172283
H,0,4.5740375379,-4.0672324902,4.8062757502
H,0,3.5246295143,-2.6862660218,4.3374925553
C,0,2.3395441657,-3.9110435355,0.852334031
C,0,3.1006406839,-4.44230695,-0.1911813813
C,0,1.4844364524,-4.7495701583,1.5655573736
C,0,3.0107548742,-5.7930252962,-0.5070920668
C,0,1.3940983244,-6.102540498,1.2499041855
C,0,2.1594409951,-6.626806572,0.213975778
H,0,3.7612463417,-3.8038161532,-0.7706974337
H,0,0.8842233123,-4.3399945456,2.3719611324

H,0,3.3483219171,-6.1566782535,-1.3050607023
H,0,0.3873806212,-6.3423389613,1.8008395069
H,0,1.6495082835,-7.4463392407,-0.0328339095
H,0,0.6910311658,1.5142569555,-3.5559777545
H,0,2.2983853586,2.2827968552,-3.5236743134

H,0,3.6056703718,-6.194473612,-1.3186632748
H,0,0.7257706787,-6.7431387391,1.8130480562
H,0,2.0920862116,-7.6794261718,-0.0336736555
H,0,0.4252868453,1.624220305,-3.1375970478
H,0,2.0680823309,2.0582371566,-3.6621136946

TS-4a (RRR), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1760.09384084 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.422527 a.u.
1 imaginary frequency = 324.1478 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6616207 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.68821 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.5813829 a.u.

0; 1
C,0,-1.0327147537,3.738246013,0.0836553781
C,0,-0.7758813661,4.6410471645,-0.9476165243
C,0,0.1780511549,4.3430912657,-1.9237003887
C,0,0.8678094902,3.1429699747,-1.8537770694
C,0,1.9362882322,2.5829418646,-2.7482619376
C,0,-0.3489997596,2.5264691377,0.1660169065
C,0,0.6070378241,2.2535489213,-0.8089778906
N,0,1.4109889563,1.1181108629,-0.9451351857
C,0,2.2932100746,1.2202244677,-2.1180018884
C,0,3.7874254776,1.1554941718,-1.6394229324
C,0,1.5258002402,0.1340787577,-0.0479117914
C,0,2.2384166495,-1.0290118437,-0.2147568037
C,0,2.4125928027,-1.9542725177,0.9511969337
O,0,4.5131590049,0.3526947007,-2.2557073621
O,0,4.0554606243,1.9271111783,-0.6895154354
H,0,-1.7821973872,3.9748538185,0.8330227705
H,0,-1.3232588709,5.5774360495,-0.9943985128
H,0,0.3779161256,5.0439583043,-2.7295181685
H,0,-0.5727427002,1.8259277783,0.9641867681
H,0,2.0895003322,0.3858493844,-2.7958547288
H,0,0.984222575,0.2935589932,0.8821647412
H,0,2.7347724202,-1.2539214449,-1.1523064009
H,0,1.8362041322,-1.5624857603,1.7964126256
C,0,6.349648338,0.1356522554,0.4888156782
C,0,7.613664282,0.7114355278,0.5755989168
C,0,6.2380206375,-1.2431339215,0.271213342
H,0,7.7022991456,1.7842279938,0.7187690344
C,0,8.7601852783,-0.0716733293,0.457692682
C,0,7.3923727636,-2.0198326038,0.1013553941
H,0,9.7417054943,0.3868398369,0.5383753092
H,0,7.2854585895,-3.0781383668,-0.118904484
C,0,8.6498240514,-1.4397691314,0.2104898543
H,0,9.5412534447,-2.0488485123,0.0943666992
H,0,5.4661194369,0.774350746,0.4755476706
C,0,4.9301992055,-1.9465625909,0.1998196721
O,0,4.7817183101,-2.9516012026,-0.4770179197
C,0,3.8268476626,-1.493934955,1.1257349914
H,0,3.9303099469,-0.5081326241,1.5693493619
S,0,4.5961739916,-2.5358724854,3.0639859727
C,0,5.3522309944,-4.0875547718,2.5467108827
H,0,6.1526441137,-3.9081346278,1.826964143
H,0,5.7431579,-4.5991250208,3.4288504318
H,0,4.5657923556,-4.6886058758,2.088419993
C,0,6.0284866513,-1.6090670279,3.6516427295
H,0,5.6874061147,-0.6020397075,3.898048951
H,0,6.4095723637,-2.0917785007,4.5544766038
H,0,6.8026431292,-1.5613827786,2.8841082395
C,0,2.0783382909,-3.4233204767,0.8032062084
C,0,1.9971240194,-4.060827726,-0.4362551807
C,0,1.7712497459,-4.1568435289,1.9537934825
C,0,1.643891668,-5.4034842763,-0.5198289791
C,0,1.4263391409,-5.5049598353,1.8740456407
C,0,1.3640779235,-6.1331237149,0.6341268984
H,0,2.2185432346,-3.5068984173,-1.3416358147
H,0,1.786593395,-3.6655028287,2.9244175542

TS-4a (RRR), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1761.58393604 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.424123 a.u.
1 imaginary frequency = 480.3612 i cm⁻¹

0; 1
C,0,-0.7795921354,3.9619895409,0.0134592572
C,0,-0.4333649226,4.8016332416,-1.0426579527
C,0,0.4516155434,4.3633518297,-2.0299850619
C,0,0.9852477844,3.0894833137,-1.941210748
C,0,1.9197053032,2.3606515453,-2.872469265
C,0,-0.2501314395,2.6759681813,0.1146508109
C,0,0.6408594025,2.266726063,-0.8692663205
N,0,1.3113087658,1.0367660975,-0.9847762279
C,0,2.2687865262,1.0657850102,-2.1026879286
C,0,3.7335379184,1.1282744453,-1.5420609828
C,0,1.3827341452,0.0987039658,-0.0397488204
C,0,2.0619788789,-1.0874093982,-0.1730301048
C,0,2.2642896508,-1.9778655402,1.0176778386
O,0,4.5894284867,0.5953543868,-2.2694697277
O,0,3.8744268719,1.7356916158,-0.4622821258
H,0,-1.4732391504,4.3087165055,0.7701509009
H,0,-0.8563221451,5.7970637442,-1.1003724507
H,0,0.7192834608,5.0116310999,-2.8568109288
H,0,-0.53700938,2.0301501717,0.9351218131
H,0,2.1554329585,0.1763228331,-2.7220497763
H,0,0.8652283657,0.3220237185,0.8895634359
H,0,2.5114814357,-1.3688418796,-1.1149975578
H,0,1.6783461892,-1.5979962363,1.8571544294
C,0,6.1810429402,0.2078795266,0.8573189373
C,0,7.4452574425,0.7610801365,1.0254161929
C,0,6.0535242735,-1.0660050498,0.2993186927
H,0,7.5431168289,1.7580462369,1.4376687052
C,0,8.5804631748,0.0461671696,0.6541762026
C,0,7.1931940791,-1.7668597171,-0.1068209638
H,0,9.5636138036,0.4799042609,0.7963639145
H,0,7.0756738654,-2.7424179962,-0.5648110718
C,0,8.4544872925,-1.2181463497,0.0814757937
H,0,9.336165788,-1.7692943742,-0.22267334
H,0,5.3030421681,0.7981712241,1.0858920044
C,0,4.7426648788,-1.7575193991,0.145830628
O,0,4.5844354425,-2.6584360885,-0.6476516926
C,0,3.6439097628,-1.4155794898,1.1311485196
H,0,3.7137198195,-0.4613160194,1.6389046976
S,0,4.6034462117,-2.6204580328,2.9113309716
C,0,5.2972145337,-4.087829212,2.1102570339
H,0,6.0930033076,-3.7948617639,1.425247599
H,0,5.6847380535,-4.7507845811,2.8830059671
H,0,4.4909464106,-4.5770181121,1.5643134275
C,0,6.1196564605,-1.8301178061,3.5109289282
H,0,5.858367452,-0.8258999034,3.8411259202
H,0,6.4898542628,-2.412127395,4.3550073882
H,0,6.8628511394,-1.7822769415,2.7160947231
C,0,2.0466112068,-3.470644985,0.9138412001
C,0,2.0864221861,-4.1658505932,-0.2938607069
C,0,1.7766634235,-4.1754807834,2.089666111
C,0,1.8950814516,-5.5432233344,-0.3185434743
C,0,1.5897196887,-5.5548389475,2.0678598325
C,0,1.656263707,-6.243531311,0.8613309496
H,0,2.2848503048,-3.6359592795,-1.2160512948
H,0,1.7115096346,-3.6411177274,3.032401333

H,0,1.5872513127,-5.8826410467,-1.4929603472
H,0,1.1914100842,-6.0561974571,2.7800896453
H,0,1.0883804937,-7.1813623251,0.5650287768
H,0,1.587991134,2.4751666362,-3.7802365183
H,0,2.8141680771,3.2371054288,-2.7607896187

H,0,1.9345440554,-6.0714004803,-1.2638797549
H,0,1.3844490735,-6.0855967204,2.9899795074
H,0,1.5103829188,-7.3169347276,0.8375666624
H,0,1.4229454877,2.1395951517,-3.8199567017
H,0,2.8182779548,2.9388561598,-3.0939123488

TS-4a (SRS), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1760.09605861 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.424526 a.u.
1 imaginary frequency = 374.1537 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6625261 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6889106 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.5773562 a.u.
0; 1
C,0,0.2653622687,4.085487241,-0.850087493
C,0,0.6420825056,4.4831435717,-2.1307851401
C,0,1.4693836641,3.6652319548,-2.9029139909
C,0,1.8897069922,2.4470878585,-2.3934187812
C,0,2.799222418,1.4182027714,-2.9925845478
C,0,0.6806986277,2.8636683435,-0.3219217841
C,0,1.4768424582,2.0399596419,-1.1176810416
N,0,2.0431661436,0.790176511,-0.8201927678
C,0,3.0580312139,0.4416296623,-1.8438748487
C,0,4.5223241158,0.4956455509,-1.2583121833
C,0,1.8063752301,-0.0411629855,0.2010838934
C,0,0.8065579011,0.0180853277,1.1494666269
C,0,0.70926777,-1.0197101309,2.2383918293
O,0,4.6508094527,-0.0696776148,-0.1480286205
O,0,5.3792470212,1.0322005113,-1.9826692295
H,0,-0.3539590875,4.7385832926,-0.2423717237
H,0,0.3051812317,5.4380414815,-2.5226404379
H,0,1.7898168907,3.9821262368,-3.8915167139
H,0,0.4209546718,2.6023805827,0.6949914174
H,0,2.8867009702,-0.5961617206,-2.1454178046
H,0,2.5339553455,-0.846732724,0.2441567766
H,0,0.0201600248,0.7593902196,1.1064065187
H,0,1.3909059334,-1.8532951105,2.0502184807
C,0,2.8018859188,2.5257561328,3.8365051636
C,0,3.4216902507,3.7671897468,3.9213224785
C,0,3.4152524261,1.4799551131,3.1331789688
H,0,2.9516472787,4.5692421553,4.4821733515
C,0,4.639831504,3.9811134726,3.2792931629
C,0,4.6383222536,1.7015510399,2.4840353999
H,0,5.1163987692,4.9555652325,3.3345419385
H,0,5.0617537682,0.9059182294,1.8763830334
C,0,5.2384166059,2.9522725435,2.5532622416
H,0,6.1734707043,3.128586912,2.030546818
H,0,1.8492609163,2.3826730537,4.3383068175
C,0,2.8372199635,0.1180956649,3.0442356912
O,0,3.5290685148,-0.8725832853,2.8694213671
C,0,1.3454500354,-0.0690710611,3.1849395572
H,0,0.7412373631,0.7837432975,3.4871791591
S,0,1.3522908158,-1.1586290551,5.2198431398
C,0,2.7674643054,-0.5276330642,6.1455513919
H,0,2.7953253981,0.5638379096,6.1339206713
H,0,2.7076605634,-0.8936961909,7.1727714496
H,0,3.6646442816,-0.9246507296,5.6688152014
C,0,-0.0145898828,-0.3759588646,6.0980424351
H,0,-0.929983417,-0.6253654333,5.5584033318
H,0,-0.0665622225,-0.7815465907,7.1105498544
H,0,0.1106579244,0.7083079439,6.1394292785
C,0,-0.6644375918,-1.5230692264,2.6003836802
C,0,-1.7448583248,-0.6531662394,2.786500627
C,0,-0.8695097049,-2.8933532759,2.7796010751
C,0,-2.9976386466,-1.1435666304,3.1435857665
C,0,-2.1226515764,-3.3863201542,3.1358370695
C,0,-3.1900738227,-2.512627332,3.3198872632
H,0,-1.6179395598,0.4180352151,2.6488600485
H,0,-0.0392048025,-3.5799375368,2.636216541

TS-4a (SRS), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1761.58252028 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.426223 a.u.
1 imaginary frequency = 522.5427 i cm⁻¹
0; 1
C,0,-2.7849853608,-1.1278167152,2.8130746426
C,0,-4.1174650002,-1.5048188714,2.6818401317
C,0,-4.6409146362,-1.8067275027,1.423250926
C,0,-3.8162193914,-1.7402674286,0.3147030371
C,0,-4.1357830335,-1.9767317239,-1.1364382734
C,0,-1.9406818233,-1.0605333503,1.7050730525
C,0,-2.4730034003,-1.3841533795,0.4611243763
N,0,-1.8659523636,-1.3213040452,-0.8143834933
C,0,-2.9219642613,-1.3995021571,-1.8702571099
C,0,-3.1164070109,0.0400401031,-2.4611072447
C,0,-0.5863474454,-1.1446870169,-1.1348951297
C,0,0.5163983555,-1.2262086149,-0.3033748389
C,0,1.871063322,-0.7880538772,-0.8043732273
O,0,-2.1645616355,0.4140946646,-3.1789552722
O,0,-4.1395589396,0.6611447179,-2.1313455817
H,0,-2.3921052793,-0.8673806841,3.7888164592
H,0,-4.7545733606,-1.5476618512,3.5569869548
H,0,-5.6845468738,-2.0773004882,1.310267216
H,0,-0.9256592255,-0.7148013251,1.8267724718
H,0,-2.5558973478,-2.0499333728,-2.6631884566
H,0,-0.4482331089,-0.8951031839,-2.184903618
H,0,0.4339887286,-1.6269030173,0.6943293649
H,0,1.8631041083,-0.6172243508,-1.8816467416
C,0,-0.3674925818,2.1035944987,1.5749648437
C,0,-1.4737982967,2.4690439456,2.3301925435
C,0,-0.495972994,1.9334133164,0.192264293
H,0,-1.3723917504,2.6204279442,3.3983105656
C,0,-2.717889615,2.6118472167,1.7170801072
C,0,-1.7346238412,2.1180857968,-0.4267759972
H,0,-3.5871500378,2.8581408226,2.3159031258
H,0,-1.8231243817,1.9652830831,-1.4977757068
C,0,-2.8496467665,2.4291117507,0.3435901037
H,0,-3.8158308052,2.5098295406,-0.1385357153
H,0,0.5878312978,1.96241763,2.0698456655
C,0,0.625677897,1.4690490915,-0.6680680987
O,0,0.7592300265,1.7983663658,-1.8229875155
C,0,1.5903591078,0.4642915334,-0.0663623023
H,0,1.6613374311,0.4020954974,1.0162158326
S,0,3.5378425686,1.7694076621,-0.2708634437
C,0,2.9515523705,3.4349887789,0.1304879516
H,0,2.3276398197,3.422573277,1.024063345
H,0,3.8114222859,4.0864062765,0.2820633456
H,0,2.3725110525,3.7823436769,-0.7238234337
C,0,4.3553637413,1.3235536349,1.2801589293
H,0,4.7637705661,0.3201651379,1.1552293496
H,0,5.1632489511,2.0289797506,1.4712609814
H,0,3.6423200063,1.3385666638,2.105698848
C,0,3.111746214,-1.513067501,-0.3574299466
C,0,3.1891404122,-2.1589512769,0.8772408747
C,0,4.253855217,-1.4417540721,-1.1572886902
C,0,4.3904924548,-2.7130599862,1.3085685182
C,0,5.4565288526,-1.9932264639,-0.7256797517
C,0,5.5286071474,-2.625919995,0.5118011806
H,0,2.3157590349,-2.2369503856,1.515250552
H,0,4.2005732534,-0.9459869455,-2.1210273009

H,0,-3.8264366703,-0.4549432373,3.2797248305
H,0,-2.2628669589,-4.4551356916,3.267682608
H,0,-4.168301149,-2.8947380672,3.5959781254
H,0,2.3332654007,0.9289968939,-3.855864924
H,0,3.7628866043,1.8304916365,-3.3082630477

H,0,4.4367843491,-3.2142451324,2.2681373471
H,0,6.3347829117,-1.9307816937,-1.3572246277
H,0,6.463674406,-3.0558012209,0.8505005522
H,0,-4.2514958302,-3.0452437656,-1.3368743562
H,0,-5.0408814914,-1.4540029825,-1.4428696149

TS-4a (SSS), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1760.09894948 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.423273 a.u.
1 imaginary frequency = 354.7532 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6623088 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6890871 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.5787811 a.u.
0; 1
C,0,4.3047786901,0.7963126864,-3.0496866122
C,0,3.7140584901,0.8950380689,-4.3069156986
C,0,2.3370844912,1.0981961441,-4.4178304644
C,0,1.5667214822,1.1870844029,-3.26947537
C,0,0.0967724299,1.439384691,-3.1238248843
C,0,3.5429479105,0.8779739191,-1.8843058971
C,0,2.1654422583,1.0554444899,-2.0100496309
N,0,1.1910958203,1.193894025,-1.0102621944
C,0,-0.1565222261,1.3603374841,-1.6173689045
C,0,-1.10946913,0.1775228799,-1.1897301091
C,0,1.2928439816,1.067298272,0.3192330379
C,0,2.3192993266,0.5921737292,1.1036891512
C,0,2.0842658737,0.4494751669,2.5856549446
O,0,-1.7214986779,-0.4030060459,-2.1003062902
O,0,-1.1609573114,-0.0310238826,0.0514476926
H,0,5.3785281326,0.6571702785,-2.9662816579
H,0,4.3262037343,0.8244018603,-5.2008097037
H,0,1.8712801093,1.1944705011,-5.3947503674
H,0,4.0357082961,0.8328319526,-0.9228783354
H,0,-0.5973123288,2.2816989208,-1.2206341804
H,0,0.3620735628,1.32203002,0.8150911965
H,0,3.2512647877,0.2108692314,0.7116620188
H,0,1.2545492541,1.0969155544,2.8818883418
C,0,0.5603876081,-2.6815471493,0.0690218587
C,0,0.087092317,-3.574262321,-0.8884413207
C,0,1.7461217439,-2.9640031832,0.7596840542
H,0,-0.8189364174,-3.3255872199,-1.4325357902
C,0,0.7780511294,-4.7532645993,-1.1526667093
C,0,2.4414383925,-4.1515784353,0.482311732
H,0,0.4034534763,-5.4473447478,-1.8997579521
H,0,3.3613782893,-4.3524729887,1.0220062851
C,0,1.9569149475,-5.0431334572,-0.4621381763
H,0,2.4966207325,-5.962901794,-0.6672232451
H,0,-0.0014427729,-1.7630790144,0.2295454667
C,0,2.3458733566,-2.0505316795,1.7641986403
O,0,3.4726708657,-2.2446767589,2.2046059488
C,0,1.5128582002,-0.9148018304,2.3140473654
H,0,0.4945364464,-0.8571286709,1.936982379
S,0,0.8321693414,-2.0697729058,4.1703420845
C,0,-0.1396724082,-0.8023254263,5.0043801229
H,0,-0.4918645274,-1.1941685496,5.9606586374
H,0,0.456552722,0.0971123915,5.1657012396
H,0,-0.9986186032,-0.5768827675,4.3698292
C,0,2.2965692123,-2.1711500774,5.2174974493
H,0,2.0315630362,-2.6859820198,6.1432122193
H,0,3.0381583409,-2.7507188894,4.6661287023
H,0,2.6930842336,-1.1765076301,5.4253447369
C,0,3.2371892211,0.7262806631,3.5222757475
C,0,4.5483206954,0.2987214399,3.2905710412
C,0,2.98657762,1.5143803855,4.6513866367
C,0,5.5670240505,0.6272988805,4.1792445599
C,0,4.0040010894,1.8403214971,5.545445769
C,0,5.3002799423,1.3928217358,5.3125134461
H,0,4.7738348413,-0.3135265002,2.4259421593
H,0,1.9829461565,1.8958446328,4.8276899466

TS-4a (SSS), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1761.58461883 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.426954 a.u.
1 imaginary frequency = 488.2972 i cm⁻¹
0; 1
C,0,3.6778878785,-0.6966395926,-2.9498370761
C,0,3.070270096,-0.5215286583,-4.1893065914
C,0,1.873290093,0.1882951612,-4.285051201
C,0,1.3025660061,0.7122926967,-3.1380065957
C,0,0.036763382,1.5105524023,-2.9855574359
C,0,3.1135845887,-0.1762125024,-1.78613853
C,0,1.9157377387,0.5248211306,-1.895654898
N,0,1.1039666886,1.0987038195,-0.8888027679
C,0,-0.1986459292,1.5155916722,-1.4695340075
C,0,-1.3857842807,0.5876772047,-1.0066167552
C,0,1.2485686717,1.1070457988,0.4347275984
C,0,2.2838948246,0.6776650637,1.2375913578
C,0,2.0271805886,0.5453108577,2.720676174
O,0,-2.3773182171,0.6198546155,-1.7489039082
O,0,-1.2296133094,-0.0239205721,0.0731923865
H,0,4.6022240863,-1.2572783605,-2.8760357612
H,0,3.5250669124,-0.9399094837,-5.0789213847
H,0,1.3896051847,0.3281488651,-5.2454186794
H,0,3.6018926158,-0.3617268296,-0.8432915821
H,0,-0.4359824598,2.5154174169,-1.1010134714
H,0,0.3652901216,1.4827490869,0.9410558156
H,0,3.2477894487,0.3680282719,0.8691793556
H,0,1.1769139276,1.1625733858,3.0136777138
C,0,0.9581966572,-2.2424269652,-0.2154507485
C,0,0.7478055537,-2.8325500711,-1.4582161706
C,0,2.109837242,-2.550653744,0.5126776599
H,0,-0.1424477138,-2.5783043162,-2.0218394723
C,0,1.680383683,-3.7224696066,-1.9780870304
C,0,3.040267893,-3.4594750377,-0.0080582761
H,0,1.519973435,-4.1688443326,-2.9528629479
H,0,3.9292447785,-3.6893854986,0.5667733012
C,0,2.8277430715,-4.0387083366,-1.2490229034
H,0,3.5541640681,-4.7335734326,-1.6535304141
H,0,0.2241185363,-1.5255046668,0.135217267
C,0,2.4442865347,-1.9018238902,1.8125063168
O,0,3.4334707188,-2.2103577936,2.4437788451
C,0,1.5242366419,-0.8194040246,2.3574620568
H,0,0.5054644808,-0.8149082293,1.9832322643
S,0,0.8477767638,-2.0743102274,4.2113019138
C,0,-0.1438777474,-0.7889070429,5.0032272267
H,0,-0.5457172417,-1.171821668,5.9401652401
H,0,0.4707732863,0.0904802792,5.190204554
H,0,-0.9626570703,-0.542944,4.3279805347
C,0,2.2709687877,-2.1408351926,5.327030443
H,0,1.9319127927,-2.5223251597,6.2900831803
H,0,2.9893711504,-2.8252004036,4.881526438
H,0,2.7178149762,-1.1537308898,5.4356531795
C,0,3.1668010626,0.7868374607,3.6779800382
C,0,4.4740796558,0.3566852294,3.4444746488
C,0,2.8981138491,1.5085679004,4.843172114
C,0,5.4740199362,0.6049720122,4.3780975443
C,0,3.897222028,1.7581989298,5.7794907409
C,0,5.18840531,1.2958064098,5.5530934236
H,0,4.7206073383,-0.1884827353,2.5431968242
H,0,1.8979998274,1.8921709027,5.0180840681

H,0,6.5780423609,0.2821338572,3.9830145844
H,0,3.7824793904,2.4526630432,6.4146655836
H,0,6.0995673199,1.6458374409,6.0028098879
H,0,-0.1834143655,2.4112266704,-3.5436078424
H,0,-0.5191412814,0.671652676,-3.6046338692

H,0,6.4818486396,0.2564830478,4.1858588491
H,0,3.6653320923,2.317957239,6.6777545048
H,0,5.9708534361,1.4830338648,6.2788072883
H,0,0.1741108064,2.5219174625,-3.3764464898
H,0,-0.8158319174,1.0617640764,-3.493716768

TS-4a (RSR) 2, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1760.09765408 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.421186 a.u.
1 imaginary frequency = 338.9498 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6646891 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6907686 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.5790205 a.u.
0; 1
C,0,1.8859683831,4.5710087263,0.2036411289
C,0,2.0935843412,5.0710121485,-1.0797078499
C,0,2.3292895214,4.1956277127,-2.1419898202
C,0,2.3320368614,2.8295159314,-1.9107864096
C,0,2.5860673707,1.6947000416,-2.8565393702
C,0,1.8878905319,3.1990210075,0.4544807493
C,0,2.0914583219,2.3345990489,-0.6210991708
N,0,2.1652218829,0.9339338019,-0.6403038281
C,0,2.7089344933,0.4769794714,-1.9373207169
C,0,4.1760689155,-0.0902536651,-1.803858645
C,0,1.9099784009,0.0424054153,0.3252137544
C,0,1.2814549749,0.2298388693,1.5347217542
C,0,1.1306661189,-0.9021749189,2.5226294107
O,0,4.4043202372,-0.7185179842,-0.7483105851
O,0,4.9036179239,0.1005320316,-2.7966903645
H,0,1.7325941828,5.2564722073,1.0319630723
H,0,2.0891993797,6.1432095885,-1.2508220687
H,0,2.5187220656,4.5797231687,-3.1405860155
H,0,1.7794380157,2.8403435032,1.4693412368
H,0,2.0922383325,-0.3574739336,-2.2860602381
H,0,2.2626170447,-0.9518205031,0.0665107371
H,0,0.8650303034,1.1817202682,1.8376676919
H,0,1.7670670402,-1.7402187374,2.2294510925
C,0,-2.3588467109,-0.4752510605,-0.0038615873
C,0,-3.3956546556,-0.2544850209,-0.9037920746
C,0,-1.5412028176,-1.6053970632,-0.1357003319
H,0,-4.0202343466,0.6272201421,-0.8001134176
C,0,-3.6258620413,-1.1567240368,-1.9398261857
C,0,-1.7739796127,-2.5007539056,-1.1898715101
H,0,-4.4371819568,-0.9811719683,-2.6399908611
H,0,-1.1241046945,-3.3643592413,-1.2871205091
C,0,-2.8113971844,-2.2801937504,-2.0834257443
H,0,-2.9865773177,-2.9799746031,-2.8946533579
H,0,-2.1794069977,0.2545911942,0.778236922
C,0,-0.41105854,-1.91139039,0.7771052584
O,0,0.3770277056,-2.8178916217,0.5305493019
C,0,-0.2625760993,-1.157551375,2.0699328488
H,0,-0.9833667461,-0.3742875941,2.2817091075
S,0,-1.2089535161,-2.6323804603,3.5050337556
C,0,-2.4454626201,-3.5456869709,2.558082857
H,0,-2.0121518961,-3.9518569773,1.642139555
H,0,-2.8287671653,-4.3551429187,3.1829971426
H,0,-3.2572827305,-2.8583083577,2.3158382595
C,0,0.113127834,-3.8531019484,3.5891950128
H,0,0.9102990252,-3.4263479622,4.1997969582
H,0,-0.2721358247,-4.7533143876,4.0720619816
H,0,0.4787582961,-4.0733776744,2.5833831213
C,0,1.3686869262,-0.5442834848,3.9679364947
C,0,0.4754017765,0.2449844577,4.6992205904
C,0,2.5401861747,-0.9853095832,4.5911138416
C,0,0.7458406472,0.5799779601,6.0233883377
C,0,2.8123176143,-0.6500151051,5.9142467181
C,0,1.9142170898,0.1328941989,6.6350057197
H,0,-0.4408507503,0.609144821,4.2409832059
H,0,3.248176757,-1.5899303891,4.0295388182

TS-4a (RRR) 2, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1760.09278983 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.422128 a.u.
1 imaginary frequency = 335.8210 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6591962 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6853919 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.5740035 a.u.
0; 1
C,0,-0.964964684,3.9152557784,-0.1999383305
C,0,-0.7768676776,4.5478348232,-1.4266384062
C,0,0.0367823616,3.9618676912,-2.398238462
C,0,0.633806556,2.7383591023,-2.1394133337
C,0,1.5688826405,1.9313852329,-2.9869967115
C,0,-0.3695699464,2.6853461211,0.0776166433
C,0,0.4137739809,2.094959711,-0.9143043844
N,0,1.1333011924,0.890609755,-0.8823295126
C,0,2.0117031224,0.7855092663,-2.0735052313
C,0,3.5458970709,0.7969461899,-1.7056754745
C,0,1.144112792,-0.0828247763,0.0379017392
C,0,0.3005721819,-0.2882706011,1.1057837497
C,0,0.5148919821,-1.4648332492,2.0194327904
O,0,4.2756287766,1.4398880911,-2.4816749472
O,0,3.8534008979,0.0992392444,-0.7130002752
H,0,-1.5772442778,4.386714694,0.5630113255
H,0,-1.2512393324,5.5048933987,-1.6212388928
H,0,0.2089846179,4.4622115079,-3.3472415616
H,0,-0.4937021448,2.2414908353,1.056092603
H,0,1.8242365604,-0.1898950571,-2.5357237515
H,0,1.97455238,-0.7673551614,-0.1260279261
H,0,-0.5589339732,0.3367984337,1.3008512632
H,0,1.5389641327,-1.8331831634,1.9137429966
C,0,-1.5980834168,-2.3382229974,-1.6031599528
C,0,-2.2065407292,-2.5469549877,-2.8358830213
C,0,-2.376600691,-2.2205870763,-0.4441742578
H,0,-1.5973209079,-2.6247120705,-3.7309162008
C,0,-3.5931120276,-2.6478222183,-2.9228195892
C,0,-3.7728030231,-2.3045442642,-0.5455454676
H,0,-4.0645499249,-2.8156531221,-3.8865852334
H,0,-4.3643970302,-2.1944676459,0.357693351
C,0,-4.3765015294,-2.5248619859,-1.7752634999
H,0,-5.4576041774,-2.597402965,-1.8433650323
H,0,-0.5192059232,-2.2304599792,-1.5610737319
C,0,-1.8058177943,-1.9780050461,0.9096185651
O,0,-2.5143699796,-1.5852971731,1.8287006219
C,0,-0.3615581871,-2.3165650514,1.1531420133
H,0,0.1730151137,-2.7158520319,0.2956178845
S,0,-0.5684657118,-4.3576452387,2.1240190449
C,0,-1.819687957,-4.1637769718,3.4069990574
H,0,-2.6695959273,-3.5905072518,3.0320299296
H,0,-2.1288166185,-5.1578097487,3.7371908589
H,0,-1.3505655243,-3.627337923,4.2324807263
C,0,-1.4654908187,-5.338684754,0.9023253371
H,0,-0.8314387237,-5.4270426319,0.0185083362
H,0,-1.6466200634,-6.3328188508,1.316488324
H,0,-2.4107065959,-4.8633972302,0.6336702485
C,0,0.2312240001,-1.3139149724,3.4964056857
C,0,-0.7450355617,-0.4593905688,4.0143312942
C,0,1.0014182297,-2.068223731,4.3882443908
C,0,-0.9560824825,-0.3778831246,5.3872791848
C,0,0.7865347335,-1.9939986431,5.7627006768
C,0,-0.1969258506,-1.1476093069,6.2662186243
H,0,-1.3605351194,0.1336271819,3.3477420408
H,0,1.7847900322,-2.7167513333,4.0024607792

H,0,0.0405698256,1.1921238103,6.5778105744
H,0,3.7277440409,-1.0012391302,6.3811522014
H,0,2.1236656222,0.3940951374,7.6679961685
H,0,1.7649845762,1.5894941707,-3.5758415736
H,0,3.5189863313,1.796490248,-3.4189177642

H,0,-1.7198920131,0.2914439929,5.7723473077
H,0,1.3968448402,-2.5877918854,6.4368465942
H,0,-0.3651982412,-1.0802679813,7.3369956257
H,0,1.0726136666,1.5678644663,-3.8940213416
H,0,2.4613346329,2.4873043724,-3.2924086252

TS-4a (SRS) 2, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -1760.10057360 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.424449 a.u.
1 imaginary frequency = 340.2271 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6672585 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6933991 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.5816794 a.u.
0; 1
C,0,1.6367181858,4.3507271218,0.1258031663
C,0,1.9998372524,4.8615336973,-1.1200668274
C,0,2.5011643484,4.0129723375,-2.1095102248
C,0,2.6260298901,2.6582675589,-1.8429000126
C,0,3.1608436058,1.5457426277,-2.6949804276
C,0,1.7582370531,2.9917713638,0.409658445
C,0,2.2488348882,2.1602678337,-0.5942096041
N,0,2.4333679909,0.7718168512,-0.5618533332
C,0,3.0043107049,0.2788289333,-1.836061419
C,0,4.3781762363,-0.4734871294,-1.6203348837
C,0,2.0404616917,-0.0334120288,0.4354427772
C,0,2.2290074946,-1.3920121387,0.4466191698
C,0,1.7844753324,-2.2704078811,1.5785223894
O,0,5.3616342279,0.2594451127,-1.4211212161
O,0,4.312650096,-1.7267769948,-1.6837914777
H,0,1.2559757572,5.0186717013,0.892703659
H,0,1.8990455314,5.9242082058,-1.318278472
H,0,2.7936040761,4.4096119341,-3.0778778241
H,0,1.4808633804,2.6125735238,1.3877718944
H,0,2.2830871675,-0.4304574442,-2.2576179989
H,0,1.5426206503,0.4610352029,1.265539194
H,0,2.7800551461,-1.8471254529,-0.374825485
H,0,1.3867475567,-1.6798224162,2.4092471674
C,0,-0.7027120557,-2.2111140598,-1.9182437617
C,0,-1.4304069085,-2.0942366555,-3.0973163601
C,0,-1.2446567789,-1.7528612829,-0.7100968431
H,0,-1.0003077081,-2.4406444891,-4.031775181
C,0,-2.7028221218,-1.5269951236,-3.0802363053
C,0,-2.5190912452,-1.1683550682,-0.7058352159
H,0,-3.2692674008,-1.4405247915,-4.0027064522
H,0,-2.9182920301,-0.8037869371,0.2352428011
C,0,-3.2466485417,-1.0626829261,-1.8825884149
H,0,-4.2356935679,-0.6151715994,-1.8706846909
H,0,0.2989480761,-2.626936315,-1.9550711637
C,0,-0.5213924897,-1.8245737316,0.5853630932
O,0,-0.8990829737,-1.1875584546,1.562219479
C,0,0.6520446043,-2.754158623,0.7339253444
H,0,0.9454872242,-3.3525010273,-0.1248047913
S,0,-0.3631862204,-4.5378361414,1.7065882262
C,0,-1.3079920422,-3.8692798967,3.0875329087
H,0,-1.8521925342,-2.9719913232,2.7866722865
H,0,-1.9917749378,-4.643074073,3.4429629154
H,0,-0.6023974232,-3.6220500079,3.8810880787
C,0,-1.6962614651,-4.9637531925,0.5650092717
H,0,-1.238997518,-5.2905857652,-0.3704006729
H,0,-2.2665662257,-5.7906103362,0.9937632436
H,0,-2.349737029,-4.1092981911,0.3806614571
C,0,2.7729794895,-3.2997268965,2.0732658051
C,0,3.8623573439,-3.7168252022,1.30223298
C,0,2.5950153572,-3.8544819232,3.344932344
C,0,4.7312537344,-4.6912697567,1.7888812486
C,0,3.4627276603,-4.8288372794,3.8289463694
C,0,4.531870956,-5.2559220281,3.04579587
H,0,4.0656357328,-3.2604463015,0.3356871197
H,0,1.7824638067,-3.5008261139,3.9761946739

TS-4a (SSS) 2, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -1760.09115453 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.422304 a.u.
1 imaginary frequency = 325.8074 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6584279 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6846526 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.5749403 a.u.
0; 1
C,0,4.2738555643,3.7980919585,0.5128917851
C,0,5.2037823513,3.9472114826,-0.515423192
C,0,5.4705521281,2.8866930751,-1.3851438235
C,0,4.7965777942,1.6865301847,-1.2200333383
C,0,4.8615545506,0.4078457965,-2.0032247271
C,0,3.5919907319,2.5959084573,0.69707504
C,0,3.8613499267,1.5560788978,-0.1883095619
N,0,3.3033104257,0.2709314953,-0.2194825384
C,0,4.0611145091,-0.5850995524,-1.1478219696
C,0,4.9725899249,-1.6552199767,-0.4228965695
C,0,2.2202351874,-0.1098809935,0.4690119451
C,0,1.7004249755,-1.3765952187,0.4986194129
C,0,0.4431973394,-1.7202940696,1.2393397981
O,0,4.5416665269,-2.085860024,0.6674621268
O,0,5.986555422,-1.9809698354,-1.0685525483
H,0,4.0852293207,4.6232195806,1.1933141921
H,0,5.7306233043,4.88915861,-0.6337041631
H,0,6.2003119595,2.9996688331,-2.1821654822
H,0,2.8952345041,2.4823733226,1.5215426552
H,0,3.3379045175,-1.1533094557,-1.7445853537
H,0,1.7312300263,0.6868394903,1.0269758338
H,0,2.2557062733,-2.1885181961,0.048523745
H,0,0.1548604802,-0.8994459233,1.9074024421
C,0,0.3366822658,-0.6797434849,-2.8420052327
C,0,0.4808874597,-0.2659933028,-4.1617615912
C,0,0.131374108,-2.034052522,-2.546156806
H,0,0.6500216726,0.7834414937,-4.3821758193
C,0,0.4185802274,-1.197051551,-5.1964217326
C,0,0.0838809183,-2.9641249725,-3.5935115601
H,0,0.5301973077,-0.8707969799,-6.22616309
H,0,-0.0623895732,-4.011033519,-3.3479979116
C,0,0.2217534057,-2.5476557485,-4.9101402593
H,0,0.1794892318,-3.2744603413,-5.7154904342
H,0,0.4222240969,0.053364688,-2.0464927409
C,0,-0.0336171632,-2.5612182199,-1.162783459
O,0,-0.0026815661,-3.7592043656,-0.9305724783
C,0,-0.3517724617,-1.603736726,-0.0335646977
H,0,-0.527638565,-0.5694102395,-0.3207811243
S,0,-2.4900590022,-2.1042378624,0.2240883346
C,0,-3.0173974176,-0.6075343575,1.0799337395
H,0,-2.6676262043,0.2866362864,0.5586028396
H,0,-4.107129447,-0.60086149,1.1438756683
H,0,-2.6031181612,-0.6353709984,2.0892727582
C,0,-3.1481180597,-1.7898315391,-1.4264144279
H,0,-2.8857456122,-2.6438493416,-2.0522875099
H,0,-4.2352438322,-1.7117571019,-1.361131408
H,0,-2.726734171,-0.8757891337,-1.8501450913
C,0,0.4770337394,-3.0147762514,2.0262573552
C,0,1.6601033153,-3.7468902518,2.1560085975
C,0,-0.6583683818,-3.4510169082,2.7170142814
C,0,1.6892458878,-4.9093636814,2.923871584
C,0,-0.6306442153,-4.6134066711,3.4798002497
C,0,0.5452824202,-5.3534065954,3.5790520312
H,0,2.5730062045,-3.3985923285,1.6791525991
H,0,-1.5785551927,-2.8735264268,2.6814560403

H,0,5.5774817205,-5.0006044638,1.1822692817
H,0,3.3098953802,-5.2440571155,4.8209582695
H,0,5.2152584338,-6.0126025086,3.4200155714
H,0,2.6304764523,1.4617039425,-3.6486855417
H,0,4.2259799513,1.6967584093,-2.8983403008

H,0,2.6180668465,-5.4655379438,3.0115648219
H,0,-1.5260854772,-4.9354810251,4.0036228981
H,0,0.5713822157,-6.2613972174,4.17451069
H,0,4.4246458635,0.5405008178,-3.0008564865
H,0,5.873066972,0.0114959416,-2.1256919755

TS-4a (RSS), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -1760.09862804 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.422448 a.u.
1 imaginary frequency = 331.5244 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6659091 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6920739 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.5819385 a.u.

0; 1
C,0,6.3599894004,2.2631149654,-2.130275602
C,0,5.7792001965,3.302954057,-2.8553049904
C,0,4.394181515,3.3503875407,-3.0345580411
C,0,3.6025136173,2.3588024061,-2.4767164468
C,0,2.115876792,2.1584285473,-2.5132146953
C,0,5.5783087143,1.2553656652,-1.5668180879
C,0,4.1991087012,1.3306886555,-1.7431673293
N,0,3.2125293186,0.4670173112,-1.2493217864
C,0,1.8923503217,0.8005491746,-1.8290138603
C,0,1.4106266839,-0.3247164309,-2.831114328
C,0,3.4191506894,-0.4419732964,-0.283582963
C,0,2.4904631234,-1.3359557304,0.1800553193
C,0,2.7732511693,-2.2376452528,1.3647209218
O,0,0.8345453021,-1.2955122115,-2.2879815955
O,0,1.6564158232,-0.1237679452,-4.0348785225
H,0,7.4387661394,2.225405212,-2.0109952657
H,0,6.4077533747,4.0724683508,-3.2930784262
H,0,3.9416304284,4.1545913667,-3.6082580696
H,0,6.0445196772,0.434864228,-1.0303631505
H,0,1.1765331462,0.8457146169,-1.0014042313
H,0,4.4223655143,-0.4306492853,0.1385414303
H,0,1.5413983298,-1.4347236406,-0.3449886945
H,0,2.0547181737,-3.0604785317,1.3425894406
C,0,1.2107082591,1.6250366541,2.3701627161
C,0,0.6941300293,2.9060926694,2.529122092
C,0,0.3652360257,0.5102103957,2.4499544619
H,0,1.3533945178,3.7654675957,2.4577174976
C,0,-0.6660542006,3.0860639464,2.7702822324
C,0,-1.0044503122,0.7034504855,2.6798018877
H,0,-1.0659284847,4.0880116873,2.8947108186
H,0,-1.6490861722,-0.1683558856,2.7235929384
C,0,-1.5158281623,1.9823212709,2.8433068274
H,0,-2.5770432289,2.1228833285,3.0237506021
H,0,2.2675382792,1.5089626382,2.154055618
C,0,0.8361347507,-0.8880302556,2.2852172588
O,0,0.0475637657,-1.8219186012,2.1966770571
C,0,2.3130151098,-1.1946856176,2.3205473657
H,0,2.9909496101,-0.3603402123,2.4679451819
S,0,2.5238605579,-1.9823263789,4.4016873629
C,0,1.1893084967,-1.2332899251,5.3587006046
H,0,0.2269784012,-1.4035640427,4.8722610425
H,0,1.1913365692,-1.674942156,6.3573957553
H,0,1.3901945795,-0.1636657546,5.4339644607
C,0,1.8694597518,-3.6428400097,4.1600624131
H,0,2.6204098116,-4.2117076491,3.6098102033
H,0,1.711069674,-4.1020680499,5.1377853867
H,0,0.9364022721,-3.5893459593,3.5944726792
C,0,4.1739897598,-2.7776226831,1.5085325056
C,0,5.1914484583,-2.1074453431,2.1944379493
C,0,4.474662429,-3.9993825923,0.8941238991
C,0,6.4772344276,-2.6438086533,2.2617454707
C,0,5.7552712597,-4.534746321,0.9606513949
C,0,6.7629060238,-3.857112083,1.6457517724
H,0,4.9951048762,-1.1611473083,2.6908895253
H,0,3.6941347575,-4.5278934581,0.3526056733

TS-4a (RRS), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -1760.09080348 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.422939 a.u.
1 imaginary frequency = 347.3531 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6561274 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6822291 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.5702568 a.u.

0; 1
C,0,6.0342547104,2.8011956357,-1.3579565835
C,0,5.3976530405,3.6394046921,-2.2732040954
C,0,4.12801069,3.3179759876,-2.7575740239
C,0,3.5021720623,2.1652675668,-2.3081034394
C,0,2.1878403011,1.5579587617,-2.6951444559
C,0,5.4202983424,1.6369075199,-0.9005122809
C,0,4.1446205501,1.3457960303,-1.3783171112
N,0,3.3176996339,0.2631364689,-1.0434792851
C,0,2.0243432373,0.342504188,-1.7684528345
C,0,1.6635440423,-0.9716554164,-2.5638823952
C,0,3.5823613969,-0.602086787,-0.0555515381
C,0,2.8510440304,-1.729943082,0.229957158
C,0,3.1297506899,-2.6047147523,1.4299657292
O,0,0.8096091804,-1.7120354921,-2.0118657755
O,0,2.2531639182,-1.1248117736,-3.6466230984
H,0,7.0271287832,3.0518634106,-0.9966793178
H,0,5.8963999079,4.5400945207,-2.6178018124
H,0,3.6358537346,3.9614179933,-3.4815804713
H,0,5.9369707866,0.9867643492,-0.2020339462
H,0,1.2547518238,0.5019283262,-1.0069598
H,0,4.46574692,-0.3704183989,0.5349387265
H,0,2.0631763994,-2.0407697559,-0.453318624
H,0,2.9101783783,-3.6430528601,1.1639456718
C,0,-0.4645114845,-0.4341245294,1.0481447306
C,0,-1.7059028869,0.1538082487,0.8249470336
C,0,0.2880710516,-0.062469456,2.1720835283
H,0,-2.2745149231,-0.1210802962,-0.0580243419
C,0,-2.2121014099,1.0956568712,1.7180247669
C,0,-0.2144150911,0.9093881209,3.0490967522
H,0,-3.1862230425,1.5421230439,1.5410518956
H,0,0.3907832769,1.2054284535,3.9004130355
C,0,-1.4628647956,1.4759593697,2.8308890035
H,0,-1.8505297006,2.21744305,3.5228440652
H,0,-0.0692524174,-1.1173470115,0.2982373854
C,0,1.6332262305,-0.6265934404,2.4850919697
O,0,2.424248052,0.011115671,3.1692281501
C,0,1.8895098652,-2.045596132,2.0504725848
H,0,1.0086709086,-2.493594774,1.5954832421
S,0,1.5020628493,-3.1851314824,4.0128193841
C,0,2.3908478004,-2.2833914489,5.2943863181
H,0,2.2180961764,-1.20964802,5.1982058045
H,0,2.0634248769,-2.648868203,6.2701512467
H,0,3.4520603904,-2.4953075765,5.1586211402
C,0,-0.2100977072,-2.790958836,4.4254114784
H,0,-0.843424791,-3.2292240931,3.6524338495
H,0,-0.4529602656,-3.2436625647,5.3891689054
H,0,-0.3677618424,-1.7116812326,4.4635300505
C,0,4.5097711271,-2.5820582704,2.0407128977
C,0,4.9899380433,-1.6038182576,2.9174744167
C,0,5.3774500158,-3.610746294,1.649384439
C,0,6.3008081674,-1.662522208,3.3913044828
C,0,6.6844951571,-3.6654890985,2.1188176798
C,0,7.1520980691,-2.6889406263,2.9957400784
H,0,4.3308536551,-0.8024865271,3.2330636757
H,0,5.0223844087,-4.3768562561,0.964316279

H,0,7.2535826193,-2.1089693862,2.8009395471
H,0,5.9675794893,-5.4839531379,0.4776392399
H,0,7.7635708261,-4.2752419951,1.699678677
H,0,1.5885801726,2.970194628,-1.9990557459
H,0,1.7499763783,2.0869852854,-3.5415523341

H,0,6.6543009708,-0.8953651359,4.0746385007
H,0,7.3366909361,-4.4742226098,1.8023417386
H,0,8.1716500268,-2.7300541309,3.3676985344
H,0,1.3527298097,2.2581010565,-2.5980988039
H,0,2.2235409326,1.197431493,-3.7293632945

TS-4a (RSS) 2, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1760.10826361 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.423676 a.u.
1 imaginary frequency = 341.4469 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6715335 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6984606 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.5902689 a.u.

0; 1
C,0,6.2456038492,2.2184323709,-2.8934592112
C,0,5.4874254408,2.9070273512,-3.8368916962
C,0,4.0935151765,2.8212500996,-3.8106856011
C,0,3.4775409764,2.039150304,-2.8475111274
C,0,2.0176878227,1.822124135,-2.580820704
C,0,5.6413756451,1.4220878443,-1.9203093127
C,0,4.2502435269,1.3283596858,-1.9185424038
N,0,3.4056492798,0.6199437361,-1.0542863084
C,0,1.9972367444,0.7429321076,-1.4943944722
C,0,1.4076839151,-0.6353270856,-1.9849055753
C,0,3.6865737906,-0.2749449964,-0.0962997081
C,0,4.8661757155,-0.8472523944,0.3084023413
C,0,4.814099396,-2.0131423213,1.2832183228
O,0,1.8197570545,-1.6614463545,-1.3795794309
O,0,0.55206527,-0.5544201552,-2.8793388698
H,0,7.3285600336,2.2986963821,-2.9080311725
H,0,5.9798189688,3.5173698906,-4.5877810858
H,0,3.4942220681,3.3671845665,-4.5342446264
H,0,6.2555386292,0.9198239522,-1.1856156092
H,0,1.3910880167,1.0442773328,-0.6323929505
H,0,2.7872047393,-0.6057011423,0.4075832373
H,0,5.8300468649,-0.633983137,-0.1299148084
H,0,5.8250198279,-2.2163044297,1.6426292933
C,0,4.1588745371,-3.2328258363,-2.8305380646
C,0,4.0035303132,-3.5091844984,-4.1863940718
C,0,5.3802206495,-3.5190505698,-2.2041077155
H,0,3.0600969004,-3.2763704454,-4.6706923655
C,0,5.0473569697,-4.0688064872,-4.9181242236
C,0,6.4333927201,-4.0713589501,-2.950497776
H,0,4.9154003339,-4.2828261134,-5.974922415
H,0,7.3738222624,-4.2744529553,-2.4479524422
C,0,6.266623656,-4.3493780659,-4.297994653
H,0,7.0826153694,-4.7816649123,-4.8692639998
H,0,3.3325635718,-2.7657082064,-2.2942153027
C,0,5.6359432517,-3.2517142418,-0.769312916
O,0,6.7621242887,-3.3478023832,-0.289762053
C,0,4.485241531,-2.9281134567,0.153780897
H,0,3.4953455539,-2.8159528695,-0.2835665952
S,0,4.1035187549,-4.9795709566,1.0089587842
C,0,4.5268935937,-6.181657363,-0.2692464777
H,0,5.5323798744,-6.0041345529,-0.6551670988
H,0,4.4598917009,-7.1824771774,0.162677234
H,0,3.7957793936,-6.081285316,-1.072690476
C,0,5.5296799674,-5.1298467741,2.0986498184
H,0,5.3493997632,-4.4826847092,2.958624244
H,0,5.6085984437,-6.165316892,2.4357816686
H,0,6.4347210578,-4.8181937463,1.571205597
C,0,3.8588171654,-1.9394012125,2.4470455257
C,0,2.4896182228,-2.2059282996,2.3294359883
C,0,4.3650632264,-1.5774000986,3.7005815793
C,0,1.6513526746,-2.1027553322,3.4381136416
C,0,3.5284541327,-1.4746562126,4.8068488789
C,0,2.1661729209,-1.7375737794,4.678127576
H,0,2.0604808051,-2.4860443767,1.37024126
H,0,5.4274260453,-1.3698368376,3.8051877959

TS-4a (RRS) 2, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1760.08696248 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.424898 a.u.
1 imaginary frequency = 367.8740 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.653484 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.680131 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.5700794 a.u.

0; 1
C,0,-0.5570449677,4.0193060056,0.224129867
C,0,-0.4806367299,4.7155022092,-0.9800508585
C,0,0.1744636804,4.1499799667,-2.0757855819
C,0,0.7221277339,2.8823794197,-1.9606253489
C,0,1.5004335301,2.0779272371,-2.9573893035
C,0,-0.0102889699,2.7434549494,0.3576111645
C,0,0.6068105296,2.1745745751,-0.7563677046
N,0,1.2506281068,0.9337309963,-0.8848796511
C,0,2.0460292924,0.9110305754,-2.1315810649
C,0,3.5947708176,0.9915211839,-1.8376881726
C,0,1.2811270289,-0.1144497291,-0.0563327001
C,0,0.5085764141,-0.3456995841,1.0613187999
C,0,0.6764832707,-1.5588848781,1.9522987635
O,0,4.2598653454,1.6389805006,-2.6655102388
O,0,3.9740403449,0.3390778297,-0.8380589264
H,0,-1.039059321,4.4775622852,1.0826618605
H,0,-0.9151643186,5.707269741,-1.0606271087
H,0,0.2639200888,4.7000432937,-3.0084333225
H,0,-0.029660884,2.2476818575,1.3189742257
H,0,1.8766688784,-0.0509467466,-2.6251037455
H,0,2.0092434204,-0.8537078907,-0.3676291257
H,0,-0.3145201772,0.3095294867,1.3140145254
H,0,-0.2906369377,-1.7837257888,2.4105971039
C,0,2.2351179542,2.1431124722,3.6897662647
C,0,2.4652176643,3.5112487389,3.778898275
C,0,2.9516760211,1.3689950126,2.7673847815
H,0,1.9226199003,4.1038627247,4.5091984949
C,0,3.3865636815,4.1188889588,2.9281289355
C,0,3.8839117331,1.9824611794,1.919092513
H,0,3.5527384284,5.1905691888,2.9873627712
H,0,4.3853796563,1.3794661436,1.1658469688
C,0,4.0862151623,3.3550040512,1.9953507168
H,0,4.7885558549,3.8320481955,1.318615697
H,0,1.5126783604,1.6878004185,4.3616757026
C,0,2.7919223932,-0.1040419005,2.6391924847
O,0,3.740175736,-0.8147480165,2.3427731555
C,0,1.4306026689,-0.6922071786,2.91332391
H,0,0.7580069938,-0.0171025983,3.437219702
S,0,1.843980971,-1.9274970899,4.8326634653
C,0,2.9428836002,-3.2386200544,4.2627146903
H,0,3.70721441,-2.8160444385,3.6079483123
H,0,3.3875649346,-3.7219680231,5.1355059637
H,0,2.3366969237,-3.9568704718,3.7103340981
C,0,3.01092454,-0.9132636297,5.7641871297
H,0,2.4792411649,-0.0349938503,6.1328649303
H,0,3.3786960295,-1.4917309974,6.6142149744
H,0,3.8463812652,-0.6104871192,5.1297821356
C,0,1.2044120312,-2.8544007526,1.3790881434
C,0,2.4543698328,-3.0218618569,0.7677729099
C,0,0.3471712679,-3.9605068372,1.4445492457
C,0,2.8228201142,-4.2582495412,0.2432056592
C,0,0.7184475766,-5.1970255846,0.9243826082
C,0,1.9619884865,-5.3496077988,0.3186405001
H,0,3.1626155254,-2.2028305284,0.7224127673
H,0,-0.6298047679,-3.8515117003,1.909812754

H,0,0.591294673,-2.3109967706,3.3274163082
H,0,3.9414095726,-1.1919938132,5.7708543232
H,0,1.5108499338,-1.6604052075,5.5406204228
H,0,1.5394782426,2.7514806903,-2.2514938447
H,0,1.4622451742,1.452288987,-3.4475565729

H,0,3.7967853831,-4.3646949133,-0.225414495
H,0,0.0337150953,-6.0374032705,0.9920979283
H,0,2.2583465785,-6.3108463673,-0.0908617222
H,0,0.8604795478,1.7395441587,-3.7808514874
H,0,2.3485524171,2.6222226941,-3.3831685567

Int-4a (RSR), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1282.38104021 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.354698 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1282.8950651 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1282.9071849 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1283.6389774 a.u.

0; 1
C,0,-0.089005031,4.1341271922,0.3403620573
C,0,-0.6245468945,4.5236723164,-0.8901517213
C,0,-0.4440747028,3.7409619057,-2.0282928168
C,0,0.2774656843,2.5577128805,-1.9243258805
C,0,0.6124183903,1.5264035462,-2.9574195765
C,0,0.6380470651,2.9544206194,0.4609621698
C,0,0.8013336433,2.1904779914,-0.688117448
N,0,1.49760034,0.9566731221,-0.824005507
C,0,1.6293162795,0.6295959435,-2.2511947112
C,0,3.1367115796,0.8662146079,-2.737488836
C,0,2.0499724079,0.3021146281,0.1478670224
C,0,2.7272507033,-0.9662843813,0.0196372505
C,0,2.6352716836,-1.9707558478,1.1657313022
O,0,3.226011951,1.0802403744,-3.9546797301
O,0,3.9992555388,0.7479920907,-1.8483976017
H,0,-0.2335724267,4.7604637356,1.2146138254
H,0,-1.1842123117,5.4513028734,-0.9592724123
H,0,-0.8582686201,4.0497255731,-2.9831903427
H,0,1.0621315548,2.6677082649,1.4175379114
H,0,1.4227334374,-0.4338398513,-2.3933602316
H,0,1.954542518,0.7277515852,1.1433760587
H,0,2.8518368877,-1.3647366606,-0.9782393684
H,0,2.0932178302,-1.5968749506,2.0334318765
C,0,6.3479424985,0.4351131698,0.5786982441
C,0,7.6118518686,1.0116637939,0.5016128697
C,0,5.7054614492,0.341679619,1.8197022298
H,0,8.1024060279,1.1050855993,-0.4623633928
C,0,8.2428187728,1.4741039382,1.6544438012
C,0,6.3298583329,0.8362389703,2.9712747001
H,0,9.2348785241,1.9117334605,1.5898967485
H,0,5.8066293088,0.76980487,3.9201838219
C,0,7.6009621804,1.387412596,2.8904237825
H,0,8.0925927892,1.7538072682,3.7866001023
H,0,5.8368290699,0.1240281007,-0.3289387608
C,0,4.3432382909,-0.2283595513,1.9441187642
O,0,3.5799064905,0.121670946,2.8351181745
C,0,3.920284804,-1.2607107371,0.9414532757
H,0,4.7193826446,-1.7769699145,0.4206610909
C,0,2.4385757467,-3.4149746686,0.8512551645
C,0,3.5092982239,-4.3062677405,0.7600737707
C,0,1.1387732816,-3.8971398509,0.6583690951
C,0,3.2873278289,-5.6510189518,0.4713793773
C,0,0.9165807352,-5.239109929,0.3724768015
C,0,1.992342268,-6.1205811229,0.2751765233
H,0,4.5228005048,-3.9543741779,0.9289167514
H,0,0.2982861291,-3.2114776245,0.7319732031
H,0,4.1304909626,-6.3323509475,0.4052115742
H,0,-0.0975763442,-5.598438919,0.2240927423
H,0,1.819846237,-7.1689960127,0.0507401481
H,0,-0.2844943145,0.9760366802,-3.2635148738
H,0,1.0798411289,1.9392039082,-3.8552295765

Int-4a (RRR), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1282.37529485 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.352629 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1282.8897877 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1282.9016318 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1283.6330952 a.u.

0; 1
C,0,-0.4505751683,4.381926643,0.1138107361
C,0,-1.1295563122,4.6792743418,-1.0705524802
C,0,-0.9731576904,3.8828804037,-2.2027518736
C,0,-0.1293149887,2.780564577,-2.1399990114
C,0,0.2095354899,1.752258149,-3.1748075258
C,0,0.3994534685,3.2835023155,0.1926113984
C,0,0.5389398446,2.5053208716,-0.9497823385
N,0,1.3348542259,1.3380981326,-1.1235107116
C,0,1.376881069,0.9932769437,-2.5473604559
C,0,2.8063875398,1.4175407864,-3.1459245947
C,0,2.0565650705,0.7751393165,-0.2074043434
C,0,2.7853903082,-0.4678321649,-0.3482442077
C,0,2.69226594,-1.4397543971,0.8182349612
O,0,2.7754681834,1.6212198211,-4.3682943101
O,0,3.7324291057,1.4342322112,-2.3181975173
H,0,-0.5807966091,5.0163228674,0.9845318512
H,0,-1.7845470328,5.5441751497,-1.1080607401
H,0,-1.5008935628,4.1186194738,-3.1217756665
H,0,0.928320176,3.0675344146,1.1148634814
H,0,1.2972026061,-0.0897018209,-2.6637802279
H,0,2.0302397033,1.2370614367,0.7769114475
H,0,2.8996259892,-0.8857509016,-1.340594056
H,0,2.1857761026,-1.037626434,1.6936503548
C,0,6.5331389684,-1.1467130754,2.0030146726
C,0,7.7590172118,-1.2426245476,2.653153315
C,0,6.4308694403,-1.46579983,0.6441281219
H,0,7.8306294392,-1.0020302422,3.7094241413
C,0,8.8914729437,-1.6459442349,1.9498024369
C,0,7.5723332552,-1.8831607246,-0.0518181164
H,0,9.8492832891,-1.7122259666,2.4575895809
H,0,7.4734623263,-2.132385961,-1.1033594204
C,0,8.7968831705,-1.9661221405,0.5952838365
H,0,9.6798458391,-2.2804319741,0.0471085785
H,0,5.6565487834,-0.8436516797,2.5670355676
C,0,5.1460800965,-1.4083531941,-0.103855427
O,0,5.0328076097,-1.9308835482,-1.20126574
C,0,3.9893946562,-0.7002089609,0.5322915107
H,0,4.2392718542,0.0811953821,1.2424815468
C,0,2.4655110257,-2.9021983464,0.6585383245
C,0,2.5739144383,-3.5865660078,-0.5569755416
C,0,2.1005422792,-3.6226629406,1.8031880279
C,0,2.334283946,-4.9564049999,-0.6169209139
C,0,1.8619887099,-4.9909812419,1.741725769
C,0,1.9790320036,-5.6639792149,0.5282167296
H,0,2.8593174434,-3.0574247426,-1.4588905506
H,0,2.0028074859,-3.1016925264,2.7526279792
H,0,2.4240914951,-5.4714806812,-1.5688264191
H,0,1.5804287823,-5.5296889215,2.6418022493
H,0,1.7907545166,-6.7321594504,0.4746750701
H,0,-0.6507164196,1.1035776938,-3.3756883328
H,0,0.5459897315,2.1773827678,-4.1241753163

Int-4a (SRS), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1282.40895808 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.356902 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1282.9098508 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1282.9232277 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1283.6620196 a.u.

0; 1
C,0,-1.5105103507,1.4095603471,-2.0138600049
C,0,-1.3723192925,2.1054529584,-3.213051154
C,0,-0.1060927385,2.2846605377,-3.7720087502
C,0,1.0051801981,1.7897555468,-3.1059230492
C,0,2.4481932038,1.7749442286,-3.5274450945
C,0,-0.4009846237,0.8962275051,-1.3417546569
C,0,0.8631389971,1.1213571927,-1.8835104338
N,0,2.1136792954,0.6424052743,-1.4125186172
C,0,3.1426269941,1.2720927296,-2.2606833519
C,0,3.672656845,2.3993177139,-1.3809825482
C,0,2.589432294,0.8848309855,-0.0641095489
C,0,1.5733936019,0.9730885711,1.0268659872
C,0,1.1336222376,-0.2561353059,1.7571861868
O,0,3.2975554958,2.1644269573,-0.1141793623
O,0,4.3150397465,3.3604688177,-1.7182285954
H,0,-2.499030479,1.2512315007,-1.5922879067
H,0,-2.2499005908,2.4942567255,-3.7203462638
H,0,0.0100239916,2.8056286863,-4.7186274449
H,0,-0.5336687411,0.3274263449,-0.4287507317
H,0,3.9688407085,0.5809437157,-2.464739007
H,0,3.3431274738,0.1291747478,0.1765433687
H,0,0.8363249829,1.7591455034,0.8838026951
H,0,1.6971116268,-1.1519573278,1.5041296983
C,0,3.6358354056,2.3608538924,4.4039119495
C,0,4.3474605858,3.0175896999,5.4024876277
C,0,4.0835697842,1.1281018618,3.9147078569
H,0,3.9997107529,3.9781461118,5.7699640373
C,0,5.5033984403,2.4452443658,5.9273556665
C,0,5.2560850383,0.5680347696,4.4385081661
H,0,6.0533491737,2.956570965,6.7120530406
H,0,5.5951471058,-0.3832417761,4.0411363912
C,0,5.9578314064,1.2182346307,5.4433331179
H,0,6.8605177078,0.7728060964,5.8505198985
H,0,2.7472079424,2.8297134096,3.9939590557
C,0,3.3837762556,0.3816306116,2.8331242091
O,0,3.940682961,-0.5471010356,2.2588668033
C,0,1.9890078719,0.7712669407,2.4744675513
H,0,1.4656812013,1.4070666611,3.180004493
C,0,-0.2811230986,-0.4930425224,2.1482229189
C,0,-1.1539897232,0.5512215492,2.4769352334
C,0,-0.7630332301,-1.8052439394,2.1933338609
C,0,-2.4695917234,0.2878791721,2.8435420355
C,0,-2.0796939354,-2.0693860867,2.5593871067
C,0,-2.9381757645,-1.0236661677,2.8866982508
H,0,-0.8097504128,1.5823791098,2.4499500263
H,0,-0.0972108031,-2.6260165563,1.9393525606
H,0,-3.131234408,1.1114595666,3.095856478
H,0,-2.4338366974,-3.0957769817,2.5881458167
H,0,-3.9656940104,-1.2277203171,3.1726380651
H,0,2.6081929124,1.0850118993,-4.3627667669
H,0,2.8416002487,2.7525329041,-3.8229399162

Int-4a (SSS), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1282.37573296 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.353748 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1282.8877096 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1282.8997952 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1283.6309192 a.u.

0; 1
C,0,4.5600888544,1.575074815,-3.0459952008
C,0,4.0901072951,1.8152490954,-4.3373045388
C,0,2.729023772,1.9988901264,-4.5701172846
C,0,1.8429860426,1.9213940065,-3.5041907009
C,0,0.3629561936,2.1511003132,-3.4809726742
C,0,3.6847452698,1.4891189591,-1.9671497804
C,0,2.3238198248,1.6370715677,-2.2232606934
N,0,1.2308424924,1.6197095752,-1.3170087639
C,0,-0.0345830403,1.7660677241,-2.0611856311
C,0,-0.8193114097,0.3858565744,-1.9685535922
C,0,1.1276907366,1.1977845904,-0.0858658027
C,0,2.1121118673,0.5173905038,0.7262183706
C,0,1.9590436588,0.5127793706,2.2232763032
O,0,-1.6100384038,0.1844346058,-2.8969046202
O,0,-0.5679161329,-0.2933694377,-0.9441775837
H,0,5.6245817378,1.4572667243,-2.8707582544
H,0,4.7923554833,1.8747474106,-5.1629222267
H,0,2.3623000586,2.2103544876,-5.5700556687
H,0,4.0804868465,1.3371876095,-0.9719950656
H,0,-0.6600749311,2.5156732742,-1.5680819506
H,0,0.1692397086,1.3947385252,0.3788191993
H,0,3.1028731184,0.3121727528,0.3435676
H,0,1.1175015495,1.1036578417,2.5845577602
C,0,0.3882417796,-3.2975289071,0.4968141731
C,0,-0.2106611699,-4.5353105049,0.2804068366
C,0,1.6143805646,-3.2307167108,1.1724377539
H,0,-1.1515619948,-4.5886575599,-0.2587816249
C,0,0.3932616016,-5.7001928863,0.7474269718
C,0,2.2307450358,-4.407930126,1.6149820861
H,0,-0.0857837163,-6.6615260112,0.5851728738
H,0,3.1890112165,-4.3347658995,2.1198288737
C,0,1.6165850318,-5.6362400153,1.4154279723
H,0,2.0896428339,-6.5452118677,1.7749091706
H,0,-0.0780798622,-2.4015876894,0.0916402793
C,0,2.3284598291,-1.9460791556,1.3988679665
O,0,3.5415190797,-1.904181836,1.5357598233
C,0,1.5067905949,-0.6987476454,1.4611595398
H,0,0.4361430592,-0.8118916848,1.3459938973
C,0,3.1466358799,0.5521889084,3.1286290627
C,0,4.2268030026,1.3946185151,2.863124335
C,0,3.1409642643,-0.1924757339,4.3111382448
C,0,5.2902809236,1.4839379973,3.7574906827
C,0,4.2017552016,-0.1029093685,5.2059402031
C,0,5.2807026943,0.735006944,4.9308580825
H,0,4.2342254011,1.9873614295,1.9520865912
H,0,2.3019470648,-0.8489583562,4.5266035771
H,0,6.1263292166,2.1412585832,3.5367861926
H,0,4.1876188054,-0.6910727547,6.1189604272
H,0,6.1101119434,0.803188932,5.628637732
H,0,0.1295473797,3.1952787753,-3.7145201332
H,0,-0.1919722617,1.5186213357,-4.1804589317

Int-4a (SSS) 2, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -1282.37925564 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.352556 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1282.8927743 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1282.9048978 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1283.6373862 a.u.

0; 1
C,0,4.7286471465,4.1823510867,0.3916253815
C,0,6.0950647188,4.1410988575,0.1025122988
C,0,6.7180814279,2.9422474369,-0.2371067797
C,0,5.9586436495,1.7796148959,-0.288268032
C,0,6.3477964506,0.3747577907,-0.6326486983
C,0,3.9548076217,3.0272287006,0.347502671
C,0,4.5987673085,1.8453852558,0.0027471344
N,0,4.0350642937,0.5434382698,-0.1144977373
C,0,5.1185288201,-0.4402798043,-0.2322647151
C,0,5.2998789901,-1.2146721909,1.1573983863
C,0,2.7795075932,0.2559034822,0.0141337684
C,0,2.1920155822,-1.0550944478,-0.1461979516
C,0,0.8967556206,-1.3604307826,0.5619568034
O,0,4.2795166249,-1.2583752533,1.8694647363
O,0,6.4301563863,-1.7004139683,1.2979058424
H,0,4.2624296925,5.1241109246,0.6623455022
H,0,6.6783575803,5.0554585275,0.1490266158
H,0,7.7809678236,2.9140483164,-0.4563332674
H,0,2.8976558873,3.067640587,0.5885925663
H,0,4.843326577,-1.191169503,-0.9761213871
H,0,2.1133915345,1.0954028219,0.1991837329
H,0,2.8492221647,-1.9041250363,-0.2875270576
H,0,0.4678875385,-0.5265166078,1.1175175442
C,0,-1.5117229882,-1.5330211169,-2.6419474249
C,0,-2.591249906,-1.6543539307,-3.5109412892
C,0,-0.4054976094,-2.3812179805,-2.7715279189
H,0,-3.4500953572,-0.9995311772,-3.4003664936
C,0,-2.5694330363,-2.6145166293,-4.5196391517
C,0,-0.3983401611,-3.352138944,-3.7809612787
H,0,-3.410613715,-2.7034989291,-5.2008581698
H,0,0.4626870837,-4.0080511989,-3.8592128103
C,0,-1.4708917631,-3.4640303006,-4.6540157345
H,0,-1.45574647,-4.2141909813,-5.4388320234
H,0,-1.5480214173,-0.7887398679,-1.8524061941
C,0,0.7677615509,-2.3223382066,-1.857078349
O,0,1.6068640117,-3.2079824741,-1.8502413502
C,0,0.8846513217,-1.1469385189,-0.9314712661
H,0,0.4446721828,-0.21615158,-1.2742780936
C,0,0.6887656299,-2.6982496658,1.1955344052
C,0,1.6892293898,-3.2751390278,1.9818880582
C,0,-0.5388164206,-3.350989339,1.0519200663
C,0,1.4579787228,-4.4964437016,2.6111931411
C,0,-0.7646764965,-4.57039266,1.6826118337
C,0,0.2348445768,-5.1457507933,2.4644846527
H,0,2.6436889619,-2.7627666499,2.0944011546
H,0,-1.3178837761,-2.9054917585,0.437759833
H,0,2.2409257264,-4.9424383668,3.2179393889
H,0,-1.719798617,-5.0730530147,1.5599999921
H,0,0.0606190447,-6.0991333104,2.9551353606
H,0,6.5758264345,0.2849269271,-1.7008713119
H,0,7.2078384327,0.0052095195,-0.0682142793

Int-4a (SRS) 2, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -1282.38334271 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.351947 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1282.8954656 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1282.9076791 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1283.6394448 a.u.

0; 1
C,0,1.8857367639,4.6124938223,-0.1209152981
C,0,2.7175749932,5.166320751,-1.0976519132
C,0,3.5185973497,4.3553970366,-1.8986143841
C,0,3.478726168,2.9785510597,-1.71468712
C,0,4.2017570482,1.8779438287,-2.4283103582
C,0,1.8359689305,3.236633127,0.0776198725
C,0,2.6423080934,2.4500542637,-0.735619634
N,0,2.765858093,1.0315155021,-0.7325427871
C,0,3.9109567404,0.6476354727,-1.5687807997
C,0,5.143566505,0.21272302,-0.6490614766
C,0,2.0606662714,0.2270038703,-0.0038121676
C,0,2.1630046567,-1.2175939446,-0.0117536201
C,0,1.7533425966,-1.9706341914,1.2261407252
O,0,6.2389400733,0.3203717614,-1.2167192834
O,0,4.8289195102,-0.217162412,0.4768450816
H,0,1.2741105362,5.2608854879,0.4980250767
H,0,2.7421860285,6.2436198339,-1.2294113598
H,0,4.1659544312,4.7905176126,-2.6537616789
H,0,1.1960589738,2.8155456535,0.8457242106
H,0,3.6403469978,-0.2289980583,-2.1620851709
H,0,1.2876652007,0.6707419996,0.6161059073
H,0,2.9760000373,-1.6533688767,-0.5777598194
H,0,1.3221588548,-1.3422656666,2.0054621209
C,0,-1.423499137,-2.9818044088,-1.69797095
C,0,-2.5200056428,-3.4487794395,-2.4150682874
C,0,-1.5880104246,-1.9829393888,-0.7298511398
H,0,-2.3827487659,-4.218787519,-3.1678660231
C,0,-3.7886019146,-2.9303477743,-2.1683194037
C,0,-2.8687081822,-1.4624940133,-0.4955957187
H,0,-4.6432669938,-3.3006248981,-2.7268348706
H,0,-2.9792935715,-0.6859483909,0.2541571251
C,0,-3.9619380419,-1.9351528023,-1.2059970708
H,0,-4.9506953996,-1.5301622184,-1.0132585228
H,0,-0.4440653174,-3.3939883232,-1.9153497156
C,0,-0.4667797153,-1.4182117183,0.0677127267
O,0,-0.6439871784,-0.4366519391,0.7821548245
C,0,0.8728153759,-2.0708880068,0.0156502212
H,0,0.9736285936,-2.9819138134,-0.5619238602
C,0,2.5556548627,-3.1427606831,1.6875217719
C,0,3.9514154935,-3.083393991,1.7300149858
C,0,1.9006305465,-4.3022915144,2.1138372953
C,0,4.6773663531,-4.1788999513,2.1934813646
C,0,2.6303858432,-5.3920373613,2.5777833347
C,0,4.0222490074,-5.3320101632,2.6179289815
H,0,4.4596296958,-2.1800710938,1.3954090386
H,0,0.8149361291,-4.3492375688,2.0782016784
H,0,5.7621879901,-4.1286508721,2.2214348335
H,0,2.1127288365,-6.2893427421,2.9047407364
H,0,4.5933584896,-6.1833226725,2.9772662167
H,0,3.8268144955,1.7664785873,-3.4521103199
H,0,5.2844045086,2.0200764793,-2.4759357649

Int-4a (RSS), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1282.38134703 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.353022 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1282.894676 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1282.9067342 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1283.63886 a.u.

O; 1
C,0,6.6252716821,2.2546676956,-2.4921243953
C,0,6.3024170469,2.7435614683,-3.7606772212
C,0,5.0480414242,2.5089911828,-4.3195491171
C,0,4.1134359672,1.7803154617,-3.5939398925
C,0,2.7056092305,1.3928296437,-3.9275793843
C,0,5.7018734522,1.5221189477,-1.7534123249
C,0,4.4573687672,1.3044965518,-2.3314014727
N,0,3.3493468175,0.5979233699,-1.7835381277
C,0,2.3504541276,0.385271575,-2.8359200142
C,0,2.420737778,-1.1386525849,-3.3324571416
C,0,3.305740057,0.0750758014,-0.5996308627
C,0,2.1623595367,-0.5882721403,-0.0129110546
C,0,2.388147549,-1.6721972057,1.0084499591
O,0,2.8274779328,-1.9486733244,-2.4804953816
O,0,2.0063176369,-1.2914833525,-4.4894538758
H,0,7.6103151196,2.4407999567,-2.0766496097
H,0,7.0420410643,3.3092419791,-4.3187542885
H,0,4.803246656,2.8866320795,-5.3075095218
H,0,5.9670089874,1.1344539944,-0.7753880495
H,0,1.3498914871,0.5340921994,-2.4247726564
H,0,4.1914042451,0.20495442,0.0161710321
H,0,1.2631683651,-0.6975608709,-0.6055193069
H,0,1.5916214453,-2.4145096463,0.9772105869
C,0,1.0511753846,1.2719792923,3.8851476727
C,0,0.6237110451,2.0481430234,4.9575252776
C,0,0.1164520151,0.6638585171,3.0385682298
H,0,1.3547205495,2.5122975932,5.6123161055
C,0,-0.7372963153,2.2279504701,5.1907273863
C,0,-1.2509942715,0.8452475352,3.2871108763
H,0,-1.0679638331,2.8370136503,6.0269242393
H,0,-1.9618611138,0.3618078137,2.625007877
C,0,-1.6756105291,1.6244719215,4.3529935884
H,0,-2.7370092656,1.7627838284,4.5350861348
H,0,2.1162465017,1.1383334427,3.7283895602
C,0,0.4908127694,-0.1919495849,1.8800753182
O,0,-0.3613390321,-0.7962304855,1.2437715076
C,0,1.9268746682,-0.3283841093,1.4876850866
H,0,2.6657745886,0.2917871053,1.9820796557
C,0,3.7537536294,-2.1909064376,1.3196462171
C,0,4.2355927129,-2.1953020371,2.6304648396
C,0,4.5420014976,-2.7237431289,0.2932331966
C,0,5.4915670457,-2.7252299026,2.9161537217
C,0,5.7972983126,-3.251369901,0.5831152518
C,0,6.2742452479,-3.2541247996,1.8927610303
H,0,3.6230812885,-1.7847880847,3.4293411825
H,0,4.1616168631,-2.7090282181,-0.7269217416
H,0,5.858267098,-2.7240841325,3.9386065063
H,0,6.4057976784,-3.6610524173,-0.2180539673
H,0,7.2544519649,-3.6660328997,2.1149525252
H,0,2.047011458,2.2688367288,-3.916515511
H,0,2.6031980947,0.9000517557,-4.8979586607

Int-4a (RRS), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1282.37792015 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.353708 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1282.8915942 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1282.9039176 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1283.6377118 a.u.

O; 1
C,0,6.1672661995,3.0044417463,-1.224656485
C,0,6.2525270998,3.4240590059,-2.5546056587
C,0,5.4514638107,2.8480832135,-3.5382938113
C,0,4.5591323305,1.845676691,-3.1778852296
C,0,3.5746460807,1.0736313149,-4.0020304352
C,0,5.2809329248,2.0005252374,-0.8477028067
C,0,4.4924975177,1.443639534,-1.8469701277
N,0,3.5132687169,0.4177256327,-1.7172624477
C,0,3.1171044223,-0.0369569298,-3.0563810078
C,0,3.7955570243,-1.451586403,-3.3677654042
C,0,3.1577645064,-0.124256117,-0.596758516
C,0,2.14465316,-1.1537100839,-0.4562524625
C,0,2.2964123061,-2.1641889493,0.6605773555
O,0,4.0648677983,-2.1412419176,-2.3665269375
O,0,3.9069829816,-1.6822041502,-4.5804350767
H,0,6.8031580742,3.4607990722,-0.4729443165
H,0,6.9554029172,4.206442951,-2.8237448711
H,0,5.522731011,3.1752241245,-4.5710796512
H,0,5.2288352678,1.6739141312,0.1855533881
H,0,2.0363120031,-0.1927397516,-3.0800700712
H,0,3.6182483549,0.2651956424,0.3017332523
H,0,1.7201251023,-1.5395427803,-1.3734100039
H,0,1.9416078,-3.1537907065,0.3784345074
C,0,-0.7784827422,-1.0696532764,2.9570296773
C,0,-1.7811019801,-0.9791919253,3.9168852621
C,0,0.0989269174,0.002865913,2.7527951527
H,0,-2.451966356,-1.8175507727,4.0767456415
C,0,-1.9233478455,0.1840646923,4.6693934594
C,0,-0.0427604636,1.1627295244,3.5256664768
H,0,-2.7122421259,0.2550757806,5.4124364471
H,0,0.651999195,1.9802674884,3.3628176081
C,0,-1.0524568487,1.2560631512,4.4725300893
H,0,-1.1625953503,2.161859553,5.0609318636
H,0,-0.672704059,-1.9876616633,2.3875146677
C,0,1.2142347055,-0.0387577571,1.7656061415
O,0,2.1043242731,0.7995547826,1.8034362926
C,0,1.1965059049,-1.1349294292,0.749094123
H,0,0.2081859622,-1.5116108883,0.5064047098
C,0,3.5010727395,-2.181465782,1.5452553693
C,0,3.3783984523,-2.1750822667,2.9360906123
C,0,4.7707070727,-2.2915739882,0.9666519687
C,0,4.5102513114,-2.2677053764,3.741862285
C,0,5.8998897715,-2.3838827464,1.7755980742
C,0,5.7727303489,-2.3716387818,3.163243464
H,0,2.3943674272,-2.0965373129,3.3914473962
H,0,4.8569969002,-2.3050105506,-0.119171831
H,0,4.4044863008,-2.2565447546,4.8227620911
H,0,6.8822924603,-2.4666727044,1.319559316
H,0,6.6553536646,-2.4424825226,3.7923136355
H,0,2.7458492206,1.7164139535,-4.3203824955
H,0,4.0097467492,0.6128966259,-4.8926317446

Int-4a (RRS) 2, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1282.36025672 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.354907 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1282.8741553 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1282.8865136 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1283.6195495 a.u.

0; 1
C,0,-1.1009421902,3.9239586199,0.1262693759
C,0,-0.8383274994,4.6926856961,-1.0079033023
C,0,-0.0109006002,4.2036692958,-2.0151416224
C,0,0.5431373714,2.9373652734,-1.8825810369
C,0,1.4455838372,2.1987552854,-2.8185639019
C,0,-0.5469075015,2.6565887719,0.2784918439
C,0,0.2726090186,2.1766319301,-0.7419221477
N,0,0.9562796465,0.9344489711,-0.8497058608
C,0,1.8454728327,0.9607217696,-2.0276396868
C,0,3.3671243347,0.9491966707,-1.5469030432
C,0,1.0612613483,-0.0774667833,-0.0406592781
C,0,0.3944279003,-0.2707387927,1.2362173292
C,0,0.584285862,-1.6104604546,1.9686304178
O,0,4.1411648129,1.5042943002,-2.338591929
O,0,3.5814033821,0.3350567985,-0.4813087239
H,0,-1.7421015622,4.3160289049,0.9091748336
H,0,-1.2792281358,5.6801474281,-1.1021837356
H,0,0.2014798103,4.8017346039,-2.8960639085
H,0,-0.7563522951,2.0924651713,1.175789667
H,0,1.7000340813,0.0346357816,-2.5890327802
H,0,1.6917132733,-0.8732180916,-0.4151133695
H,0,-0.5827391044,0.1865421453,1.3396717121
H,0,-0.3221389522,-1.8870479018,2.5015225744
C,0,2.2243328357,2.3971663843,2.6859076222
C,0,2.6877953415,3.7074970485,2.7328956172
C,0,3.1270282321,1.3293245798,2.6753960612
H,0,1.9804215484,4.5311724182,2.7399618011
C,0,4.056962336,3.9595211705,2.7652337483
C,0,4.5016814101,1.5922069025,2.7124875524
H,0,4.4189932316,4.9830747864,2.7962077957
H,0,5.1884472878,0.7525522674,2.6983380159
C,0,4.9638054396,2.8993178675,2.754543053
H,0,6.0312846296,3.0965703254,2.7738108948
H,0,1.1556338572,2.2137120051,2.664153481
C,0,2.6903427324,-0.0920143258,2.6564063225
O,0,3.4804837504,-1.0013752452,2.8318048233
C,0,1.2106985335,-0.3784621441,2.529413036
H,0,0.6692589286,0.0431785803,3.3758351333
C,0,1.2334730596,-2.8088051381,1.3571504502
C,0,2.4846347108,-2.8316883903,0.7237482899
C,0,0.4926892933,-3.9981583111,1.3987051385
C,0,2.9618123363,-4.0071803353,0.14920955
C,0,0.9756467612,-5.172707112,0.8325765593
C,0,2.2156417447,-5.180951962,0.200561566
H,0,3.109124602,-1.9460239765,0.6827278681
H,0,-0.4790602728,-4.0025445881,1.8865478794
H,0,3.9335319271,-4.0001376811,-0.3358091821
H,0,0.380750587,-6.079910663,0.8860201554
H,0,2.599057889,-6.0943509381,-0.2445489948
H,0,0.9276620029,1.9494977537,-3.7509186343
H,0,2.3516275978,2.7559458031,-3.0753288179

Int-4a (RSS) 2, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1282.38088969 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.353285 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1282.8924124 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1282.9045011 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1283.6353137 a.u.

0; 1
C,0,6.1435008816,3.0702696247,-1.9904057605
C,0,6.081640433,3.2391907837,-3.373631065
C,0,5.0965155114,2.5956556255,-4.1196953355
C,0,4.1898444726,1.7668111495,-3.4731120623
C,0,3.0034173248,1.0390922968,-4.0278451832
C,0,5.245128084,2.2387833961,-1.3272970609
C,0,4.2944174847,1.5690952895,-2.0936426367
N,0,3.2552932931,0.6988441557,-1.6738452718
C,0,2.5134344065,0.2062487638,-2.8486503463
C,0,2.8184449387,-1.3449659363,-2.9923155117
C,0,3.0772661717,0.0273649378,-0.5652927952
C,0,3.963146214,-0.0705654049,0.5728449411
C,0,3.3885812761,-0.3729420109,1.9462407572
O,0,3.1183168511,-1.9200697287,-1.9166142123
O,0,2.6804517262,-1.7962690151,-4.1341040139
H,0,6.8965967094,3.5979736191,-1.4140252956
H,0,6.7945905966,3.8912160599,-3.8684917755
H,0,5.0278542811,2.7478228982,-5.192668397
H,0,5.2877704284,2.1583629253,-0.2491572809
H,0,1.4385572412,0.2998381987,-2.6685135505
H,0,2.120751212,-0.472486027,-0.4831018922
H,0,4.9316609532,0.4092308845,0.5454595615
H,0,4.0424758018,-0.0055300143,2.7361016523
C,0,5.2893346085,-3.7939469011,-0.2039666211
C,0,5.8139879846,-4.9735961224,-0.7245615356
C,0,5.8285598514,-3.2591951509,0.9739785409
H,0,5.4068211986,-5.3799719843,-1.6453809243
C,0,6.8572038376,-5.6277316873,-0.0738445216
C,0,6.8924874026,-3.910073288,1.6125997336
H,0,7.2547507462,-6.5527525634,-0.4817187243
H,0,7.3033393432,-3.4699396696,2.5158527752
C,0,7.3979677965,-5.0945316065,1.0970680579
H,0,8.2136915431,-5.6032772139,1.6019944529
H,0,4.4984052245,-3.2793470079,-0.7466175307
C,0,5.3407400687,-1.9883473233,1.5638456793
O,0,6.0202986932,-1.3400798414,2.3471240893
C,0,3.97939079,-1.494469254,1.1753560681
H,0,3.3107908752,-2.1922688857,0.6838382379
C,0,1.9223110931,-0.2853378996,2.2195872475
C,0,1.308347328,0.9699142022,2.2941547658
C,0,1.1531270735,-1.4292611383,2.4407819364
C,0,-0.0483675448,1.0771633811,2.5787660804
C,0,-0.2067628827,-1.3222489287,2.7254968939
C,0,-0.8103225785,-0.0703440115,2.7940301882
H,0,1.9008156622,1.8658086796,2.1259447658
H,0,1.620919319,-2.4087252407,2.395769596
H,0,-0.5128746122,2.057508896,2.6316391436
H,0,-0.7931382211,-2.2206381642,2.8941567015
H,0,-1.8704709838,0.0127849386,3.0142524081
H,0,2.2480361955,1.7471178015,-4.3846546176
H,0,3.2461556676,0.364279172,-4.8544385658

Int-4a (RRR) 2, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1282.37539171 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.352406 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1282.8887954 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1282.900818 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1283.6322731 a.u.

0; 1
C,0,0.4858289165,4.0945255046,1.2957867162
C,0,1.3066816621,5.1142643614,0.8122691396
C,0,2.0345138606,4.9421851021,-0.36304785
C,0,1.9159488224,3.7487040483,-1.0617658088
C,0,2.6037545488,3.3033116263,-2.3145129789
C,0,0.3578806954,2.8895851187,0.6115894018
C,0,1.0684638076,2.747980893,-0.5783657263
N,0,1.1303809524,1.6367185939,-1.4617925621
C,0,2.2441127634,1.8259663745,-2.404448461
C,0,3.4268946892,0.8279348729,-2.0050996537
C,0,0.5343537872,0.485592593,-1.4299909974
C,0,-0.4698106297,0.0480982693,-0.4678154756
C,0,-0.0136327536,-0.9243609385,0.612884971
O,0,4.5535455216,1.2432746342,-2.3091129709
O,0,3.0523615203,-0.2501172838,-1.5005401868
H,0,-0.0540511114,4.2307269621,2.2272286767
H,0,1.3913303416,6.0434077618,1.3673142603
H,0,2.6929464665,5.7253716775,-0.7261509683
H,0,-0.2482044116,2.097303027,1.0291940684
H,0,1.9132239312,1.5262773648,-3.4015487696
H,0,0.8455379805,-0.2008432316,-2.2081446784
H,0,-1.2385599045,0.7604556928,-0.1803456505
H,0,1.0081233937,-1.2691514058,0.4728754755
C,0,-1.9535227982,-4.1418979049,-0.3404546123
C,0,-2.4386465383,-5.4450357656,-0.3635859182
C,0,-2.8433861564,-3.0613500131,-0.3238568335
H,0,-1.7446401023,-6.2798092466,-0.3681834932
C,0,-3.812044754,-5.6771323406,-0.3794208101
C,0,-4.2228931294,-3.304261615,-0.3276531771
H,0,-4.1885154328,-6.6956089135,-0.4034463106
H,0,-4.8977794597,-2.4545522741,-0.306064374
C,0,-4.7046485815,-4.6048801761,-0.3613461934
H,0,-5.7748972875,-4.7875094275,-0.3717956587
H,0,-0.8814464807,-3.9736960975,-0.3141168446
C,0,-2.3812774883,-1.6505171168,-0.2764987216
O,0,-3.1589670626,-0.735638861,-0.0456944711
C,0,-0.9288602521,-1.3765974814,-0.5207444565
H,0,-0.4444355081,-2.0221570757,-1.2487490556
C,0,-0.3964165384,-0.7986167267,2.0444992352
C,0,-1.5062806375,-0.0758861585,2.5003720302
C,0,0.4223813111,-1.4335005825,2.9867830492
C,0,-1.7879367259,-0.0020327902,3.8614385138
C,0,0.1384527803,-1.3591356302,4.3459273049
C,0,-0.9697249725,-0.6418310147,4.7888148175
H,0,-2.1677670938,0.416059407,1.7948305436
H,0,1.2929535506,-1.9889832783,2.6476337575
H,0,-2.6535928745,0.561657064,4.1968885772
H,0,0.7878588057,-1.8583080238,5.0590158458
H,0,-1.1922334645,-0.5782783349,5.8497930887
H,0,2.2547215466,3.8713058201,-3.1839002902
H,0,3.6928088888,3.3937475598,-2.2622258231

Int-4a (RSR) 2, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1282.37577409 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.352090 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1282.8891098 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1282.9009843 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1283.6311147 a.u.

0; 1
C,0,2.8263843951,4.5884692106,0.8266093821
C,0,3.4577920017,5.2554679632,-0.2233945331
C,0,3.6921409927,4.6067158831,-1.4334172236
C,0,3.2605482498,3.2971105712,-1.59334104
C,0,3.4394137038,2.370780334,-2.7552655819
C,0,2.390779471,3.2742129372,0.6850896643
C,0,2.5880989266,2.6562441006,-0.548660099
N,0,2.2619807485,1.3346445503,-0.9655823475
C,0,3.0165979699,1.0210988516,-2.1911271442
C,0,4.2228436661,0.0421147033,-1.8238277441
C,0,1.5787607715,0.389680455,-0.3945972316
C,0,0.82314484,0.485503639,0.8367613301
C,0,1.0686050853,-0.5870703377,1.8961745744
O,0,3.9671085229,-0.7614870462,-0.9071249054
O,0,5.223082171,0.1815247048,-2.5435546542
H,0,2.6865775233,5.089535156,1.7790209961
H,0,3.7919003484,6.2791559615,-0.0858591189
H,0,4.2177066514,5.1103779974,-2.2389680632
H,0,1.9649645172,2.7633367699,1.5378015184
H,0,2.3631835853,0.4624840909,-2.8648044204
H,0,1.5832548405,-0.5610441631,-0.9155419572
H,0,0.5946499904,1.4746544914,1.2113499991
H,0,1.7217726423,-1.3837338075,1.5475315157
C,0,-3.0553033093,-1.223359381,0.3378321207
C,0,-4.3544367445,-1.6055999972,0.0206955994
C,0,-1.9718793848,-2.0219154691,-0.0489462832
H,0,-5.1887991955,-0.9779802127,0.3179553805
C,0,-4.5835133918,-2.7893347597,-0.6760308293
C,0,-2.2131036817,-3.2065309501,-0.7587170427
H,0,-5.5994645873,-3.0880259383,-0.9171302629
H,0,-1.3625333132,-3.811142304,-1.0560788861
C,0,-3.5099287874,-3.5905175947,-1.0658662074
H,0,-3.6879035128,-4.5132578861,-1.6095431741
H,0,-2.8998886978,-0.2908733729,0.8700833407
C,0,-0.5541573608,-1.6739086404,0.2332138684
O,0,0.3597480756,-2.298409125,-0.2901331121
C,0,-0.2465730876,-0.5558246213,1.1783088544
H,0,-1.0764512508,-0.1351808921,1.7342731038
C,0,1.2192775042,-0.2177701327,3.3265022283
C,0,0.4223932095,0.753245084,3.9436012265
C,0,2.1993231864,-0.865573743,4.0846959833
C,0,0.6013473553,1.0651911424,5.2869216021
C,0,2.3774857701,-0.5537500618,5.42914316
C,0,1.5793722605,0.4123937094,6.0348867551
H,0,-0.3491818867,1.2733370461,3.3803740403
H,0,2.826415943,-1.6183101976,3.6147829113
H,0,-0.0265018231,1.8198697571,5.7513432858
H,0,3.1434057566,-1.06740023,6.0025165755
H,0,1.7176220595,0.6570251442,7.0837106822
H,0,2.8252309585,2.6772184249,-3.6095577763
H,0,4.4795555641,2.2980552753,-3.0858867983

4a (RSR), optimization in solv. CHCl₃
PBE1PBE/6-311G(d,p), E = -805.752809324 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.219525 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -806.0749493 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -806.0819583 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -806.5431123 a.u.
0; 1
O,0,0.7441755617,0.6604957152,-0.6742305504
C,0,1.3986784091,0.1639894502,0.2197171327
C,0,2.2679631423,-1.0135630876,0.0073239449
C,0,2.3693890919,-2.0514788036,1.1039916943
H,0,1.3611836821,0.5580447785,1.2523865017
H,0,2.2778722082,-1.3706518713,-1.0190207617
H,0,1.8946516597,-1.7526114096,2.0369032288
C,0,6.2079643649,0.1915790948,0.5903414971
C,0,7.4837107858,0.745728327,0.5703050829
C,0,5.3951638758,0.3363155343,1.7209225461
H,0,8.1051265519,0.6375009551,-0.3132813764
C,0,7.9611483826,1.4379087216,1.6804180886
C,0,5.8794451956,1.0466806884,2.8272407096
H,0,8.9601859373,1.8636661366,1.6649706967
H,0,5.2331823434,1.1577404532,3.6919333203
C,0,7.1566276155,1.5880756144,2.8103332694
H,0,7.5281614479,2.1294465325,3.6751156779
H,0,5.8455359915,-0.3310536431,-0.2888611
C,0,4.0118820828,-0.2078771075,1.8013085893
O,0,3.2531737352,0.1472194863,2.6937468568
C,0,3.5709462926,-1.211303318,0.7828140686
H,0,4.3514239265,-1.6946854369,0.2052768415
C,0,2.3172831442,-3.5068483066,0.8088530415
C,0,2.8583297623,-4.0595003396,-0.3573696335
C,0,1.7085718881,-4.3610646527,1.7335172292
C,0,2.7938564034,-5.4292073788,-0.5889099767
C,0,1.6427445981,-5.7320067491,1.5020367984
C,0,2.1858242342,-6.2717359236,0.3397170425
H,0,3.3339345364,-3.4212292098,-1.0981945698
H,0,1.2830745147,-3.9451833374,2.6431925341
H,0,3.2192722645,-5.8397998431,-1.5000596743
H,0,1.1652545265,-6.3781692328,2.2329278799
H,0,2.1354548432,-7.340899837,0.1566253703

4a (RSR), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -806.543938407 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.218566 a.u.
0; 1
C,0,-0.1361354791,2.6426208064,-0.5187999313
C,0,-0.6530325318,1.2744663816,-0.7416107783
C,0,-1.3055493735,0.5646004472,0.4283985614
H,0,0.286462784,2.8470583396,0.4804470211
H,0,-1.0679457716,1.1038022428,-1.7283186514
H,0,-1.2340886327,1.0997371793,1.3702624822
C,0,2.725708836,-0.6266649959,-1.0329326067
C,0,3.9629810002,-1.1093415887,-1.4462288945
C,0,2.5242669008,-0.2783488499,0.3041999311
H,0,4.1220174711,-1.3662293992,-2.4863547289
C,0,4.9940015772,-1.2599484691,-0.5241911945
C,0,3.5674251777,-0.4191349698,1.2235835896
H,0,5.9549562509,-1.642703284,-0.8473961264
H,0,3.3965684543,-0.1373649664,2.255631619
C,0,4.795333796,-0.916786295,0.8124102846
H,0,5.5988532758,-1.0353338981,1.5291488723
H,0,1.9319213661,-0.5004700558,-1.7599921848
C,0,1.2275650803,0.28447405,0.7842024403
O,0,1.1588520222,0.8969125417,1.8292095918
C,0,0.011483315,0.0726268125,-0.0718162742
H,0,0.007715145,-0.825073012,-0.6773639054
C,0,-2.5601491716,-0.2143662745,0.2343640011
C,0,-2.8063006877,-0.9555903464,-0.9241286206
C,0,-3.5250843322,-0.2012814151,1.2422684642
C,0,-3.9927905367,-1.6649921694,-1.0694107162
C,0,-4.7130143652,-0.9112383933,1.0976841044
C,0,-4.9511535059,-1.6450672139,-0.059249705
H,0,-2.0744528382,-0.9826794954,-1.7253259651
H,0,-3.3433377853,0.370828167,2.14560938
H,0,-4.1704955188,-2.2328530164,-1.9750724136
H,0,-5.4517204916,-0.8881243601,1.8901681231
H,0,-5.8765227876,-2.1963054275,-0.1751866404
O,0,-0.1862642631,3.5063610676,-1.3604973891

4a (RRR), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -805.751531866 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.219093 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -806.0746305 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -806.0816461 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -806.54293 a.u.

O; 1
O,0,1.4523214271,1.3950926713,-1.1237742438
C,0,2.0156137031,0.8225274974,-0.2177532541
C,0,2.7362726533,-0.4577890252,-0.3596486966
C,0,2.6852424347,-1.4164256553,0.8035125573
H,0,2.0176797121,1.2428419179,0.8138224216
H,0,2.7812185596,-0.8732514806,-1.3615138385
H,0,2.1984985959,-1.0134073703,1.6907637048
C,0,6.4801241641,-1.1762437823,1.9856187422
C,0,7.6915743929,-1.3042839248,2.6571183451
C,0,6.398751406,-1.4679195763,0.6191914616
H,0,7.7465077725,-1.0844456966,3.7189103461
C,0,8.8306023699,-1.7145087845,1.9684267807
C,0,7.5463750684,-1.8927021873,-0.0617837492
H,0,9.7769300063,-1.8071973084,2.4933427213
H,0,7.4629453905,-2.1235902571,-1.118935384
C,0,8.7566642391,-2.0093136934,0.6068407858
H,0,9.6442888337,-2.3312129302,0.0706028285
H,0,5.5968136434,-0.8697536658,2.5371194748
C,0,5.1278738636,-1.3715028459,-0.1510556584
O,0,5.0348642475,-1.8567645751,-1.2688186378
C,0,3.9720942975,-0.6686391312,0.4844757018
H,0,4.2248321504,0.1179113842,1.1899686462
C,0,2.4889864567,-2.8854712686,0.6644273424
C,0,2.5957127065,-3.5763884198,-0.5475470283
C,0,2.1615025398,-3.6071161883,1.8192324998
C,0,2.3899328106,-4.9522902845,-0.5947581228
C,0,1.9547441106,-4.9812872577,1.7707993214
C,0,2.0695654062,-5.6603106589,0.5604238008
H,0,2.8513638149,-3.0451804503,-1.45736567
H,0,2.0654721664,-3.0813982316,2.7662329353
H,0,2.4770682562,-5.4720019816,-1.5445288495
H,0,1.6997541435,-5.5201098702,2.6787792067
H,0,1.906234657,-6.7331129689,0.5170935088

4a (RRR), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -806.544234897 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.218062 a.u.

O; 1
C,0,1.9265847335,3.3618881269,-0.4174590534
C,0,1.4622346432,2.0867076272,0.1687313669
C,0,1.3603153287,0.9084096329,-0.7707214994
H,0,1.6081102606,3.538935508,-1.4649778527
H,0,1.734411976,1.9109165751,1.2016406817
H,0,1.5721802571,1.1341950923,-1.8118772035
C,0,-2.1296278969,-0.1107938857,-1.0864553711
C,0,-3.2695083831,-0.7868977177,-1.5083876852
C,0,-1.945758075,0.1695802399,0.269083334
H,0,-3.4064040665,-1.0125698297,-2.5589332566
C,0,-4.2311668486,-1.1728527389,-0.5800498557
C,0,-2.9078241198,-0.2325223285,1.1988673032
H,0,-5.1221004275,-1.6942163569,-0.9100781204
H,0,-2.7449189367,-0.0149175473,2.2476610684
C,0,-4.0507889874,-0.8945088782,0.7742219303
H,0,-4.8007432532,-1.1981725313,1.4945981464
H,0,-1.3774452303,0.1791315247,-1.8115131235
C,0,-0.7192177349,0.8638369324,0.762032653
O,0,-0.3924174551,0.8194244285,1.927875318
C,0,0.106416034,1.5892637112,-0.2584475908
H,0,-0.4470004549,2.1695811687,-0.9882572067
C,0,1.7183757778,-0.4865282463,-0.3784154939
C,0,2.1057183504,-0.8494264375,0.9122930479
C,0,1.6359515051,-1.4782838665,-1.3610366229
C,0,2.3999303422,-2.1768178989,1.2111606103
C,0,1.9307534748,-2.8029274794,-1.06271088
C,0,2.3138903077,-3.156591018,0.2280569708
H,0,2.1801188206,-0.1030397183,1.6931219508
H,0,1.3395003924,-1.2047503731,-2.3686319959
H,0,2.6999350517,-2.4425881241,2.2178915098
H,0,1.8613008841,-3.5574815757,-1.8373907851
H,0,2.5456152664,-4.1883178229,0.4647630064
O,0,2.6020564635,4.1716008068,0.1642466987

4a (SRS), optimization in solv. CHCl₃
PBE1PBE/6-311G(d,p), E= -805.751921040 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.218622 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -806.0744293 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -806.0814396 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -806.542651 a.u.

O; 1
O,0,2.7503588227,0.7436183705,-0.8956933582
C,0,1.9958727905,0.1080846398,-0.1881116659
C,0,2.0561736739,-1.3652381571,-0.0787900565
C,0,1.7542653473,-2.0221447039,1.2407545828
H,0,1.227942295,0.6072491782,0.4327567603
H,0,2.8136393092,-1.8255181038,-0.7074389861
H,0,1.3723290821,-1.3380946025,1.999882821
C,0,-1.4072015806,-2.7676974508,-1.8382148275
C,0,-2.464876522,-3.1299003363,-2.6659927333
C,0,-1.6420101499,-1.9983292649,-0.6925217624
H,0,-2.2748203779,-3.7183894563,-3.5583024854
C,0,-3.7634475266,-2.7374494435,-2.3508888921
C,0,-2.9498935199,-1.5959419175,-0.3921576448
H,0,-4.5884060547,-3.02771757,-2.9949644177
H,0,-3.1126138426,-0.9912923059,0.4942813201
C,0,-4.0053215625,-1.9690307072,-1.2118252464
H,0,-5.0175635018,-1.6612183188,-0.9676537202
H,0,-0.3992505071,-3.0677147163,-2.1060864545
C,0,-0.5534466176,-1.5546707291,0.2207956297
O,0,-0.7549633372,-0.6794085261,1.0527337325
C,0,0.7860474009,-2.2113219655,0.1169421698
H,0,0.8280297708,-3.1632211403,-0.4011748676
C,0,2.5887030682,-3.1556120464,1.7384652479
C,0,3.9806926434,-3.1303021801,1.6297807542
C,0,1.9772393495,-4.2508133293,2.356982592
C,0,4.7482385144,-4.1813011615,2.1260787616
C,0,2.7430015178,-5.3003134443,2.8543575669
C,0,4.1315834883,-5.2685530128,2.7390757585
H,0,4.4652161537,-2.2808242238,1.1558025241
H,0,0.8940673693,-4.2780372349,2.4440917599
H,0,5.8299613953,-4.1491810774,2.0331094343
H,0,2.2549088195,-6.1461101513,3.3300676026
H,0,4.7296272887,-6.0889199108,3.1249571002

4a (SRS), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -806.543939114 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.218597 a.u.

O; 1
C,0,1.0467354201,2.0876741206,-0.3254333691
C,0,1.2665021738,0.6795120326,-0.7207844156
C,0,1.7886831753,-0.2794121707,0.3337134315
H,0,0.6983805206,2.2530845342,0.7098240881
H,0,1.6115134707,0.5418875096,-1.7390149834
H,0,1.8582719979,0.1480820362,1.3291410188
C,0,-2.4163477845,-0.2830443809,-1.0847390377
C,0,-3.7351747984,-0.376728596,-1.516295261
C,0,-2.1326334149,-0.2180010217,0.2810962032
H,0,-3.9547663227,-0.4126463766,-2.5763116286
C,0,-4.7690599764,-0.4224054332,-0.5862940884
C,0,-3.1755409509,-0.2512518108,1.2105640608
H,0,-5.795480772,-0.5026127863,-0.9243882478
H,0,-2.9387265872,-0.1930149894,2.2661351365
C,0,-4.4888932886,-0.3625746075,0.7782344103
H,0,-5.2958901821,-0.3999864812,1.4999001125
H,0,-1.6156620234,-0.2361120989,-1.8139844146
C,0,-0.7356690595,-0.0701844849,0.785766659
O,0,-0.512881181,0.3332630309,1.907597345
C,0,0.3863528136,-0.4295461051,-0.1478899596
H,0,0.1789947906,-1.2307816792,-0.8465653045
O,0,1.2504665299,3.0177528998,-1.0670538422
C,0,2.851437245,-1.266058833,-0.0064200188
C,0,3.8519939054,-1.5279576088,0.9304095289
C,0,2.8843880137,-1.9362111053,-1.2318730115
C,0,4.8660587554,-2.4388630002,0.6512940872
H,0,3.8357386847,-1.0124838373,1.8845102206
C,0,3.8969457895,-2.846732369,-1.5114322733
H,0,2.1202189164,-1.7512640178,-1.9804480938
C,0,4.8920604267,-3.1014769135,-0.5710027354
H,0,5.6353934774,-2.6283617543,1.3906331565
H,0,3.909254233,-3.3584646541,-2.4665153251
H,0,5.6810354919,-3.8105566084,-0.7909756086

4a (SSS), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -805.751504529 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.218698 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -806.0746443 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -806.0816549 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -806.5429846 a.u.

O; 1
O,0,2.2371744979,3.1765555788,-0.8710585048
C,0,1.7366875635,2.3588892621,-0.1315343561
C,0,2.488419448,1.305874983,0.5792636454
C,0,2.002871879,0.9122858259,1.9515303755
H,0,0.6404546875,2.3588788941,0.0659416112
H,0,3.5550629831,1.2638546559,0.3820429435
H,0,1.0635262633,1.3808557782,2.2426594347
C,0,0.6710762276,-2.7484550104,1.1256556444
C,0,0.1059064265,-4.0182819344,1.1808006606
C,0,1.9932007222,-2.5846421331,0.696381508
H,0,-0.9174458075,-4.1397271491,1.5225162669
C,0,0.8521337072,-5.1308604307,0.799834645
C,0,2.7397076482,-3.7107472974,0.3277525425
H,0,0.4067398744,-6.1207429998,0.8377392157
H,0,3.7660568808,-3.5660599641,0.0060253348
C,0,2.1712620881,-4.9757446046,0.3730913672
H,0,2.7535154509,-5.8434994653,0.0780566858
H,0,0.0828580987,-1.8918485205,1.43964979
C,0,2.662858323,-1.2558115159,0.6356495845
O,0,3.8722759812,-1.1704625006,0.4820352782
C,0,1.8145778812,-0.0331532534,0.7735479249
H,0,0.7901636719,-0.1227998226,0.4237953461
C,0,2.9004407477,0.6620142238,3.1127424589
C,0,4.2893246417,0.5305228499,3.0105568471
C,0,2.3110591509,0.5687415594,4.3798570198
C,0,5.0615061811,0.3018858148,4.1459887081
C,0,3.083138875,0.3415866712,5.5137333582
C,0,4.4645243606,0.2060028368,5.4000395991
H,0,4.7726250397,0.5955006367,2.0424096008
H,0,1.2333434512,0.6775703509,4.4754010787
H,0,6.1385968724,0.202571453,4.0470612131
H,0,2.6050052331,0.2744516602,6.4866884262
H,0,5.0719980814,0.031331937,6.2831750249

4a (SSS), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -806.544234891 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.218062 a.u.

O; 1
C,0,-1.9266287953,3.3618606578,-0.4174816431
C,0,-1.4622617185,2.0866905229,0.1687178709
C,0,-1.3603253656,0.908387344,-0.7707269634
H,0,-1.6081553321,3.5389054236,-1.4650011991
H,0,-1.7344370651,1.9109030403,1.2016283277
H,0,-1.5721930582,1.1341628838,-1.8118842581
C,0,2.1296171433,-0.1107877698,-1.0864531639
C,0,3.2695034151,-0.78688353,-1.508382749
C,0,1.9457532307,0.1696051909,0.2690824446
H,0,3.4063946236,-1.01257054,-2.5589256926
C,0,4.2311734176,-1.1728113149,-0.580045585
C,0,2.9078307093,-0.2324704758,1.1988660554
H,0,5.122111548,-1.6941683263,-0.910071978
H,0,2.7449300371,-0.0148514534,2.2476575813
C,0,4.0508013451,-0.8944486678,0.7742230768
H,0,4.8007648359,-1.1980906594,1.4945987915
H,0,1.3774251418,0.1791158891,-1.8115100166
C,0,0.7192078374,0.8638549043,0.7620287065
O,0,0.3924122467,0.819452688,1.9278730741
C,0,-0.1064361619,1.5892624886,-0.2584570377
H,0,0.4469729455,2.1695820257,-0.9882706467
C,0,-1.7183656828,-0.4865532953,-0.3784123599
C,0,-2.1056998002,-0.8494501766,0.9122991336
C,0,-1.6359302923,-1.4783129827,-1.3610284999
C,0,-2.3998927053,-2.1768441251,1.2111744179
C,0,-1.9307131672,-2.8029591157,-1.0626950363
C,0,-2.3138418212,-3.1566212182,0.2280756234
H,0,-2.1801086614,-0.1030603002,1.6931242426
H,0,-1.3394859416,-1.2047807625,-2.3686262239
H,0,-2.6998912225,-2.4426131756,2.2179074905
H,0,-1.8612522193,-3.5575163128,-1.8373711809
H,0,-2.545552281,-4.1883499237,0.4647875169
O,0,-2.6021121856,4.1715680666,0.1642178804

4a (RSS), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -805.753066243 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.218756 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -806.0757106 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -806.0826993 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -806.5442759 a.u.

O; 1
O,0,3.3992147032,-1.0741721288,-2.2936297128
C,0,3.4782527845,-1.1204087024,-1.0846556301
C,0,2.3899278765,-1.6045430513,-0.2128754402
C,0,2.7083044274,-2.315558464,1.0784727364
H,0,4.3967853263,-0.7879299216,-0.5565496814
H,0,1.4701516003,-1.8886954219,-0.7153111546
H,0,1.9374067916,-3.0388294038,1.3419323967
C,0,1.2839079289,1.7357541286,2.2488006434
C,0,0.8645556797,2.9138706694,2.8584721819
C,0,0.4467539401,0.6138835102,2.232510081
H,0,1.5168232237,3.7817500211,2.8600132456
C,0,-0.3877841873,2.9795578835,3.4636441484
C,0,-0.8160700802,0.6943358473,2.8347709333
H,0,-0.7103313513,3.898815555,3.9437879437
H,0,-1.455649439,-0.181920574,2.8065497083
C,0,-1.228957383,1.8665898038,3.4509713228
H,0,-2.2063717893,1.9173515409,3.9211846857
H,0,2.2580621492,1.7108660007,1.7719900259
C,0,0.817850816,-0.6755684499,1.5870763926
O,0,-0.013917828,-1.5584588316,1.428271461
C,0,2.2248773244,-0.9018929159,1.1394324345
H,0,2.9700026559,-0.1476089249,1.3687484906
C,0,4.1029807865,-2.6830639645,1.4725249193
C,0,4.7176850157,-2.1022451575,2.5837972737
C,0,4.7933776783,-3.6653943248,0.7546191016
C,0,5.9998385556,-2.4889593638,2.9672709953
C,0,6.0732311393,-4.0532085916,1.1373497863
C,0,6.6809613776,-3.4645540518,2.2448967654
H,0,4.186691928,-1.3457476155,3.1556595771
H,0,4.3224241742,-4.124753996,-0.1108759555
H,0,6.4654521326,-2.0269897684,3.8330585881
H,0,6.5984654465,-4.8145432285,0.5679449757
H,0,7.681263878,-3.7653199097,2.5421786165

4a (RRS), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -805.746161239 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.220231 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -806.069008 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -806.0761995 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -806.5394756 a.u.

O; 1
O,0,3.2318525549,0.5919494811,-1.7304501631
C,0,3.1499009454,-0.022217822,-0.6857306553
C,0,2.1550464577,-1.1155276213,-0.5061118973
C,0,2.2999952195,-2.1390840679,0.5930950847
H,0,3.8395593305,0.1713776859,0.1512951307
H,0,1.7316514995,-1.4485111673,-1.4496670394
H,0,1.9544135341,-3.1333294811,0.3125119564
C,0,-0.6764939059,-1.1098989411,2.9725382426
C,0,-1.6247441181,-1.0576874933,3.9890872575
C,0,0.1382562267,-0.0011524183,2.7117628022
H,0,-2.2487993233,-1.9229847047,4.1903787563
C,0,-1.7730977029,0.1027724984,4.7448300977
C,0,-0.0108298331,1.1570219539,3.4848752001
H,0,-2.5187270602,0.1437237773,5.5334968929
H,0,0.633637273,2.004294578,3.2739229867
C,0,-0.9644330818,1.2110471424,4.4915489219
H,0,-1.0797816581,2.114958753,5.0819641407
H,0,-0.5645583593,-2.0235337118,2.3968498918
C,0,1.185502967,-0.0006069178,1.6503239125
O,0,2.0090570842,0.9003455764,1.5887887771
C,0,1.1824391689,-1.1231470328,0.664680197
H,0,0.198386098,-1.5157748028,0.427188656
C,0,3.463154367,-2.1617889733,1.5348895576
C,0,3.2753087781,-2.1072607141,2.9180631174
C,0,4.7590134092,-2.33722893,1.0381665556
C,0,4.3592760234,-2.2117406448,3.7859498747
C,0,5.8429198164,-2.4439303908,1.903823849
C,0,5.6458411393,-2.3793703387,3.281540758
H,0,2.2733040024,-1.9855317387,3.3204818017
H,0,4.9172869212,-2.3899533581,-0.0361387815
H,0,4.1960351985,-2.1618482044,4.8585756906
H,0,6.8431867819,-2.574555481,1.5012430615
H,0,6.4915852462,-2.4588654902,3.9581853656

TS-3b (RS), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1494.85470888 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.408738 a.u.
1 imaginary frequency = 190.4566 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1495.3089906 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1495.3346671 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1496.0706702 a.u.
0; 1
C,0,2.0988525703,1.4771316665,-3.8375919287
N,0,1.547089203,0.9333846876,-1.6227538143
C,0,2.0798555474,0.3156949835,-2.837935085
C,0,3.5210902365,-0.2656888684,-2.5968020848
C,0,1.4604014592,0.2841134674,-0.4825673219
C,0,1.5454794714,-1.1025374057,-0.33162676
C,0,1.8317652788,-1.6441486814,0.9106387257
O,0,3.8601932637,-1.1265729499,-3.4316448733
O,0,4.1744401307,0.1950628334,-1.6293009994
H,0,1.4360205753,-0.5029565472,-3.1708601845
H,0,1.3234437526,0.9019366644,0.4039821882
H,0,1.5545696589,-1.7390706594,-1.2122827636
H,0,1.795974085,-0.9608930178,1.7587895922
C,0,3.9346820381,1.2731867747,1.7802529871
C,0,3.6912596519,2.577625394,2.2040598278
C,0,4.098695536,0.2496685528,2.7246925274
H,0,3.5806871368,3.3696820948,1.468325026
C,0,3.6040500006,2.8736772205,3.5627932146
C,0,4.0187229843,0.5580344489,4.0867983207
H,0,3.4156376131,3.8933136943,3.8869277232
H,0,4.1608025503,-0.2482219161,4.7997176672
C,0,3.7681305049,1.8591370674,4.5051033271
H,0,3.704281041,2.085682349,5.5656676149
H,0,4.0118552465,1.0649237783,0.7149952192
C,0,4.3765598839,-1.1748005039,2.3478660227
O,0,4.7036952791,-2.0007302581,3.2256114459
C,0,4.195253686,-1.5451209068,0.9849979463
H,0,4.2554533431,-0.8587120117,0.1413162079
S,0,4.8512871253,-3.1294994873,0.6463706771
C,0,4.6082418824,-3.2654712716,-1.1326607298
H,0,3.5559465794,-3.4961574144,-1.3007637936
H,0,4.8611698595,-2.3354285408,-1.651216595
H,0,5.2177317852,-4.1006224375,-1.4820609505
C,0,6.6515517358,-2.9395796735,0.7329731369
H,0,6.8711482285,-2.6921955002,1.7721249498
H,0,7.1155478769,-3.8906311375,0.463015874
H,0,6.9670135362,-2.1383846373,0.0633203181
H,0,1.1307810054,1.5634522226,-4.344508532
H,0,2.8672371292,1.3278626464,-4.5988433805
C,0,1.6351887016,-3.0868054344,1.2522813414
C,0,0.1780279649,-3.3572024699,1.6587468814
H,0,2.2946692727,-3.3665111945,2.0816718539
H,0,1.8860047887,-3.7257620165,0.3960746751
C,0,-0.0462874504,-4.8109890753,2.0537183561
H,0,-0.4821220692,-3.0849520052,0.8267977161
H,0,-0.0902220029,-2.6992350054,2.4948595859
H,0,-1.0876343368,-4.9849622104,2.3407280387
H,0,0.1890009796,-5.4872351097,1.2247486524
H,0,0.5865024259,-5.0923014982,2.9021306201
C,0,2.3451173166,2.6942469878,-2.9458073112
H,0,2.0802616136,3.6428928855,-3.4178519235
H,0,3.396288032,2.7268826904,-2.6461936179
C,0,1.4777181218,2.3926801234,-1.7293046551
H,0,1.8279703092,2.8566517497,-0.803011352
H,0,0.4371301207,2.6972961529,-1.8981350444

TS-3b (RS), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1496.07251144 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.406818 a.u.
1 imaginary frequency = 256.6609 i cm⁻¹
0; 1
C,0,-4.7598365967,-0.4340524539,0.1328609548
N,0,-2.6975937046,0.2056768068,1.0603038962
C,0,-3.32325529,-0.9235376442,0.3641484324
C,0,-2.6016870033,-1.2313979112,-0.9941784908
C,0,-1.4310967779,0.2121955667,1.392736442
C,0,-0.5809522515,-0.8980355915,1.3627508219
C,0,0.7883666473,-0.693896964,1.3551446582
O,0,-2.8508018915,-2.3601688641,-1.4538238307
O,0,-1.882872955,-0.3331303035,-1.4830731704
H,0,-3.2891242095,-1.8221374026,0.9816017056
H,0,-1.0240396009,1.1754339391,1.6958732054
H,0,-0.9836535684,-1.8855909305,1.1634650235
H,0,1.1324868429,0.3093871558,1.601667775
C,0,0.3247495798,2.4506508194,-0.482740045
C,0,-0.101920538,3.7250076971,-0.1179168725
C,0,1.6714584417,2.0957240559,-0.3391748708
H,0,-1.1415540838,4.001790112,-0.2503182195
C,0,0.8022941285,4.6481427314,0.4001827455
C,0,2.5734583251,3.0302961667,0.1745770547
H,0,0.465505806,5.6387954034,0.6824208628
H,0,3.6133949041,2.7425585387,0.2719215183
C,0,2.1420986765,4.2971708,0.5479827951
H,0,2.8497507796,5.0131779339,0.9495802922
H,0,-0.3979478407,1.750471159,-0.8922167976
C,0,2.2009551182,0.7354880112,-0.7106689493
O,0,3.4253401853,0.5393754503,-0.7715436775
C,0,1.2373836792,-0.2929624662,-0.8822214658
H,0,0.2002230374,-0.1196691354,-1.1390024271
S,0,1.8833484998,-1.7599081632,-1.5887194484
C,0,0.3784027894,-2.7480120585,-1.7275553718
H,0,0.1025488179,-3.0662756083,-0.7238678171
H,0,-0.4230151305,-2.1450320228,-2.1555131198
H,0,0.6143763847,-3.6165409757,-2.3402012683
C,0,2.1543216399,-1.3364286641,-3.3321215023
H,0,2.9575486387,-0.6018524791,-3.3414818566
H,0,2.4546363929,-2.2405281455,-3.8606601371
H,0,1.232725891,-0.9212781148,-3.7363999442
H,0,-5.3795442854,-0.6661333433,1.0029078455
H,0,-5.20198269,-0.9083444837,-0.7418984636
C,0,1.7821140034,-1.7852990854,1.6109332651
C,0,1.9595949462,-2.0009576128,3.1233817396
H,0,2.749654541,-1.5211515379,1.1735063182
H,0,1.4489635762,-2.72625475,1.1588779918
C,0,3.0196004943,-3.0598577975,3.4143144107
H,0,0.9998206514,-2.2950694787,3.5571616439
H,0,2.2416221105,-1.0519333334,3.5899810191
H,0,3.1362541695,-3.21524357,4.4883713094
H,0,2.7471758806,-4.0172083924,2.9626813269
H,0,3.9890701904,-2.7604880106,3.0085472923
C,0,-4.5938779584,1.0830910203,-0.0114535805
H,0,-5.5212760889,1.6320499105,0.1467762108
H,0,-4.2016666733,1.3238426467,-1.0009117563
C,0,-3.5468401502,1.4083340729,1.0511886815
H,0,-2.9395114913,2.2858567126,0.8254904205
H,0,-4.0054569898,1.5340095844,2.0363524243

TS-3b (RR), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1494.85447705 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.407877 a.u.
1 imaginary frequency = 221.9535 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1495.3085564 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1495.334025 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1496.0704616 a.u.

0; 1
C,0,-5.389824145,0.0610359107,-1.2024117887
N,0,-3.107826574,-0.4677962125,-1.3536198233
C,0,-3.9902072104,0.6454236102,-0.9801317342
C,0,-3.7358822818,1.0707781429,0.50744613
C,0,-1.7949173307,-0.3854782193,-1.3642872585
C,0,-1.0474923836,0.7650026868,-1.0982391144
C,0,0.3450883148,0.714025153,-1.0664691094
O,0,-3.4651763237,2.2790065636,0.6773826132
O,0,-3.8200768102,0.1507075559,1.3556417948
H,0,-3.78447604,1.5030175833,-1.6276181155
H,0,-1.2695000557,-1.3097331097,-1.6007865556
H,0,-1.5636443081,1.6854292032,-0.8342133052
H,0,0.8090780247,-0.1858014186,-1.4676539103
C,0,4.005501038,0.3001189374,0.7102178143
C,0,5.3508730903,0.4435062295,0.3848598163
C,0,3.2953662171,-0.8366327022,0.3050718229
H,0,5.8931676844,1.3261144306,0.710983843
C,0,6.0015997149,-0.5445869517,-0.3505624679
C,0,3.9624370722,-1.8281986251,-0.4229159374
H,0,7.051478098,-0.4303861425,-0.6044155174
H,0,3.4009007228,-2.7094390517,-0.7162224633
C,0,5.3039483593,-1.6824997429,-0.7531920074
H,0,5.8089762175,-2.4568577469,-1.3233637851
H,0,3.5209561149,1.071390676,1.3010543807
C,0,1.8520773623,-1.0704962365,0.6270896753
O,0,1.3602914685,-2.2054688784,0.4630660018
C,0,1.0354321686,0.0286331239,1.0296330254
H,0,1.4206669435,0.946938905,1.4576898941
S,0,-0.5157435782,-0.4941024774,1.6565892367
C,0,-0.1497561122,-1.4976912441,3.1142026246
H,0,0.3956337392,-2.3682806796,2.7496165069
H,0,0.4475689196,-0.928229178,3.8272774043
H,0,-1.1023994264,-1.8004029442,3.5533311439
C,0,-1.1380537392,1.0046447545,2.4229326453
H,0,-1.2766602942,1.7504419478,1.6394562914
H,0,-2.1371944738,0.7653051863,2.7921304766
H,0,-0.4478186627,1.3432506698,3.1977380994
H,0,-5.7165877766,0.2442777167,-2.232625652
H,0,-6.1246441732,0.5104022632,-0.5306881126
C,0,1.1602170076,1.9692820259,-1.1543695809
C,0,1.216676094,2.4928549779,-2.597173597
H,0,2.1816166579,1.7842643307,-0.8060671344
H,0,0.7250876237,2.7413374545,-0.5075972105
C,0,2.0783752857,3.7429542138,-2.7190717981
H,0,0.1977345986,2.701012599,-2.9435889595
H,0,1.610952804,1.7048946945,-3.2514486401
H,0,2.1083304984,4.1028669085,-3.7518766757
H,0,1.688845319,4.5538196664,-2.0940719447
H,0,3.1087269332,3.5453851969,-2.4038957463
C,0,-5.2001776783,-1.436102793,-0.9576612856
H,0,-5.993104875,-2.0524693884,-1.3877913484
H,0,-5.1350970648,-1.6141045793,0.1178020414
C,0,-3.8463371851,-1.7101669407,-1.5983212205
H,0,-3.3122116135,-2.5592059329,-1.1639899345
H,0,-3.9405948461,-1.871597073,-2.6800775481

TS-3b (RR), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1496.07281171 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.407594 a.u.
1 imaginary frequency = 278.5657 i cm⁻¹

0; 1
C,0,5.2140630736,0.605805626,0.9467353792
N,0,2.9115308567,0.3766378532,1.3581193755
C,0,3.8334448368,0.8645626434,0.3242072674
C,0,3.6513711224,0.0741929371,-1.0122142792
C,0,1.6097338472,0.4838028377,1.2674608329
C,0,0.9148948837,1.1392195184,0.2448414561
C,0,-0.4764122277,1.1004891147,0.2144714501
O,0,3.718299411,0.7621770865,-2.0491244172
O,0,3.4788942369,-1.1574709837,-0.9017288331
H,0,3.6506211013,1.9239161387,0.1377450318
H,0,1.0389202967,0.0118907216,2.0654449284
H,0,1.4620727193,1.6158675182,-0.5630163115
H,0,-0.9714462192,0.768229333,1.1251102002
C,0,-4.1034106474,-0.45626051,-0.6956180632
C,0,-5.4102934026,-0.0146739118,-0.5186425655
C,0,-3.3312853423,-0.8326401452,0.4067039218
H,0,-6.0063786144,0.2626785348,-1.3799994724
C,0,-5.9522909225,0.0658258646,0.7610859155
C,0,-3.8867501011,-0.762433479,1.6860833554
H,0,-6.968929821,0.4150386357,0.8979941881
H,0,-3.282513879,-1.0689342394,2.5317074451
C,0,-5.1878057201,-0.307681963,1.8638540289
H,0,-5.6078869611,-0.246722749,2.8608696348
H,0,-3.6998788457,-0.5292382727,-1.6988258461
C,0,-1.9149453003,-1.316366779,0.2809155475
O,0,-1.4204114086,-2.0203333088,1.1741476375
C,0,-1.1392894777,-0.8241772905,-0.8074843038
H,0,-1.5640208387,-0.4536426619,-1.7302478296
S,0,0.4230385565,-1.6133246392,-0.9560759434
C,0,0.0437495751,-3.315968673,-1.4382432642
H,0,-0.4758211842,-3.7612004809,-0.5919025073
H,0,-0.5768027231,-3.3174072196,-2.3321626015
H,0,0.9944768597,-3.8194651913,-1.6108192031
C,0,0.9846281849,-0.9322579989,-2.5239439428
H,0,1.1658884666,0.1293331732,-2.3667743474
H,0,1.9371260826,-1.4067278327,-2.7469208286
H,0,0.2257167648,-1.1083267746,-3.2851911262
H,0,5.516378173,1.4669136567,1.5485854476
H,0,5.972239478,0.439024539,0.1817937903
C,0,-1.2557121292,2.0544062113,-0.6443698356
C,0,-1.3137648825,3.4474261956,0.0016484054
H,0,-2.2758558479,1.68683488,-0.7820658499
H,0,-0.7892537786,2.1299755685,-1.6327956186
C,0,-2.1646066257,4.408954152,-0.8237899597
H,0,-0.2980381592,3.8375799032,0.1088124383
H,0,-1.7265750522,3.3561119422,1.0115174506
H,0,-2.2083043442,5.3957563174,-0.3594324343
H,0,-1.7517166112,4.5270759316,-1.8288699706
H,0,-3.187368479,4.036083703,-0.9217508641
C,0,4.9850175501,-0.6162918497,1.8442326875
H,0,5.7447739982,-0.7242669168,2.6177925758
H,0,4.9551003055,-1.5207652102,1.23722387
C,0,3.6033780645,-0.3499350568,2.4365489428
H,0,3.0481131662,-1.2534962022,2.6889289569
H,0,3.6643449351,0.2935968025,3.3195230576

TS-3b (SR), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1494.85132736 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.405190 a.u.
1 imaginary frequency = 229.4119 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1495.3036809a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1495.3291331a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1496.063728 a.u.

0; 1
C,0,2.1204865326,1.7743932935,-4.1477332297
N,0,2.0531487397,1.2755625321,-1.8648327166
C,0,2.4769789199,0.6950654989,-3.137987138
C,0,4.0221322439,0.3439019296,-3.1053519575
C,0,2.1346305852,0.5901072205,-0.7452905379
C,0,2.1294969224,1.0845552258,0.5603813896
C,0,2.5219151723,0.2339126794,1.5906807313
O,0,4.6020764035,0.422340288,-4.1993748317
O,0,4.4748551448,-0.0153810204,-1.9876611713
H,0,1.9405467356,-0.2449290142,-3.3111117567
H,0,2.2715924817,-0.4773861723,-0.8886709204
H,0,2.0593055808,2.1530741918,0.7447164718
H,0,2.4143276607,-0.8370928667,1.428784807
C,0,4.3613758783,-3.1312695697,1.1871958227
C,0,4.0002243749,-4.4658757791,1.3490722255
C,0,4.9153468463,-2.4121525651,2.2536506061
H,0,3.5825280495,-5.0154161321,0.5105064195
C,0,4.1807418317,-5.0971878724,2.5773538959
C,0,5.106767608,-3.0621227482,3.4783288071
H,0,3.8951584871,-6.1378091281,2.7017760572
H,0,5.5544366032,-2.4970529485,4.2897476838
C,0,4.7376226572,-4.3912719579,3.6428300832
H,0,4.8857756969,-4.880347394,4.6014852789
H,0,4.2368103994,-2.6692113209,0.2123671719
C,0,5.3451537333,-0.9712037399,2.1636846519
O,0,6.1070622345,-0.5222583862,3.0384671151
C,0,4.7362445673,-0.1942925016,1.1272726384
H,0,4.3807818582,-0.6704953737,0.2216354805
S,0,5.3660656528,1.3522533655,0.6156828385
C,0,6.9388774779,0.9904129604,-0.1940008672
H,0,7.4150545794,1.9346115442,-0.4678218038
H,0,7.5741027671,0.4027612438,0.4699526936
H,0,6.6496953117,0.4349504881,-1.0899823413
C,0,5.8900384811,2.2393191726,2.0945725618
H,0,6.3702736232,3.1587773937,1.7547266027
H,0,4.9880226651,2.4833369286,2.6569130416
H,0,6.5453054857,1.6103207475,2.6931782299
H,0,1.0658542759,1.7073791301,-4.4377128507
H,0,2.7477233174,1.671239124,-5.0331557794
C,0,2.3896019763,3.0622348802,-3.3673795183
H,0,1.872495991,3.9352043914,-3.7717273944
H,0,3.4639682292,3.2718012411,-3.3717847904
C,0,1.93048859,2.7321580546,-1.9461401917
H,0,2.5452432649,3.2096680614,-1.1761036513
H,0,0.8854704858,3.0148333843,-1.7725282254
C,0,2.496380809,0.6643059253,3.0248514648
C,0,1.1291204769,0.3779049086,3.6638974128
H,0,2.7058219907,1.7389684208,3.0990234013
H,0,3.273124176,0.1417635503,3.5933515336
C,0,1.0853848237,0.785772133,5.1307909799
H,0,0.90550404,-0.6920966518,3.56936576
H,0,0.3506863391,0.9075644966,3.1019538789
H,0,0.1055093787,0.5758542893,5.5698525762
H,0,1.8369069699,0.2430182121,5.7139605514
H,0,1.2824616225,1.8566953753,5.2501094692

TS-3b (SR), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1496.06706375 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.404889 a.u.
1 imaginary frequency = 347.8450 i cm⁻¹

0; 1
C,0,5.3037209681,-0.2060309092,-1.0320383497
N,0,3.1047983651,0.5931049965,-1.0272787295
C,0,3.8684909534,-0.6239696418,-1.3359129234
C,0,3.3715111501,-1.8519665455,-0.4704540404
C,0,1.8122723099,0.6641998816,-1.2258377875
C,0,0.9215277086,1.6149468418,-0.7195789818
C,0,-0.4304903959,1.2612866486,-0.7090724287
O,0,4.2073595239,-2.7583293665,-0.3389338256
O,0,2.1936783909,-1.7993669008,-0.0534473853
H,0,3.7182710874,-0.895045331,-2.3836717515
H,0,1.4012477447,-0.1600766376,-1.8014678074
H,0,1.2724801342,2.4578720973,-0.1344560744
H,0,-0.7527705893,0.5377445792,-1.4538688283
C,0,-2.5327335463,-1.5887245282,-1.1824823067
C,0,-3.4701058205,-1.7622178108,-2.1957605342
C,0,-2.8769134201,-0.9021953364,-0.0149316601
H,0,-3.1978020293,-2.3063513021,-3.0923059719
C,0,-4.7532721656,-1.2392044735,-2.058811626
C,0,-4.1734019063,-0.4005859396,0.1243527416
H,0,-5.4786586833,-1.3662064267,-2.8538380599
H,0,-4.4298247246,0.1255639449,1.0363280673
C,0,-5.1043032739,-0.5593554234,-0.8949118198
H,0,-6.1024782074,-0.1520937882,-0.783343304
H,0,-1.54075983,-2.0090545745,-1.3041196514
C,0,-1.8962099615,-0.5976817377,1.0874816437
O,0,-2.3227196923,-0.3023567489,2.2105604914
C,0,-0.5308329401,-0.4773684763,0.6817556634
H,0,-0.1026967204,-1.119406767,-0.0745928551
S,0,0.7245019393,-0.1252791463,1.8593876624
C,0,0.6344094376,-1.4681716345,3.0660441919
H,0,1.3230069419,-1.2354944543,3.877517122
H,0,-0.3920286129,-1.557524833,3.4163223751
H,0,0.9638624036,-2.3577203167,2.5319258732
C,0,0.1005026409,1.2708044663,2.8243945679
H,0,0.8666502815,1.4959151125,3.5655223834
H,0,0.0003318579,2.1072512864,2.1338117186
H,0,-0.8531205108,1.020917977,3.2780362767
H,0,5.7287794587,0.3413164521,-1.8777039937
H,0,5.9202855095,-1.07565073,-0.8190222567
C,0,5.1287665843,0.7243647411,0.1728962647
H,0,5.9825887176,1.3780775806,0.3457473568
H,0,4.961150244,0.1286035422,1.0737971299
C,0,3.8613071896,1.5134033018,-0.1676461724
H,0,3.266089734,1.7733663545,0.7109218919
H,0,4.0820971471,2.4284591489,-0.724826306
C,0,-1.5125402154,2.2096822747,-0.2595104518
C,0,-2.51739035,2.4654085854,-1.3908544488
H,0,-1.0614840553,3.1535510574,0.0654203347
H,0,-2.0592990879,1.8102447366,0.6012783601
C,0,-3.6800860687,3.3364794334,-0.9264688547
H,0,-2.8992343521,1.5010693003,-1.744517722
H,0,-2.0030819117,2.9349487793,-2.235204191
H,0,-4.3894927358,3.5145055419,-1.7367145678
H,0,-4.2175229764,2.8486705457,-0.108257559
H,0,-3.3269086401,4.3066155726,-0.5669878897

TS-3b (SS), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1494.85548558 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.408503 a.u.
1 imaginary frequency = 218.8840 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1495.3080347a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1495.3337158 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1496.0692682 a.u.
0; 1
C,0,1.5233420832,0.3607583689,-3.8425499086
N,0,1.7250470668,0.5899113696,-1.51700487
C,0,1.791146237,-0.4280227748,-2.5659203829
C,0,3.1778905643,-1.1854768275,-2.5729469983
C,0,1.9554837454,0.2694071422,-0.2611915711
C,0,2.2523754931,1.1169149136,0.8054287993
C,0,2.7587388528,0.5408512714,1.9674981321
O,0,3.4088714041,-1.8044266666,-3.6230483209
O,0,3.8599051101,-1.1288845795,-1.5158468983
H,0,1.0278837215,-1.1942367329,-2.3864421744
H,0,1.954604044,-0.799443357,-0.0734906154
H,0,2.3128700028,2.1923884865,0.668234368
H,0,2.5338232436,-0.5137081695,2.1231757524
C,0,5.2822546463,2.2995114909,-0.3175609483
C,0,5.3370316184,3.5052691294,-1.0132017434
C,0,5.7035315164,2.239879223,1.0174730909
H,0,5.0273464498,3.5399688421,-2.0541938245
C,0,5.7981950974,4.6597619136,-0.3848966111
C,0,6.178239739,3.4023936482,1.6358188843
H,0,5.8381049754,5.5976273224,-0.9315830856
H,0,6.5138752855,3.3314506095,2.6656992505
C,0,6.2180271484,4.6061713851,0.9440225876
H,0,6.5815209637,5.5035715691,1.4365299047
H,0,4.9361129049,1.4047582411,-0.8280626431
C,0,5.6994808379,0.9779301685,1.8196626915
O,0,6.3536814674,0.9083843176,2.8805263495
C,0,4.8824769227,-0.10225213,1.3694133081
H,0,4.6041308331,-0.2609833508,0.3306779272
S,0,5.271091607,-1.590966536,2.2127282356
C,0,4.3246974204,-2.7905660485,1.2532259816
H,0,4.3649956001,-2.5356386206,0.1882859214
H,0,4.7438953587,-3.7776473317,1.4539539748
H,0,3.2943577068,-2.7638446935,1.6110524228
C,0,6.9594843443,-2.0180367199,1.7129247913
H,0,7.2244864751,-2.9742820112,2.1683919737
H,0,7.0166271824,-2.0643358718,0.6245316972
H,0,7.5903983323,-1.2205833689,2.1065574492
H,0,0.4470282531,0.4494201886,-4.0287516538
H,0,1.9885188343,-0.142939499,-4.6904212006
C,0,2.9958935219,1.3320175285,3.2156768091
C,0,1.7041263251,1.4699837454,4.0335493811
H,0,3.372028946,2.3291325023,2.9567041139
H,0,3.7662291778,0.8529669889,3.8301082259
C,0,1.9211871284,2.2514446377,5.3230939139
H,0,1.3136476491,0.4708660176,4.2664183401
H,0,0.9408207977,1.9622330172,3.4192006639
H,0,0.990799346,2.3416376633,5.8919200524
H,0,2.6598051719,1.7591178369,5.9646116175
H,0,2.2853733499,3.2631484122,5.1150261408
C,0,2.1263390373,1.7314708106,-3.5318988115
H,0,1.7403924107,2.5323094152,-4.1666090826
H,0,3.2143220548,1.6953773542,-3.6541627943
C,0,1.7791290372,1.9472361126,-2.0600128629
H,0,2.5225902736,2.5437417836,-1.5227391578
H,0,0.8003220231,2.4271354124,-1.9379027031

TS-3b (SS), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1496.07144376 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.408820 a.u.
1 imaginary frequency = 261.3775 i cm⁻¹
0; 1
C,0,-4.7148973253,0.6478119034,0.6191311068
N,0,-2.4914242029,0.3359325057,1.3079459109
C,0,-3.6467502701,-0.4293936216,0.8160686791
C,0,-3.3143375992,-1.2142351806,-0.5106664303
C,0,-1.3464665158,-0.2513704076,1.551460528
C,0,-0.0913142315,0.33911572,1.7163039895
C,0,1.009979676,-0.5013779714,1.6190749753
O,0,-4.3091713543,-1.706781176,-1.0618629053
O,0,-2.1103291046,-1.2922168205,-0.846069211
H,0,-3.9405210642,-1.1762946802,1.5574088998
H,0,-1.395100711,-1.3365335829,1.5632204402
H,0,0.0401855864,1.4142348254,1.6720443664
H,0,0.8386050251,-1.5556276121,1.8245517506
C,0,0.0299545028,1.5699153842,-1.3715884098
C,0,-0.420375084,2.8745649381,-1.5619707336
C,0,1.4027850139,1.3128645078,-1.2902253023
H,0,-1.4837100982,3.0683334017,-1.6503946348
C,0,0.4848630844,3.9274590384,-1.6478477264
C,0,2.3067869427,2.3745352931,-1.3861948611
H,0,0.1266658888,4.9400184457,-1.7930404256
H,0,3.3664626399,2.1561605861,-1.3284615297
C,0,1.8524208432,3.675812301,-1.5543468741
H,0,2.5611370006,4.492910925,-1.6213287256
H,0,-0.6946589704,0.7621118971,-1.3084684015
C,0,1.9631334228,-0.0687881066,-1.1118883327
O,0,3.166012997,-0.2879564417,-1.3286464054
C,0,1.0800983046,-1.0632862735,-0.6085025959
H,0,0.0052159397,-1.036180389,-0.7418824806
S,0,1.7444741251,-2.6852050964,-0.7160024557
C,0,0.2784187413,-3.6475292865,-0.2782436305
H,0,-0.59471073,-3.2027472272,-0.7594754931
H,0,0.4483893361,-4.6720404902,-0.6047440678
H,0,0.1766738812,-3.6232740507,0.8052234559
C,0,1.8360986456,-3.0336805646,-2.49538037
H,0,2.1743873671,-4.0609720894,-2.6244667751
H,0,0.8515312143,-2.8730321145,-2.9315627912
H,0,2.566896529,-2.3337261472,-2.896046779
H,0,-5.2377962291,0.8424687821,1.5591779284
H,0,-5.4382647057,0.3387929304,-0.1318054357
C,0,2.4092429736,-0.0189898742,1.8424949869
C,0,2.7243367155,0.0527832005,3.3451837218
H,0,2.5349627716,0.9736053511,1.3961251178
H,0,3.1230690156,-0.6866042684,1.3513114121
C,0,4.1620942065,0.5012414922,3.5928684634
H,0,2.5565543554,-0.9297189637,3.7984005918
H,0,2.0251075897,0.7440295277,3.8242332467
H,0,4.377909324,0.560952674,4.6612065232
H,0,4.871094903,-0.1979857998,3.1427377545
H,0,4.3409168407,1.4867903363,3.1556545968
C,0,-3.8871519451,1.8720313044,0.2122559708
H,0,-4.4202688979,2.8150678717,0.3255543068
H,0,-3.5702411331,1.7734724675,-0.8300660468
C,0,-2.6695623126,1.7837723334,1.131422639
H,0,-1.7665965593,2.2234965182,0.7068915329
H,0,-2.862431359,2.2432627746,2.1055069356

TS-3b down (SR), optimization in solv. CHCl_3
 PBE1PBE/6-31G(d,p), $E = -1494.84278798$ a.u.
 Thermal correction to Gibbs Free Energy at $25^\circ\text{C} = 0.407892$ a.u.
 1 imaginary frequency = $215.3631 \text{ i cm}^{-1}$
 SP at B2PLYP/6-311+G(d,p) in CHCl_3 , $E = -1495.2969321$ a.u.
 SP at mPW2PLYP/6-311+G(d,p) in CHCl_3 , $E = -1495.3219433$ a.u.
 SP at M06-2X/6-311+G(d,p) in CHCl_3 , $E = -1496.0543739$ a.u.
 0; 1
 C,0,2.4176798466,1.3833936638,-4.6874808838
 N,0,2.278113267,1.4967301527,-2.3433396041
 C,0,2.5838369568,0.5375848268,-3.4200504442
 C,0,4.0191140012,-0.0938456657,-3.2920176316
 C,0,2.1342792351,1.1732365268,-1.072059843
 C,0,2.5141949002,-0.0431409542,-0.5059470342
 C,0,2.1424935427,-0.397909283,0.7845084794
 O,0,4.9693939219,0.658983163,-3.572082281
 O,0,4.0345338952,-1.2962452534,-2.9256573401
 H,0,1.8528889529,-0.2749982528,-3.356104472
 H,0,1.7098825167,1.9530010264,-0.4390474834
 H,0,3.1153956433,-0.7233230358,-1.1068519338
 H,0,1.5830282001,0.3348550043,1.3683158066
 C,0,-1.2747779029,0.6499479665,1.7412549346
 C,0,-1.9674414622,1.6950846179,2.3438778558
 C,0,-1.0331404934,-0.5380523982,2.4422246645
 H,0,-2.1486157295,2.612031209,1.7908657285
 C,0,-2.4283576564,1.5662296145,3.6524108979
 C,0,-1.4982035336,-0.655197859,3.7565338625
 H,0,-2.9707830186,2.382592192,4.1203668224
 H,0,-1.2995180196,-1.5812485579,4.2862730285
 C,0,-2.1915343915,0.3876504007,4.3579670133
 H,0,-2.5483852747,0.2833692594,5.3784635607
 H,0,-0.9244209702,0.7701126492,0.7203559514
 C,0,-0.2996554292,-1.7074848193,1.8641884537
 O,0,-0.0716556208,-2.7096185601,2.5741299701
 C,0,0.1857192232,-1.6337616935,0.5248656576
 H,0,-0.2709157146,-1.0173690758,-0.2404889897
 S,0,0.7608685961,-3.1964273858,-0.0310794722
 C,0,1.0450964418,-2.9387368745,-1.7919983356
 H,0,1.1394275812,-3.9303474809,-2.2384250113
 H,0,0.2003137141,-2.4068899664,-2.2347506096
 H,0,1.9787940773,-2.3897379763,-1.9473091859
 C,0,-0.6951669391,-4.2716926681,-0.0836623085
 H,0,-0.3809847059,-5.2497411598,-0.4538226239
 H,0,-1.0383678166,-4.3484933813,0.948219879
 H,0,-1.4618578771,-3.8334176027,-0.7240015638
 H,0,1.3874643411,1.3183725849,-5.0570883005
 H,0,3.0922503339,1.046168426,-5.4762115364
 C,0,2.9305231545,-1.3871468517,1.585380903
 C,0,4.0595819802,-0.6755196628,2.3479390301
 H,0,3.3725338618,-2.142915568,0.9249149276
 H,0,2.2879830956,-1.909321764,2.3034845623
 C,0,4.8689749689,-1.64490987,3.1995813412
 H,0,3.6284365089,0.107572012,2.9847188681
 H,0,4.7134034372,-0.1682353084,1.6292440983
 H,0,5.6712435735,-1.1254676157,3.7322550622
 H,0,4.2368885349,-2.1399196818,3.944543161
 H,0,5.3279304967,-2.4236137289,2.581290046
 C,0,2.7303261189,2.804426627,-4.2219407645
 H,0,2.3560264675,3.5807920702,-4.8933240856
 H,0,3.8126563465,2.9034618408,-4.1100279613
 C,0,2.0691127545,2.8557541544,-2.8535960681
 H,0,2.5104854821,3.5885252732,-2.1739081359
 H,0,0.9921858358,3.0562752346,-2.9361418325

Int-3b (RS), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1494.88379242 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.413132 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1495.3304136 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1495.3578142 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1496.1009812 a.u.

O, 1
C,0,-4.693075853,-0.5751281521,0.2542345219
N,0,-2.7592484477,-0.1217628982,1.5078590031
C,0,-3.2353877841,-1.016806999,0.4514501045
C,0,-2.4091474947,-0.8638415075,-0.8639341528
C,0,-1.417789003,0.0414778713,1.6741176743
C,0,-0.4764451144,-0.9038952627,1.4528621159
C,0,0.9187945986,-0.4984435889,1.0890324535
O,0,-2.2471466049,-1.9209839648,-1.5274158815
O,0,-1.9888418193,0.2797164086,-1.1662811185
H,0,-3.1816948285,-2.067559506,0.7570554259
H,0,-1.1075334939,1.0528740878,1.9476900914
H,0,-0.7905040092,-1.9190881838,1.2252138538
H,0,1.0437471362,0.5470967418,1.4075583178
C,0,0.3518689744,2.4857196143,-0.5661064803
C,0,0.0874159491,3.8456709681,-0.4314438362
C,0,1.6746525612,2.0569947236,-0.7517393941
H,0,-0.9371152144,4.1807128572,-0.3007875685
C,0,1.1249674881,4.7739465571,-0.470248236
C,0,2.7134574971,2.9967936327,-0.8051160846
H,0,0.909026161,5.8326969257,-0.3591282416
H,0,3.7276433543,2.6423021458,-0.9598563659
C,0,2.4408244913,4.3485438677,-0.6579909228
H,0,3.2490454657,5.0727881885,-0.6909245588
H,0,-0.4773229762,1.7786316884,-0.5596037658
C,0,2.0358344434,0.6287179476,-0.9295747709
O,0,3.1169359632,0.2888489141,-1.3899471567
C,0,1.0174807976,-0.4093618379,-0.479577577
H,0,0.0161964543,-0.1691990392,-0.8727424734
S,0,1.5289031486,-1.9676926252,-1.3125226691
C,0,0.3744170532,-3.246029591,-0.7775794539
H,0,0.6076292591,-3.5162478357,0.2514625701
H,0,-0.6621607618,-2.9025276246,-0.9097771054
H,0,0.5883909709,-4.1008147043,-1.4243427041
C,0,0.8435773788,-1.649755263,-2.9524275903
H,0,1.3459429509,-0.770558571,-3.3566548934
H,0,1.0690380766,-2.5185781931,-3.5730232675
H,0,-0.2377480602,-1.5017904595,-2.8435658348
H,0,-5.3424988644,-1.0994438082,0.9652824598
H,0,-5.0529073289,-0.796942365,-0.7538830385
C,0,2.0656507052,-1.2923885174,1.723998639
C,0,2.1264817992,-1.1074910757,3.2367102598
H,0,3.0201617686,-0.9832699637,1.2764231367
H,0,1.9581802867,-2.3648385872,1.5091021533
C,0,3.2297673162,-1.9288065513,3.8899739779
H,0,1.1516880861,-1.3740555539,3.6628487743
H,0,2.2756385846,-0.0425331357,3.4594110082
H,0,3.2542581064,-1.7722449325,4.972645178
H,0,3.0838506732,-3.0001763696,3.7128023101
H,0,4.214542793,-1.6596002132,3.4922345565
C,0,-4.6499249396,0.9187739455,0.5731485698
H,0,-5.6312123653,1.3427321761,0.8028788403
H,0,-4.2149401531,1.4575178441,-0.2731335407
C,0,-3.6875898741,0.9746708769,1.7558933063
H,0,-3.1484191418,1.927034189,1.8250660216
H,0,-4.2218150105,0.8292016486,2.7064931897

Int-3b (RR), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1494.87702938 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.410758 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1495.3266976 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1495.3536052 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1496.0948860 a.u.

O, 1
C,0,-5.1800756091,-0.8417663844,-1.0857001854
N,0,-2.8498191991,-1.0199581896,-1.2365933816
C,0,-3.8863740756,-0.0173525413,-1.0064344026
C,0,-3.7124323905,0.6968983131,0.3699339223
C,0,-1.5351489735,-0.7335609135,-1.1466203577
C,0,-0.9955070167,0.4939928525,-0.9230754037
C,0,0.4752512935,0.7298886055,-0.7517195358
O,0,-3.6547248672,1.9549987506,0.3209006466
O,0,-3.627100406,-0.036296605,1.379492366
H,0,-3.8416497414,0.7534500738,-1.7866490855
H,0,-0.8820829439,-1.6000752887,-1.2555823724
H,0,-1.6502550821,1.3557048087,-0.8171551224
H,0,1.0378456566,0.0385399482,-1.3948756735
C,0,3.8457859622,0.114930353,-0.1143386
C,0,5.1326493662,-0.045254148,-0.6157128491
C,0,3.0699651143,-1.0064923399,0.2037144902
H,0,5.7304734214,0.8281747147,-0.8561382662
C,0,5.6523255769,-1.3232930507,-0.8063638233
C,0,3.6045554926,-2.2887924376,0.0148458367
H,0,6.6568361495,-1.4455842634,-1.2003676982
H,0,2.9921026149,-3.1475004976,0.269687392
C,0,4.886582159,-2.4458066415,-0.4901717421
H,0,5.292439169,-3.4416163482,-0.638664623
H,0,3.4610822696,1.1181049004,0.0353597671
C,0,1.69595645,-0.9172197214,0.7565034706
O,0,1.1164796863,-1.906729161,1.1810601688
C,0,0.9666132849,0.4184221498,0.7231135156
H,0,1.5908523004,1.2281377161,1.1166533201
S,0,-0.4610240855,0.2273639878,1.860482862
C,0,0.4293394373,0.0968680906,3.435046979
H,0,0.9625360427,-0.852885205,3.4408129049
H,0,1.1115617753,0.9371263421,3.5771279202
H,0,-0.3296209262,0.0912050142,4.2192279168
C,0,-1.0849448476,1.9121429098,2.039592072
H,0,-1.9266887264,2.0544592688,1.3456799326
H,0,-1.4694319103,1.9719006551,3.0597541724
H,0,-0.2780740591,2.6342694093,1.9028477467
H,0,-5.5465756181,-0.8683303286,-2.1189495482
H,0,-5.9713312237,-0.4212829174,-0.4598456538
C,0,0.8672872028,2.1569805281,-1.156335325
C,0,0.659086904,2.4294512144,-2.6419129326
H,0,1.9196268448,2.3459227805,-0.9053557542
H,0,0.2758054291,2.8720888364,-0.5673440674
C,0,1.0275598998,3.8542709128,-3.0344178686
H,0,-0.3867962258,2.2273332489,-2.8999128101
H,0,1.2601560831,1.716578083,-3.2225011442
H,0,0.8736723099,4.0237880915,-4.1043115578
H,0,0.4166331091,4.5836499598,-2.4914684148
H,0,2.0784353891,4.0708005369,-2.8112879371
C,0,-4.7445867791,-2.2377626391,-0.6396767283
H,0,-5.4376161725,-3.0289276278,-0.9392190412
H,0,-4.628701414,-2.242048518,0.4471174962
C,0,-3.372972858,-2.3776913724,-1.2889959288
H,0,-2.7136043406,-3.0700144503,-0.7551148236
H,0,-3.4621620931,-2.7288948859,-2.3289936305

Int-3b (SR), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1494.88013385 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.411026 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1495.3274159 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1495.3547093 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1496.0958025 a.u.

0; 1
C,0,-5.0651170641,0.5653995526,-0.9039832825
N,0,-2.9864344568,-0.3055629708,-1.4618212113
C,0,-3.585213946,0.9191818095,-0.9263234077
C,0,-3.0291839472,1.3258360561,0.4834030342
C,0,-1.6366471343,-0.3694745385,-1.5812552024
C,0,-0.8124357209,-1.4393604935,-1.515632422
C,0,0.6636645813,-1.187962845,-1.3384723188
O,0,-3.8171764049,1.9019085799,1.2492375714
O,0,-1.8048387414,1.0614012122,0.6989935982
H,0,-3.3725040988,1.7551903414,-1.6065846535
H,0,-1.1873884026,0.6123474048,-1.7192633015
H,0,-1.1858318204,-2.4449484415,-1.3390640331
H,0,1.006640464,-0.4388568164,-2.0692786779
C,0,1.2050484963,2.5218176452,0.2950635216
C,0,1.3894909667,3.9016167786,0.2799759415
C,0,2.3185039945,1.6726139254,0.1937668568
H,0,0.5276643291,4.5559073652,0.3673742598
C,0,2.6665096776,4.4416119352,0.1560354334
C,0,3.6035373637,2.2264561208,0.079068996
H,0,2.7996977782,5.5194760891,0.1397349123
H,0,4.4516295764,1.5530735388,0.0074062428
C,0,3.7766263141,3.6010630808,0.0551137736
H,0,4.7727621757,4.0221293221,-0.0411939943
H,0,0.1927472414,2.1355880054,0.4082854944
C,0,2.224799351,0.1908964427,0.2286888824
O,0,3.2213465463,-0.5089418953,0.3516272842
C,0,0.8605004597,-0.4513019868,0.032364102
H,0,0.0490297807,0.2825790631,0.0858399364
S,0,0.3319753319,-1.5183556727,1.4217145744
C,0,-0.0036181006,-0.3036166042,2.7072461436
H,0,-0.367018338,-0.848718732,3.5800300423
H,0,0.9012646264,0.2559971873,2.9516500882
H,0,-0.7885086667,0.3479132357,2.2910611409
C,0,1.7760299256,-2.3819826278,2.0699874577
H,0,1.4264574713,-2.9204005623,2.9534127705
H,0,2.1123248759,-3.090476204,1.3137282497
H,0,2.5764717689,-1.6861697334,2.3164051349
H,0,-5.4934425058,0.6596196159,-1.9081544447
H,0,-5.605692278,1.2159405634,-0.2160200512
C,0,-5.0487417465,-0.8992648909,-0.455657867
H,0,-5.9397916955,-1.4543814047,-0.7602346964
H,0,-4.9894212408,-0.9402409241,0.6365818883
C,0,-3.7625407102,-1.4737916057,-1.0700018772
H,0,-3.2027978227,-2.0863954197,-0.3466523282
H,0,-3.9589983264,-2.1051668459,-1.9462316024
C,0,1.519273421,-2.4408377593,-1.5187100861
C,0,1.5147951057,-2.9453517323,-2.9588395984
H,0,1.1312679727,-3.2394119004,-0.866839793
H,0,2.5484984768,-2.2413313473,-1.1996825105
C,0,2.3224642479,-4.2239398016,-3.1383441779
H,0,1.9171548188,-2.1587427641,-3.6109714619
H,0,0.4789002134,-3.1063052523,-3.2810819846
H,0,2.3116146979,-4.559880634,-4.1796506202
H,0,3.3683181005,-4.076785483,-2.8466469473
H,0,1.9193854271,-5.0364223314,-2.5234159995

Int-3b (SS), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1494.87980418 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.411120 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1495.328969 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1495.3563177 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1496.0988755 a.u.

0; 1
C,0,-4.7852677524,-0.2095116182,0.8003579248
N,0,-2.5836546502,-0.3306488983,1.5639339929
C,0,-3.5226134872,-1.0618927792,0.7098875326
C,0,-3.0495401087,-1.2890835309,-0.7700371837
C,0,-1.2909858093,-0.7326594932,1.5835439887
C,0,-0.1520984422,-0.0500631394,1.8484242482
C,0,1.1251948984,-0.6743550436,1.354023161
O,0,-3.9444523818,-1.6571282596,-1.5478352317
O,0,-1.8167356792,-1.1389780875,-1.0374440953
H,0,-3.6945209145,-2.0649621342,1.1238117664
H,0,-1.1876100425,-1.7733064073,1.2840905373
H,0,-0.147533902,1.0073554978,2.0994586606
H,0,1.095847116,-1.7470944734,1.5964524424
C,0,-0.3010578497,1.9893886379,-0.8469860493
C,0,-0.9146964838,3.2351205798,-0.9497229669
C,0,1.0986422386,1.9108176986,-0.8293757898
H,0,-1.9982789502,3.2983852807,-0.9825235615
C,0,-0.14724257,4.395038603,-1.0147698778
C,0,1.86705494,3.0810660355,-0.9168691609
H,0,-0.6346020251,5.3631166573,-1.0863528116
H,0,2.9490283169,2.9943644479,-0.9153670008
C,0,1.2466974487,4.318312217,-0.9967786646
H,0,1.8434736288,5.2237140758,-1.0500481417
H,0,-0.9117279988,1.0888153039,-0.8178744279
C,0,1.8179298025,0.6201217999,-0.7795688684
O,0,2.9829539865,0.5129780638,-1.1457494597
C,0,1.0967775307,-0.5920298829,-0.2248654599
H,0,0.0457375773,-0.6625656054,-0.5403748076
S,0,1.8851936179,-2.0571827974,-1.0138803016
C,0,0.6376665175,-3.31117413773,-0.6506789285
H,0,-0.3567998341,-2.8920099697,-0.8459474228
H,0,0.8493850414,-4.1658289497,-1.2966087275
H,0,0.748711435,-3.6172487595,0.3899320894
C,0,1.4720255904,-1.752963291,-2.744394361
H,0,1.6924368759,-2.6652841949,-3.3002778287
H,0,0.4101574808,-1.500889582,-2.8083451964
H,0,2.1037069099,-0.9387407121,-3.0972606257
H,0,-5.3419497389,-0.4461882392,1.7145114439
H,0,-5.4292792338,-0.3881792411,-0.0614624536
C,0,2.4013344541,-0.1025884548,1.9695430136
C,0,2.5099412542,-0.4009992038,3.4608479965
H,0,2.4209917008,0.9856778132,1.8165665701
H,0,3.282728773,-0.4989971126,1.4483156917
C,0,3.7537375168,0.2069697767,4.0955444045
H,0,2.5126790378,-1.4893370078,3.6107026949
H,0,1.6093719508,-0.0291800556,3.9645959679
H,0,3.8095715892,-0.0227132516,5.1639797268
H,0,4.6670126944,-0.1737315935,3.6247627586
H,0,3.7582559764,1.2973361109,3.9889206094
C,0,-4.2284607462,1.213386342,0.8712070181
H,0,-4.9330954419,1.9370700316,1.2892884175
H,0,-3.9613541496,1.5515098564,-0.1366700766
C,0,-2.9644256557,1.0661741874,1.7232134542
H,0,-2.1557641845,1.7293842575,1.3889019651
H,0,-3.1558681682,1.2907518422,2.7815968447

TS-4b (RSR), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1494.86549070 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.410398 a.u.
1 imaginary frequency = 314.0351 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1495.3154696 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1495.3411467 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1496.0776953 a.u.

0; 1
C,0,-4.3357996909,-1.9669817791,0.0792333382
N,0,-2.2357343741,-1.3242108299,0.89703057
C,0,-2.8884961049,-1.7364526162,-0.3557407186
C,0,-2.734463201,-0.6306486749,-1.4618820337
C,0,-0.9139354637,-1.2700146035,1.0831699048
C,0,0.0331156283,-1.518331268,0.1201815261
C,0,1.5142630062,-1.3910008111,0.3382347891
O,0,-1.7450437943,-0.7751906721,-2.2267645752
O,0,-3.5818484576,0.2843307702,-1.4568027304
H,0,-2.4012172454,-2.6498480828,-0.717891874
H,0,-0.6079847383,-1.004722388,2.0947473258
H,0,-0.3061088393,-1.6805526409,-0.9020504875
H,0,1.7688598791,-1.377464997,1.4035807413
C,0,-0.6995245799,1.9873756801,-0.8628267961
C,0,-1.5604537192,3.0150973971,-1.2370086836
C,0,0.144711527,2.1596732205,0.2413059006
H,0,-2.2560668287,2.8412239082,-2.0510606449
C,0,-1.5567927062,4.2222850296,-0.5443586481
C,0,0.121108188,3.367718207,0.956472761
H,0,-2.2255614899,5.0233471364,-0.8465111626
H,0,0.7629385858,3.4737144022,1.8259661506
C,0,-0.710118235,4.4009603831,0.5523699335
H,0,-0.7140391326,5.3404495103,1.0970822645
H,0,-0.7560474427,1.0415853034,-1.400155651
C,0,1.0212432604,1.0785181685,0.7474814206
O,0,1.4180097883,1.0674517993,1.9088508738
C,0,1.5103856939,0.0029864461,-0.1968323656
H,0,1.2018390615,0.0918473428,-1.2366917718
S,0,3.5759460399,0.6667357037,-0.5769436076
C,0,3.472425668,2.4592686872,-0.7534730566
H,0,3.0288222258,2.9136082626,0.133996322
H,0,4.4798618941,2.8476815479,-0.9153620998
H,0,2.8554222726,2.6700127662,-1.6283464385
C,0,4.3468130534,0.5180761911,1.0439333922
H,0,4.5294509612,-0.5425942991,1.2231594148
H,0,5.2999241354,1.0505394003,1.0265959632
H,0,3.6788905908,0.917710007,1.8097666314
H,0,-4.4687937414,-2.9982273843,0.4280352668
H,0,-5.0266216807,-1.781677617,-0.7448896659
C,0,-3.1959665187,-1.0642355783,1.9688760988
H,0,-2.9359681982,-0.1457293529,2.5043466858
H,0,-3.1911513454,-1.8952647453,2.6888584185
C,0,-4.525088004,-0.9803119151,1.2311433166
H,0,-4.6503051179,0.0189629673,0.8078392475
H,0,-5.3736432172,-1.2152604212,1.8787109215
C,0,2.3483856994,-2.4203378769,-0.4157146431
C,0,2.1232696874,-3.838361106,0.0974199755
H,0,3.4161957825,-2.1732945851,-0.3343564743
H,0,2.1013344188,-2.3708243513,-1.4850312566
C,0,2.932041315,-4.8781456605,-0.6665735033
H,0,1.0535751709,-4.0722628031,0.0306987181
H,0,2.3786491658,-3.8801157014,1.1647865665
H,0,2.7528256239,-5.8853123117,-0.2784803264
H,0,2.6685972476,-4.8795550893,-1.7298066251
H,0,4.0071302959,-4.6795660759,-0.5926295988

TS-4b (RSR), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1496.07910557 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.407861 a.u.
1 imaginary frequency = 472.9743 i cm⁻¹

0; 1
C,0,-4.3422912058,-1.9206348292,0.1165594378
N,0,-2.2321864785,-1.2992098536,0.9376773239
C,0,-2.8805787108,-1.7375273872,-0.3085176877
C,0,-2.6903384865,-0.6651136238,-1.4354601073
C,0,-0.9125582919,-1.2473303714,1.1048930854
C,0,0.0203963253,-1.5559648958,0.1445776958
C,0,1.5115344883,-1.4209804223,0.3450771698
O,0,-1.8541883009,-0.9503316382,-2.3236877562
O,0,-3.368196446,0.3732655428,-1.3279306925
H,0,-2.418290916,-2.6723657569,-0.6375403022
H,0,-0.5869464834,-0.9292100575,2.093778862
H,0,-0.3099618752,-1.8160035682,-0.855313892
H,0,1.7891151956,-1.4058713538,1.4014339987
C,0,-0.7145453896,1.9662090588,-0.9004324272
C,0,-1.532207067,3.0105094082,-1.3230119815
C,0,0.1237346563,2.1505249707,0.2004039342
H,0,-2.2191754425,2.8385899095,-2.1412816144
C,0,-1.4882542438,4.2379540372,-0.673656063
C,0,0.142033955,3.3795691372,0.8739223319
H,0,-2.1207471675,5.0509283193,-1.0111491208
H,0,0.7816837837,3.4966985558,1.7413081081
C,0,-0.6477771377,4.4250152364,0.426463873
H,0,-0.6233225779,5.380417765,0.9366458839
H,0,-0.7881565901,1.0080562402,-1.4051971311
C,0,0.9667301113,1.0522979322,0.73538216
O,0,1.3487015909,1.0377243822,1.8899957848
C,0,1.4226088694,-0.0464550278,-0.2021527539
H,0,1.1380958606,0.0343189928,-1.2458498091
S,0,3.5129748383,0.7192864541,-0.5917821335
C,0,3.3970168103,2.5246541399,-0.5212200671
H,0,2.9990885039,2.8354613197,0.4445694574
H,0,4.3938373934,2.9368785473,-0.6725901149
H,0,2.7354371872,2.8467115135,-1.3241205358
C,0,4.2945482123,0.3948347817,1.0043782302
H,0,4.414549566,-0.6831095074,1.1008924133
H,0,5.273428387,0.8729391005,1.0113127405
H,0,3.6628030119,0.7781026217,1.8048257618
H,0,-4.4962759501,-2.9433694332,0.472127173
H,0,-5.0254033939,-1.7309651448,-0.710164053
C,0,-3.1930918587,-1.0092631682,2.0100865205
H,0,-2.9210544567,-0.0843579477,2.5211684322
H,0,-3.1924718386,-1.8297467998,2.7366762086
C,0,-4.525385648,-0.9260827057,1.2699496924
H,0,-4.6602492198,0.0750491458,0.8624001631
H,0,-5.366823425,-1.174176537,1.9170208311
C,0,2.3332766869,-2.4242366667,-0.4534148554
C,0,2.1620091263,-3.8491243683,0.065902679
H,0,3.3948303605,-2.1520144755,-0.4186495996
H,0,2.032322413,-2.3739330881,-1.5067873959
C,0,2.9904674108,-4.8552484648,-0.7279878475
H,0,1.1024913355,-4.1188025011,0.0207641138
H,0,2.4482052039,-3.8816716992,1.1229801837
H,0,2.8600780049,-5.8679263964,-0.3423432789
H,0,2.6957578285,-4.8554235772,-1.7805335072
H,0,4.0551114848,-4.6113218458,-0.6788835224

TS-4b (RRR), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1494.85610463 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.406818 a.u.
1 imaginary frequency = 310.9984 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1495.3088644 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1495.3344021 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1496.0702218 a.u.
0; 1
C,0,4.839319483,-0.6141199476,-0.8258455654
N,0,3.2215417707,0.7672449231,0.1230049124
C,0,3.3338634751,-0.3546065485,-0.7956493261
C,0,2.5660480939,-1.621126673,-0.2555951543
C,0,2.067993955,1.3687965063,0.4068730175
C,0,0.9299373506,1.4144691618,-0.3636781644
C,0,-0.3417335325,1.9595846885,0.2168593497
O,0,2.5287185872,-2.5640193414,-1.0685169636
O,0,2.1188800851,-1.5512465276,0.9157259413
H,0,2.9359041494,-0.1012393197,-1.782663061
H,0,2.063397221,1.9064083923,1.3565066135
H,0,0.9070452519,1.0109961498,-1.370852097
H,0,-0.1198485577,2.3901612558,1.2027354505
C,0,-0.7654820724,-2.4600977318,0.2670862242
C,0,-0.9864313423,-3.8319774405,0.3625599655
C,0,-1.5943722716,-1.6877692427,-0.5575382565
H,0,-0.3241228497,-4.4340938429,0.9767776363
C,0,-2.0276247197,-4.4337973718,-0.3386419001
C,0,-2.6168305082,-2.3057587683,-1.2954975718
H,0,-2.1956351569,-5.5033312187,-0.2495737017
H,0,-3.2227916365,-1.6960559683,-1.9592525937
C,0,-2.8423189137,-3.6690274431,-1.1750590474
H,0,-3.6439650947,-4.1391953066,-1.7366514037
H,0,0.1137640538,-2.0337388809,0.7548307051
C,0,-1.4357561953,-0.2194758662,-0.7257718259
O,0,-1.8263367784,0.3392894755,-1.7417912213
C,0,-0.9249483426,0.5987460746,0.4395369022
H,0,-0.4277630607,0.0337872349,1.2250879169
S,0,-2.8201621324,0.8713958508,1.578411963
C,0,-4.1929664163,0.6235831592,0.4357631228
H,0,-4.1612809481,-0.3805551679,0.0090143487
H,0,-5.1275103918,0.7763476957,0.9794130365
H,0,-4.099065852,1.3670393556,-0.3568659984
C,0,-2.9152865835,-0.6196059788,2.5874739786
H,0,-2.1133707212,-0.5637056261,3.3252164991
H,0,-3.878120853,-0.6334902253,3.1019841735
H,0,-2.7937856248,-1.5121282966,1.9704820693
H,0,5.3418663197,0.0834366251,-1.5065902903
H,0,5.0495416851,-1.6332377489,-1.1547163493
C,0,-1.1088007675,2.9911763782,-0.606197932
C,0,-0.3758694586,4.3277071117,-0.6478783921
H,0,-2.1063604866,3.1406109078,-0.1671459888
H,0,-1.2680899964,2.6130303324,-1.6188101043
C,0,-1.0976794014,5.370099074,-1.4914686665
H,0,0.6349030656,4.1627114812,-1.0422829032
H,0,-0.2457334767,4.7060159493,0.3754290851
H,0,-0.5504460582,6.3175481832,-1.5111641977
H,0,-1.2115287413,5.0292567776,-2.5262367518
H,0,-2.1003975116,5.5736928901,-1.0990572727
C,0,5.2430597092,-0.3378348041,0.623940674
H,0,6.3107609783,-0.1451279714,0.7535111625
H,0,4.9650254491,-1.1899102808,1.2506015448
C,0,4.3887253951,0.8732905037,0.9977410172
H,0,4.0826595505,0.8735715356,2.0493987674
H,0,4.9193778249,1.8134158655,0.7968386233

TS-4b (RRR), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1496.07185019 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.406378 a.u.
1 imaginary frequency = 469.9703 i cm⁻¹
0; 1
C,0,4.8393974489,-0.9112881661,-0.6380004333
N,0,3.289034932,0.4360296661,0.477125537
C,0,3.3869182088,-0.4213170962,-0.6987880375
C,0,2.3940693035,-1.6318377457,-0.6018831261
C,0,2.1822469236,1.101776694,0.777564316
C,0,1.1215384129,1.3417396552,-0.065432758
C,0,-0.1235072798,2.013372128,0.4489180672
O,0,2.1243607416,-2.1613165917,-1.6965228779
O,0,2.0277133871,-1.9646105412,0.5446973804
H,0,3.176582758,0.1390037262,-1.6114860402
H,0,2.1449852881,1.4970347524,1.7921343341
H,0,1.1489098892,1.0429528414,-1.1059009134
H,0,0.055677143,2.3846903446,1.4625785116
C,0,-1.0617247472,-2.3302996942,0.4375481876
C,0,-1.5263890726,-3.6343230797,0.5742564431
C,0,-1.6306314356,-1.4948769542,-0.5258071182
H,0,-1.0686514035,-4.2919433922,1.303090511
C,0,-2.5615813793,-4.0991178124,-0.2311939119
C,0,-2.6397382657,-1.9792772363,-1.3656083359
H,0,-2.9269176789,-5.1123885147,-0.1115146568
H,0,-3.0438137508,-1.3292942503,-2.1333849476
C,0,-3.1143978248,-3.2734058513,-1.2089993327
H,0,-3.9052005322,-3.6421450076,-1.8508279626
H,0,-0.2059517112,-2.0026946909,1.0165230497
C,0,-1.2298749258,-0.0697374632,-0.6934004415
O,0,-1.3733973809,0.5096512844,-1.7481051001
C,0,-0.7960430062,0.6901329852,0.5453367576
H,0,-0.5131423948,0.0914028599,1.4036034451
S,0,-2.8864741721,1.0903596861,1.3584978513
C,0,-3.9660671298,1.2358833188,-0.0848838581
H,0,-3.973312422,0.2986682216,-0.6399331281
H,0,-4.9693520385,1.4865052126,0.2574605292
H,0,-3.5707332677,2.035023758,-0.7096523578
C,0,-3.4789756379,-0.4654836553,2.0701034446
H,0,-2.7627481812,-0.7692457644,2.8324147811
H,0,-4.4495866366,-0.2816619498,2.5295762034
H,0,-3.5536602402,-1.2310308041,1.2986739444
H,0,5.5042794217,-0.1689900971,-1.0884515237
H,0,4.9654519491,-1.8553867019,-1.1668438422
C,0,-0.7237008293,3.1305867313,-0.3992294963
C,0,0.1665862851,4.3714402885,-0.3810074856
H,0,-1.7105769579,3.395335062,0.0020805867
H,0,-0.8686026246,2.789386892,-1.4249402286
C,0,-0.4119143662,5.5042713426,-1.2242700174
H,0,1.1591120991,4.0993325738,-0.7533778714
H,0,0.301154359,4.7083858484,0.6529288982
H,0,0.234949417,6.3834480837,-1.2086924518
H,0,-0.5283480945,5.1909447055,-2.2648627169
H,0,-1.3957684219,5.8046933635,-0.8540033481
C,0,5.1016160719,-1.0167280772,0.8694699464
H,0,6.1621880627,-1.0180362042,1.1204234839
H,0,4.64099219,-1.9241427507,1.2608593235
C,0,4.3806748824,0.2094853638,1.4332723501
H,0,3.9767431445,0.0492498885,2.4347090153
H,0,5.0389254905,1.0841838144,1.4530903056

TS-4b (SRS), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1494.86270292 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.408733 a.u.
1 imaginary frequency = 334.9327 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1495.3131583 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1495.3387311 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1496.0745333 a.u.
0; 1
C,0,-4.1873228441,2.2989903967,-0.1307821129
N,0,-1.9070819928,1.7471781327,-0.1059766017
C,0,-3.0605685205,1.8755366407,0.8020882781
C,0,-3.3100191182,0.522804165,1.5644166541
C,0,-0.6622971186,1.5429761263,0.3081648203
C,0,0.4515416346,1.4420512467,-0.5036033444
C,0,1.8290321703,1.1607548007,0.0336056386
O,0,-2.3359951686,0.1560675125,2.2664025935
O,0,-4.4161407191,-0.0255194245,1.3996310321
H,0,-2.8335264594,2.6358586282,1.5580557012
H,0,-0.5766736924,1.4252600821,1.3853677698
H,0,0.3673113982,1.567838213,-1.5795723982
H,0,1.839669452,1.2538259641,1.1245626661
C,0,0.0240049249,-2.5446376975,-1.494459828
C,0,-0.9354566521,-3.3630063972,-2.0797492413
C,0,-0.2104639666,-1.9803305749,-0.2332828835
H,0,-0.7417470527,-3.8154481925,-3.0476841575
C,0,-2.1479189012,-3.5897058136,-1.4298475017
C,0,-1.4266058972,-2.2184976468,0.4218677087
H,0,-2.9047199892,-4.2114431873,-1.8995851181
H,0,-1.6287194146,-1.7151372127,1.3660568559
C,0,-2.395085688,-3.006760784,-0.1879345845
H,0,-3.3511857678,-3.15114226,0.3056400363
H,0,0.9574816135,-2.3696247879,-2.0224228587
C,0,0.771367559,-1.1135666353,0.4629589145
O,0,0.8260757824,-1.0552757098,1.6838271592
C,0,1.7209418439,-0.2728317715,-0.3570395201
H,0,1.7251684913,-0.4470082364,-1.4314761565
S,0,3.6864685689,-1.2868089168,0.0383948533
C,0,3.9740821674,-0.7553945611,1.737776723
H,0,3.0515878109,-0.8613151082,2.3126194579
H,0,4.779018065,-1.3596513503,2.1607315867
H,0,4.2866493312,0.2894005559,1.7113831237
C,0,3.286069754,-3.0267280499,0.3087806292
H,0,2.9743034349,-3.4542741642,-0.645034217
H,0,4.1853649863,-3.5393441372,0.6568178704
H,0,2.4871444454,-3.1240999183,1.0463460138
H,0,-4.2145066936,3.3891852639,-0.2443116763
H,0,-5.1409640677,1.9470664406,0.2641275572
C,0,2.9488380261,1.9699457599,-0.6083856235
C,0,2.8711243105,3.4512858116,-0.2545734604
H,0,2.9014438091,1.8469941819,-1.699606065
H,0,3.9267993736,1.574205669,-0.3007998393
C,0,3.9633894984,4.2763253045,-0.9217042012
H,0,2.9342562583,3.5638959255,0.8357190938
H,0,1.8836729253,3.8325344191,-0.5426420895
H,0,3.8842851252,5.3334247649,-0.6511768008
H,0,4.9600420004,3.9309343984,-0.625304535
H,0,3.9009171175,4.2065765039,-2.0132536543
C,0,-3.8183139825,1.6280652341,-1.4524559741
H,0,-4.3131709175,2.0636255208,-2.3238748154
H,0,-4.0769600293,0.566337975,-1.3957063551
C,0,-2.3027166858,1.786066715,-1.5086622416
H,0,-1.8014849046,0.9847541411,-2.0629883441
H,0,-2.0075206341,2.7454170439,-1.9571265375

TS-4b (SRS), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1496.07691916 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.407136 a.u.
1 imaginary frequency = 487.4341 i cm⁻¹
0; 1
C,0,-4.0132617236,2.2227295395,-0.1773888901
N,0,-1.7399206585,1.6517719152,-0.0736778311
C,0,-2.8916679385,1.936024483,0.8155155085
C,0,-3.1286329132,0.7073902441,1.7554468523
C,0,-0.4872304913,1.5526424007,0.3410704361
C,0,0.6131003827,1.4046748801,-0.4854728478
C,0,1.9822336655,1.056295417,0.0530337057
O,0,-2.2407853289,0.5562145682,2.6224892001
O,0,-4.1255721398,-0.0023238369,1.5320187927
H,0,-2.6459857945,2.7968869943,1.4399871329
H,0,-0.3705687,1.5625997155,1.4223539062
H,0,0.5099401706,1.4962859411,-1.560731151
H,0,2.0122877315,1.1693412026,1.1397347847
C,0,-0.2937889171,-2.2538916083,-1.567941526
C,0,-1.3895384429,-2.7863378032,-2.2340963215
C,0,-0.4437467184,-1.7576477112,-0.2681687805
H,0,-1.2709221577,-3.1882713486,-3.2331711764
C,0,-2.6430241977,-2.7851964049,-1.6233665618
C,0,-1.69391256,-1.7864545668,0.3543312693
H,0,-3.5022221985,-3.173509154,-2.1580807326
H,0,-1.8032923083,-1.375069339,1.3524893679
C,0,-2.7956004908,-2.2816624413,-0.3341862636
H,0,-3.7681649122,-2.244224561,0.1408702895
H,0,0.6706691306,-2.2409534729,-2.0638388184
C,0,0.6692943732,-1.1050930335,0.4726157301
O,0,0.7484313721,-1.1149986856,1.6814201228
C,0,1.6922729823,-0.3425837195,-0.3419757915
H,0,1.7035334943,-0.5227497205,-1.4111346095
S,0,3.5533096097,-1.6222264846,0.0417453231
C,0,3.9274233733,-1.0748401897,1.7244456871
H,0,3.0188226907,-1.1057979906,2.3241288737
H,0,4.6966531078,-1.7267049447,2.1365339789
H,0,4.3088189123,-0.0567036582,1.6629829681
C,0,2.9127106226,-3.2801327955,0.392651863
H,0,2.5026475004,-3.6823477609,-0.532437724
H,0,3.7407010527,-3.904562416,0.7258903412
H,0,2.1417472559,-3.2275518905,1.1607370744
H,0,-3.9936040889,3.2756955217,-0.4736733815
H,0,-4.9831749139,1.9878037771,0.2560394615
C,0,3.1579184285,1.7270068239,-0.640532941
C,0,3.2226338484,3.2242790949,-0.3517944009
H,0,3.0737131496,1.5618496278,-1.7219580927
H,0,4.0953778148,1.2521026235,-0.3267354481
C,0,4.3957079298,3.8970729776,-1.0592860232
H,0,3.301335328,3.3786532473,0.7295293956
H,0,2.2814229096,3.6863589845,-0.6650658131
H,0,4.4220408721,4.9681860398,-0.8517853435
H,0,5.3471004493,3.4684306454,-0.7334508529
H,0,4.3234361975,3.7659239268,-2.1421708024
C,0,-3.6678746063,1.3273635666,-1.3711054554
H,0,-4.1620991387,1.6245104644,-2.2957230138
H,0,-3.9367997077,0.2967028296,-1.1324389144
C,0,-2.1473595783,1.4493670879,-1.4658453612
H,0,-1.6607555052,0.5491032982,-1.8561343172
H,0,-1.8411432247,2.3083286996,-2.0748828784

TS-4b (SSS), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1494.86525567 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.408236 a.u.
1 imaginary frequency = 313.8056 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1495.3143427 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1495.3402049 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1496.0764981 a.u.
0; 1
C,0,4.2303373663,-2.2137039106,-0.1037273831
N,0,1.9109217439,-1.903873119,-0.1322492862
C,0,3.0309558528,-2.0195118069,0.8122097895
C,0,3.1074061981,-0.7378483137,1.7254958298
C,0,0.6501525193,-1.7861551461,0.2731828744
C,0,-0.4515866399,-1.4668536902,-0.4889968781
C,0,-1.7691233701,-1.1683874915,0.1770109732
O,0,4.2141451473,-0.1755268535,1.8150202238
O,0,2.0192981168,-0.4287415654,2.2779430144
H,0,2.8617804741,-2.8797745617,1.4712260763
H,0,0.5316050445,-1.9145445059,1.3452426824
H,0,-0.3835256052,-1.2992899032,-1.5597609453
H,0,-1.8415970208,-1.7056986986,1.1300894407
C,0,1.2575527809,1.7509242754,0.1013204043
C,0,2.4089183856,2.5257103371,-0.0152929155
C,0,0.1763669443,1.971397275,-0.7627608794
H,0,3.2449784879,2.3205074401,0.6467722231
C,0,2.4852360846,3.5280769902,-0.9787447273
C,0,0.2638566403,2.9809487394,-1.7342913553
H,0,3.384854009,4.1308804274,-1.0657672005
H,0,-0.5808865723,3.1363127394,-2.3977704083
C,0,1.4078946583,3.7576206551,-1.837321822
H,0,1.4662889662,4.5403761821,-2.587886663
H,0,1.2526395217,0.9665292451,0.8560985376
C,0,-1.0714630999,1.1672864228,-0.7314761565
O,0,-1.9220996696,1.279764888,-1.6076290768
C,0,-1.3452339153,0.2510678767,0.446773441
H,0,-0.6094584314,0.3113952103,1.2471199276
S,0,-2.7554341762,1.522095046,1.5341176933
C,0,-3.311671547,0.3671412406,2.7990195687
H,0,-4.0724876749,0.8544788281,3.4114592039
H,0,-3.7142490221,-0.5406219731,2.346313316
H,0,-2.4491369811,0.1265321165,3.4227131885
C,0,-4.2362088992,1.7291665303,0.5253754454
H,0,-3.9118478543,2.1247612802,-0.4378814731
H,0,-4.7443899198,0.7763465444,0.3780987792
H,0,-4.8963822943,2.4404761537,1.0253262781
H,0,4.3530554206,-3.2704213431,-0.3686161504
H,0,5.1341565571,-1.8527827521,0.3881199667
C,0,-3.0012126154,-1.4633831672,-0.6688924916
C,0,-3.150930996,-2.9563163124,-0.9466645968
H,0,-2.9483845826,-0.9037860503,-1.6079151916
H,0,-3.8996122346,-1.1095773396,-0.1473086797
C,0,-4.3825315493,-3.2763065266,-1.7833727508
H,0,-3.1986194673,-3.5003211787,0.0064468536
H,0,-2.2492569065,-3.3180722886,-1.455848192
H,0,-4.4676615113,-4.3504972674,-1.9731604777
H,0,-5.3006526176,-2.9540542013,-1.2794495202
H,0,-4.3432773381,-2.7685333068,-2.7532172089
C,0,2.3603831766,-1.635864255,-1.4933458848
H,0,1.8236553101,-0.7741266853,-1.9065164523
H,0,2.1523150532,-2.5037444252,-2.1339450435
C,0,3.8591196301,-1.3868906163,-1.335483085
H,0,4.0354926785,-0.3279643247,-1.1216030833
H,0,4.4207277441,-1.6568438639,-2.2330007525

TS-4b (SSS), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1496.07893182 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.410171 a.u.
1 imaginary frequency = 466.3235 i cm⁻¹
0; 1
C,0,4.1733664497,-2.1162994946,-0.1786886869
N,0,1.8660879439,-1.7313006438,-0.1031044302
C,0,3.0132797899,-1.9592399245,0.798061725
C,0,3.1496519071,-0.7595018241,1.8030524505
C,0,0.6078038756,-1.7042858895,0.309036789
C,0,-0.4955430935,-1.3825749082,-0.4523489613
C,0,-1.8397060294,-1.1411516031,0.1944851106
O,0,4.247346684,-0.1813436727,1.856140059
O,0,2.1083707798,-0.5156199546,2.4562631919
H,0,2.8298199741,-2.8606024006,1.3883905056
H,0,0.4806603167,-1.915929077,1.3667101247
H,0,-0.4097770359,-1.1699649375,-1.5119243491
H,0,-1.934555128,-1.7118800827,1.1218968272
C,0,1.3024811654,1.5778678075,0.1911329082
C,0,2.5485927755,2.1793546771,0.0357497447
C,0,0.2714174584,1.859383811,-0.7101988251
H,0,3.3406355268,1.9285305062,0.7331284591
C,0,2.7666373272,3.0644764839,-1.0153487747
C,0,0.4963164867,2.7570468611,-1.7611105409
H,0,3.738880736,3.5274616052,-1.1403794346
H,0,-0.3087834438,2.9646675337,-2.4553901279
C,0,1.7374540275,3.3570668737,-1.9110596055
H,0,1.9079868686,4.0495079129,-2.7267066922
H,0,1.1844993938,0.8789114499,1.0098914928
C,0,-1.0626365972,1.1951758266,-0.6485181579
O,0,-1.9164784633,1.3988203809,-1.4879609917
C,0,-1.3700215476,0.2471513232,0.4998075411
H,0,-0.7019180056,0.3016160074,1.352434515
S,0,-2.8750921011,1.548849563,1.5686190693
C,0,-3.6233617721,0.2581439767,2.5884607622
H,0,-4.4310716093,0.6986840702,3.1710317769
H,0,-4.0003993859,-0.5520649189,1.9665028014
H,0,-2.8495379319,-0.1102148816,3.2604248108
C,0,-4.2120648983,1.9042928456,0.4029416691
H,0,-3.882861765,2.7397844271,-0.2105895889
H,0,-4.4106367805,1.0431828693,-0.2297910397
H,0,-5.0945257572,2.1861916463,0.9768593109
H,0,4.2196035937,-3.1452741901,-0.5467223393
H,0,5.117008717,-1.8571939143,0.2956272337
C,0,-3.04056621,-1.387878874,-0.7097746563
C,0,-3.1650387433,-2.8662980281,-1.0759528467
H,0,-2.9607018493,-0.7812449754,-1.6155493265
H,0,-3.9563467249,-1.075150612,-0.19736489
C,0,-4.4074655452,-3.1424284873,-1.9181646123
H,0,-3.1958397934,-3.4656148184,-0.1593060194
H,0,-2.2686113039,-3.1779027055,-1.6200899356
H,0,-4.477695584,-4.1976989615,-2.1879496977
H,0,-5.3165665441,-2.8736136604,-1.3737374658
H,0,-4.3873662378,-2.5593325299,-2.8425307185
C,0,2.2866539976,-1.3635007605,-1.4581115566
H,0,1.7600092351,-0.4600582965,-1.7794734661
H,0,2.043252054,-2.1763067018,-2.1518202911
C,0,3.7957796882,-1.1609486396,-1.3155501969
H,0,3.9982685676,-0.1327371863,-1.0060399399
H,0,4.3264375416,-1.3598879035,-2.2461047131

4b (RSR), optimization in solv. CHCl₃
PBE1PBE/6-311G(d,p), E= -692.770435343 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.224127 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -693.0401987 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -693.0469825 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -693.4421561 a.u.

O; 1
C,0,1.0771720018,0.2051218218,0.237042632
C,0,1.937191549,-0.9665065606,-0.0203690709
C,0,2.1277552919,-2.0006525756,1.0604215466
H,0,1.0974674544,0.6000359312,1.2705845833
H,0,1.910581698,-1.3168590309,-1.0492790268
H,0,1.6909513585,-1.7236946128,2.0197677186
C,0,5.8429889481,0.3698613595,0.2856395499
C,0,7.0945405065,0.9658004054,0.1680091104
C,0,5.1279579639,0.4649159933,1.4852405323
H,0,7.6392480674,0.8968325294,-0.7686347714
C,0,7.6459649914,1.6497980559,1.2486084616
C,0,5.6844109403,1.1686219933,2.5610828251
H,0,8.6265763932,2.1076834393,1.1567220968
H,0,5.1115391855,1.2420797981,3.4799411718
C,0,6.9386571154,1.750883588,2.446860854
H,0,7.3675268829,2.2862193288,3.2886115235
H,0,5.4196121324,-0.1453924386,-0.5705522531
C,0,3.7734234311,-0.1272159487,1.6710478995
O,0,3.0775402575,0.2027999839,2.6228624714
C,0,3.2924352573,-1.1454020219,0.6888629847
H,0,4.0458703845,-1.600041212,0.0540773262
C,0,2.0883740572,-3.4672531352,0.7125735034
C,0,0.6664463559,-4.0140065766,0.6102496415
H,0,2.6446258542,-4.026709036,1.4763797332
H,0,2.6160025411,-3.6315762354,-0.2366778122
C,0,0.6316051977,-5.4997395934,0.27724354
H,0,0.118228231,-3.4476670817,-0.1533106897
H,0,0.1428119912,-3.8347009959,1.558147118
H,0,-0.396027903,-5.8690373691,0.2100027734
H,0,1.1213860672,-5.7018770816,-0.6817396192
H,0,1.1481243671,-6.0891405577,1.042767004
O,0,0.3675643192,0.7003904159,-0.6158324277

4b (RSR), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -693.442823042 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.222223 a.u.

O; 1
C,0,-1.1227848634,2.1220356818,-0.2997702973
C,0,-1.3414964808,0.7017520301,-0.6382418788
C,0,-1.8029620547,-0.2398490485,0.4499728871
H,0,-0.7411096589,2.3256413376,0.7163746569
H,0,-1.7028223071,0.525500761,-1.6454189889
H,0,-1.8602602797,0.2108903216,1.4373755837
C,0,2.3651629946,-0.3725245026,-1.085187035
C,0,3.6689546347,-0.5385753732,-1.5403912337
C,0,2.1181459497,-0.1970688599,0.2780243935
H,0,3.8592535413,-0.6619962334,-2.5995483978
C,0,4.725591939,-0.5450944401,-0.6353455976
C,0,3.1847955975,-0.1890334906,1.1807669106
H,0,5.7400056683,-0.6823252337,-0.9909289956
H,0,2.9775645035,-0.0425526315,2.2340041311
C,0,4.4830978189,-0.3713944747,0.726534478
H,0,5.3075488362,-0.3760620414,1.4291609114
H,0,1.5484684328,-0.355217807,-1.7972943875
C,0,0.737083637,0.0219812186,0.8055059885
O,0,0.5588759044,0.5133008489,1.9013420696
C,0,-0.4160608698,-0.3833077293,-0.0629360972
H,0,-0.2236036253,-1.191614863,-0.757348702
C,0,-2.8631146286,-1.2639498538,0.1233304578
C,0,-4.2706255693,-0.6701455491,0.1541419292
H,0,-2.7935515909,-2.0885607237,0.840837791
H,0,-2.6640023576,-1.6891386609,-0.867326738
C,0,-5.3416030711,-1.7115020026,-0.1579427796
H,0,-4.3269779125,0.152634935,-0.566267263
H,0,-4.4524412013,-0.2332307695,1.141517553
H,0,-6.3416329519,-1.2752787782,-0.1282105348
H,0,-5.1906276848,-2.1393733167,-1.1526038404
H,0,-5.3100009878,-2.5302447075,0.5655996932
O,0,-1.3625853623,3.0273429565,-1.0632906673

4b (RRR), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -692.771035735 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.224581 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -693.0408049 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -693.0475607 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -693.4428694 a.u.
0; 1
C,0,1.8433254866,-0.6943345487,-2.3551125137
C,0,2.9548367231,-1.1780203115,-1.5186227433
C,0,2.6578570789,-2.1927009976,-0.4450727401
H,0,0.8634347136,-0.6295338708,-1.8286459522
H,0,3.9352351808,-1.2239097014,-1.9847071117
H,0,1.6030237545,-2.4474573706,-0.3381620833
C,0,3.1716982539,0.3976179907,2.6820270735
C,0,3.2591680843,1.0456083292,3.909998037
C,0,4.2968381935,0.3005371391,1.8551181866
H,0,2.3847257553,1.1094805289,4.5503404757
C,0,4.4656892199,1.609975938,4.3166583763
C,0,5.5089658362,0.8600802355,2.2790016879
H,0,4.5298689822,2.121457955,5.2726674648
H,0,6.3736781612,0.7678761667,1.6296555227
C,0,5.5919049,1.5166564894,3.4987394565
H,0,6.5330945139,1.9554931032,3.8160099967
H,0,2.228128333,-0.0496224175,2.3860996925
C,0,4.2794009548,-0.4049295161,0.5418839287
O,0,5.3261579443,-0.6861909659,-0.0254255076
C,0,2.9580020214,-0.7669700685,-0.0528509074
H,0,2.1054176546,-0.1846727544,0.2829289365
C,0,3.6017842597,-3.3438464382,-0.2017459312
C,0,3.3746845982,-4.4920919762,-1.1832544022
H,0,3.4578235313,-3.7060023516,0.8251321099
H,0,4.6364723853,-2.9931856815,-0.2714056192
C,0,4.3019981362,-5.6723380417,-0.9243277161
H,0,3.5193985637,-4.1229934432,-2.2064808911
H,0,2.3293827485,-4.8226541388,-1.1221220169
H,0,4.124835249,-6.4825151796,-1.6380121763
H,0,5.3525195579,-5.3747106463,-1.0113106052
H,0,4.1555729585,-6.0772374206,0.0831200267
O,0,1.9422154059,-0.3925051307,-3.5247286947

4b (RRR), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -693.443646497 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.223075 a.u.
0; 1
C,0,2.3965737257,2.5887498139,-0.1411546328
C,0,1.7957279164,1.3229835207,0.3169243066
C,0,1.5684667583,0.2396037128,-0.710800141
H,0,2.1083833675,2.8998320276,-1.1661850079
H,0,2.0323702229,1.008786595,1.3270185358
H,0,1.8323714781,0.5064228958,-1.7311737442
C,0,-2.2052281582,-0.0206999351,-1.0788718566
C,0,-3.484667973,-0.3587682976,-1.5075112863
C,0,-1.9139732841,0.0218391697,0.2861668664
H,0,-3.7049972988,-0.4023472382,-2.5671732528
C,0,-4.4781215214,-0.6403974432,-0.574960156
C,0,-2.9121213236,-0.2744056413,1.2179022174
H,0,-5.4763790607,-0.8968216145,-0.9096797317
H,0,-2.6685666782,-0.2441912234,2.2732157908
C,0,-4.1919575077,-0.5958597798,0.7887322675
H,0,-4.9673038802,-0.8135084195,1.513398253
H,0,-1.4324984533,0.1865502665,-1.8103556454
C,0,-0.5412839987,0.3399481922,0.7867637309
O,0,-0.2010660414,0.0386763737,1.9110107293
C,0,0.3949978316,1.0133255227,-0.1686225614
H,0,-0.0605098818,1.7231779735,-0.8492400822
C,0,1.8421694961,-1.1994083825,-0.3416136479
C,0,3.3217984351,-1.5478516542,-0.5018196816
H,0,1.2378576064,-1.8530424301,-0.981037245
H,0,1.5303170042,-1.3828706423,0.6905365887
C,0,3.6104571138,-3.0047493623,-0.150135768
H,0,3.9145676596,-0.8847163517,0.1366040366
H,0,3.629767624,-1.3469672855,-1.53338341
H,0,4.6676346846,-3.2426921058,-0.2807655042
H,0,3.3439545334,-3.21397149,0.8889804099
H,0,3.0317441625,-3.6799061424,-0.7859663802
O,0,3.1556634408,3.2612043753,0.5114870023

4b (SRS), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -692.770435341 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.224127 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -693.0401987 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -693.0469825 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -693.4421561 a.u.

O; 1
C,0,-0.9266634632,-2.5586112607,0.0127160715
C,0,0.2781150286,-2.1439215192,0.7577980944
C,0,1.5286375766,-1.7721818895,0.001564254
H,0,-1.0937308282,-2.0491478712,-0.9553298251
H,0,0.4020946053,-2.6475948393,1.7133357495
H,0,1.3949097641,-1.7259348882,-1.0790957363
C,0,-0.3922815658,1.7561250012,1.9722834572
C,0,-0.8137797108,2.9572938419,2.5334378882
C,0,-0.3404703745,1.608818193,0.5812533492
H,0,-0.8612672251,3.0613002343,3.6131101144
C,0,-1.1748350995,4.0224286897,1.712010604
C,0,-0.7208607629,2.6808331157,-0.2362821012
H,0,-1.4962743351,4.9617233291,2.1525823303
H,0,-0.6854160173,2.5456332913,-1.3125456047
C,0,-1.1280302826,3.8827975409,0.3247024147
H,0,-1.411821536,4.7124484436,-0.3157659263
H,0,-0.1301096971,0.9300452467,2.6254728174
C,0,0.0765682622,0.3432017856,-0.0852304777
O,0,-0.147237675,0.1663728388,-1.2759265211
C,0,0.7914744574,-0.6924480453,0.7204245812
H,0,1.2093291077,-0.3665252606,1.6672541343
C,0,2.8713390783,-2.2606397892,0.4832555405
C,0,3.1755912229,-3.6899137643,0.0406539206
H,0,2.9111325342,-2.1974222778,1.5791077859
H,0,3.6496707724,-1.5840864461,0.1060520033
C,0,4.5405178016,-4.1726087661,0.513401639
H,0,3.121587067,-3.746859556,-1.0541948134
H,0,2.3918011807,-4.357704464,0.4201755143
H,0,4.7367622939,-5.1973357548,0.1842287829
H,0,5.3424879315,-3.537359598,0.1215928573
H,0,4.609490298,-4.1552092249,1.606714731
O,0,-1.6831822494,-3.4210807567,0.4127868206

4b (SRS), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -693.442823043 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.222223 a.u.

O; 1
C,0,1.1227845174,2.1220364847,-0.2997623569
C,0,1.3414975169,0.7017543136,-0.6382392365
C,0,1.8029642283,-0.2398503464,0.4499719705
H,0,0.7411086393,2.325638017,0.7163831639
H,0,1.7028236281,0.5255072473,-1.6454169685
H,0,1.8602619966,0.2108853749,1.4373763591
C,0,-2.3651606689,-0.3725242161,-1.0851884486
C,0,-3.6689521806,-0.5385742244,-1.5403933341
C,0,-2.1181438351,-0.1970731094,0.278023602
H,0,-3.859250914,-0.6619915765,-2.5995509379
C,0,-4.7255895742,-0.5450968831,-0.635347829
C,0,-3.1847935816,-0.1890413593,1.1807660347
H,0,-5.7400031979,-0.6823269655,-0.9909318002
H,0,-2.977562681,-0.0425639895,2.234003776
C,0,-4.4830956684,-0.3714014316,0.7265328579
H,0,-5.3075467464,-0.3760718076,1.4291592013
H,0,-1.5484660663,-0.3552146415,-1.7972956863
C,0,-0.7370817065,0.0219759409,0.8055061075
O,0,-0.5588743985,0.5132915205,1.901344073
C,0,0.4160631861,-0.3833086546,-0.0629374984
H,0,0.2236068011,-1.1916133985,-0.7573531306
C,0,2.8631180861,-1.2639484957,0.1233253684
C,0,4.2706281398,-0.6701421544,0.1541379199
H,0,2.6640057741,-1.6891341596,-0.8673331737
H,0,2.7935567963,-2.088561968,0.8408298784
C,0,5.3416070372,-1.7114957761,-0.1579513572
H,0,4.4524438489,-0.2332306087,1.141514961
H,0,4.3269786105,0.1526410118,-0.5662683556
H,0,6.3416362265,-1.2752710025,-0.128218524
H,0,5.310007017,-2.5302410443,0.5655883026
H,0,5.1906314519,-2.1393639225,-1.1526137464
O,0,1.3625847172,3.0273468251,-1.0632791919

4b (SSS), optimization in solv. CHCl₃
PBE1PBE/6-311G(d,p), E= -692.771035734 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.224581 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -693.0408049 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -693.0475607 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -693.4428694 a.u.

O; 1
C,0,1.3217125193,2.3847025552,0.2362911393
C,0,2.2298511336,1.3438406156,0.7471869741
C,0,1.9586801413,0.7584420944,2.1088293467
H,0,0.2605175891,2.2690374585,0.5557259926
H,0,3.2678667747,1.4007250567,0.4312611069
H,0,1.0521203534,1.1260336995,2.5905236983
C,0,0.7012728663,-2.8796303771,0.7174870452
C,0,0.2182674706,-4.1710875512,0.5322858703
C,0,1.992298838,-2.543023309,0.2942963346
H,0,-0.7808367951,-4.4276794486,0.8709874041
C,0,1.0149655926,-5.1320590057,-0.08529563
C,0,2.7904915624,-3.5202113547,-0.3139896533
H,0,0.6332304771,-6.1377939347,-0.2350938118
H,0,3.7922093967,-3.2447156454,-0.6279048472
C,0,2.3031603731,-4.8048155765,-0.5090070456
H,0,2.9250853219,-5.5541263672,-0.989442923
H,0,0.0735058906,-2.146286192,1.213507928
C,0,2.5815177487,-1.1874223857,0.4885537848
O,0,3.7821182186,-1.0054785517,0.339878463
C,0,1.6738022326,-0.0672003968,0.8784689947
H,0,0.623936582,-0.1929198251,0.6321050519
C,0,3.0963764316,0.4789828207,3.0590360096
C,0,3.53515788,1.7311041241,3.8160464966
H,0,3.9440981234,0.061383724,2.506429572
H,0,2.7756170253,-0.2887866235,3.7759765409
C,0,4.6622297839,1.451439661,4.8016584833
H,0,2.6741382379,2.1551816595,4.3494018231
H,0,3.8533784606,2.4935681406,3.0938605513
H,0,4.962752521,2.3601301195,5.3318346152
H,0,4.3581778654,0.712792582,5.5515168675
H,0,5.545765771,1.0567992097,4.2884657777
O,0,1.6624264023,3.3119484139,-0.4658576708

4b (SSS), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -693.443646497 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.223075 a.u.

O; 1
C,0,-2.3965709782,2.5887539716,-0.14114469
C,0,-1.7957266275,1.3229854069,0.3169299174
C,0,-1.5684667188,0.2396088815,-0.7107982666
H,0,-2.1083802344,2.8998393342,-1.1661740176
H,0,-2.0323691673,1.0087853012,1.3270230922
H,0,-1.8323713024,0.506431806,-1.7311709224
C,0,2.2052286906,-0.0206952369,-1.0788713032
C,0,3.4846683926,-0.3587624744,-1.5075119437
C,0,1.9139735465,0.0218380563,0.2861675582
H,0,3.7049979424,-0.4023368227,-2.5671740574
C,0,4.4781215415,-0.6403963828,-0.5749618417
C,0,2.9121211839,-0.2744115202,1.2179018091
H,0,5.4763789987,-0.8968196879,-0.9096823281
H,0,2.6685663211,-0.2442015467,2.2732154642
C,0,4.1919572475,-0.5958646177,0.7887307253
H,0,4.9673033313,-0.8135170135,1.5133958857
H,0,1.4324992846,0.1865586721,-1.8103543485
C,0,0.5412844047,0.3399459847,0.7867655638
O,0,0.2010661673,0.0386700404,1.9110113659
C,0,-0.3949969107,1.013327609,-0.1686181946
H,0,0.06051136,1.723181967,-0.849233337
C,0,-1.8421707676,-1.1994042334,-0.3416167054
C,0,-3.321799908,-1.5478458251,-0.5018245008
H,0,-1.5303187814,-1.3828702064,0.6905330344
H,0,-1.2378591485,-1.8530366306,-0.9810422487
C,0,-3.6104598941,-3.00474442,-0.1501453397
H,0,-3.6297684587,-1.3469579808,-1.5333877494
H,0,-3.9145689245,-0.8847120613,0.1366010097
H,0,-4.667637533,-3.2426860025,-0.280776641
H,0,-3.0317469288,-3.6798996296,-0.7859776099
H,0,-3.3439582674,-3.2139699982,0.8889703953
O,0,-3.1556598614,3.2612072597,0.5114992248

Int-2c cis, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -938.837615005 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.281660 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -939.1992322 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -939.2078202 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -939.7378583 a.u.

1; 1
C,0,-4.2663370897,-2.3522331049,0.4728293746
C,0,-5.2544446219,-1.4728973698,0.0229200262
C,0,-4.9193887074,-0.2138880002,-0.4719657067
C,0,-3.5818475493,0.1538701685,-0.5115501626
C,0,-2.9395323694,1.4116355174,-1.0170471343
C,0,-2.9220770573,-1.9967200394,0.4404874395
C,0,-2.6121409043,-0.7376726561,-0.0602728983
N,0,-1.3295119138,-0.1492207601,-0.1981091073
C,0,-1.481984544,1.2770432127,-0.5329820325
C,0,-1.1618154311,2.1214802904,0.7053323185
C,0,-0.1828899542,-0.762536299,-0.0308033862
C,0,1.0954053191,-0.1839985607,-0.1513251494
C,0,2.1934587834,-0.9804757999,0.0125282442
O,0,-0.6523170861,1.6893765169,1.7098939421
H,0,-4.547828217,-3.3242856112,0.8639142859
H,0,-6.2963662916,-1.7732945032,0.0647223472
H,0,-5.6894513566,0.467399181,-0.8195558465
H,0,-2.1654083393,-2.6796589188,0.8113307441
H,0,-0.7696153982,1.5475372933,-1.3173300062
H,0,-0.2515711813,-1.8209673744,0.2050770395
H,0,1.1946520511,0.8756568547,-0.3547145899
H,0,2.0175224582,-2.0327199509,0.2354075103
C,0,3.5782259307,-0.5947013516,-0.0682919969
C,0,4.5545243706,-1.5832826974,0.1605319607
C,0,3.9960375422,0.7187585283,-0.3626517852
C,0,5.9045797077,-1.2720977721,0.0997811113
C,0,5.344540664,1.0246363924,-0.4226961335
C,0,6.3006398359,0.0317994382,-0.1917927875
H,0,4.2395559426,-2.5977565004,0.3890057055
H,0,3.2651123691,1.4996281854,-0.5460373382
H,0,6.6481517837,-2.0416627212,0.2792148904
H,0,5.6595425775,2.0379497505,-0.6497848367
H,0,7.3568048554,0.2785707282,-0.2400683133
H,0,-3.4016812969,2.3215835033,-0.6303040254
H,0,-2.9773295643,1.4597462051,-2.1099300547
O,0,-1.4884660398,3.3861341083,0.483608913
C,0,-1.198898374,4.3004006671,1.5542647432
H,0,-0.129008483,4.2995032994,1.7700020036
H,0,-1.5193685598,5.2768804053,1.1973266144
H,0,-1.7525905811,4.0161326949,2.450528197

Int-2c cis, optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -939.738508358 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.279383 a.u.
Thermal correction to Gibbs Free Energy at 20 °C = 0.280572 a.u.

1; 1
C,0,-4.2975157945,-2.3737904044,0.4533958395
C,0,-5.2832691493,-1.4733275062,0.0461491477
C,0,-4.9439194846,-0.2095124984,-0.4295434254
C,0,-3.603632181,0.1403745287,-0.4938554786
C,0,-2.9606499674,1.4069434412,-0.9916078233
C,0,-2.9504977336,-2.0347039978,0.3964255539
C,0,-2.6399989959,-0.7713758206,-0.0852835499
N,0,-1.344882912,-0.1898117971,-0.232987749
C,0,-1.4862892539,1.2438529273,-0.5572991164
C,0,-1.1488618248,2.0673489575,0.688259726
C,0,-0.2069506133,-0.7975510143,-0.0539888684
C,0,1.0709732728,-0.1954405799,-0.1615624756
C,0,2.1685511064,-0.975217537,0.0212739448
O,0,-0.8311493981,1.5996412733,1.7459643346
H,0,-4.5822858697,-3.3486242152,0.8282139352
H,0,-6.3254653971,-1.7612884276,0.105732414
H,0,-5.7105707143,0.4881005982,-0.7442462931
H,0,-2.1948331001,-2.7331549194,0.7322720087
H,0,-0.794377709,1.513554389,-1.3550363913
H,0,-0.2650670294,-1.8543514418,0.1883814933
H,0,1.1557410095,0.8618458461,-0.3756118893
H,0,2.0059633456,-2.0277429387,0.2458004407
C,0,3.555041684,-0.5626859121,-0.0480249698
C,0,4.5447712159,-1.530955227,0.1812889069
C,0,3.9429624341,0.7568552723,-0.3367432147
C,0,5.8890162118,-1.1924113172,0.1248420004
C,0,5.2845577925,1.0912506607,-0.3916586751
C,0,6.2591148626,0.1181146343,-0.1612327641
H,0,4.2501653996,-2.5503088724,0.405440017
H,0,3.1982258064,1.5218573664,-0.5192946756
H,0,6.6457716734,-1.9461933367,0.3022760277
H,0,5.5782043246,2.1094188481,-0.61463721
H,0,7.3080855331,0.3857852648,-0.205486585
H,0,-3.4018210147,2.3073811484,-0.5655643038
H,0,-3.0305691487,1.4784327584,-2.0782441393
O,0,-1.2545100717,3.356156005,0.4136381562
C,0,-0.9822110354,4.259178233,1.5026444625
H,0,0.0318856606,4.1028634743,1.8671533221
H,0,-1.0961406076,5.2553406479,1.0874307676
H,0,-1.696677327,4.0898024889,2.3068210987

Int-2c trans, optimization in solv. CHCl₃
PBE1PBE/6-311G(d,p), E = -938.833971281 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.281631 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -939.1953881 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -939.2039635 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -939.7330439 a.u.

1; 1
N,0,-1.326080471,-0.5592850248,0.422519674
C,0,-1.8835175807,0.6952203046,0.0621945326
C,0,-3.2157557231,0.7347987131,0.48093155
C,0,-3.5906310487,-0.5505741845,1.1565158262
C,0,-2.4267536111,-1.4776645044,0.7782964464
C,0,-2.6851059914,-2.4129235021,-0.409086716
O,0,-1.8632030319,-2.6441387826,-1.2627702617
C,0,-3.9842165724,1.8621245756,0.2349958102
C,0,-3.4074215409,2.9334877754,-0.4451229546
C,0,-2.0876902248,2.8645845956,-0.8930625613
C,0,-1.3040276261,1.7396784582,-0.6537152043
H,0,-4.5471220376,-0.9522338779,0.8190892833
H,0,-3.641434529,-0.4272207643,2.2431988562
H,0,-2.1151240505,-2.1054130188,1.6179209242
H,0,-5.0197593347,1.9032203288,0.5577170008
H,0,-3.9969433975,3.8215849189,-0.6485477706
H,0,-1.6649485605,3.6916676432,-1.4536844677
H,0,-0.3039356434,1.6830921708,-1.0622834471
C,0,-0.0783206675,-0.9680518209,0.4567917921
H,0,0.0388004914,-2.0228514209,0.6893129662
C,0,1.091521065,-0.2033066658,0.2757239933
H,0,1.0303361623,0.8691427577,0.1499743985
C,0,2.2983469379,-0.8436288552,0.3150042648
H,0,2.2856260093,-1.9250527716,0.4510627727
C,0,3.6060175225,-0.254865879,0.1871474569
C,0,4.7256532739,-1.106323859,0.2533396651
C,0,3.8119938773,1.1268272451,-0.0007200563
C,0,6.0100621802,-0.5966261266,0.1349422071
H,0,4.5745888362,-2.1725330261,0.3982560138
C,0,5.0956047611,1.6309314465,-0.1178632831
H,0,2.9675987636,1.806563368,-0.0547093568
C,0,6.195935849,0.7718607572,-0.0511736949
H,0,6.865572826,-1.2620351503,0.1866199495
H,0,5.247115948,2.6956899221,-0.2624923958
H,0,7.2000677133,1.1739606132,-0.1449842857
O,0,-3.884120635,-2.9650252889,-0.3189138479
C,0,-4.2033607845,-3.9280260733,-1.3373062544
H,0,-5.1962647458,-4.2965402775,-1.0886252276
H,0,-4.2035504675,-3.4488774682,-2.3176929199
H,0,-3.4745738713,-4.7401615309,-1.3272845581

Int-2c trans, optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -939.734042863 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.280996 a.u.

1; 1
N,0,-1.2904855378,-0.6344210314,0.4137656214
C,0,-1.842463709,0.6312886678,0.0424753585
C,0,-3.1523879107,0.701231755,0.511961801
C,0,-3.5190692524,-0.5691163588,1.2339994588
C,0,-2.4103387981,-1.5320471234,0.7741756185
C,0,-2.7678961477,-2.3700649562,-0.4593479659
O,0,-2.0506724072,-2.4848798634,-1.4146640673
C,0,-3.9118218282,1.8318962704,0.2618605471
C,0,-3.3457419282,2.8683692356,-0.4779508247
C,0,-2.0500257852,2.7612884659,-0.9808231444
C,0,-1.2751878605,1.6317128597,-0.7361544547
H,0,-4.5073281684,-0.9425106461,0.9730084073
H,0,-3.4730905335,-0.4326258375,2.3163819967
H,0,-2.0932763692,-2.2162698257,1.5616759922
H,0,-4.9307872223,1.9010512574,0.6230571613
H,0,-3.9275016887,3.7570933056,-0.6888582351
H,0,-1.6416745654,3.5580536135,-1.5893624446
H,0,-0.2974099926,1.5366140777,-1.18530509
C,0,-0.0490484856,-1.029552989,0.4659506225
H,0,0.0854061033,-2.0806537229,0.7062764253
C,0,1.1123878159,-0.2361825677,0.2922899839
H,0,1.0259147217,0.8346832691,0.1867213195
C,0,2.3200868617,-0.8575084708,0.3284511295
H,0,2.3276453328,-1.9382390273,0.4580809265
C,0,3.622919533,-0.2362558543,0.2064249394
C,0,4.7586071865,-1.0546421769,0.3056513044
C,0,3.7895684247,1.1429560226,-0.0061121206
C,0,6.0309141894,-0.5109406457,0.2004620904
H,0,4.634406582,-2.1199911113,0.4670161921
C,0,5.0599754034,1.6815694943,-0.1116204733
H,0,2.9292676581,1.7958593259,-0.0913859819
C,0,6.1814907098,0.8565022842,-0.0084389461
H,0,6.9015744859,-1.1499404541,0.2775636434
H,0,5.1836659769,2.7446194583,-0.2766386753
H,0,7.1733500247,1.284117877,-0.0939743514
O,0,-3.9320606002,-2.9709939033,-0.2924103465
C,0,-4.3503563936,-3.845544738,-1.358262378
H,0,-5.3022679046,-4.2567382531,-1.037980512
H,0,-4.4629508434,-3.2746484114,-2.278667194
H,0,-3.6123590776,-4.6340642715,-1.4977753338

TS-3c up (SR), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1799.81445218 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.460187 a.u.
1 imaginary frequency = 224.9715 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1800.3783538 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1800.405948 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1801.3189975 a.u.

1; 1
C,0,4.6342368296,3.8459330886,-2.8758724298
C,0,4.340094872,4.1209910731,-4.2116853275
C,0,3.634174871,3.2005066382,-4.9883923918
C,0,3.2243953455,2.0100342633,-4.4080402036
C,0,2.4337513779,0.8665904452,-4.9797220056
C,0,4.233066687,2.6513569982,-2.2803436378
C,0,3.5212314361,1.7568095535,-3.0700735271
N,0,3.0121054651,0.493965559,-2.7021962804
C,0,2.5761563336,-0.2296153648,-3.8964666162
C,0,3.5850241223,-1.3119020114,-4.2794997685
C,0,2.9180500916,0.0381664884,-1.4544965102
C,0,2.5140070801,-1.225143809,-1.0679224854
C,0,2.4530621036,-1.5447587827,0.3002414238
O,0,4.5689582018,-1.6075297866,-3.6426744009
H,0,5.1964761116,4.5657501544,-2.2894572866
H,0,4.6702729988,5.0558966752,-4.6530940108
H,0,3.4101900659,3.412744748,-6.029510709
H,0,4.4969675044,2.4284005973,-1.2511740124
H,0,1.6199007974,-0.7247275424,-3.6995122528
H,0,3.2067308727,0.7511850894,-0.686880205
H,0,2.3080331647,-1.982900535,-1.8155727946
H,0,2.4141342358,-0.7069312838,0.9884662793
C,0,4.1013464775,-1.454644993,3.9676502329
C,0,3.7185867303,-1.2541401933,5.2898755988
C,0,4.3349939445,-0.3596833724,3.126010716
H,0,3.545832007,-2.1089320187,5.936697426
C,0,3.563545163,0.0392088468,5.7840893963
C,0,4.1838218967,0.9358893342,3.6349577058
H,0,3.2654703341,0.1931867063,6.8169615652
H,0,4.3798189761,1.7733294988,2.9732610979
C,0,3.7971078661,1.1347214394,4.9537782865
H,0,3.6795978042,2.1434998404,5.3380197612
H,0,4.2263889796,-2.4696164901,3.6044263508
C,0,4.761032429,-0.4966264588,1.7037019802
O,0,5.1237999383,0.5091152509,1.058256015
C,0,4.6704588587,-1.7665681304,1.0462910746
H,0,4.6565414582,-2.7238337548,1.5543552516
S,0,5.5245027605,-1.7129360472,-0.481134021
C,0,7.2776890986,-1.5619175293,-0.0652895703
H,0,7.3882687053,-0.5796804039,0.3949007623
H,0,7.5779148755,-2.354483142,0.6208175635
H,0,7.8459082647,-1.6069175762,-0.9963065456
C,0,5.4333193,-3.4214592955,-1.0280198886
H,0,4.3784958346,-3.6672143936,-1.1488681652
H,0,5.931696423,-3.4800532605,-1.9960818793
H,0,5.8981464154,-4.0877456138,-0.2993431495
C,0,1.8630576159,-2.7822181036,0.814492878
C,0,1.7036348667,-3.9338434087,0.0265660987
C,0,1.4113516508,-2.8128454587,2.1436534768
C,0,1.1206394413,-5.0776453116,0.5548625233
C,0,0.8240316663,-3.9567743121,2.669580184
C,0,0.680345922,-5.0940142616,1.878056557
H,0,2.0270720976,-3.9417694191,-1.0101846183
H,0,1.5182558358,-1.9269526648,2.7631209429
H,0,1.0040165019,-5.959310414,-0.0678058072

TS-3c up (SR), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1801.32585916 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.464826 a.u.
1 imaginary frequency = 253.4894 i cm⁻¹

1; 1
C,0,3.7545934866,4.1676237847,-3.3292125146
C,0,3.6140936795,4.223453286,-4.7147956393
C,0,3.2466555732,3.0877844314,-5.4372909297
C,0,3.0301098569,1.9022008115,-4.7551698331
C,0,2.5896205697,0.5551190877,-5.268719323
C,0,3.5375205596,2.981493664,-2.6322541862
C,0,3.1829384764,1.8647168919,-3.3742927372
N,0,2.913489903,0.5554321896,-2.9015222537
C,0,2.7367768988,-0.3689883137,-4.0373784682
C,0,3.9949801344,-1.2334474331,-4.1609657457
C,0,2.8713011322,0.1836103902,-1.6316716412
C,0,2.5372796039,-1.0768868409,-1.1540911649
C,0,2.5819742222,-1.2898771831,0.2227521753
O,0,5.0783329502,-0.7770247449,-4.4038084238
H,0,4.0398124128,5.0572435046,-2.7809100194
H,0,3.7921175606,5.156755767,-5.2343308668
H,0,3.1324421687,3.1317633409,-6.514036863
H,0,3.6588035454,2.9482384922,-1.5568115663
H,0,1.8624719285,-0.9962905779,-3.8705845336
H,0,3.0852809568,0.9722351104,-0.9160675643
H,0,2.282549851,-1.8755202129,-1.8393430322
H,0,2.8108282455,-0.4252872099,0.840687317
C,0,5.5069003055,0.7519686176,1.0281503812
C,0,5.8164729242,2.1039358042,1.1335567607
C,0,5.6744307076,0.0853037613,-0.1891955141
H,0,5.6853109814,2.6140709874,2.0802413053
C,0,6.2999198007,2.7975218923,0.0267161959
C,0,6.1439754545,0.7920372487,-1.3014204222
H,0,6.5459526594,3.8494595229,0.1130801424
H,0,6.2447730802,0.2689075621,-2.2463222307
C,0,6.4613399413,2.1403358057,-1.1907466307
H,0,6.8226705438,2.6812201883,-2.0574361818
H,0,5.1342435289,0.2284860447,1.9010755544
C,0,5.3273472013,-1.3569238239,-0.3874288744
O,0,5.4074649287,-1.8526992794,-1.5201328009
C,0,4.757233228,-2.0977587076,0.6858540925
H,0,4.9258309708,-1.8909570332,1.7347071717
S,0,4.6229279438,-3.8115047996,0.2817819896
C,0,6.329253151,-4.375670589,0.0339938487
H,0,6.6837593503,-3.88344803,-0.8683413874
H,0,6.9257960721,-4.0970439401,0.9007983378
H,0,6.2965311624,-5.4564580942,-0.1006164278
C,0,4.2863794947,-4.549422189,1.8934960175
H,0,3.2977596775,-4.22721869,2.2133742896
H,0,4.3020543524,-5.629258707,1.7575944327
H,0,5.0528592625,-4.2355460926,2.6002760024
C,0,1.8511601332,-2.3592350409,0.9164397455
C,0,1.3834013956,-3.5037522632,0.2586127304
C,0,1.5978387741,-2.2123369546,2.2869378955
C,0,0.6941744392,-4.4839522063,0.963943513
C,0,0.8967499348,-3.1852642127,2.9862568329
C,0,0.4492687311,-4.3285122603,2.3262932483
H,0,1.5580147279,-3.6367656632,-0.8025692669
H,0,1.9560666177,-1.326105848,2.8008580554
H,0,0.3406719798,-5.3679137506,0.4470655231

H,0,0.4745849015,-3.9595246603,3.6974111612
H,0,0.2224683009,-5.9892531219,2.2874950101
H,0,1.3810976233,1.140525992,-5.1054803696
H,0,2.8009498952,0.5209622645,-5.9479221907
O,0,3.2026245027,-1.9025165843,-5.4070676514
C,0,4.0541880702,-2.9554380127,-5.8794516174
H,0,4.1070301925,-3.758592999,-5.141565387
H,0,3.5965591128,-3.3119529936,-6.8000984059
H,0,5.0578945932,-2.5723099696,-6.0723205367

H,0,0.701004164,-3.0548835165,4.0435762028
H,0,-0.093045748,-5.0926598993,2.8698477598
H,0,1.550200726,0.586006065,-5.5999766967
H,0,3.2040697681,0.2089977107,-6.0996916377
O,0,3.7191446598,-2.522371905,-4.0172908736
C,0,4.837805181,-3.4157599548,-4.159036972
H,0,5.583620643,-3.1764185112,-3.4035879785
H,0,4.4324581254,-4.4132355802,-4.0143525264
H,0,5.2621483084,-3.3156429039,-5.1578167932

TS-3c up (SS), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1799.81107646 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.462587 a.u.
1 imaginary frequency = 157.3857 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1800.3789316 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1800.4065465 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1801.3196106 a.u.

1; 1
C,0,5.0905016266,1.8298591696,-0.9652877562
C,0,6.1396019791,0.9365292204,-0.7483984265
C,0,5.8851884203,-0.4220910105,-0.5559777966
C,0,4.5734483326,-0.8694022271,-0.5819494162
C,0,4.0228909963,-2.2604063476,-0.446845079
C,0,3.7676593512,1.3930479282,-0.9929552889
C,0,3.5364439591,0.0370350499,-0.7963894771
N,0,2.3023519975,-0.6451413763,-0.782031382
C,0,2.4977856886,-2.0279703429,-0.3343123806
C,0,2.0426313255,-2.1524629641,1.1194158602
C,0,1.1101163075,-0.1222590515,-1.0510992104
C,0,-0.0962402282,-0.8036814055,-1.0812216754
C,0,-1.2702924098,-0.1042265037,-1.365978787
O,0,2.1762701995,-1.279463395,1.9423659908
H,0,5.3020120247,2.8845131553,-1.1101908342
H,0,7.16129176,1.3017652619,-0.7268792344
H,0,6.7015315033,-1.1181997498,-0.3886429245
H,0,2.9616141388,2.1011840071,-1.1527764782
H,0,1.9318496398,-2.7167194062,-0.9636681416
H,0,1.1213109841,0.9323201125,-1.3142649477
H,0,-0.129525831,-1.8652971099,-0.8646851831
H,0,-1.1633288694,0.9582606843,-1.5762727392
C,0,-4.6495533345,-0.9792642542,0.8402029529
C,0,-5.8165024629,-1.7330035739,0.7881253583
C,0,-3.4524006845,-1.5581719229,1.2768214009
H,0,-6.7391188514,-1.2745995236,0.4450979104
C,0,-5.8033075731,-3.0718300885,1.1732425392
C,0,-3.4511672872,-2.9027917109,1.6666301114
H,0,-6.7167715553,-3.6579902808,1.1324471253
H,0,-2.5168806582,-3.3365195186,2.0081619912
C,0,-4.6165923758,-3.6558905983,1.6140816503
H,0,-4.602972897,-4.6985240706,1.9178777505
H,0,-4.6819220011,0.0595974602,0.5294783011
C,0,-2.1623207512,-0.814860457,1.3650775826
O,0,-1.1448062942,-1.3737417771,1.8286806231
C,0,-2.0649547443,0.5242878679,0.887534005
H,0,-2.9003793878,1.1906518076,0.7081471883
S,0,-0.5854805848,1.2799952312,1.4247967745
C,0,-0.8790460481,3.0071635319,1.0090144235
H,0,-0.880004002,3.0980480232,-0.0782819459
H,0,-1.8296923665,3.3481768139,1.4225071393
H,0,-0.0530185196,3.5909395831,1.4175897465
C,0,-0.6272942358,1.3430279651,3.233033162
H,0,-0.6159063212,0.3027119105,3.5577751372
H,0,0.2774576786,1.85389519,3.5682680535
H,0,-1.5272154753,1.8572429901,3.5719373081
C,0,-2.5011064472,-0.6909383359,-1.8774922689
C,0,-2.7122558241,-2.0777070616,-1.9413240559
C,0,-3.4926836003,0.1651221994,-2.3855679705
C,0,-3.8773378317,-2.586648193,-2.4982212304
C,0,-4.6562176261,-0.3456711908,-2.9427026119
C,0,-4.8511421616,-1.7250404205,-3.0004763162
H,0,-1.9625414044,-2.763852667,-1.5615916846
H,0,-3.3389743572,1.2407004898,-2.3423717693
H,0,-4.0269896579,-3.6608432082,-2.5425393724

TS-3c up (SS), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1801.32461071 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.461960 a.u.
1 imaginary frequency = 228.4226 i cm⁻¹

1; 1
C,0,5.1070720856,1.7439715189,-1.1345885245
C,0,6.1212137294,0.8716072083,-0.7445455936
C,0,5.8314514174,-0.4558132681,-0.4277724474
C,0,4.5189241224,-0.8901126299,-0.5027569239
C,0,3.9351437835,-2.2608814917,-0.2709903957
C,0,3.7825059216,1.3186754448,-1.213154139
C,0,3.5181261573,-0.0027393406,-0.8856602316
N,0,2.2673171437,-0.6705728587,-0.8800695702
C,0,2.4116625511,-1.9859201494,-0.2453183821
C,0,1.9302020923,-1.8870484223,1.2038665595
C,0,1.0993756225,-0.1453435124,-1.2196876937
C,0,-0.1134093183,-0.8178254753,-1.263512837
C,0,-1.2795920531,-0.0945114415,-1.4963594426
O,0,1.9159345092,-0.8658224332,1.8384959157
H,0,5.3466607171,2.7714502401,-1.3797507659
H,0,7.1422220105,1.2277589923,-0.6885576104
H,0,6.6201240548,-1.1367694325,-0.1301867195
H,0,3.0045393099,2.0062041883,-1.5192766899
H,0,1.8450529561,-2.7476239251,-0.7771184132
H,0,1.1330959794,0.8977369857,-1.5206044639
H,0,-0.1562147499,-1.8777659249,-1.0512440293
H,0,-1.1653717159,0.9705785496,-1.6895260693
C,0,-4.5549038312,-1.0129870679,0.7238206117
C,0,-5.7335377594,-1.7369278958,0.5945471228
C,0,-3.3612358346,-1.6617425003,1.0489665798
H,0,-6.651283474,-1.2257889976,0.3288721065
C,0,-5.7346660874,-3.1137277996,0.7976420517
C,0,-3.3728231908,-3.0430517151,1.2639113364
H,0,-6.6551242662,-3.6763054115,0.6937157042
H,0,-2.4416333925,-3.5358692845,1.5159189096
C,0,-4.5516995004,-3.7655998576,1.1392724017
H,0,-4.5499131777,-4.836592133,1.303815132
H,0,-4.5790836202,0.0560246286,0.5545999395
C,0,-2.0421757655,-0.9558898137,1.1416628082
O,0,-1.0203956171,-1.5886921942,1.4588850011
C,0,-1.9561452194,0.4173668558,0.7785186693
H,0,-2.7981555523,1.0912140827,0.7091349926
S,0,-0.4458955956,1.1708791915,1.260725931
C,0,-0.8988941353,2.9142265541,1.1576186695
H,0,-1.1213761074,3.1333145096,0.1145372731
H,0,-1.7647107284,3.1073078491,1.788987638
H,0,-0.0386035031,3.494823096,1.484863699
C,0,-0.3006358033,0.9627302444,3.0539459146
H,0,-0.1525255999,-0.1020903495,3.2134799956
H,0,0.5823473639,1.5187625511,3.3667294572
H,0,-1.2077311435,1.3311804037,3.5292382557
C,0,-2.550021805,-0.6640549656,-1.9457208343
C,0,-2.7774510436,-2.045344632,-1.9889444613
C,0,-3.5724144775,0.2047903935,-2.3489800074
C,0,-4.0017141006,-2.5407502369,-2.4165815015
C,0,-4.7932188186,-0.2916094771,-2.7827365466
C,0,-5.0107729144,-1.6672981516,-2.8126863848
H,0,-2.0041876998,-2.7385248734,-1.6796756107
H,0,-3.4031355101,1.2764790932,-2.3146711241
H,0,-4.1711164825,-3.6105271163,-2.4352360945

H,0,-5.4095647718,0.3291759272,-3.3372730152
H,0,-5.7590563364,-2.1279213595,-3.4389949721
H,0,4.2519892647,-2.8636253745,-1.3313460086
H,0,4.4168867612,-2.7928086827,0.42266735
O,0,1.5508646767,-3.3647205077,1.3430062522
C,0,1.1215914476,-3.6199640995,2.6901841518
H,0,0.2562470918,-2.9938971481,2.9130863707
H,0,0.8568896669,-4.6758085117,2.716013709
H,0,1.9311699473,-3.4105621529,3.3918704611

H,0,-5.5749289565,0.3902954604,-3.0949798342
H,0,-5.9656498519,-2.0576514667,-3.1447271604
H,0,4.1855791227,-2.9323995948,-1.0944187902
H,0,4.2762856745,-2.7220047382,0.6563527704
O,0,1.6268204141,-3.0875747008,1.6667329987
C,0,1.2127711328,-3.1490436575,3.0421602999
H,0,0.2741691274,-2.6079798965,3.1503173104
H,0,1.0790863808,-4.2048803755,3.2586107075
H,0,1.9829365429,-2.7194099126,3.6819250498

TS-3c up (RS), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1799.81086915 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.462050 a.u.
1 imaginary frequency = 187.8699 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1800.3767009 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1800.4042496 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1801.3175159 a.u.

1; 1
C,0,3.3348940878,3.4427099964,-2.8779337144
C,0,2.5163875572,3.4284826823,-4.0063067294
C,0,1.578844832,2.4102163502,-4.191922371
C,0,1.4608794803,1.425575888,-3.2245692367
C,0,0.5704647354,0.2150718982,-3.1639799335
C,0,3.2263232681,2.4589369018,-1.8960050259
C,0,2.2631829489,1.4740220298,-2.0816918807
N,0,1.9769501371,0.3578263892,-1.2648374497
C,0,1.2578530129,-0.6341441325,-2.0719891255
C,0,2.232482971,-1.6466132569,-2.671417912
C,0,2.1801516348,0.2015826514,0.0431533334
C,0,2.5153246456,1.1854617426,0.9619620901
C,0,2.6432084328,0.8707861799,2.3148971823
O,0,3.4302339393,-1.6321588416,-2.5271053401
H,0,4.0827346915,4.2214488834,-2.7658188955
H,0,2.6227945849,4.2044573883,-4.7577287624
H,0,0.9602862901,2.3851083983,-5.0839814506
H,0,3.9050138405,2.4364725085,-1.0517477989
H,0,0.5352306729,-1.1732757834,-1.4553151419
H,0,1.9768063179,-0.803495956,0.4063645612
H,0,2.6243117112,2.2088420782,0.625892041
H,0,2.4196861511,-0.1511534124,2.6120203187
C,0,4.3002178323,-2.6126249145,2.9183348534
C,0,3.9118996939,-3.9459136054,2.9917150441
C,0,4.5282629188,-2.0086718209,1.6751599137
H,0,3.7417624138,-4.4059396796,3.960494357
C,0,3.7456999818,-4.6907483592,1.8254397147
C,0,4.3605412292,-2.7649100068,0.5084568588
H,0,3.4444299036,-5.7324876549,1.8851670111
H,0,4.5339457321,-2.2836903402,-0.4488097185
C,0,3.9703206289,-4.0968803716,0.5847432955
H,0,3.8437708114,-4.6752473433,-0.3261173712
H,0,4.432241413,-2.0533206582,3.8395466082
C,0,4.9386895132,-0.5815534847,1.5157329615
O,0,5.1728196217,-0.1175541344,0.3811904805
C,0,4.9375048206,0.281967857,2.6433425623
H,0,4.9871774531,-0.0376068288,3.6776620347
S,0,5.6839681561,1.8328226342,2.3032684384
C,0,5.9813975634,2.4675563018,3.9627019557
H,0,6.5700992751,1.7502686359,4.5373128271
H,0,6.518860823,3.4113525869,3.8600739197
H,0,5.0138179355,2.6447836188,4.4332677378
C,0,7.3790229043,1.4806304888,1.7753005908
H,0,7.886883787,2.4363496207,1.6323710482
H,0,7.8821951196,0.8706866232,2.5262492043
H,0,7.2887547715,0.9462014541,0.8299660694
C,0,2.5502593035,1.8600212375,3.3926019082
C,0,2.600990757,3.2441975668,3.1611611654
C,0,2.385301658,1.4068427409,4.712123246
C,0,2.5016643442,4.1410761765,4.2194656342
C,0,2.2835551779,2.303706405,5.766731547
C,0,2.3454431337,3.6762716647,5.5238377195
H,0,2.7142375876,3.6301495717,2.1533736405
H,0,2.3395015722,0.3375161203,4.9029635138
H,0,2.5411618768,5.2082145004,4.0236154848

TS-3c up (RS), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1801.31974785 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.464051 a.u.
1 imaginary frequency = 234.6322 i cm⁻¹

1; 1
C,0,3.4570024336,3.242274791,-2.8042150938
C,0,2.6453626016,3.2422629908,-3.9363461634
C,0,1.6742482493,2.255238427,-4.1177403547
C,0,1.5151930771,1.2910527141,-3.1379684143
C,0,0.5913430894,0.097917685,-3.0726642035
C,0,3.3066723753,2.2771961898,-1.8092092539
C,0,2.3064996394,1.3335890824,-1.9913368785
N,0,1.9786165074,0.2311986061,-1.159375599
C,0,1.2616009027,-0.7618829092,-1.9711476655
C,0,2.2448414445,-1.7431100164,-2.6033462169
C,0,2.1296362551,0.1229526928,0.1546357441
C,0,2.4567275767,1.1436151554,1.0388658142
C,0,2.6390479771,0.8465713537,2.385466923
O,0,3.4353106987,-1.6003039869,-2.6400891754
H,0,4.2310582651,3.9927314815,-2.6996909164
H,0,2.7852068912,4.0019428566,-4.6956170352
H,0,1.0655241961,2.2381494539,-5.0141344278
H,0,3.9755797063,2.2328789071,-0.9592570487
H,0,0.5416059802,-1.3089792399,-1.3654141207
H,0,1.9058928033,-0.8643097458,0.5550330666
H,0,2.5644139057,2.1534934956,0.6700612464
H,0,2.4272681071,-0.1712436151,2.7021299401
C,0,4.0616144502,-2.466940415,2.6569797632
C,0,3.5977203221,-3.7774801701,2.6350663008
C,0,4.478483045,-1.8474489962,1.4748345193
H,0,3.276063962,-4.250665832,3.5550205547
C,0,3.5444934841,-4.4789769657,1.4330803335
C,0,4.4232413258,-2.5574240999,0.2726784214
H,0,3.1826288231,-5.5002794161,1.4184895058
H,0,4.7351858209,-2.0615535591,-0.6379920012
C,0,3.9582375935,-3.8666606469,0.2525014115
H,0,3.922294979,-4.4116246824,-0.6835366235
H,0,4.0877242982,-1.936692046,3.602258862
C,0,4.9222007759,-0.4175502605,1.4095025721
O,0,5.1191092703,0.1166097018,0.3083535001
C,0,4.9295774852,0.355402346,2.6013816294
H,0,5.0590721548,-0.0484925378,3.5964292835
S,0,5.6071342577,1.9647498744,2.3606186571
C,0,5.9177711139,2.4791091858,4.0637257337
H,0,6.5536839632,1.7398449588,4.5484108093
H,0,6.4091654701,3.4495122992,4.0215225872
H,0,4.9577555883,2.5677214635,4.5688037649
C,0,7.3100864505,1.6909417718,1.798967842
H,0,7.7937922091,2.6654105498,1.7409934398
H,0,7.813356147,1.0327065935,2.5045917875
H,0,7.2315266111,1.2366380598,0.8143848842
C,0,2.5857347026,1.8520447363,3.4593783711
C,0,2.6295258328,3.2284466042,3.205268811
C,0,2.4862981803,1.4114508902,4.7860272144
C,0,2.5932317842,4.1379629471,4.2568520664
C,0,2.4431068835,2.3203435657,5.8338227501
C,0,2.5032144753,3.6885760313,5.571233439
H,0,2.6894655724,3.6002010646,2.189714125
H,0,2.4465861544,0.345763596,4.9889914181
H,0,2.6288068901,5.2003016468,4.0480576413

H,0,2.1532187049,1.9345938144,6.7793436793
H,0,2.2657820329,4.3795508672,6.3470185628
H,0,-0.4445149932,0.4841623264,-2.850820087
H,0,0.4968944134,-0.3258329264,-4.1090791588
O,0,1.5562120156,-2.5521868068,-3.3742943172
C,0,2.3505016502,-3.5701028383,-3.9984628161
H,0,1.6469068746,-4.2050540007,-4.53347727
H,0,3.0669419046,-3.1219546629,-4.6893833384
H,0,2.8888404202,-4.1461072094,-3.2426990195

H,0,2.3627539844,1.9648544438,6.8538414245
H,0,2.4716038844,4.3998427362,6.3876256812
H,0,-0.4124592343,0.3931048118,-2.7585131537
H,0,0.5122802096,-0.4414287984,-4.0159292416
O,0,1.5813006117,-2.7597754718,-3.1451635326
C,0,2.3782581947,-3.7191783414,-3.8588862267
H,0,1.6791352187,-4.4612556878,-4.2320270872
H,0,2.8983591519,-3.229644565,-4.6813835699
H,0,3.1034552192,-4.1750057557,-3.1860908355

TS-3c up (RR), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1799.80762369 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.463203 a.u.
1 imaginary frequency = 215.4505 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1800.3743352 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1800.4019158 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1801.3144422 a.u.
1; 1
C,0,-3.0509852117,-3.1310522413,0.8033777831
C,0,-4.3183848389,-3.2089050093,0.2294658958
C,0,-4.7107462053,-2.2910739295,-0.7468215396
C,0,-3.8137365682,-1.313994126,-1.1460151762
C,0,-3.9672298729,-0.2120905806,-2.1569163506
C,0,-2.1379345965,-2.1527468059,0.4108921375
C,0,-2.5350360528,-1.2645078999,-0.582550306
N,0,-1.8240366722,-0.1783049512,-1.1419788574
C,0,-2.7803928662,0.7116068492,-1.8095184513
C,0,-3.2071246855,1.8409544702,-0.8736373495
C,0,-0.5088264572,0.0361913056,-1.2137213689
C,0,0.5173258263,-0.8298387452,-0.874919519
C,0,1.8443389847,-0.4482364397,-1.1066123787
O,0,-2.901202689,1.9434136464,0.2888220496
H,0,-2.7683584838,-3.8318273122,1.5826405355
H,0,-5.0116096475,-3.9778356999,0.5553853544
H,0,-5.7049799218,-2.3368095908,-1.1811316332
H,0,-1.1800810708,-2.0692319576,0.9085047917
H,0,-2.3292274492,1.1524376246,-2.701067147
H,0,-0.2436347872,0.9968058552,-1.6478084527
H,0,0.3053439104,-1.8178522141,-0.4871200393
H,0,1.9842992826,0.4601742985,-1.6897883079
C,0,1.2673623382,-0.8004860428,2.8152205027
C,0,0.5559803453,-1.5734339266,3.7271755714
C,0,0.6510210428,0.2818131319,2.1730919073
H,0,1.0434449945,-2.4064243956,4.2248622779
C,0,-0.775453556,-1.2718296601,4.0096560864
C,0,-0.6889621181,0.5719971432,2.4571690223
H,0,-1.327220333,-1.8732626707,4.7262768563
H,0,-1.1628444352,1.3953472763,1.9336793127
C,0,-1.3962093141,-0.1993752234,3.3714257889
H,0,-2.4360783541,0.0317674139,3.5816396678
H,0,2.307467759,-1.0432916156,2.6216978513
C,0,1.3510459847,1.1611382984,1.1947885063
O,0,0.7745033233,2.1569432641,0.7164394385
C,0,2.652699979,0.8039848498,0.7290877004
H,0,3.3290650412,0.143553115,1.2594218361
S,0,3.4348725565,2.1432224007,-0.0965998453
C,0,5.1406554024,1.5711751022,-0.1651516519
H,0,5.7324599757,2.3451828771,-0.654976714
H,0,5.5126632437,1.3805277235,0.8430734315
H,0,5.1596730971,0.6565189671,-0.7594241057
C,0,3.5749587294,3.4920393022,1.1027562259
H,0,4.1239648315,4.3065328478,0.6261036372
H,0,2.5530939096,3.7990850001,1.3250938467
H,0,4.0856329784,3.1390576962,1.999699699
C,0,2.9316845279,-1.429156053,-1.1854273226
C,0,2.9694379107,-2.5683727513,-0.3676105081
C,0,3.948586804,-1.2448243571,-2.1343407466
C,0,3.9991589625,-3.4913676951,-0.4943656805
C,0,4.973455639,-2.1762409682,-2.2658118147
C,0,5.0032898572,-3.2999103852,-1.4434975395
H,0,2.2004286127,-2.7204711746,0.3845176294
H,0,3.9172526093,-0.3784925257,-2.7912880986
H,0,4.0206095854,-4.365172828,0.1497784

TS-3c up (RR), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1801.31560492 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.461668 a.u.
1 imaginary frequency = 259.7990 i cm⁻¹
1; 1
C,0,-2.8914884997,-3.0503396116,1.0294360825
C,0,-4.1817732559,-3.1967262999,0.5272623523
C,0,-4.6529121326,-2.3477302947,-0.4758001016
C,0,-3.809276099,-1.3704556176,-0.9723510674
C,0,-4.0528527587,-0.3247696618,-2.0322261943
C,0,-2.0314036946,-2.0706121297,0.5358105263
C,0,-2.5088425595,-1.2560531165,-0.4807180431
N,0,-1.8623552042,-0.169278745,-1.1297417781
C,0,-2.8851929907,0.6588448557,-1.7870949187
C,0,-3.322102026,1.7933751543,-0.8638475408
C,0,-0.5639454544,0.0627741521,-1.2811757344
C,0,0.4892527305,-0.7745042278,-0.9410208538
C,0,1.7921494987,-0.3616670874,-1.2129312989
O,0,-3.0169883444,1.9013092881,0.2912127913
H,0,-2.5484006364,-3.6935725437,1.8309249267
H,0,-4.8317280288,-3.9635382392,0.9302839693
H,0,-5.6638825662,-2.4453907589,-0.853315336
H,0,-1.0538737202,-1.9309341427,0.9766723023
H,0,-2.4953049432,1.0821906423,-2.7116190075
H,0,-0.3341801051,1.0032374445,-1.7768362468
H,0,0.3062103061,-1.7434964846,-0.5027002419
H,0,1.8924144807,0.5330281463,-1.8175023092
C,0,1.0903224157,-0.8056374514,2.536119047
C,0,0.3416592213,-1.6046428209,3.3958442496
C,0,0.5353585099,0.358875667,1.9939723726
H,0,0.7831714469,-2.4991196584,3.8187805346
C,0,-0.9641874367,-1.2476046761,3.7227190157
C,0,-0.7838382141,0.6969097649,2.3111003224
H,0,-1.5429085927,-1.8680344817,4.3971807074
H,0,-1.2163370191,1.582065182,1.8640917411
C,0,-1.5275571231,-0.0988904884,3.1729427592
H,0,-2.5503524457,0.1720151613,3.4074160914
H,0,2.1105681883,-1.0958252223,2.3168406967
C,0,1.2841796996,1.2913948233,1.0856560187
O,0,0.7379239471,2.3250799353,0.6866259274
C,0,2.575739344,0.8860538847,0.6150643139
H,0,3.1344384172,0.0927193129,1.0869468529
S,0,3.6934352322,2.101580271,0.0382990952
C,0,3.6100548304,3.4665673014,1.2322609901
H,0,4.277606486,4.2491545931,0.8744601406
H,0,2.5800705979,3.8086778374,1.3026737098
H,0,3.9657798827,3.069416211,2.1806073773
C,0,2.9518870659,2.9289696924,-1.3948980382
H,0,3.5211095955,3.8467816141,-1.5384336181
H,0,3.0835143648,2.2898342359,-2.2645544913
H,0,1.9061034138,3.1357201183,-1.1823649769
C,0,2.9363794614,-1.2839577993,-1.2342897407
C,0,2.9499325929,-2.4620976539,-0.4771947997
C,0,4.0432361621,-0.9772238553,-2.0333362148
C,0,4.0481024962,-3.3096172542,-0.5208986993
C,0,5.1377751661,-1.8315557248,-2.0834447787
C,0,5.1435873953,-2.9980290916,-1.3245321773
H,0,2.1075756841,-2.7142399637,0.1578525931
H,0,4.0400372204,-0.0729670546,-2.633911739
H,0,4.0510463316,-4.2163558697,0.0718593031

H,0,5.7458683832,-2.0265845336,-3.0140306608
H,0,5.8045078501,-4.0258700313,-1.5417997831
H,0,-3.8638896786,-0.5949837718,-3.1783543136
H,0,-4.9217553576,0.3137993862,-2.0933242098
O,0,-3.9822968657,2.694781984,-1.53874514
C,0,-4.4811129217,3.8012491609,-0.774914541
H,0,-5.0760530559,4.3925610956,-1.4684027939
H,0,-5.0981020526,3.4437083593,0.0518000762
H,0,-3.6524491588,4.3913606674,-0.3788494724

H,0,5.9842161916,-1.5875483918,-2.7137877696
H,0,5.9978568625,-3.6632383782,-1.3583574214
H,0,-3.9758818857,-0.7574518023,-3.0322416789
H,0,-5.0215063244,0.1657537164,-1.9441463467
O,0,-4.1126301077,2.6310375369,-1.5256157512
C,0,-4.6405473758,3.7300675843,-0.7640024842
H,0,-5.2546084697,4.297337894,-1.456517311
H,0,-5.2392533902,3.3535367944,0.0644783005
H,0,-3.8241168344,4.3409077838,-0.3808743026

TS-4c up (RRR), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1799.82105881 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.461618 a.u.
1 imaginary frequency = 365.1420 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1800.3840397 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1800.4115467 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1801.3261164 a.u.

1; 1
C,0,5.2563543638,-1.525120986,-2.5122357019
C,0,6.332856821,-1.2915635195,-1.6566635191
C,0,6.1167468693,-1.012851712,-0.3062503259
C,0,4.8159737379,-0.9718426027,0.1708643602
C,0,4.3006101598,-0.7399506782,1.56317735
C,0,3.9437591925,-1.4845268152,-2.046248424
C,0,3.750470665,-1.2058939494,-0.6985356853
N,0,2.5355586502,-1.1114618453,0.0077922672
C,0,2.7760662871,-0.5824373862,1.3488573347
C,0,2.3625746858,0.8869442559,1.3977516809
C,0,1.3193318233,-1.3865884535,-0.4708271635
C,0,0.1312177033,-1.2685309676,0.213142587
C,0,-1.1697617531,-1.6455626593,-0.4370128419
O,0,2.1837098675,1.5828927725,0.4278866283
H,0,5.4379114924,-1.7353527512,-3.5614955361
H,0,7.3457256468,-1.3236632508,-2.0449178466
H,0,6.9542091953,-0.8316524816,0.3607367875
H,0,3.1167634544,-1.6535831217,-2.727614202
H,0,2.2041816231,-1.1436515587,2.0919007439
H,0,1.3045645798,-1.7533514972,-1.4943391953
H,0,0.1012977936,-0.9210048271,1.2388005674
H,0,-0.9736638509,-2.1844397146,-1.3677400488
C,0,-0.4588010636,2.6736033462,-1.1193286403
C,0,-0.2547760674,4.0243493147,-1.3774230945
C,0,-1.3240580297,2.2778869923,-0.090795569
H,0,0.4273687414,4.3244454018,-2.1663938535
C,0,-0.9153020683,4.9889342312,-0.6202579524
C,0,-1.9679880125,3.2570835215,0.6809117571
H,0,-0.7580672484,6.0427266341,-0.8297449348
H,0,-2.6222275933,2.9367460397,1.4855497114
C,0,-1.7714246687,4.6041573094,0.4120226961
H,0,-2.2820668151,5.355939255,1.005720814
H,0,0.0951527713,1.9402654815,-1.6948102652
C,0,-1.5896091772,0.8589540112,0.2618300012
O,0,-2.0791729984,0.5552616216,1.3408090469
C,0,-1.3163849069,-0.2010118022,-0.7658735389
H,0,-0.8148110703,0.1044038535,-1.6772713274
S,0,-3.4665460332,-0.0125120544,-1.8542649641
C,0,-4.6740990765,0.1493012338,-0.5254340651
H,0,-4.3620418196,0.8990676504,0.204821392
H,0,-5.6391373046,0.4177376747,-0.9610216018
H,0,-4.7478548123,-0.8249217236,-0.040474922
C,0,-3.5697066758,1.6130426737,-2.6325893878
H,0,-2.8036299648,1.6551197796,-3.4087841043
H,0,-4.5543496607,1.7191719548,-3.0935516097
H,0,-3.4029453253,2.4104719363,-1.9066045244
C,0,-2.2179090962,-2.4089943264,0.3377480762
C,0,-2.3046491245,-2.416344064,1.730977223
C,0,-3.1275578405,-3.1773382156,-0.3968027955
C,0,-3.2905101896,-3.1604757198,2.3714739375
C,0,-4.1216654133,-3.9140679349,0.2426544108
C,0,-4.2057197442,-3.9062326736,1.6317778569
H,0,-1.6134600432,-1.8301776224,2.325143694
H,0,-3.0539518553,-3.2054902343,-1.4815475624
H,0,-3.3441320502,-3.1555089652,3.4560738976

TS-4c up (RRR), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1801.33008124 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.463702 a.u.
1 imaginary frequency = -468.0005 i cm⁻¹

1; 1
C,0,5.3836710727,-1.5465635431,-2.5294075652
C,0,6.4221656365,-1.1067590481,-1.7111007446
C,0,6.1752779737,-0.7522584066,-0.3847748424
C,0,4.8822121971,-0.8400240567,0.1030221162
C,0,4.3541856631,-0.5627225597,1.4877258268
C,0,4.0783569402,-1.6377736789,-2.0505411333
C,0,3.8555651178,-1.2725704163,-0.7306963992
N,0,2.6333936073,-1.2713469029,-0.0205770854
C,0,2.8190036983,-0.7231947892,1.3247399
C,0,2.1216460678,0.6317455647,1.4180361992
C,0,1.4278923929,-1.5627107468,-0.5153332758
C,0,0.2541038014,-1.4857483625,0.1923976639
C,0,-1.0745930142,-1.7386243971,-0.4618273509
O,0,1.8774961619,1.3344080696,0.4736079481
H,0,5.5890787117,-1.8221349312,-3.5565541411
H,0,7.427782202,-1.042088603,-2.1072504564
H,0,6.9822584319,-0.4158392096,0.2556489732
H,0,3.2819419995,-1.9844258135,-2.6964797086
H,0,2.3989881749,-1.395946199,2.0733505649
H,0,1.4119690194,-1.8675697268,-1.5578586642
H,0,0.2460947309,-1.1960753695,1.2340044098
H,0,-0.9428115195,-2.2628278307,-1.408576535
C,0,-0.415258456,2.6261918126,-1.2138685518
C,0,-0.41585079,3.9649794181,-1.5841197471
C,0,-1.1581226407,2.2101837358,-0.1062198852
H,0,0.1716913556,4.287046013,-2.4350510758
C,0,-1.1646960458,4.8903739306,-0.8613261063
C,0,-1.8800926212,3.148445853,0.637900646
H,0,-1.1722358485,5.9314544266,-1.1617091954
H,0,-2.43360714,2.8187686817,1.5100680918
C,0,-1.8928100439,4.4831188787,0.2541628991
H,0,-2.4667577413,5.2041140184,0.8231149445
H,0,0.1983048313,1.926184584,-1.7671071021
C,0,-1.2398010915,0.7874034088,0.328901327
O,0,-1.5046735646,0.4882878115,1.4734270218
C,0,-1.0815195301,-0.2748728966,-0.7334683189
H,0,-0.6015579102,0.019695732,-1.6586673593
S,0,-3.282972146,0.1125713025,-1.6464124928
C,0,-4.3134296779,0.3834190758,-0.1830565758
H,0,-3.9574625768,1.2530921159,0.3699619943
H,0,-5.3415381078,0.537715399,-0.5094420665
H,0,-4.248736034,-0.511262266,0.436222444
C,0,-3.4043759971,1.7363280909,-2.4408662997
H,0,-2.6464819384,1.7787976921,-3.2216095117
H,0,-4.3956333833,1.8231472588,-2.8855882961
H,0,-3.2386384782,2.531518954,-1.7147715444
C,0,-2.20394453,-2.3809302014,0.3075584271
C,0,-2.3009486181,-2.3727915602,1.6982098821
C,0,-3.2097699839,-3.000199364,-0.4388959194
C,0,-3.4016144668,-2.947464721,2.3264377462
C,0,-4.3136002038,-3.5685214375,0.1882675301
C,0,-4.4147313759,-3.5364481174,1.5753811806
H,0,-1.5328728797,-1.9046799753,2.2989116322
H,0,-3.1299473336,-3.0365560305,-1.5204646873
H,0,-3.4673155999,-2.9317841176,3.4077189584

H,0,-4.8189958811,-4.5027566806,-0.3458310958
H,0,-4.9738920656,-4.4844001192,2.1364317068
H,0,4.5062869794,-1.5996731902,2.2090919442
H,0,4.7330670222,0.1402345976,2.0452436343
O,0,2.2608301112,1.2861148562,2.6617444514
C,0,1.9293110989,2.6700405101,2.8481440705
H,0,1.8924687169,2.8197851214,3.9254642962
H,0,2.6931112326,3.3065775258,2.3973479262
H,0,0.9603620142,2.8896735475,2.3950014477

H,0,-5.0865286714,-4.0417553384,-0.405316512
H,0,-5.2712143126,-3.979521514,2.0691507757
H,0,4.7378285796,-1.2848423268,2.2095446866
H,0,4.6178206421,0.4348901799,1.8429390994
O,0,1.8567633677,0.9332192804,2.6805058208
C,0,1.2568541653,2.2222802251,2.9083251727
H,0,1.1453564802,2.3043494603,3.9851539459
H,0,1.909066195,3.0056831032,2.524347646
H,0,0.2863490547,2.2674153815,2.4143996754

TS-4c up (RSR), optimization in solv. CHCl₃
PBE1PBE/6-311G(d,p), E = -1799.82742583 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.462816 a.u.
1 imaginary frequency = 369.3231 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1800.3883721 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1800.4157983 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1801.3294179 a.u.

1; 1
C,0,0.4654085678,3.9890526426,0.13247263
C,0,0.0427724458,4.4264596249,-1.1226020347
C,0,0.1771159512,3.6047559147,-2.2434755366
C,0,0.7340778393,2.3451692889,-2.089132027
C,0,0.9702128937,1.2538732146,-3.0962063002
C,0,1.029801847,2.7258539437,0.3017484153
C,0,1.144271932,1.9221466807,-0.8257597211
N,0,1.6638620703,0.6140907551,-0.9091122667
C,0,1.8211328732,0.2272139979,-2.3237936359
C,0,3.3130581131,0.2429775532,-2.6667288385
C,0,1.9067078743,-0.1977140161,0.1271045958
C,0,2.4312975986,-1.4662591218,0.0527034891
C,0,2.5627866075,-2.3463093372,1.274237083
O,0,4.0107525861,-0.7471991708,-2.6463923922
H,0,0.3655232771,4.6429563664,0.993011022
H,0,-0.3872196146,5.4171326715,-1.2299829301
H,0,-0.1488277722,3.9476372639,-3.2209509625
H,0,1.3793075815,2.4044888019,1.2774842618
H,0,1.4736662287,-0.7998365249,-2.4562425344
H,0,1.6453892503,0.2150333808,1.0979599234
H,0,2.7472832066,-1.8833357203,-0.8977334886
H,0,1.9979482658,-1.9406965489,2.1159685716
C,0,6.2116906317,-0.1066489732,0.4352458773
C,0,7.3557510749,0.6264934814,0.138158016
C,0,5.4931362615,0.1624297611,1.6085238171
H,0,7.9103839883,0.4146608728,-0.7707561588
C,0,7.7894342569,1.6288885429,1.0034909171
C,0,5.9263714482,1.1866479259,2.4632093421
H,0,8.6868460787,2.1939028,0.7701952741
H,0,5.3504283886,1.3924848693,3.3599417787
C,0,7.0704664409,1.9119904113,2.1649277595
H,0,7.4053280451,2.6973376496,2.8351438525
H,0,5.8697579721,-0.8544109666,-0.273040559
C,0,4.2689215761,-0.577733391,1.993946457
O,0,3.5180056169,-0.1719238291,2.8741504328
C,0,3.9649980135,-1.886991915,1.3257883175
H,0,4.6453505417,-2.2641517107,0.5713048546
S,0,5.0447461438,-3.2535828124,2.9878653354
C,0,6.4480412366,-2.3544890736,3.6836161162
H,0,6.1494423402,-1.3612951561,4.0243943029
H,0,6.8518981633,-2.9313174672,4.5187099916
H,0,7.2058115253,-2.265425812,2.9039393998
C,0,3.8424817483,-3.0751665749,4.3179085117
H,0,2.972777325,-3.6781268337,4.052252751
H,0,4.2759393956,-3.4579733551,5.2441803606
H,0,3.556255339,-2.0257533591,4.4287929212
C,0,2.2717185807,-3.8089913759,1.0719482012
C,0,3.004174254,-4.5934513133,0.1758430425
C,0,1.22134425,-4.3957909685,1.7820402975
C,0,2.6944766415,-5.9382931268,0.0000750371
C,0,0.9110696042,-5.7418711051,1.6065983847
C,0,1.6480432721,-6.5163577197,0.7154453285
H,0,3.8207436373,-4.1614743455,-0.3974855812
H,0,0.6382672049,-3.791754572,2.4730584465
H,0,3.2726247639,-6.5360540997,-0.6980193663

TS-4c up (RSR), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1801.33162624 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.463119 a.u.
1 imaginary frequency = 473.6090 i cm⁻¹

1; 1
C,0,4.6007547465,-0.8300760182,-2.8135244571
C,0,5.6823886738,-1.3445497878,-2.1026099307
C,0,5.5112086049,-1.8336673488,-0.8063760547
C,0,4.2488380226,-1.8022416726,-0.2405022599
C,0,3.7716917046,-2.2878912528,1.1060911269
C,0,3.3248270566,-0.7896771575,-2.25362996
C,0,3.1793717836,-1.2889739275,-0.9681576752
N,0,1.9978745064,-1.3642294925,-0.1898586608
C,0,2.3412703327,-1.7215424915,1.2021435705
C,0,2.2165736518,-0.4416037052,2.0327978497
C,0,0.749602197,-1.1812463144,-0.6317605868
C,0,-0.3895710843,-1.2682148064,0.1285337042
C,0,-1.7670166194,-1.1069331523,-0.489204629
O,0,1.222095775,-0.1393692668,2.6425830777
H,0,4.7493202557,-0.4443050158,-3.8145585936
H,0,6.6650698449,-1.3591203707,-2.5571743359
H,0,6.352737505,-2.2318380916,-0.2515597583
H,0,2.4943626108,-0.3697218267,-2.8075346254
H,0,1.6183190927,-2.440979919,1.5851777122
H,0,0.6679543783,-0.9529600496,-1.6905298849
H,0,-0.3490820906,-1.4773873315,1.1894788768
H,0,-1.7181048272,-1.1584902841,-1.5765032508
C,0,-0.1996824869,2.6204741702,1.1304724155
C,0,0.2929099633,3.8057623716,1.6672292437
C,0,-0.4075531649,2.5165471105,-0.2482654626
H,0,0.4550421692,3.8842168355,2.7355502394
C,0,0.5792979972,4.8835138183,0.835521841
C,0,-0.0992138536,3.598035623,-1.0822337096
H,0,0.9567855836,5.8070463234,1.2584335344
H,0,-0.2565138663,3.4989276907,-2.1498512508
C,0,0.3873823843,4.777735789,-0.5417780278
H,0,0.6170387508,5.6158768815,-1.1880828793
H,0,-0.3799918946,1.7825173795,1.7933450847
C,0,-0.9553081233,1.2909073666,-0.8850534911
O,0,-0.904275035,1.1035532573,-2.0839836794
C,0,-1.6602367409,0.2816457447,-0.0146345369
H,0,-1.7254376982,0.4646281853,1.0481383955
S,0,-3.8067104701,1.2909966626,-0.3440156816
C,0,-3.5784442159,2.9691925377,-0.9879441763
H,0,-2.8732098813,2.9602742128,-1.8198521589
H,0,-4.5491560782,3.3351688809,-1.3212713937
H,0,-3.2043370447,3.5928461477,-0.1777532166
C,0,-4.1798084987,0.438629464,-1.8925637061
H,0,-4.409212131,-0.5984898899,-1.6520694642
H,0,-5.0498131849,0.9111559736,-2.3468486633
H,0,-3.3181259925,0.5019285864,-2.5595510136
C,0,-2.8370677685,-2.0102005381,0.0634045213
C,0,-3.4951850387,-1.7478229475,1.2641071741
C,0,-3.1664461189,-3.1599500708,-0.6569280453
C,0,-4.4731567559,-2.620768695,1.7341314337
C,0,-4.1414318029,-4.031703176,-0.1874909676
C,0,-4.7983619336,-3.7626618958,1.010455139
H,0,-3.2614372048,-0.8623792219,1.8448891475
H,0,-2.6575309606,-3.367936174,-1.5926356392
H,0,-4.9814339116,-2.4043419075,2.6659922697

H,0,0.0922899067,-6.1832861701,2.1667105628
H,0,1.4085394823,-7.5662834058,0.5773964792
H,0,0.0252205198,0.7990691081,-3.4113413321
H,0,1.4850248465,1.6088557035,-3.9909968004
O,0,3.7416065321,1.4672949442,-2.9429554236
C,0,5.141720255,1.594999982,-3.2259960831
H,0,5.2880206691,2.6335424986,-3.5161839921
H,0,5.7261702782,1.3619397464,-2.3334796329
H,0,5.4268761363,0.9226669844,-4.0369921909

H,0,-4.3911873947,-4.9184289771,-0.7576484475
H,0,-5.5612056058,-4.4390915052,1.376461683
H,0,3.7434419424,-3.3791452991,1.1335304699
H,0,4.3972667053,-1.9392821628,1.9265102173
O,0,3.3065639367,0.3060222758,1.9492945817
C,0,3.2706949147,1.56602224,2.6390067456
H,0,4.2527096576,2.005726569,2.4944214666
H,0,2.4968533068,2.1994952189,2.2073038436
H,0,3.0709884231,1.4025904276,3.6973289095

TS-4c up (SSS), optimization in solv. CHCl₃
PBE1PBE/6-311G(d,p), E = -1799.81625400 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.461493 a.u.
1 imaginary frequency = 382.7294 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1800.3776482 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1800.405105 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1801.3181285 a.u.

1; 1
C,0,2.7615964661,-0.9816690486,-3.283750468
C,0,4.0665274865,-1.467646783,-3.2495368965
C,0,4.6181717285,-1.918759893,-2.0496122359
C,0,3.8440333018,-1.8893925631,-0.9017828133
C,0,4.1920126565,-2.3073438843,0.4976534886
C,0,1.9703467744,-0.9467174957,-2.1361878893
C,0,2.525863417,-1.4222244783,-0.9509991721
N,0,1.9667296031,-1.4800139462,0.3445307666
C,0,3.0408868345,-1.7056080365,1.3204723832
C,0,3.3772485302,-0.3873702653,2.0238067625
C,0,0.7055059937,-1.3140734463,0.7604408209
C,0,-0.4425640815,-1.1637088051,0.0160349186
C,0,-1.7727148277,-0.9562486589,0.6921730645
O,0,2.6461134805,0.5766482209,2.0467149613
H,0,2.3483058013,-0.6105694238,-4.2162059835
H,0,4.6610022012,-1.4830643459,-4.1573370412
H,0,5.6406895684,-2.2823014683,-2.0126885963
H,0,0.9780282478,-0.5202697056,-2.1876611572
H,0,2.6973183342,-2.3969597401,2.0962934772
H,0,0.611006391,-1.317081431,1.8443058542
H,0,-0.4466034095,-1.2379012965,-1.0621348865
H,0,-1.6938151343,-1.2070454645,1.753045925
C,0,0.7304579191,2.4640446504,-0.0261847559
C,0,1.6145579237,3.5249938486,-0.1881481467
C,0,-0.3992949815,2.3641801915,-0.8490387224
H,0,2.4957368276,3.5870427635,0.4427211174
C,0,1.3743292875,4.4958140743,-1.157391537
C,0,-0.6222976667,3.3334288089,-1.8376632833
H,0,2.0629695297,5.3273543704,-1.2745272297
H,0,-1.4939414655,3.234392517,-2.4766450459
C,0,0.254276495,4.398470777,-1.9837398093
H,0,0.0687761491,5.153410901,-2.7414547026
H,0,0.9641619159,1.7047531185,0.7133618198
C,0,-1.3708629731,1.2445185631,-0.7622930215
O,0,-2.1140252558,0.9725905485,-1.6943150401
C,0,-1.465907436,0.4972047304,0.5447121829
H,0,-0.8489820572,0.8892031782,1.3467444052
S,0,-3.2590021118,1.9302506147,1.2969500778
C,0,-3.7267300627,1.1195062693,2.8387967906
H,0,-4.6071266547,1.6180558057,3.249782225
H,0,-3.943731195,0.0631731072,2.6700240046
H,0,-2.8958948769,1.2285372312,3.5378774508
C,0,-4.6405931158,1.4809861661,0.2276986204
H,0,-5.5291936284,2.0300686511,0.5459615575
H,0,-4.3684505957,1.7722638994,-0.7874237
H,0,-4.8176081442,0.4049936071,0.2612679309
C,0,-2.9839964716,-1.6594061884,0.1283789035
C,0,-3.2705643903,-1.7524557884,-1.2370454845
C,0,-3.8329429181,-2.3041611237,1.035063878
C,0,-4.3909746377,-2.4515576401,-1.6745790676
C,0,-4.9576720284,-2.9992174558,0.5975969455
C,0,-5.2413413952,-3.0722950522,-0.7621237827
H,0,-2.6374317355,-1.2564220225,-1.9624568398
H,0,-3.6055760992,-2.2778675391,2.0985982864
H,0,-4.6003767585,-2.5100783239,-2.7385399918

TS-4c up (SSS), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1801.32095218 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.462140 a.u.
1 imaginary frequency = 479.8393 i cm⁻¹

1; 1
C,0,3.51767978,-0.6239378799,-2.8946667806
C,0,3.1340106294,-0.126214315,-4.1359039861
C,0,2.0950855145,0.8000424869,-4.2320075826
C,0,1.4642502098,1.2209001937,-3.075347546
C,0,0.3314524045,2.1995093314,-2.9029298639
C,0,2.8900206103,-0.2080886261,-1.7212516765
C,0,1.8673987654,0.7274249277,-1.8325312744
N,0,1.0272695548,1.2715446428,-0.8252135818
C,0,-0.1340317909,1.9109567315,-1.4633136652
C,0,-1.342145376,0.9738229452,-1.3819777292
C,0,1.1017172034,1.1711458969,0.5037102466
C,0,2.1463492913,0.7072906838,1.269525026
C,0,1.9906764557,0.5610299725,2.7651176819
O,0,-1.3852952186,-0.0185399715,-0.7022455168
H,0,4.3130374652,-1.3562537896,-2.8291445923
H,0,3.6373149986,-0.4669689717,-5.0320901598
H,0,1.7812476796,1.1815148299,-5.1966293416
H,0,3.186313687,-0.6464977156,-0.7808853345
H,0,-0.3989008641,2.824880654,-0.9292963766
H,0,0.2037778249,1.5104293732,1.0166176066
H,0,3.113013284,0.4796043024,0.8477949303
H,0,1.1145175969,1.1100572109,3.1114427295
C,0,0.7717699522,-2.3987988209,-0.0313211581
C,0,0.3387713266,-3.2293294712,-1.0583054096
C,0,1.9071369207,-2.7417433356,0.7091407996
H,0,-0.5328812276,-2.9502277248,-1.6379751953
C,0,1.0248671177,-4.4062455234,-1.3410734663
C,0,2.6001529903,-3.9205886299,0.413585675
H,0,0.6821444994,-5.0538319187,-2.1393993455
H,0,3.4836808233,-4.1695346236,0.9890293387
C,0,2.155559639,-4.7530453606,-0.6024712736
H,0,2.6886151705,-5.6696328382,-0.8232477051
H,0,0.2335456441,-1.4748431741,0.1411995268
C,0,2.4753350507,-1.8607968127,1.7687071351
O,0,3.6189165472,-1.9782273072,2.15083407
C,0,1.5671068737,-0.8160371733,2.3818871564
H,0,0.5144415131,-0.9048794776,2.1438789702
S,0,1.199282627,-2.2522960649,4.2982106235
C,0,0.2414332029,-1.0869316171,5.2925988281
H,0,0.0755747363,-1.5147420261,6.2804501299
H,0,0.7765730839,-0.1427221744,5.3795631551
H,0,-0.7158068879,-0.9388905483,4.7945683639
C,0,2.783114047,-2.2198469649,5.1743221793
H,0,2.6519683953,-2.7055521975,6.1407978055
H,0,3.4946506809,-2.7770447547,4.5681046824
H,0,3.126948834,-1.1940539652,5.298967428
C,0,3.1654240898,0.8858127243,3.654671165
C,0,4.4903340712,0.5879087777,3.3324812047
C,0,2.8974424355,1.5505092652,4.8534523148
C,0,5.5151509731,0.9100180498,4.2150629204
C,0,3.9221907889,1.8707459207,5.7387839057
C,0,5.2353654974,1.5407447339,5.4244817667
H,0,4.7317012957,0.0861548914,2.4054697611
H,0,1.8782453788,1.8335349604,5.0968614985
H,0,6.5384432228,0.6660687446,3.9553543328

H,0,-5.6027303617,-3.4896977974,1.3203243876
H,0,-6.1146012459,-3.6153141276,-1.1106678058
H,0,4.198425832,-3.3981867335,0.5936709287
H,0,5.1619019667,-1.9377996154,0.8342570592
O,0,4.5394948344,-0.4727711159,2.6543343133
C,0,4.9263075321,0.6846101287,3.4108742895
H,0,5.8820931969,0.4310468017,3.864775927
H,0,5.030628421,1.5474417208,2.7506189298
H,0,4.1800420689,0.9002614385,4.1775986523

H,0,3.6931407546,2.3839226209,6.6648979051
H,0,6.0385492209,1.7854031154,6.1089786178
H,0,0.6933597998,3.2268233096,-2.980459075
H,0,-0.4726739553,2.0644545608,-3.6240190741
O,0,-2.3403314964,1.4316078603,-2.1183279901
C,0,-3.5605821782,0.6697977864,-2.0815167444
H,0,-4.2558893257,1.2048417918,-2.7205188289
H,0,-3.3796001631,-0.3345869336,-2.4617872787
H,0,-3.933604516,0.6182323019,-1.0596575591

TS-4c up (SRS), optimization in solv. CHCl₃
PBE1PBE/6-311G(d,p), E = -1799.82289626 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.460492 a.u.
1 imaginary frequency = 376.7209 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1800.3844116 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1800.4117133 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1801.3245758 a.u.

1; 1
C,0,-0.2730443506,3.6177336058,-1.6470511046
C,0,0.1108788029,3.8041880406,-2.9728530447
C,0,1.0647436263,2.9665264674,-3.553754886
C,0,1.6094721518,1.9426005966,-2.7976130643
C,0,2.6395315542,0.9153441557,-3.1712046817
C,0,0.2673286062,2.5903214366,-0.8741359693
C,0,1.1995291364,1.7478553487,-1.4734721739
N,0,1.9114258003,0.6614876191,-0.9237419478
C,0,3.0432129376,0.3423978593,-1.8015796009
C,0,4.3235497666,0.950359452,-1.2241009282
C,0,1.7245762597,-0.0235638633,0.2126161242
C,0,0.693546958,0.063843099,1.1167049147
C,0,0.6149683368,-0.8664116505,2.3065592769
O,0,4.4224600452,1.3992420019,-0.1076561605
H,0,-0.9980084411,4.2882189969,-1.196364322
H,0,-0.3238114404,4.6120638928,-3.5526617141
H,0,1.3810354909,3.1176769312,-4.5815008801
H,0,-0.0122028188,2.4981670285,0.166457836
H,0,3.1905935824,-0.7408768308,-1.8438254716
H,0,2.5047707729,-0.7550239384,0.4044786841
H,0,-0.1456551073,0.7318055683,0.9767075276
H,0,1.3112025125,-1.7005148579,2.1992923308
C,0,2.6822411824,2.817533719,3.5831746366
C,0,3.3632511879,3.9869017435,3.9011655321
C,0,3.3861585695,1.6169204811,3.4166086911
H,0,2.8132081304,4.9142156152,4.0251630545
C,0,4.7475814482,3.969219755,4.0558020592
C,0,4.7812889811,1.6130348681,3.5629399431
H,0,5.2753824043,4.8845360101,4.3062183778
H,0,5.3132271031,0.6787168501,3.4177611881
C,0,5.4568535298,2.7803289689,3.884003538
H,0,6.5361434035,2.7685036982,3.998631588
H,0,1.6061823935,2.8616905005,3.4528200967
C,0,2.7393480551,0.3270636159,3.0832601216
O,0,3.3952230629,-0.6808163544,2.8455130633
C,0,1.2389967125,0.2171788955,3.0912692535
H,0,0.639137027,1.0943403292,3.3009618117
S,0,1.0785881553,-0.4754911326,5.3863894315
C,0,1.7176676178,-2.1509923327,5.2128197542
H,0,2.6287737691,-2.1461046384,4.6083325083
H,0,1.9148617234,-2.560745448,6.2056798083
H,0,0.9432764675,-2.7456060346,4.7254460373
C,0,2.4016244019,0.2864913333,6.3508736634
H,0,2.1909045183,1.3545413293,6.4198446937
H,0,2.3964539995,-0.1500011875,7.3522539989
H,0,3.373315121,0.1313576326,5.8784358575
C,0,-0.7625740731,-1.3494502842,2.6715716668
C,0,-1.7616638336,-0.4815878933,3.1225628266
C,0,-1.0611553422,-2.7069141064,2.5261191675
C,0,-3.031668132,-0.9639768236,3.4238452792
C,0,-2.3315322939,-3.1900117749,2.8275501746
C,0,-3.3198534795,-2.3188411121,3.2773764331
H,0,-1.5592696363,0.5799324919,3.2428017555
H,0,-0.2921446311,-3.3886465867,2.1697599512
H,0,-3.7974221766,-0.2790988371,3.7752945721

TS-4c up (SRS), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1801.32179560 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.465259 a.u.
1 imaginary frequency = 508.5735 i cm⁻¹

1; 1
C,0,-2.8695181383,-1.0493457236,2.7541402312
C,0,-4.1714357666,-1.5252349381,2.6304151499
C,0,-4.6508602158,-1.9586897875,1.3932075356
C,0,-3.8089504602,-1.9157723988,0.2967826836
C,0,-4.0698588106,-2.3018309784,-1.1357026345
C,0,-2.0089119889,-1.0067678019,1.6584346764
C,0,-2.5001506662,-1.4535328487,0.4381786092
N,0,-1.8699535581,-1.4350314594,-0.834301501
C,0,-2.9011636873,-1.6474006162,-1.8857105645
C,0,-3.1909435142,-0.2931175561,-2.5386222582
C,0,-0.586831507,-1.2639794685,-1.1509148201
C,0,0.5026247109,-1.2840320267,-0.2980808344
C,0,1.8588894061,-0.8624287309,-0.8184585726
O,0,-2.431498636,0.2013546561,-3.3312058601
H,0,-2.5142130987,-0.694778937,3.7141823513
H,0,-4.8200621997,-1.5479033082,3.4973860325
H,0,-5.6684780692,-2.315921141,1.2889281755
H,0,-1.0156655604,-0.5975473936,1.7678641335
H,0,-2.4834505064,-2.2833533357,-2.6641540263
H,0,-0.422565057,-1.0811546614,-2.2108833713
H,0,0.4072485486,-1.658848969,0.7092341239
H,0,1.8486323453,-0.730895251,-1.9004785598
C,0,-0.4104718378,2.1162000952,1.4636303482
C,0,-1.5010887563,2.5351175397,2.2156568034
C,0,-0.5541837644,1.8987057273,0.0906623915
H,0,-1.3851391948,2.7203506187,3.2765211216
C,0,-2.7444353294,2.6949409243,1.6096584332
C,0,-1.7934938878,2.1032223592,-0.5219908198
H,0,-3.6006118877,2.9897671237,2.2045645055
H,0,-1.8723997298,1.9403159267,-1.5917753715
C,0,-2.8911400232,2.4781998373,0.2416556271
H,0,-3.8614098929,2.6073007471,-0.2232128687
H,0,0.5446887931,1.9732034736,1.9568589814
C,0,0.5379025358,1.3606211644,-0.7679715383
O,0,0.6210496619,1.5925224557,-1.9509847676
C,0,1.4954722667,0.3843710742,-0.1214078166
H,0,1.5894634291,0.3828425522,0.9593755305
S,0,3.4619531945,1.8018389788,-0.3450561157
C,0,2.8639441107,3.4669955102,0.0458340418
H,0,2.2755166667,3.4653847537,0.9628893362
H,0,3.7181008245,4.1350139033,0.1516462919
H,0,2.2491011633,3.7925693577,-0.7923688242
C,0,4.305756364,1.3828624982,1.2005782199
H,0,4.7422067422,0.3916871948,1.073647361
H,0,5.0953846422,2.1112506562,1.3819935101
H,0,3.6031996453,1.3779947866,2.0351160372
C,0,3.1086748129,-1.5411676142,-0.3325228983
C,0,3.1875642414,-2.1487995898,0.9206556678
C,0,4.2545451058,-1.4635163739,-1.1259457068
C,0,4.3982712223,-2.6607095513,1.3774407516
C,0,5.4656560947,-1.9733939396,-0.6681229074
C,0,5.5405537436,-2.5687484314,0.5874875187
H,0,2.3107454131,-2.2324271072,1.5533378322
H,0,4.1988296087,-0.9966471107,-2.1037100451
H,0,4.4484321974,-3.1332664216,2.3510652731

H,0,-2.5476873377,-4.2476633947,2.7108629803
H,0,-4.3109706283,-2.6935587052,3.5141042268
H,0,2.2033597603,0.1308551591,-3.7992198301
H,0,3.4976144304,1.3296152167,-3.7029750726
O,0,5.3144037909,0.8646589011,-2.106134838
C,0,6.5869933255,1.3498611148,-1.656255198
H,0,7.2735109002,1.1850905735,-2.4844825971
H,0,6.522674652,2.4128366326,-1.4162855079
H,0,6.9106704575,0.7976116315,-0.7718941527

H,0,6.3480849744,-1.9076975513,-1.2932083371
H,0,6.482360155,-2.9662959027,0.9461937864
H,0,-4.0255678943,-3.3866027008,-1.2559421541
H,0,-5.0329394148,-1.9511878357,-1.5012925343
O,0,-4.3180568348,0.2652447466,-2.1258562832
C,0,-4.671947392,1.511404102,-2.7513837758
H,0,-5.5850387033,1.8346684778,-2.2606863015
H,0,-3.8766968798,2.2441208579,-2.6177281938
H,0,-4.8403831064,1.3505025526,-3.8155176604

TS-3c down (RS), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1799.81602092 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.460672 a.u.
1 imaginary frequency = 235.8492 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1800.3820189 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1800.4094206 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1801.3234043 a.u.

1; 1
C,0,2.1297666017,3.428809908,-3.4722159134
C,0,1.944422621,2.904986419,-4.7514294403
C,0,1.6767878438,1.5466965745,-4.9281633145
C,0,1.5989722398,0.7275159114,-3.8125619459
C,0,1.2868641647,-0.7385967894,-3.7083238541
C,0,2.0585418709,2.6157318811,-2.3423909419
C,0,1.7899146131,1.2666254864,-2.541192302
N,0,1.6651721808,0.250955642,-1.5716517452
C,0,1.5788863288,-1.0555141255,-2.2216478011
C,0,2.892616518,-1.8160111344,-2.0526827294
C,0,1.6112746336,0.4330149227,-0.2549473662
C,0,1.5356399246,-0.5596056468,0.7064924747
C,0,1.480462009,-0.2208794047,2.0644096286
O,0,3.9039510149,-1.3595878084,-1.5795873289
H,0,2.3435203669,4.485874759,-3.3490991379
H,0,2.0127195667,3.5578524308,-5.6156683646
H,0,1.5306138274,1.1375088783,-5.9234100445
H,0,2.2205911283,3.0353659486,-1.3550973924
H,0,0.7729855029,-1.6431853243,-1.7728952598
H,0,1.6545168167,1.4704565072,0.063560949
H,0,1.5068877389,-1.6001992387,0.405011774
H,0,1.696228551,0.8135157089,2.3200463381
C,0,-0.0520362992,3.1608881339,2.9576338887
C,0,0.3180823171,4.4952263661,3.0860791389
C,0,-0.4576126422,2.6557523971,1.7154797999
H,0,0.6295258476,4.8776582823,4.0532836847
C,0,0.2876970407,5.3397843363,1.978042965
C,0,-0.4855700145,3.5133796817,0.6083292751
H,0,0.5757272246,6.3816227729,2.081939325
H,0,-0.8050211441,3.1085358728,-0.3467564164
C,0,-0.1153911833,4.8463112485,0.7383287446
H,0,-0.1435770848,5.5026069485,-0.1263812529
H,0,-0.025617834,2.5225944954,3.835631055
C,0,-0.8533052337,1.2342801017,1.490743424
O,0,-1.1768980268,0.8477716574,0.349456047
C,0,-0.7269052678,0.2843931541,2.5445847688
H,0,-0.7183002075,0.534529509,3.5995933106
S,0,-1.4943105514,-1.250886296,2.1592962019
C,0,-1.655387522,-1.997896143,3.7910170743
H,0,-2.19776295,-1.3255256278,4.4581699899
H,0,-2.1987098262,-2.9355956514,3.6648430841
H,0,-0.6535166626,-2.202033726,4.169334717
C,0,-3.2300443026,-0.8835499378,1.8027112968
H,0,-3.7394965116,-1.8351751313,1.6401927176
H,0,-3.6723951927,-0.3358068069,2.6354719671
H,0,-3.2292142335,-0.2854766464,0.892215109
C,0,1.7366041196,-1.1814043774,3.1462901778
C,0,1.7421428384,-2.5704076677,2.9433065322
C,0,1.998336418,-0.6924239616,4.4362980841
C,0,1.9900709561,-3.4384825776,4.0015049475
C,0,2.248925661,-1.5600540977,5.4907184994
C,0,2.2414661643,-2.9382492696,5.2775601962
H,0,1.5543315249,-2.9842061576,1.9577835385
H,0,2.0062524583,0.3812434139,4.6066763379
H,0,1.9922817153,-4.5100829939,3.827167042

TS-3c down (RS), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1801.32672548 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.463507 a.u.
1 imaginary frequency = 279.7204 i cm⁻¹

1; 1
C,0,2.746953462,3.787649556,-2.8981435767
C,0,2.1386952869,3.5314335237,-4.1260477222
C,0,1.4964044808,2.3152264114,-4.3620788017
C,0,1.4685506068,1.3666814996,-3.3527388833
C,0,0.8300040988,0.0007346731,-3.3195146188
C,0,2.725658505,2.8420235637,-1.8757599208
C,0,2.0693469725,1.6471492032,-2.1301659026
N,0,1.8787384549,0.5593741151,-1.2464344566
C,0,1.3068142513,-0.5824327485,-1.9632154228
C,0,2.3500646929,-1.6814887393,-2.1270610802
C,0,1.9692983811,0.621846393,0.074848418
C,0,1.7920626847,-0.4360645038,0.9517706578
C,0,1.6036962828,-0.1519283034,2.307304226
O,0,3.4780318839,-1.6250852564,-1.7198436333
H,0,3.2524747852,4.7316993441,-2.7358332763
H,0,2.1745156817,4.2799864229,-4.9078915022
H,0,1.0283631595,2.1157193457,-5.3191498149
H,0,3.2139963006,3.0380984645,-0.9291500409
H,0,0.4715817193,-0.9771584652,-1.3763872391
H,0,2.1839265027,1.6109385554,0.472212845
H,0,1.705066262,-1.4473020295,0.5766040869
H,0,1.7647362726,0.8807129474,2.6084524631
C,0,-0.1330997439,3.0387064836,2.1827273915
C,0,0.2329342419,4.3602392855,1.9543645435
C,0,-0.5005673586,2.2148815181,1.1140611723
H,0,0.5150580505,4.9919756087,2.7879309164
C,0,0.2389523307,4.8698387355,0.6580621977
C,0,-0.4950443748,2.7365773617,-0.183351318
H,0,0.5291579688,5.8990658738,0.4826682133
H,0,-0.7680406674,2.0862906953,-1.0067097538
C,0,-0.1258323901,4.0556499637,-0.4113713595
H,0,-0.1106201421,4.4435892614,-1.4233109069
H,0,-0.1274122379,2.6618951137,3.1987109762
C,0,-0.8310651226,0.7647036459,1.2779357085
O,0,-1.0779239242,0.0717968526,0.2803995889
C,0,-0.6632962833,0.1571442246,2.5587866142
H,0,-0.7602064103,0.6844233566,3.4988667498
S,0,-1.2814126769,-1.4999532255,2.5842235588
C,0,-1.4150047683,-1.8228242082,4.3557678512
H,0,-1.9963456896,-1.029007397,4.8227190548
H,0,-1.9133866348,-2.7847869683,4.4633248687
H,0,-0.4107559838,-1.8756131003,4.7699242278
C,0,-3.0425734096,-1.3529494926,2.1733857077
H,0,-3.4823430455,-2.3422870417,2.2937514526
H,0,-3.5021443655,-0.625763621,2.8401988232
H,0,-3.0895906488,-1.0313146399,1.136318309
C,0,1.7813188369,-1.1362592202,3.3876056541
C,0,1.7796632306,-2.5168673327,3.1546834659
C,0,1.9677813408,-0.6692512064,4.6953507372
C,0,1.9446103285,-3.4061300811,4.2109247942
C,0,2.1423959818,-1.5581876248,5.7473400722
C,0,2.1242100846,-2.9313171273,5.5076614478
H,0,1.6506803839,-2.9047754762,2.1514936929
H,0,1.9747728004,0.3998774415,4.881727695
H,0,1.9397385294,-4.4723447559,4.0197997271

H,0,2.453830227,-1.1625078898,6.4799694929
H,0,2.4375374067,-3.618387143,6.1006674773
H,0,0.2352448573,-0.9352230577,-3.9404650237
H,0,1.8891262085,-1.3581331191,-4.3771014986
O,0,2.7526231582,-3.0561529646,-2.5171255981
C,0,3.9308864729,-3.8721973871,-2.4625580523
H,0,3.6412301786,-4.834826126,-2.8797733439
H,0,4.7309273013,-3.4227705658,-3.0539445217
H,0,4.2655570004,-3.9855550143,-1.4295234055

H,0,2.292016037,-1.1824238952,6.7521908587
H,0,2.2570338917,-3.6279862896,6.3263738722
H,0,-0.2588927715,0.0767777068,-3.335070488
H,0,1.1336221634,-0.62884223,-4.1557506268
O,0,1.8262336464,-2.7171216082,-2.773884513
C,0,2.7093092768,-3.8279466396,-3.0013993212
H,0,2.116511273,-4.56989059,-3.5273594532
H,0,3.5568879513,-3.5102645543,-3.6074421425
H,0,3.0655475733,-4.2209367755,-2.0498628653

TS-3c down (RR), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1799.81276045 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.462276 a.u.
1 imaginary frequency = 218.3659 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1800.3803139 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1800.4079118 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1801.3233355 a.u.

1; 1
C,0,1.1149991879,5.0640623841,-1.6673277001
C,0,1.204449752,5.4034993516,-3.0174111512
C,0,1.6364632485,4.4667586274,-3.9577617937
C,0,1.9753176142,3.1931230345,-3.5279215681
C,0,2.4160213661,1.9877039146,-4.3087394201
C,0,1.4566311809,3.7888638311,-1.2211889072
C,0,1.8804633842,2.8714893423,-2.1746473681
N,0,2.2749304348,1.531946283,-1.9785336239
C,0,2.8768392257,1.0090486323,-3.2041372615
C,0,4.3979702881,0.9664788473,-3.0673072165
C,0,2.1208419486,0.8323502583,-0.8589818154
C,0,2.5737123496,-0.4539207463,-0.6201058234
C,0,2.3042757344,-1.0587783553,0.6120191149
O,0,5.0187744476,1.3466407637,-2.1054540299
H,0,0.7865355865,5.8057220033,-0.9461374344
H,0,0.9417296077,6.4064949395,-3.3381086432
H,0,1.7058039584,4.7311704641,-5.0087198006
H,0,1.4081835982,3.544920565,-0.1652431164
H,0,2.5145610574,-0.0062644701,-3.3899748726
H,0,1.5798238113,1.3486979647,-0.0702739433
H,0,3.1574279831,-0.9835299777,-1.3649284152
H,0,1.8809457197,-0.4191959529,1.385113522
C,0,-0.3124316207,-1.2328412078,-2.2485441529
C,0,-0.5254380168,-0.802733834,-3.5541803124
C,0,-0.7325658877,-0.4465894932,-1.1672291651
H,0,-0.2050884618,-1.4230207835,-4.3861608606
C,0,-1.1569038159,0.4170469294,-3.7945656211
C,0,-1.3657765045,0.7766470667,-1.4208980521
H,0,-1.3285330554,0.7475804652,-4.8149557219
H,0,-1.6827933549,1.3736302462,-0.5718569737
C,0,-1.576089387,1.2069627893,-2.7243999395
H,0,-2.0678345224,2.1571742422,-2.908922291
H,0,0.1840844419,-2.1836490734,-2.0835161157
C,0,-0.5222015493,-0.8289403396,0.2586730681
O,0,-0.8697743114,-0.0558852223,1.1737603826
C,0,0.1596249739,-2.0463367644,0.5614199463
H,0,0.2418610008,-2.8790484201,-0.1277018577
S,0,-0.026548481,-2.5109360373,2.2463122475
C,0,0.4267797295,-4.2523846942,2.1922794521
H,0,0.2763383084,-4.660986887,3.1921210588
H,0,-0.196427356,-4.7747477988,1.4644553439
H,0,1.4808289253,-4.3177509052,1.9218095894
C,0,-1.8061757141,-2.6433692076,2.5531640088
H,0,-1.93816725,-3.0028485736,3.5756054384
H,0,-2.2025354348,-1.6337967911,2.4467496933
H,0,-2.2586421074,-3.3235850867,1.830611188
C,0,3.0579529209,-2.2166982058,1.100480099
C,0,3.5278677267,-3.2254050817,0.2442952362
C,0,3.3415166853,-2.3068530172,2.4722141541
C,0,4.2554170976,-4.2939533298,0.7501491473
C,0,4.0807743224,-3.3736873905,2.9743204931
C,0,4.5355798658,-4.3712123845,2.1160972828
H,0,3.3027608704,-3.1839090453,-0.8176019717
H,0,2.9941034525,-1.5248425058,3.141849783
H,0,4.6065811078,-5.0722115421,0.0795285212

TS-3c down (RR), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1801.32782173 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.464426 a.u.
Thermal correction to Gibbs Free Energy at 20 °C = 0.466024 a.u.
1 imaginary frequency = 267.3933 i cm⁻¹

1; 1
C,0,0.9459971831,5.0718509836,-0.0753527352
C,0,0.7737520266,5.6577866666,-1.3284469489
C,0,1.0794196967,4.9496101055,-2.4910659668
C,0,1.5538196372,3.6530243928,-2.3789813964
C,0,1.9018441444,2.6557436598,-3.4540948602
C,0,1.4218686356,3.7685902547,0.0500805202
C,0,1.7112375678,3.083947052,-1.1204869769
N,0,2.1497695565,1.7442482472,-1.2580102876
C,0,2.4816619511,1.4603935604,-2.6560637956
C,0,3.995839239,1.3551586376,-2.8192616466
C,0,2.2154225168,0.8466633282,-0.287146025
C,0,2.6238253545,-0.4719850122,-0.4234296522
C,0,2.5299950651,-1.3269903515,0.6751000208
O,0,4.7992163065,1.6302448168,-1.9720918271
H,0,0.7107003594,5.6364800867,0.8184242678
H,0,0.4041427713,6.6731745224,-1.3991916242
H,0,0.9460290909,5.4047134566,-3.4658177234
H,0,1.5558902367,3.3244795395,1.0288097623
H,0,2.0272344584,0.5147866589,-2.9591234384
H,0,1.8957336186,1.1962569465,0.6907496084
H,0,2.9821579003,-0.8487399498,-1.373480788
H,0,2.3690937051,-0.8666857086,1.6484947611
C,0,-0.4688939525,-0.5881196159,-1.465436857
C,0,-0.7824182188,0.1908258692,-2.5734901451
C,0,-0.6143547101,-0.0663611327,-0.1752972691
H,0,-0.6657809818,-0.2188611088,-3.5706691839
C,0,-1.2416115254,1.4959393355,-2.4041357085
C,0,-1.0790671031,1.243008123,-0.0159339275
H,0,-1.4858812812,2.1020301077,-3.2695368169
H,0,-1.1740493066,1.640473589,0.9875699831
C,0,-1.3928881024,2.0201609944,-1.1231715413
H,0,-1.7379439795,3.0390653731,-0.9897790447
H,0,-0.0916664776,-1.5919805878,-1.6191579685
C,0,-0.2044588466,-0.8117293289,1.0568597397
O,0,-0.2410713598,-0.250859307,2.1624791042
C,0,0.3520838419,-2.1167221273,0.908998748
H,0,0.1585261828,-2.7594243486,0.0611671713
S,0,0.4946530111,-2.9761619645,2.4449396749
C,0,0.6917565481,-4.6810357716,1.881457751
H,0,0.7199125289,-5.3096115773,2.7695732957
H,0,-0.1489978508,-4.9453933308,1.2417166006
H,0,1.6354535068,-4.7515937855,1.3441768719
C,0,-1.1945297468,-3.053564866,3.1040083329
H,0,-1.1684852841,-3.6854432465,3.9908273105
H,0,-1.4647278133,-2.0328366363,3.3640180491
H,0,-1.8551788431,-3.4600271681,2.3405225495
C,0,3.1891282276,-2.6429348175,0.6892790413
C,0,3.239353792,-3.4491868466,-0.4552642096
C,0,3.7737501001,-3.1006717091,1.8746283593
C,0,3.8591951841,-4.689467871,-0.4102749525
C,0,4.4026611412,-4.3418721744,1.9145684039
C,0,4.44297611297,-5.138906705,0.7753445622
H,0,2.7648800511,-3.115038363,-1.3721663734
H,0,3.7456549189,-2.477601069,2.7620946247
H,0,3.8848024362,-5.311533796,-1.2968733887

H,0,4.3018734164,-3.4238498597,4.0359451007
H,0,5.1078849839,-5.2070340445,2.5064939275
H,0,1.5754802643,1.5570500298,-4.8636456634
H,0,3.2151990636,2.1938009518,-5.0237535515
O,0,4.9308244271,0.4412169114,-4.168219427
C,0,6.3629916314,0.3598980594,-4.1826975933
H,0,6.621314718,-0.1032866838,-5.1330963284
H,0,6.7995016076,1.3579623062,-4.1112897048
H,0,6.7159369448,-0.2494363216,-3.3485397403

H,0,4.8596647343,-4.6843491807,2.8350474551
H,0,4.9275423325,-6.1071999812,0.8075491275
H,0,1.010535801,2.3452632825,-4.0037173211
H,0,2.6221478074,3.0440117898,-4.1749940842
O,0,4.2900822713,0.9300010635,-4.0427394904
C,0,5.690925342,0.8328097463,-4.3539176317
H,0,5.7382912069,0.4888418079,-5.3824536305
H,0,6.1617529775,1.8094964937,-4.250016687
H,0,6.1702658583,0.1196809483,-3.6844509727

TS-3c down (SR), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1799.81224567 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.461730 a.u.
1 imaginary frequency = 256.1576 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1800.3771029 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1800.4044733 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1801.3177221 a.u.

1; 1
C,0,5.4388490075,4.4857447985,0.711196283
C,0,5.1416757556,5.7053290329,0.1070443863
C,0,3.912330624,5.896978687,-0.5261649056
C,0,2.9882057894,4.8652097899,-0.5264703
C,0,1.6164065566,4.8031672742,-1.1351221224
C,0,4.5184151742,3.4380045071,0.7171482879
C,0,3.2847533196,3.6561319334,0.1100809602
N,0,2.2029013257,2.765736898,-0.0528234278
C,0,1.2799361395,3.3011702398,-1.0596808441
C,0,1.4483464629,2.5472537239,-2.3784922869
C,0,1.9116611144,1.6322317081,0.5907048969
C,0,2.5277952744,1.1018655237,1.7092606772
C,0,2.0776895331,-0.1128596782,2.2486310293
O,0,2.039413773,1.5007582127,-2.4952854713
H,0,6.4088836023,4.3359691907,1.1748169675
H,0,5.876165731,6.5043213402,0.1134340207
H,0,3.6853364459,6.8381669519,-1.0181662625
H,0,4.7902538673,2.4807871013,1.1433841524
H,0,0.2508471372,3.1396635225,-0.7233112587
H,0,1.0835934307,1.0862322808,0.1491040016
H,0,3.3022935966,1.6630445828,2.2142614917
H,0,1.4333729994,-0.7216301756,1.6196398855
C,0,-1.5419377179,-1.2929677779,1.729963547
C,0,-2.3464274403,-2.0349127215,0.8722235941
C,0,-1.3818287177,0.0851756814,1.5360695946
H,0,-2.4618506626,-3.1027054108,1.030805045
C,0,-3.0047969569,-1.4104693797,-0.185136272
C,0,-2.0521900777,0.7028349409,0.4729404787
H,0,-3.634428377,-1.9920275284,-0.8518081625
H,0,-1.9347696579,1.7741811944,0.3446913964
C,0,-2.8582083494,-0.0384380589,-0.3816002283
H,0,-3.3761998211,0.4527359279,-1.1998464929
H,0,-1.0466295351,-1.8002529244,2.5518294674
C,0,-0.5285510767,0.9483529727,2.4048512769
O,0,-0.3731509458,2.1562920833,2.1299394908
C,0,0.2070548049,0.3715612166,3.4826035276
H,0,-0.0576562789,-0.5658842243,3.959401857
S,0,0.859060069,1.5871971013,4.5772096161
C,0,-0.5459138125,2.5763989435,5.1446331474
H,0,-1.3174367555,1.9262294891,5.5585029929
H,0,-0.1699104779,3.2738610855,5.8954858751
H,0,-0.910466875,3.1129955447,4.269511167
C,0,1.1874005803,0.6133381286,6.0570503412
H,0,1.99113628,-0.0864914528,5.8265550025
H,0,1.515654711,1.3078943399,6.8318729054
H,0,0.2846206954,0.0864507174,6.3709786111
C,0,2.8445427621,-0.873636834,3.2468967861
C,0,3.8961261871,-0.306973487,3.984108498
C,0,2.5310438671,-2.2252328331,3.4589923224
C,0,4.6009585434,-1.0680140735,4.9106521061
C,0,3.2381312035,-2.9850712374,4.3816231287
C,0,4.2738097134,-2.4072819924,5.1144495023
H,0,4.1724493978,0.7325922259,3.8386214496
H,0,1.730152577,-2.6825105532,2.8834866329
H,0,5.4130812883,-0.6150290283,5.4709602674

TS-3c down (SR), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1801.32046896 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.462273 a.u.
1 imaginary frequency = 278.2296 i cm⁻¹

1; 1
C,0,5.3053345996,4.5114249452,0.6335166586
C,0,4.9333519257,5.7221427937,0.0567494232
C,0,3.684160485,5.8612656331,-0.5502621493
C,0,2.8160770051,4.7842080833,-0.5490668855
C,0,1.4317515367,4.6597112064,-1.1331805071
C,0,4.440612576,3.4174586672,0.6387013932
C,0,3.1888090777,3.5857470704,0.0602833113
N,0,2.1485975541,2.6373889405,-0.1037408471
C,0,1.1955743799,3.1339323421,-1.1048591992
C,0,1.4529671701,2.4553932415,-2.4495469694
C,0,1.9113116504,1.5097800632,0.5566332781
C,0,2.556590136,1.0215112455,1.6811475999
C,0,2.1111681212,-0.1761141571,2.248200675
O,0,2.2382521206,1.5647784458,-2.6265847408
H,0,6.2895626514,4.4048847042,1.0731321658
H,0,5.6248987387,6.5554372799,0.0616488998
H,0,3.399973259,6.7945765194,-1.022226511
H,0,4.7679781907,2.4688632596,1.039205336
H,0,0.1790248764,2.884793508,-0.794029186
H,0,1.0914750977,0.9276796649,0.1415717342
H,0,3.3100600415,1.6159464206,2.1734754081
H,0,1.4811703085,-0.8121296532,1.6336663741
C,0,-1.3395125502,-1.11572609,1.4845336843
C,0,-2.128665889,-1.7702877472,0.5458076778
C,0,-1.256940252,0.2797872635,1.4870114068
H,0,-2.1817036282,-2.8521327872,0.5476195067
C,0,-2.8467224487,-1.0375097059,-0.3949699534
C,0,-1.9795488715,1.0075250576,0.5372264825
H,0,-3.4629383837,-1.5495254713,-1.1242643885
H,0,-1.9178023899,2.0892093967,0.5537565536
C,0,-2.7730454472,0.3532401882,-0.3965307607
H,0,-3.3366121873,0.9259840092,-1.123242554
H,0,-0.7864001606,-1.7059327837,2.2061635992
C,0,-0.3917739557,1.0463998981,2.4422304661
O,0,-0.1457017025,2.242390285,2.2269323063
C,0,0.2627870028,0.34340534,3.4917174028
H,0,-0.1020567013,-0.5904013861,3.8999449716
S,0,1.0355719162,1.3943735352,4.6843878808
C,0,-0.276569367,2.4903986326,5.2881693138
H,0,-1.1321269175,1.8896748083,5.5901799794
H,0,0.1369427579,3.0505172169,6.1259821283
H,0,-0.5252532395,3.1527878957,4.463055338
C,0,1.1713243932,0.2640283927,6.0891185311
H,0,1.822139586,-0.5576073545,5.7943960538
H,0,1.620170961,0.8204454662,6.9100464144
H,0,0.1773574591,-0.093858952,6.3538817982
C,0,2.8519829626,-0.8779597839,3.3139547397
C,0,3.8976630357,-0.2710023538,4.0191880192
C,0,2.4823772154,-2.1875323847,3.6482879833
C,0,4.5450407932,-0.9538986236,5.0442439946
C,0,3.1306991895,-2.8691659005,4.6687069622
C,0,4.1613432907,-2.2496949492,5.3750620482
H,0,4.2175014625,0.7348410189,3.7768998223
H,0,1.6769855222,-2.6689839851,3.1022986089
H,0,5.3527036719,-0.472087434,5.5818664001

H,0,2.9853664428,-4.0308598156,4.5266085923
H,0,4.8284447857,-2.9999584257,5.8353059363
H,0,0.8973059956,5.3834672316,-0.5474001918
H,0,1.5803031151,5.1718327872,-2.1616968774
O,0,0.8050683556,3.1757430478,-3.3578723305
C,0,0.8384906776,2.5266691132,-4.636496523
H,0,0.2616722265,3.163718573,-5.3042845544
H,0,1.8681394213,2.4354523099,-4.9872056976
H,0,0.3898123752,1.5337015177,-4.5685803772

H,0,2.8361824499,-3.8822498407,4.9141627471
H,0,4.6675019823,-2.77915086,6.1732190246
H,0,0.697430148,5.1641134098,-0.5016401484
H,0,1.3503927702,5.0629506258,-2.141296133
O,0,0.6610744231,2.9692925462,-3.3827399043
C,0,0.7728198747,2.3903895011,-4.6937623564
H,0,0.053230631,2.921307637,-5.3093061164
H,0,1.783574189,2.5283672972,-5.0752771674
H,0,0.536473902,1.3278367471,-4.6513696252

TS-3c down (SS), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1799.80948202 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.462287 a.u.
1 imaginary frequency = 208.4325 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1800.3757517 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1800.4033423 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1801.3177752 a.u.

1; 1
C,0,2.878212166,3.8962085496,-2.7238547848
C,0,2.3706226101,3.7137341281,-4.0086558831
C,0,1.7680921086,2.5060814513,-4.3639458306
C,0,1.6659570396,1.5018932898,-3.4151528234
C,0,1.082136183,0.1237970368,-3.5340159426
C,0,2.782411592,2.8944545899,-1.7590058644
C,0,2.1499606551,1.7075618308,-2.1190362794
N,0,1.942075603,0.5370146378,-1.3565592454
C,0,1.5981670495,-0.5682086224,-2.2610948533
C,0,2.8242475477,-1.4581860708,-2.4709283491
C,0,2.0032773762,0.3349303289,-0.0416405605
C,0,2.1902998277,1.2568661824,0.9748370496
C,0,2.262418933,0.8096609179,2.2983120797
O,0,3.8060505882,-1.437118337,-1.7682874271
H,0,3.3729675033,4.8275013465,-2.4668322089
H,0,2.4609136989,4.5085030573,-4.7422263956
H,0,1.3927643794,2.3505430377,-5.3709429595
H,0,3.2350772039,3.0384035009,-0.786973203
H,0,0.8222420099,-1.1869571769,-1.7983735073
H,0,1.8749754386,-0.7072119932,0.2385019507
H,0,2.2717203247,2.3139781105,0.7628735663
H,0,2.3382952546,-0.2648761527,2.4539721751
C,0,-1.1812132659,1.1884677565,0.5483695754
C,0,-1.7863580503,1.4355053768,-0.6793519583
C,0,-0.983956093,-0.1264346166,0.9893172007
H,0,-1.9332931491,2.4582848222,-1.0125297961
C,0,-2.2080579243,0.3736973385,-1.4774987341
C,0,-1.4063695969,-1.1870804245,0.1764795198
H,0,-2.6927192018,0.5691128651,-2.4297731378
H,0,-1.2509371409,-2.1992795258,0.5361724738
C,0,-2.0171028609,-0.940139618,-1.0469303293
H,0,-2.3526307028,-1.7692490274,-1.6629836056
H,0,-0.8588787435,2.0291322345,1.1537925226
C,0,-0.3455202719,-0.4746049693,2.2922982056
O,0,-0.1314760608,-1.6685969321,2.5831556515
C,0,0.0647621221,0.5706037811,3.1760468655
H,0,-0.3346825071,1.5779106885,3.144534146
S,0,0.3772444718,-0.0423720982,4.7943391662
C,0,0.3388400715,1.4616076838,5.7836093977
H,0,-0.6012254658,1.9922143104,5.6212494804
H,0,0.4369802365,1.1641810785,6.8286788275
H,0,1.1887579321,2.0801431493,5.4955382582
C,0,-1.1579740187,-0.8272996559,5.3484439291
H,0,-1.0120739895,-1.1426449618,6.3833782751
H,0,-1.9865261805,-0.1233001965,5.2612067701
H,0,-1.3036063209,-1.6913864557,4.7007560906
C,0,2.820025383,1.6389787074,3.3696472163
C,0,2.6840682778,3.0368033615,3.3859073707
C,0,3.5429636119,1.0178571387,4.4003426485
C,0,3.2504126454,3.7867420518,4.4075251831
C,0,4.1185372657,1.7739053022,5.4172090707
C,0,3.970760549,3.1582442008,5.4257626878
H,0,2.1123271808,3.5359600835,2.6089696656
H,0,3.6670555833,-0.0615600979,4.3905123096
H,0,3.1311204279,4.8658098283,4.4135774157

TS-3c down (SS), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1801.32167062 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.46290 a.u.
1 imaginary frequency = 256.7842 i cm⁻¹

1; 1
C,0,2.0500009397,3.8658493263,-2.7322589509
C,0,1.5830759403,3.5694510951,-4.0082168036
C,0,1.2602147694,2.2557282941,-4.3476329686
C,0,1.396186728,1.2631178114,-3.3939321786
C,0,1.093555154,-0.2053273628,-3.5172223353
C,0,2.1918456069,2.873450715,-1.7623719245
C,0,1.8406033096,1.5734215746,-2.1076562424
N,0,1.8480743422,0.3888680116,-1.3221517503
C,0,1.6355240752,-0.7792098538,-2.1946942476
C,0,2.9485067518,-1.5474504813,-2.3513820744
C,0,2.0144048229,0.2087231713,-0.0178152469
C,0,2.2746398388,1.1318233809,0.9860369291
C,0,2.2963751479,0.6882960987,2.3071224883
O,0,3.9470080982,-1.3268942033,-1.7223740209
H,0,2.3214249727,4.884017666,-2.4814882712
H,0,1.4828232152,4.3579401053,-4.7436820243
H,0,0.9100519605,2.0117155626,-5.3439822764
H,0,2.5888277068,3.1409128254,-0.7974912599
H,0,0.9184703666,-1.455730842,-1.7233730081
H,0,1.914270872,-0.8314960212,0.2862308894
H,0,2.4294302994,2.1770445583,0.7812335854
H,0,2.3063899246,-0.3869542986,2.4756995285
C,0,-0.8159457879,1.5659841952,0.5342866299
C,0,-1.2024687527,1.9728643204,-0.7372502194
C,0,-0.8630008496,0.2130029292,0.8883778543
H,0,-1.1433545732,3.0195618316,-1.0116258732
C,0,-1.6450784672,1.0331590265,-1.6644182368
C,0,-1.3215880056,-0.7216737788,-0.0440940268
H,0,-1.9369165401,1.3517634475,-2.6589484716
H,0,-1.3519853262,-1.7663357882,0.2420197686
C,0,-1.7161244484,-0.3131392086,-1.3121324186
H,0,-2.0763469008,-1.043904563,-2.027845514
H,0,-0.4492633823,2.3081430853,1.2334193425
C,0,-0.3544697774,-0.3049105651,2.1980312569
O,0,-0.241783091,-1.5274788949,2.3789604993
C,0,0.1073395316,0.6336020016,3.1644427641
H,0,-0.212756275,1.6662435645,3.2049930086
S,0,0.3949527752,-0.0982405593,4.7447793877
C,0,0.403874917,1.3562210817,5.8139641913
H,0,-0.520531194,1.9125698937,5.6654390185
H,0,0.4833397894,0.9982289686,6.8388019303
H,0,1.2729295985,1.9592525014,5.5593936204
C,0,-1.1924523658,-0.8288453635,5.232835549
H,0,-1.0846721977,-1.1751481446,6.2602202687
H,0,-1.971405595,-0.0743396336,5.1408373576
H,0,-1.363576565,-1.6635651242,4.5577187991
C,0,2.8576016117,1.511268452,3.3904236395
C,0,2.7006818464,2.9031814148,3.4119794263
C,0,3.5644048525,0.8872968302,4.4242152649
C,0,3.2379635331,3.6522584717,4.448391316
C,0,4.1093844422,1.642381243,5.4589647003
C,0,3.9449140849,3.0233125886,5.4748382662
H,0,2.130717835,3.3956254647,2.6311279435
H,0,3.6957566761,-0.1893406703,4.4101012896
H,0,3.1038792271,4.727042108,4.4624385216

H,0,4.6834784462,1.2801773291,6.2017521004
H,0,4.4149140031,3.7489662805,6.2209344371
H,0,-0.0131390687,0.1588120521,-3.5240057217
H,0,1.3944588612,-0.4054492713,-4.4355910622
O,0,2.6289765995,-2.2890229767,-3.48920551
C,0,3.6896934712,-3.2231809691,-3.736453254
H,0,3.3592671595,-3.8255415926,-4.5804182968
H,0,4.6112006396,-2.6915896872,-3.9808521171
H,0,3.8544065813,-3.8489209876,-2.8572956418

H,0,4.6610013752,1.1502274399,6.2507962645
H,0,4.3643644671,3.6109920001,6.2823538584
H,0,0.0182679724,-0.3770251592,-3.5977841844
H,0,1.5741562171,-0.664308255,-4.3805213577
O,0,2.8107594476,-2.5137876677,-3.2488043456
C,0,3.9612633638,-3.3512607654,-3.4570679435
H,0,3.6681677754,-4.0627114909,-4.2229205679
H,0,4.8039141071,-2.7474942716,-3.7909442405
H,0,4.217778058,-3.8639270899,-2.530799174

7, optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -592.822978956 a.u.
Thermal correction to Gibbs Free Energy = 0.159504 a.u.
0; 1
C,0,-4.618715515,-1.9469806702,0.7010542702
C,0,-5.5611187139,-1.0273252715,0.2467767526
C,0,-5.1456175169,0.1452377004,-0.3912853188
C,0,-3.791659756,0.3761442608,-0.5572943499
C,0,-3.0490446426,1.5080273451,-1.2259353313
C,0,-3.2512731578,-1.7259562511,0.5314391063
C,0,-2.8538218819,-0.5552596104,-0.1016348631
N,0,-1.5472955164,-0.1413169351,-0.4174080769
C,0,-1.6114616899,1.2926946324,-0.6931121096
C,0,-1.3513885496,2.1054623757,0.5730314206
O,0,-1.0398537555,1.6371661675,1.6372405725
H,0,-4.9498343526,-2.8505072539,1.199979986
H,0,-6.6170747379,-1.21908922,0.3924621405
H,0,-5.8744937518,0.8661110204,-0.7458536708
H,0,-2.521761256,-2.4431654579,0.8893051608
H,0,-0.8604648682,1.5947242009,-1.4258669747
H,0,-3.4327215656,2.500247177,-0.9917062568
H,0,-3.0588538878,1.3842764728,-2.3123391122
O,0,-1.4784111422,3.4120393924,0.3442990771
C,0,-1.22212704,4.2744978728,1.4609064117
H,0,-0.2040855003,4.1285092416,1.8209838423
H,0,-1.3555203124,5.2856321056,1.0877247029
H,0,-1.9274378335,4.0651254505,2.2646592912
H,0,-0.8462059661,-0.3932903956,0.2695843993

2-H⁺, optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -862.018147683 a.u.
Thermal correction to Gibbs Free Energy = 0.168751 a.u.
Charge = 1 Multiplicity = 1
C,0,1.1504507371,-2.4698273165,-7.4675447208
C,0,2.1793135692,-3.3626838191,-7.739524166
C,0,1.3451304273,-1.0993140257,-7.6654974017
H,0,2.0260545668,-4.4235983919,-7.5867881586
C,0,3.4025426955,-2.8912731119,-8.206424912
C,0,2.5770572572,-0.6311327532,-8.1357987734
H,0,4.2036297328,-3.5898752187,-8.4164756885
H,0,2.7135832639,0.43305808,-8.2838549601
C,0,3.6013425255,-1.5255945014,-8.4043196839
H,0,4.5547587135,-1.1625144548,-8.7675936142
H,0,0.2062755717,-2.8578658339,-7.1041123535
C,0,0.2838962234,-0.0981169061,-7.3925562981
O,0,0.43915067,1.0867711057,-7.5712426075
C,0,-1.046336431,-0.640344127,-6.8625322513
H,0,-0.8983984107,-1.1965103709,-5.9340927133
C,0,-1.5208695276,1.7404946123,-5.34852316
H,0,-0.6782816807,2.2178452878,-5.8392908302
H,0,-2.2870757375,2.4583269121,-5.0595826701
H,0,-1.2131454074,1.1616516637,-4.478967789
C,0,-2.5175206848,1.5453216645,-7.9976198661
H,0,-2.7966688262,0.8423641114,-8.7810538925
H,0,-3.3394339109,2.2344089864,-7.811669951
H,0,-1.5922366379,2.0632689084,-8.2293653627
S,0,-2.3236714714,0.5834906406,-6.4794839351
H,0,-1.506643908,-1.3193196119,-7.5846892205

7-H⁺, optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -593.239599247 a.u.
Thermal correction to Gibbs Free Energy = 0.174808 a.u.
1; 1
C,0,-4.7204539026,-1.8975247561,0.9558044256
C,0,-5.6211192383,-0.9895221027,0.3976978526
C,0,-5.1800748866,0.1525662249,-0.2663638062
C,0,-3.813283356,0.3781467117,-0.3657931535
C,0,-3.0520282131,1.4922715941,-1.035739871
C,0,-3.3476030559,-1.6846068818,0.8627830277
C,0,-2.9509196639,-0.5420909436,0.198430901
N,0,-1.551205034,-0.1210965007,-0.0209141654
C,0,-1.6338632957,1.3226892396,-0.4612172182
C,0,-1.3694016965,2.1469563911,0.7977885596
O,0,-0.9613961489,1.6513671833,1.817059455
H,0,-5.0883491706,-2.77543023,1.4710453258
H,0,-6.6842074254,-1.1755197562,0.4869535692
H,0,-5.8874499293,0.852780311,-0.6934775562
H,0,-2.633614481,-2.3759766797,1.2922704258
H,0,-0.8429107491,1.5251478561,-1.1821714776
H,0,-3.4453653641,2.4830335544,-0.8129916235
H,0,-3.044485706,1.3629490874,-2.1196403896
O,0,-1.6193005473,3.4179218662,0.5992902979
C,0,-1.3654397471,4.3003569634,1.7142167356
H,0,-0.3072603771,4.2700166027,1.9681707414
H,0,-1.655339215,5.2873201903,1.3697746234
H,0,-1.9661614573,3.9915480799,2.5676345132
H,0,-1.0889240734,-0.7040665225,-0.7244772905
H,0,-1.0022768956,-0.1608504825,0.851428428

8, optimization in solv. CHCl_3
M06-2X/6-311+G(d,p), E= -690.875122491 a.u.
Thermal correction to Gibbs Free Energy = 0.252927 a.u.
0; 1
N,0,-1.3687240933,-0.5628483011,-0.3110436164
C,0,-1.4537268976,0.6147299667,-1.2013179696
C,0,-2.70439243,-1.1174611083,-0.0818945311
H,0,-2.7697908095,-2.1518386686,-0.432471662
C,0,-1.0689559908,1.8978895687,-0.4650092201
H,0,-0.0553865765,1.7923668811,-0.0743683679
H,0,-1.0932009016,2.7583722046,-1.1385690774
H,0,-1.7484749226,2.0768346256,0.3693890915
C,0,-0.5683147988,0.4167445128,-2.4293855039
H,0,0.4676397796,0.2799925222,-2.1095152952
H,0,-0.8886437443,-0.4632578306,-2.9917752485
H,0,-0.5996161101,1.2883843563,-3.0856253294
N,0,-2.8751333258,0.6474864259,-1.578141271
C,0,-3.6286728845,-0.2744144687,-0.9488802814
O,0,-4.840048538,-0.4100597725,-1.0359014719
C,0,-3.4485053559,1.7115346964,-2.3738681202
H,0,-2.9036609207,1.8241013748,-3.3127348414
H,0,-4.4824898788,1.4470419647,-2.5893381379
H,0,-3.4293341077,2.6601569475,-1.8303700386
C,0,-3.1531002787,-1.0879284011,1.3924484377
H,0,-4.1842044299,-1.4499126428,1.4305668318
H,0,-2.5284989522,-1.7895596342,1.9494877804
C,0,-3.0517454138,0.2850858907,2.002792243
C,0,-4.0508796773,1.2391598542,1.7887374372
C,0,-1.9284275332,0.6484227609,2.7474424937
C,0,-3.9217225629,2.5290555713,2.2964114634
H,0,-4.9315784892,0.9668841938,1.2155848052
C,0,-1.7985194792,1.9349759941,3.2618260504
H,0,-1.1453520938,-0.0834159501,2.914790099
C,0,-2.7931944024,2.8815809619,3.0327556658
H,0,-4.7052033641,3.2577916092,2.1221109459
H,0,-0.9191441252,2.2001539476,3.837726976
H,0,-2.6933265578,3.8846740425,3.4307859215
H,0,-0.7721657633,-1.2603320455,-0.7365027685

8- H^+ , optimization in solv. CHCl_3
M06-2X/6-311+G(d,p), E= -691.299457475 a.u.
Thermal correction to Gibbs Free Energy = 0.268657 a.u.
1; 1
N,0,-1.3789440121,-0.4558482962,-0.2335804416
C,0,-1.4767904434,0.7030546488,-1.2456048976
C,0,-2.7213599275,-1.1250688189,-0.0820862267
H,0,-2.6567913192,-2.1346367564,-0.4859511047
C,0,-1.0434459741,1.9894011683,-0.5586347227
H,0,-0.0050563903,1.9110468077,-0.2296719842
H,0,-1.1042756554,2.8161078584,-1.2674080127
H,0,-1.6870882785,2.2112652884,0.2969721876
C,0,-0.6239049901,0.3639282134,-2.4594669748
H,0,0.43182247,0.3174744422,-2.1839347381
H,0,-0.9332168977,-0.585500892,-2.9015923395
H,0,-0.7350050114,1.1464071558,-3.2100715274
N,0,-2.898844944,0.6936399398,-1.5485431832
C,0,-3.6304143397,-0.2789755848,-0.9646248373
O,0,-4.8206005867,-0.4679829499,-1.0714524274
C,0,-3.5043552778,1.7382912799,-2.3600487359
H,0,-2.9658722672,1.852814744,-3.300883027
H,0,-4.5282628901,1.4350763811,-2.568415244
H,0,-3.511312333,2.686819411,-1.8193996726
C,0,-3.1998088368,-1.1360032418,1.3773181115
H,0,-4.2394168768,-1.4690566719,1.3495702423
H,0,-2.6261656407,-1.8758017188,1.938492572
C,0,-3.0754816378,0.2315647424,2.0048309794
C,0,-4.0062343885,1.2361415513,1.7201247659
C,0,-1.9781162382,0.5357916934,2.8150418545
C,0,-3.831588475,2.519633636,2.2251515303
H,0,-4.8736749479,1.0060329804,1.1097535226
C,0,-1.8004261754,1.8242740356,3.3165937732
H,0,-1.2691214864,-0.244666692,3.0789487543
C,0,-2.724068667,2.8185743264,3.017094147
H,0,-4.5646827146,3.287005884,2.0068281783
H,0,-0.9478134825,2.0445269562,3.9476047455
H,0,-2.5918311741,3.8191075531,3.4105333495
H,0,-0.6622319795,-1.1197574974,-0.5321556039
H,0,-1.0818820409,-0.0682026775,0.6705164575

10, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1036.79703937 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.376397 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1037.1735432 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1037.1860172 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1037.7946113 a.u.

1; 1
N,0,-1.3738543624,-0.5256295961,-0.3004734554
C,0,-1.4231332185,0.6491647969,-1.2330130563
C,0,-0.2452330873,-0.9862635303,0.1639522767
C,0,-0.0706863335,-2.1529145052,0.939092347
C,0,1.1909233342,-2.4748141736,1.3551997692
H,0,0.6422408204,-0.4136777188,-0.0964172861
H,0,-0.921822445,-2.7828856917,1.1682630837
H,0,1.9937881336,-1.7909585217,1.0795623472
C,0,1.5989376427,-3.6200122075,2.1240238253
C,0,2.9662764107,-3.7540245012,2.4339357131
C,0,0.6969583882,-4.6051056071,2.5749199493
C,0,3.4207287431,-4.8373535367,3.1703636034
C,0,1.1554888244,-5.6844954931,3.309418603
C,0,2.515857445,-5.8027015289,3.6081854424
H,0,3.6663900716,-2.99798525,2.0891924191
H,0,-0.3619149332,-4.5253100198,2.3511148948
H,0,4.4759831627,-4.9317835757,3.4040831981
H,0,0.4569918165,-6.4399720399,3.6539797219
H,0,2.868439815,-6.652125095,4.18516555
C,0,-2.6939051058,-1.1079089452,-0.0551738204
H,0,-2.7022527847,-2.1510982486,-0.3916671209
C,0,-0.9935456867,1.925837818,-0.5180729953
H,0,0.0565211879,1.864409365,-0.2196283995
H,0,-1.0841692865,2.7731949288,-1.2019382108
H,0,-1.6112299945,2.1070004305,0.3637184436
C,0,-0.5701396786,0.3722200772,-2.4683068705
H,0,0.4913896275,0.3242989251,-2.2142577929
H,0,-0.871366444,-0.5631615341,-2.9455440516
H,0,-0.6901238128,1.1888095399,-3.1835902878
N,0,-2.8387249231,0.6607694956,-1.5685130251
C,0,-3.5895354512,-0.2899504377,-0.9693622766
O,0,-4.7885497452,-0.4649557151,-1.0918695117
C,0,-3.4180220429,1.6393779493,-2.4612332492
H,0,-2.9696491419,1.5843869912,-3.4567259649
H,0,-4.4804564656,1.4066626225,-2.5370053941
H,0,-3.3018277115,2.6518862803,-2.0650449234
C,0,-3.1943531654,-1.031802214,1.4026707852
H,0,-4.2345188476,-1.3706402877,1.3531000061
H,0,-2.6527399752,-1.7552454145,2.0171799498
C,0,-3.1062156765,0.3390152188,2.0193366329
C,0,-4.0822923262,1.3074135365,1.7578165779
C,0,-2.0338198889,0.6721331168,2.8522611673
C,0,-3.9770542119,2.5831175252,2.3049284138
H,0,-4.9299593594,1.0559632489,1.125698392
C,0,-1.9287148276,1.9474593671,3.4020686268
H,0,-1.2783494612,-0.0759520734,3.0822333375
C,0,-2.8983023883,2.9077661749,3.1253774093
H,0,-4.7447474907,3.3226041287,2.0969150388
H,0,-1.0923894787,2.1883857821,4.051703064
H,0,-2.820461671,3.9015121435,3.5561331034

10, optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1037.79596295 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.374909 a.u.
Thermal correction to Gibbs Free Energy at 20 °C = 0.376191 a.u.

1; 1
N,0,-1.3942221782,-0.5513641919,-0.3218284056
C,0,-1.4672251824,0.6565228572,-1.2153599399
C,0,-0.270063035,-0.9812734441,0.1574051793
C,0,-0.0866938466,-2.1663359893,0.9189737332
C,0,1.1603444528,-2.4383600266,1.3835774061
H,0,0.6072317273,-0.3781354626,-0.0653272328
H,0,-0.9220061934,-2.8313730313,1.091531435
H,0,1.9473853071,-1.7220069698,1.1550384286
C,0,1.5754579364,-3.5848248697,2.1642140041
C,0,2.9307699918,-3.6870203052,2.5135056576
C,0,0.6824171767,-4.5868529994,2.5804623587
C,0,3.387426468,-4.7644623026,3.258420682
C,0,1.1412551292,-5.6594205696,3.3245675523
C,0,2.4927492034,-5.7502213887,3.6635371523
H,0,3.622130406,-2.9152396634,2.1930449986
H,0,-0.3691000272,-4.5277684668,2.3269798041
H,0,4.4347974868,-4.8360130712,3.5230492215
H,0,0.4503632354,-6.4288853895,3.6455657241
H,0,2.8442997416,-6.5929339201,4.2467804494
C,0,-2.7077872234,-1.173924831,-0.1012967138
H,0,-2.6973149613,-2.2037655794,-0.4667909491
C,0,-1.0427110773,1.9179650487,-0.4714941559
H,0,-0.0072602365,1.8322091623,-0.1369849896
H,0,-1.0958286682,2.7681191087,-1.1535792159
H,0,-1.6879762875,2.1033049225,0.3874189954
C,0,-0.6251058453,0.4177291293,-2.4664870989
H,0,0.4369925368,0.3837346193,-2.2187124073
H,0,-0.9169459341,-0.5135699888,-2.9536351031
H,0,-0.7706182999,1.244492245,-3.1622353226
N,0,-2.8899789241,0.6633023991,-1.5329737574
C,0,-3.6192716096,-0.3276007095,-0.980250497
O,0,-4.8107433166,-0.5162973297,-1.0982462831
C,0,-3.4908441838,1.7332466869,-2.3106719776
H,0,-2.9599671077,1.8681182286,-3.2533328937
H,0,-4.5200044385,1.4478636538,-2.518079127
H,0,-3.4829298895,2.6679950125,-1.7459545395
C,0,-3.1946309205,-1.1167502589,1.3639361261
H,0,-4.2403771527,-1.431661111,1.3333659033
H,0,-2.6508461459,-1.8430838712,1.9679377074
C,0,-3.0591936384,0.2608925877,1.9610488905
C,0,-4.0091352726,1.2512374453,1.6973471743
C,0,-1.9495548206,0.5783931135,2.7461624378
C,0,-3.8414927968,2.5386552315,2.1980263366
H,0,-4.8845758487,1.0093675343,1.1025201763
C,0,-1.7815674601,1.8653111295,3.2496751114
H,0,-1.2156179466,-0.1900165299,2.9721985364
C,0,-2.7248824586,2.8494049053,2.9708999014
H,0,-4.587638351,3.2972495939,1.9929215936
H,0,-0.9184907064,2.0979856171,3.8622161088
H,0,-2.5981646043,3.8507247492,3.3646676036

11, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -943.182321095 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.338662 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -943.5137075 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -943.5245315 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -944.0889749 a.u.

1; 1
N,0,-1.4416536159,0.0598427911,0.6200839845
C,0,-1.6049664312,1.4126623113,0.0709088624
C,0,-0.3362937357,-0.6328302804,0.5488777374
C,0,0.892971643,-0.2550550303,-0.0434535548
C,0,1.9224188535,-1.1497204051,-0.0201023034
H,0,-2.4909901425,1.3883806257,-0.5695464013
H,0,-0.3844470603,-1.6179973056,1.0092794023
H,0,1.0130698578,0.7229540312,-0.4937165474
H,0,1.7401441221,-2.1104478266,0.4616276912
C,0,3.2471967345,-0.9784829443,-0.5626988531
C,0,4.1796738419,-2.0153084342,-0.3719300171
C,0,3.6443780782,0.1725303331,-1.2713473061
C,0,5.4709735923,-1.9054216152,-0.8666560016
C,0,4.9332541862,0.2767904873,-1.765709037
C,0,5.8485189116,-0.759619329,-1.563852703
H,0,3.8800186033,-2.9068443566,0.1722232197
H,0,2.9430813581,0.9829305812,-1.4423702802
H,0,6.1822340916,-2.7101039135,-0.7117645179
H,0,5.2319605938,1.1650271152,-2.3129392138
H,0,6.857700226,-0.6714635543,-1.9544203897
H,0,-0.7508180164,1.6354345003,-0.5680880701
C,0,-2.6269635417,-0.4953852332,1.3002712953
H,0,-2.3318115467,-1.4514194468,1.7387154466
H,0,-2.8796772622,0.1853182405,2.1182809566
C,0,-3.7982516368,-0.6596314525,0.3650476086
C,0,-3.735378314,-1.5695932766,-0.6945367158
C,0,-4.9616936574,0.0866539344,0.5593263198
C,0,-4.8212435881,-1.7273382358,-1.5483630747
H,0,-2.8361723304,-2.1608156373,-0.8513687885
C,0,-6.0517375472,-0.0759536051,-0.2927892031
H,0,-5.0165943006,0.7943418937,1.3828003049
C,0,-5.9816910873,-0.9809150681,-1.3476156532
H,0,-4.7656936308,-2.4377508773,-2.3675069987
H,0,-6.9543232179,0.5053830608,-0.1312399413
H,0,-6.8305418269,-1.1078010917,-2.0126064087
C,0,-1.769257099,2.4489896469,1.1566444373
C,0,-2.8888180609,3.2821180141,1.1557816679
C,0,-0.8002428246,2.6032675898,2.1523479551
C,0,-3.0370592534,4.2630941497,2.1334893113
H,0,-3.6460842111,3.1660081686,0.3847953612
C,0,-0.953067745,3.577451848,3.132975688
H,0,0.0780432736,1.9622924971,2.1655629857
C,0,-2.0709993097,4.4101469472,3.1241661034
H,0,-3.9101548917,4.9083266766,2.1217382067
H,0,-0.1962561158,3.6901412037,3.9033345693
H,0,-2.1871709664,5.1714722719,3.889498865

11, optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -944.089727777 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.340330 a.u.

1; 1
N,0,-1.0238614931,0.2168387258,0.0584434522
C,0,-1.0450985413,1.2867634519,-0.9592945603
C,0,0.0195539735,-0.5032590274,0.3380592375
C,0,1.3209874198,-0.4098292133,-0.2363066958
C,0,2.2672770086,-1.2839280434,0.1860385951
H,0,-1.8575658799,1.0526589476,-1.6492349948
H,0,-0.1293655894,-1.2578864816,1.1065172897
H,0,1.5441901746,0.3433145709,-0.9783022344
H,0,1.9829613387,-2.0173171855,0.9385549943
C,0,3.6454922064,-1.3582592767,-0.2630239187
C,0,4.4644029073,-2.3622538647,0.2735095719
C,0,4.1834038569,-0.4699100913,-1.2091423981
C,0,5.7882988953,-2.4814562652,-0.1260065379
C,0,5.5048132857,-0.5893234168,-1.6031153688
C,0,6.308572025,-1.5951558472,-1.0641211415
H,0,4.0540506313,-3.0496555419,1.0051883775
H,0,3.5727620478,0.3153694467,-1.6377403708
H,0,6.4126401646,-3.2610053012,0.2920672598
H,0,5.9143179825,0.0993734647,-2.3316218943
H,0,7.3416536098,-1.6845513595,-1.3778822417
H,0,-0.1149926007,1.2567211058,-1.5194858688
C,0,-2.2925143117,0.0283087974,0.8015845961
H,0,-2.1378257551,-0.784804304,1.5103599415
H,0,-2.4771358025,0.9473317679,1.3618521925
C,0,-3.4427002409,-0.260852686,-0.1313091138
C,0,-3.4318077849,-1.4090090563,-0.9251307028
C,0,-4.5163857412,0.6221947684,-0.2108865457
C,0,-4.4845621475,-1.6664006107,-1.7942532519
H,0,-2.5991613734,-2.1034883387,-0.8640733331
C,0,-5.5746274217,0.361366373,-1.0779171973
H,0,-4.5250089014,1.515285184,0.4055476503
C,0,-5.5571268205,-0.7799182699,-1.8718720739
H,0,-4.472906873,-2.5594924006,-2.4073358735
H,0,-6.4086754089,1.0504132812,-1.133101301
H,0,-6.378393229,-0.9825151191,-2.5486696283
C,0,-1.2650967523,2.6378121245,-0.3189340369
C,0,-2.346950953,3.4248394119,-0.7045639853
C,0,-0.3839059429,3.1040497391,0.6573821273
C,0,-2.5459387022,4.6739653519,-0.1216062384
H,0,-3.0357521256,3.0596772938,-1.4593733964
C,0,-0.5856913731,4.3478149612,1.243189587
H,0,0.4629507119,2.4953476265,0.9608546594
C,0,-1.6678746628,5.1344090666,0.8531215203
H,0,-3.3881558198,5.2830346655,-0.4270309797
H,0,0.1019957588,4.7065806194,1.9994003194
H,0,-1.823511661,6.1048014553,1.3090561723

12, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -634.079639461 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.230687 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -634.3091479 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -634.3160918 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -634.6803562 a.u.

1; 1
C,0,-2.5888596132,0.9131691157,-1.7628942152
N,0,-1.4140825606,-0.2936672315,-0.0034209109
C,0,-1.5987558191,1.0280796727,-0.6056929097
C,0,-0.2660900909,-0.8903114106,0.173200365
C,0,1.0212486795,-0.3897219759,-0.1320175565
C,0,2.1038710684,-1.1724872554,0.1437287438
H,0,-0.6476203383,1.4268328727,-0.9532618751
H,0,-0.3294560844,-1.8817749089,0.6172513798
H,0,1.1404740423,0.5971878406,-0.5626394576
H,0,1.9149761891,-2.1535804368,0.579542936
C,0,3.4939155172,-0.8565718608,-0.0717606554
C,0,4.4553045173,-1.8142528561,0.3016575097
C,0,3.9277171364,0.3600481976,-0.6343460659
C,0,5.8080839918,-1.5671002139,0.1193843779
C,0,5.2786072377,0.6023341092,-0.8150542676
C,0,6.2204907921,-0.3590940469,-0.4392657341
H,0,4.1277890778,-2.7538054951,0.738322309
H,0,3.2082235322,1.1165413565,-0.9306735225
H,0,6.5406735371,-2.3123515719,0.4113130445
H,0,5.6060112948,1.5412279035,-1.249740658
H,0,7.2784553537,-0.1627266661,-0.5837440756
H,0,-2.8042473863,1.9109602708,-2.150577652
H,0,-2.1467488911,0.3083853019,-2.5692865164
H,0,-2.0019166831,1.6902204362,0.1675496214
C,0,-2.6792476083,-0.9341787199,0.3687146089
H,0,-2.4809353886,-1.9443203908,0.730799644
H,0,-3.1271646213,-0.3450965954,1.1756965522
C,0,-3.6112729822,-0.9500019436,-0.8380481181
H,0,-4.5868094592,-1.3373223053,-0.5369897306
H,0,-3.196536232,-1.604713358,-1.6193073469
O,0,-3.8067692085,0.3546231653,-1.3320978242

12, optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -634.680779188 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.229373 a.u.
Thermal correction to Gibbs Free Energy at 20 °C = 0.230291 a.u.

1; 1
C,0,-2.5545772643,0.9076642461,-1.7850962277
N,0,-1.405625498,-0.2913302305,-0.0022842538
C,0,-1.5738699954,1.0335549646,-0.6203260679
C,0,-0.2735027715,-0.8985822715,0.1778863214
C,0,1.0256320014,-0.4093465979,-0.1408005659
C,0,2.0931637908,-1.1923904704,0.1497934714
H,0,-0.6190468385,1.4177545392,-0.965018538
H,0,-0.343099343,-1.8833038818,0.6335640426
H,0,1.1511508622,0.5673325438,-0.5857565681
H,0,1.9039217903,-2.1631784903,0.6043655101
C,0,3.492192303,-0.8763039863,-0.0740096689
C,0,4.4547721592,-1.8108023404,0.3343398086
C,0,3.9141066395,0.3214716562,-0.6743580504
C,0,5.8071742564,-1.5570357047,0.1516630999
C,0,5.2633263719,0.5709261931,-0.8570053787
C,0,6.2114330411,-0.3666537753,-0.4441410782
H,0,4.1335133269,-2.7365351272,0.7991619288
H,0,3.1916950303,1.0591121281,-1.0017925888
H,0,6.5427925084,-2.2836362594,0.4731399377
H,0,5.5830377061,1.4953939451,-1.3216236365
H,0,7.266064571,-0.165461483,-0.5892531217
H,0,-2.7565366461,1.8958440488,-2.1949580468
H,0,-2.1188404258,0.2746618702,-2.5689341322
H,0,-1.9795326698,1.6994248843,0.1448597009
C,0,-2.6879137707,-0.9058187697,0.3835461599
H,0,-2.5039278668,-1.9082602955,0.7661899609
H,0,-3.1228793506,-0.2863056133,1.1712846861
C,0,-3.6130769007,-0.9322679087,-0.8295924378
H,0,-4.5942139196,-1.2961557033,-0.5291785501
H,0,-3.2017979488,-1.5984571601,-1.5983045398
O,0,-3.7830572286,0.36827828,-1.3509716969

13, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -558.953314833 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.225144 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -559.137175 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -559.143674 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -559.4753293 a.u.

1; 1
C,0,-2.9235520553,0.7012282617,-1.4766142601
N,0,-1.2851158538,-0.6287341754,-0.416566454
C,0,-1.43988436,0.656527709,-1.124430197
C,0,-0.1505343842,-1.1475662187,-0.0506472292
C,0,1.1247376091,-0.5746542972,-0.276393594
C,0,2.2318460551,-1.2370265696,0.1634967578
H,0,-0.7789225452,0.6857996665,-1.9936617843
H,0,-0.2104851686,-2.1007942072,0.4714071336
H,0,1.197150422,0.377227044,-0.7907827404
H,0,2.0740508084,-2.1853129081,0.6773074777
C,0,3.6101308051,-0.8329668259,0.0302358783
C,0,4.6019774623,-1.6729356084,0.5695060852
C,0,4.0024841244,0.3565402933,-0.6143977756
C,0,5.9444427926,-1.3373996242,0.4700961964
C,0,5.3432873733,0.6875245731,-0.7117199229
C,0,6.3159188815,-0.1571978329,-0.1705376421
H,0,4.3068626891,-2.5923987312,1.067689908
H,0,3.2582080572,1.0210930477,-1.0412158646
H,0,6.7007265059,-1.9926063886,0.8897707297
H,0,5.6387733896,1.6049205104,-1.210508466
H,0,7.3656837197,0.10812428,-0.2505033676
H,0,-3.29131048,1.7267584462,-1.5364291497
H,0,-3.0942788935,0.2214970732,-2.4452719374
H,0,-1.1584459674,1.461905794,-0.4374329223
C,0,-2.596316261,-1.2560418145,-0.1555072058
H,0,-2.750176505,-2.0500852417,-0.8944960305
H,0,-2.607637743,-1.6923604308,0.8449159692
C,0,-3.5776009036,-0.1102185991,-0.3585929054
H,0,-3.6546794757,0.4859317547,0.556075683
H,0,-4.5740110993,-0.4721139803,-0.61705737

13, optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -559.475774410 a.u.
Thermal correction to Gibbs Free Energy at 25 °C= 0.224724 a.u.
Thermal correction to Gibbs Free Energy at 20 °C= 0.225609a.u.

1; 1
C,0,-2.9082938022,0.7034183396,-1.4811810178
N,0,-1.2797673475,-0.644556782,-0.419004786
C,0,-1.4214523565,0.6476736328,-1.1334022092
C,0,-0.1581228353,-1.1633785582,-0.0444851649
C,0,1.1253739164,-0.5826405977,-0.2671776979
C,0,2.2209884667,-1.2445372773,0.1753037092
H,0,-0.7639109164,0.6611424078,-2.0019186996
H,0,-0.218433448,-2.1147555627,0.4791909123
H,0,1.1948098754,0.3677172222,-0.7804661044
H,0,2.0646916471,-2.1923683434,0.6869794698
C,0,3.6073988981,-0.8333304654,0.0398765823
C,0,4.6005389894,-1.6656369754,0.5754472867
C,0,3.986883261,0.3531837221,-0.6084767012
C,0,5.9417275313,-1.3245149611,0.4673831648
C,0,5.3252431652,0.6907284447,-0.7151614131
C,0,6.3043432773,-0.146717498,-0.1781081548
H,0,4.3129232904,-2.5829755031,1.0774357526
H,0,3.2392289069,1.0121515955,-1.0327909058
H,0,6.7008102326,-1.9745844925,0.8839763968
H,0,5.6120870137,1.6056241665,-1.2185096074
H,0,7.3502459355,0.1221127356,-0.2652921468
H,0,-3.2647764152,1.729390142,-1.54721877
H,0,-3.0853435737,0.2130178219,-2.4404742652
H,0,-1.1324176688,1.4460369043,-0.4454586502
C,0,-2.6052257921,-1.2620491679,-0.1647532233
H,0,-2.7667184009,-2.0343927406,-0.9205468495
H,0,-2.6160101341,-1.7109198172,0.8268733625
C,0,-3.5654623625,-0.0930720706,-0.3502213519
H,0,-3.6072328175,0.5043089742,0.5631305603
H,0,-4.5708002363,-0.4314134458,-0.5932144983

12 counterion CCl_3COO^- , optimization in solv. CHCl_3
M06-2X/6-311+G(d,p), E= -2242.09822006 a.u.
Thermal correction to Gibbs Free Energy at 25 °C= 0.235192 a.u.
Thermal correction to Gibbs Free Energy at 20 °C= 0.236464 a.u.
0; 1
C,0,-2.7752116363,1.3590408269,-1.5453193784
N,0,-1.6372116772,-0.0020711471,0.1186548306
C,0,-1.7005858372,1.3450874147,-0.4599179574
C,0,-0.5831115473,-0.7576180665,0.1792050307
C,0,0.7357424274,-0.427625991,-0.2587102274
C,0,1.6828411185,-1.3826981505,-0.0973009488
H,0,-0.7369219202,1.6326982356,-0.8700255557
H,0,-0.7475762737,-1.7445666757,0.6169696376
H,0,0.9595996412,0.5386168588,-0.6898505019
H,0,1.366225706,-2.3257589395,0.3501160564
C,0,3.0904906919,-1.2869568413,-0.455415386
C,0,3.908258753,-2.392092345,-0.182074593
C,0,3.6573699561,-0.1502311377,-1.0521874535
C,0,5.2617282017,-2.3639768678,-0.4929113092
C,0,5.0072904456,-0.1245019035,-1.3622823776
C,0,5.8116965943,-1.2306199934,-1.0828528299
H,0,3.4697785882,-3.2711610944,0.2781565039
H,0,3.0454407747,0.7154242196,-1.2768075804
H,0,5.8845118048,-3.2228547704,-0.2750141625
H,0,5.4387591416,0.7558822185,-1.8226860733
H,0,6.8671388697,-1.2051902117,-1.3271344349
H,0,-2.8973554237,2.372877584,-1.9239936337
H,0,-2.4729562526,0.7017709391,-2.371232202
H,0,-1.9718973137,2.0341144293,0.343577471
C,0,-2.9441980321,-0.4803317527,0.6061367819
H,0,-2.8308981411,-1.5063845825,0.9555729408
H,0,-3.2414242484,0.1703714172,1.4326719111
C,0,-3.9557270894,-0.3758083416,-0.5276747577
H,0,-4.9476793152,-0.6326587662,-0.1594577979
H,0,-3.6829094198,-1.0676893468,-1.3346323342
O,0,-4.0209833449,0.9482000722,-1.0267484922
C,0,-0.8805792232,-4.1437829069,1.4793894518
O,0,0.3104729882,-3.9472388008,1.23184234
O,0,-1.8625387182,-3.3976413084,1.3604657732
C,0,-1.2572541686,-5.5917599661,2.0349592517
Cl,0,0.1661134279,-6.6242745778,2.2849961025
Cl,0,-2.122115075,-5.4182990979,3.5882096353
Cl,0,-2.3405944629,-6.3829492525,0.8514130492

13 counterion CCl_3COO^- , optimization in solv. CHCl_3
M06-2X/6-311+G(d,p), E= -2166.89366212 a.u.
Thermal correction to Gibbs Free Energy at 25 °C= 0.228679 a.u.
Thermal correction to Gibbs Free Energy at 20 °C= 0.229948 a.u.
0; 1
C,0,-3.197678354,1.1234154053,-1.0311569537
N,0,-1.7029524645,-0.6907679326,-0.7808484728
C,0,-1.7289372403,0.7890262185,-0.7666605764
C,0,-0.6535824645,-1.4201229682,-0.6017938039
C,0,0.6680918861,-0.9093946531,-0.4039813339
C,0,1.6461697572,-1.800704054,-0.1247065241
H,0,-1.0440538515,1.1800239017,-1.5192564013
H,0,-0.8006418968,-2.4973380258,-0.5734495134
H,0,0.8429210291,0.1591207448,-0.430251529
H,0,1.3600213024,-2.8497931698,-0.0647835356
C,0,3.0442258224,-1.5062009133,0.1595863507
C,0,3.8522288884,-2.551547967,0.6260197273
C,0,3.605590665,-0.2310746031,-0.0050608327
C,0,5.1884440833,-2.3292596135,0.9322176215
C,0,4.9408673858,-0.0125655792,0.2952490441
C,0,5.7334346657,-1.0595319502,0.7671226791
H,0,3.4179420895,-3.5373358945,0.7560697979
H,0,3.0018163454,0.5875442639,-0.3788233842
H,0,5.802701589,-3.1431301649,1.2971768279
H,0,5.3697957474,0.9732258613,0.1615985615
H,0,6.7764834656,-0.8826533045,1.0016701486
H,0,-3.4825822102,2.0670966625,-0.5693019342
H,0,-3.3761997766,1.1971231773,-2.106140066
H,0,-1.407037571,1.1242172586,0.2223507662
C,0,-3.0670585678,-1.2562113971,-0.8790399098
H,0,-3.2494185096,-1.5343222891,-1.9203569225
H,0,-3.1194582721,-2.1300091437,-0.2315800117
C,0,-3.9443970608,-0.0842808542,-0.4540354736
H,0,-3.9788129217,-0.0267733886,0.6362766661
H,0,-4.9609584133,-0.1781732032,-0.8319595703
C,0,-0.8809015637,-3.5286283552,1.7164961892
O,0,-0.306613851,-4.165831846,0.8252317847
O,0,-1.8306943933,-2.7427757997,1.6598964524
C,0,-0.2127612634,-3.6775284022,3.1600085847
Cl,0,-1.3453229136,-3.2828689793,4.471952507
Cl,0,0.4255940853,-5.3165116172,3.4245436548
Cl,0,1.1526814321,-2.5106403748,3.2011573855

14, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -598.224732610 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.254045 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -598.4188479 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -598.4265212 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -598.7838403 a.u.

1; 1
C,0,-2.5101501167,1.0730912749,-1.7695844529
N,0,-1.5038318741,-0.2047882119,0.0656183461
C,0,-1.6680394257,1.1396023925,-0.4987175192
C,0,-0.3624855084,-0.8140384186,0.2266957431
C,0,0.9317293252,-0.3254893822,-0.08083785
C,0,2.0042125348,-1.1295404965,0.1643989306
H,0,-0.6924201151,1.5836407264,-0.6846870999
H,0,-0.4322653989,-1.8159001223,0.6462189444
H,0,1.0603231143,0.660488188,-0.5105187009
H,0,1.8071427699,-2.1107809852,0.5961744901
C,0,3.3953551987,-0.8392520869,-0.0874649068
C,0,4.3458980628,-1.8283040284,0.2255851865
C,0,3.8384337714,0.3803377701,-0.6352739821
C,0,5.6968402646,-1.6095346034,-0.0029843048
C,0,5.1874241757,0.5947972609,-0.861653939
C,0,6.1185440801,-0.3983690634,-0.5473147663
H,0,4.0121697212,-2.7715753551,0.6496620957
H,0,3.1275980676,1.1615919236,-0.8846289873
H,0,6.4206916943,-2.3800217217,0.2415444634
H,0,5.5212336634,1.5365815426,-1.2852278283
H,0,7.1748066207,-0.2243743732,-0.7284332837
H,0,-2.6508037104,2.0938509456,-2.1373814617
H,0,-1.9517397302,0.5252597999,-2.5380350443
H,0,-2.1727908449,1.7422838938,0.2653965928
C,0,-2.7739724341,-0.8698741505,0.3876483541
H,0,-2.5539051532,-1.8499366677,0.8143761146
H,0,-3.2693427437,-0.2645570874,1.1557366325
C,0,-3.6449975423,-0.9733298502,-0.8609057133
H,0,-4.6008258446,-1.4214950653,-0.5732589291
H,0,-3.1663565021,-1.6574780211,-1.5718837288
C,0,-3.8509386544,0.3958587321,-1.5028689764
H,0,-4.452670276,1.0271094351,-0.8362941075
H,0,-4.41398219,0.2932988056,-2.4350293115

14, optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -598.784279732 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.252528 a.u.

1; 1
C,0,-0.2020842104,-0.4892724847,0.9407427267
C,0,1.0801591367,-0.0739838825,-0.4704110203
C,0,2.034434525,-1.0220090048,0.31650918
H,0,-0.3279537096,-1.5448896884,1.1694581129
H,0,1.2746407,0.9639506635,0.2415308851
H,0,1.7686030351,-2.0521004174,0.5471810874
C,0,3.3996296113,-0.8234867892,-0.1404935728
C,0,4.1998933944,-1.9563477702,-0.343706513
C,0,3.9432500223,0.4488091119,-0.3799487997
C,0,5.5094425838,-1.8257888406,-0.7855633296
C,0,5.2517999052,0.5763947034,-0.8146058582
C,0,6.0356947703,-0.5596866848,-1.0207319744
H,0,3.7858318508,-2.9413819651,-0.1573863505
H,0,3.3502205751,1.3404566139,-0.2159786239
H,0,6.1177608786,-2.7073553253,-0.9446361596
H,0,5.6677897357,1.5605273411,-0.9917234855
H,0,7.0582530456,-0.4539298245,-1.362591271
C,0,-2.5193907017,-0.3417753236,1.6084596384
C,0,-1.3353081599,1.6924132319,0.862990072
C,0,-3.6096116053,-0.1237844912,0.5626328576
H,0,-2.7746187362,0.1650723692,2.5434483505
H,0,-2.3519868252,-1.3973181581,1.8152181561
C,0,-2.4064234057,1.9454459065,-0.1979069913
H,0,-1.6047485741,2.1724241631,1.8080452843
H,0,-0.3645992377,2.0656448577,0.5529051805
C,0,-3.7515635282,1.3610332129,0.2318385394
H,0,-4.5439413401,-0.5297012641,0.9543368713
H,0,-3.3550080875,-0.6906318753,-0.3379252685
H,0,-2.4791869636,3.0228296515,-0.3557825413
H,0,-2.0812626784,1.4947582037,-1.1408249701
H,0,-4.4910583613,1.5014703051,-0.5577890666
H,0,-4.1159848681,1.8967302423,1.1150352245
N,0,-1.2491832569,0.2466894617,1.1375025892

15, optimization in solv. CHCl₃
PBE1PBE/6-311G(d,p), E= -711.208353703 a.u.
Thermal correction to Gibbs Free Energy at 25 °C =0.245186 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -711.4518441 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -711.4592465 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -711.8805282 a.u.

1; 1
C,0,-4.2848138858,-2.3648679606,0.4167515461
C,0,-5.268108257,-1.4412346497,0.0515391111
C,0,-4.9209586639,-0.1669992024,-0.3917079768
C,0,-3.5772495681,0.1743304684,-0.4668224076
C,0,-2.9348788394,1.4529530724,-0.9177207702
C,0,-2.9354795878,-2.0379855402,0.3476155655
C,0,-2.6124636815,-0.7607522409,-0.1001923897
N,0,-1.3230758026,-0.1971314901,-0.2537391767
C,0,-1.4377476016,1.2211633854,-0.667511022
C,0,-0.1853136431,-0.8135486916,-0.0573901528
C,0,1.0912251397,-0.2271185815,-0.1899525432
C,0,2.1982511943,-0.9957275009,0.0323245509
H,0,-4.5741657235,-3.3512616415,0.7637467
H,0,-6.314664623,-1.7208111067,0.1166812508
H,0,-5.6871515999,0.5483407012,-0.6734824579
H,0,-2.1828896518,-2.7618500954,0.6416187809
H,0,-0.8281600449,1.3789099862,-1.5590927339
H,0,-0.2523014844,-1.8588891679,0.2302729128
H,0,1.175368767,0.8203922237,-0.4576455531
H,0,2.0341292769,-2.0388146826,0.3027072533
C,0,3.5791009514,-0.5931554247,-0.0470430051
C,0,4.5662993379,-1.5546370072,0.2417838947
C,0,3.9822679427,0.7107929517,-0.39797511
C,0,5.9125981633,-1.2262339566,0.1850241143
C,0,5.3270605584,1.0340374795,-0.4535816516
C,0,6.2941791031,0.068235245,-0.1621968295
H,0,4.2632885154,-2.5625193073,0.5120412053
H,0,3.2429437468,1.4708288273,-0.6292277611
H,0,6.6644756862,-1.9754701373,0.4101862398
H,0,5.6302894418,2.0401367343,-0.7246700551
H,0,7.3472411165,0.3284964612,-0.2073672611
H,0,-3.3037204347,2.3159281208,-0.3573620009
H,0,-3.1350878353,1.6414501191,-1.9769607604
H,0,-1.0496008633,1.845332979,0.1414187431

15, optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -711.880981441 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.243094 a.u.
Thermal correction to Gibbs Free Energy at 20 °C = 0.244091 a.u.

1; 1
C,0,-4.2906041868,-2.3589969579,0.4216473792
C,0,-5.2680921975,-1.4331834866,0.0517981949
C,0,-4.9152115717,-0.1631502836,-0.3953457113
C,0,-3.5705555309,0.1707209802,-0.4703073522
C,0,-2.9228212875,1.448926434,-0.9306605658
C,0,-2.9403594934,-2.0378641941,0.353074759
C,0,-2.6156500749,-0.7657056004,-0.0990666458
N,0,-1.3136027587,-0.204228776,-0.2506080128
C,0,-1.4256197333,1.2236849877,-0.6575627497
C,0,-0.1880024473,-0.8236814761,-0.0563032915
C,0,1.0960693323,-0.230001379,-0.1841696906
C,0,2.1911048602,-1.0026359158,0.0320513847
H,0,-4.5845789252,-3.3405094142,0.7710513413
H,0,-6.313708353,-1.707557792,0.1163039647
H,0,-5.6757164396,0.5536658393,-0.6808995555
H,0,-2.1913386787,-2.760352123,0.6514770544
H,0,-0.8037061145,1.3858997476,-1.5364258553
H,0,-0.253607702,-1.870088511,0.2254629811
H,0,1.1765275497,0.8183672205,-0.4407968881
H,0,2.0264766964,-2.0465157543,0.2929571977
C,0,3.5802700705,-0.5953790489,-0.0457187325
C,0,4.5664111229,-1.5528119135,0.2358504389
C,0,3.9728339014,0.7085216246,-0.3918942714
C,0,5.9118841367,-1.2189245759,0.1756050766
C,0,5.3156916163,1.0383600738,-0.4511392141
C,0,6.2868599225,0.0763903361,-0.1674699412
H,0,4.2686093445,-2.5610225309,0.5023350982
H,0,3.2307447272,1.4649894618,-0.6163639426
H,0,6.6657719516,-1.9650866336,0.3931397594
H,0,5.6126052,2.0447086427,-0.7189544166
H,0,7.3366118925,0.3402593953,-0.2153433692
H,0,-3.2991386428,2.3136877745,-0.3845086737
H,0,-3.1081833397,1.6152901444,-1.9929413361
H,0,-1.0570908472,1.8365417042,0.1657965859

TS-3 10 and 2 (SR), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1897.77663963 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.556959 a.u.
1 imaginary frequency = 228.3574 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1898.3555511 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1898.3869674 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1899.3791878 a.u.

1; 1
C,0,2.7903690934,0.1409834154,-1.2356929778
C,0,2.6271262803,-1.2315999099,-1.1011285592
C,0,2.5049691868,-1.8121414997,0.1658521576
H,0,2.8131695589,0.7503293894,-0.3361018726
H,0,2.6216408503,-1.858271169,-1.9844981961
H,0,2.3762846669,-1.1327646083,1.0047230749
C,0,4.0514310675,-0.5019448003,3.3356301035
C,0,3.8130085503,0.2988479419,4.4473668078
C,0,4.7080830135,0.0209453185,2.2144678338
H,0,3.3001552107,-0.1147117088,5.310300193
C,0,4.2329709124,1.6275039591,4.4549734616
C,0,5.1273196579,1.3563685097,2.2335328811
H,0,4.0492608265,2.2495954732,5.3258334954
H,0,5.64850393,1.7430063396,1.3637085031
C,0,4.8929613782,2.1546057508,3.3462136002
H,0,5.2281512008,3.1874391318,3.3524588188
H,0,3.7197208695,-1.5359864063,3.350801419
C,0,4.9933564464,-0.7741626857,0.9838923951
O,0,5.4356568298,-0.2127280174,-0.039736427
C,0,4.6691016463,-2.1611646332,0.9435343695
H,0,4.5625823146,-2.7865964825,1.8232357684
S,0,5.3828289478,-2.9603841468,-0.449292682
C,0,7.1718812168,-2.7341182352,-0.3013498846
H,0,7.3492039744,-1.6646255041,-0.4098922072
H,0,7.5105468056,-3.0955577705,0.6703966126
H,0,7.6435040664,-3.286369093,-1.1162564953
C,0,5.2354605021,-4.6972165456,0.0059733469
H,0,4.1734909851,-4.9375360055,0.0659897892
H,0,5.7012844011,-5.2829259533,-0.7882194825
H,0,5.7323869238,-4.8792130628,0.9603341264
C,0,1.9646393968,-3.159668518,0.3938799425
C,0,1.7993091761,-4.0978756097,-0.6369742343
C,0,1.5702236891,-3.5160147228,1.6927833633
C,0,1.2728304571,-5.3568812421,-0.3685697894
C,0,1.0410119842,-4.7717766805,1.958813321
C,0,0.8954531447,-5.6995474591,0.9286139201
H,0,2.0767693251,-3.8503747416,-1.6568925086
H,0,1.675417457,-2.7926321268,2.4976538533
H,0,1.1495404688,-6.0705655265,-1.1773363679
H,0,0.7376178894,-5.027053242,2.9694314064
H,0,0.4816065716,-6.681952998,1.1337339212
N,0,2.8838724614,0.8119199479,-2.3746223364
C,0,3.1529531434,2.275827962,-2.4115279247
C,0,2.8995998447,0.1975804303,-3.6932127918
C,0,1.9274010607,3.0689339592,-1.9646222722
C,0,4.383477785,2.6264032876,-1.5796535257
N,0,3.4237266395,2.46082327,-3.8325258344
H,0,3.6767742724,-0.5770489343,-3.7332385341
C,0,3.3141602983,1.3489725256,-4.5908287901
C,0,1.5660581119,-0.4082521554,-4.1804894582
H,0,1.6811464223,2.8281889949,-0.9268587153
H,0,2.1358226582,4.1411324665,-2.0100435677
H,0,1.0667425271,2.8413973596,-2.5968197362
H,0,4.1974313463,2.4680150299,-0.5154620369
H,0,5.2377496584,2.0154927558,-1.8776968533

TS-3 10 and 2 (SR), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1899.38353507 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.557167 a.u.
Thermal correction to Gibbs Free Energy at 20 °C = 0.558903 a.u.
1 imaginary frequency = 273.6841 i cm⁻¹

1; 1
C,0,2.663272038,0.107942726,-1.1378950443
C,0,2.531689452,-1.2751798999,-1.0702545392
C,0,2.3988915214,-1.8987624549,0.1697636508
H,0,2.6166728466,0.678414563,-0.2122729724
H,0,2.6064008148,-1.8622457586,-1.9740668657
H,0,2.1886080238,-1.2625897606,1.0248544915
C,0,3.9192780457,-0.158415177,3.0038203704
C,0,3.759571252,0.7877635798,4.0101614404
C,0,4.7277740003,0.1178495183,1.8973814399
H,0,3.1245686049,0.5680161204,4.859864098
C,0,4.4159057181,2.0124420132,3.9255937732
C,0,5.3811294116,1.3504380825,1.8193752771
H,0,4.294641532,2.747181916,4.7126624068
H,0,6.0101558318,1.5525908231,0.9604462808
C,0,5.2307183961,2.2909056892,2.8308118139
H,0,5.7495206872,3.240014985,2.7675923005
H,0,3.4030308067,-1.1080711022,3.0884707008
C,0,4.9208611434,-0.8488761776,0.7687568157
O,0,5.3123263101,-0.4432775465,-0.3349809507
C,0,4.5269800933,-2.2027147044,0.9587575723
H,0,4.4489504066,-2.6594582477,1.9372598765
S,0,5.102454581,-3.2983936252,-0.301632603
C,0,6.9022107019,-3.0878731376,-0.3554963719
H,0,7.0813862372,-2.0846531633,-0.7340681937
H,0,7.309060714,-3.2172438548,0.6454926914
H,0,7.287156924,-3.8379020389,-1.0456458062
C,0,5.000416143,-4.8870760517,0.5534382971
H,0,3.951361449,-5.0891766197,0.76272162
H,0,5.4000274866,-5.6394299336,-0.1238869462
H,0,5.5842485455,-4.8351562855,1.4711208316
C,0,1.9591894668,-3.3010639103,0.3183354423
C,0,1.8822398293,-4.1804252623,-0.7680787595
C,0,1.618892828,-3.7728070073,1.5928864221
C,0,1.4949617814,-5.5032524785,-0.5773889555
C,0,1.2300458022,-5.0913310954,1.7820147079
C,0,1.1740649383,-5.9637667885,0.6956121794
H,0,2.1202635059,-3.844454546,-1.7697080862
H,0,1.6634739254,-3.0962590809,2.4405646186
H,0,1.4409464833,-6.1729925855,-1.4271046376
H,0,0.968441988,-5.4401138786,2.7735171965
H,0,0.8725239331,-6.9938873865,0.8411445354
N,0,2.8148564998,0.8201410409,-2.2364431209
C,0,3.0462437227,2.2927357448,-2.2074422953
C,0,2.9619912276,0.2428896748,-3.5681816957
C,0,1.7766102584,3.0508617414,-1.8279591041
C,0,4.2047982364,2.6296639339,-1.2726995542
N,0,3.4159514869,2.5293915326,-3.601690733
H,0,3.7549552826,-0.5125350524,-3.560313909
C,0,3.4119111099,1.4389295652,-4.3942676057
C,0,1.6673033447,-0.3501212092,-4.166239814
H,0,1.4166702927,2.7080409354,-0.8555974748
H,0,1.9957925546,4.1171325345,-1.745022252
H,0,0.9942853074,2.8989704012,-2.5724235584
H,0,3.9217898695,2.462005627,-0.232050724
H,0,5.0723458089,2.0100103382,-1.5033247274

H,0,4.6274234177,3.6831460292,-1.7140032316
C,0,3.7465578004,3.7458982055,-4.4054430317
O,0,3.4803965857,1.2647214727,-5.7972749651
H,0,1.7457228689,-0.6818755371,-5.2256838283
H,0,1.3620657376,-1.3343072168,-3.6374703309
C,0,0.3849351858,0.5185269102,-4.0701538982
H,0,4.6844473655,4.1389159189,-4.0027504693
H,0,3.8566380263,3.5948415861,-5.4797904222
H,0,2.9456447125,4.4688257306,-4.2264087679
C,0,0.1437250921,1.4913769169,-5.0469228548
C,0,-0.4815663178,0.4362796877,-2.9759810343
C,0,-0.9291998665,2.3696675694,-4.9227471723
H,0,0.8033888864,1.5578755736,-5.9082218294
C,0,-1.5578590197,1.3115337907,-2.852185656
H,0,-0.3121169808,-0.3224752253,-2.2152526142
C,0,-1.7816674193,2.2839915432,-3.8237703053
H,0,-1.1049480759,3.1174229095,-5.6907628748
H,0,-2.2236628487,1.2313993982,-1.9976231411
H,0,-2.6216502537,2.9659937128,-3.7299909967

H,0,4.4629067646,3.6847422045,-1.3745736924
C,0,3.6396676002,3.8664505221,-4.117813887
O,0,3.671496244,1.3946389264,-5.5809631416
H,0,1.8954032615,-0.5753214319,-5.2108452151
H,0,1.4256363353,-1.2906011796,-3.670669063
C,0,0.50229663,0.6004861933,-4.0629395441
H,0,4.4269040787,4.3731883054,-3.5582350354
H,0,3.9475034711,3.7676559612,-5.1567830638
H,0,2.7196915913,4.4537237046,-4.0703839512
C,0,0.3389747544,1.6303303897,-4.9933154874
C,0,-0.3982372436,0.5002279972,-3.0013847456
C,0,-0.6963689006,2.549591453,-4.8546784421
H,0,1.0267101016,1.7096451333,-5.8292964083
C,0,-1.4384536823,1.4151737767,-2.8642259506
H,0,-0.2822746538,-0.300332701,-2.2764718686
C,0,-1.5855301593,2.4460999817,-3.7877317983
H,0,-0.8135990239,3.3422101198,-5.5844047824
H,0,-2.1329534644,1.3235264734,-2.0373423237
H,0,-2.3935759066,3.160147905,-3.6820751493

TS-3 10 and 2 (SS), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -1897.77054661 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.555631 a.u.
1 imaginary frequency = 166.6251 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1898.3500129 a.u.
1;

1;
C,0,1.9275568141,0.3187508414,-0.7264113519
C,0,2.032450566,-1.0549455668,-0.5840115677
C,0,2.1852574991,-1.6120092619,0.6938168592
H,0,2.0150387705,0.9333173377,0.1677204266
H,0,1.9886834166,-1.6959516318,-1.4568501411
H,0,2.0914346171,-0.9270967399,1.5318338744
C,0,4.3885496837,1.3053922625,2.1874313427
C,0,4.0995735795,2.5935011419,2.6289044853
C,0,4.139450154,0.2027357699,3.014140487
H,0,4.3191326712,3.4452366372,1.9915841855
C,0,3.5487365598,2.7928290487,3.8933967545
C,0,3.6037933561,0.41552901,4.289342305
H,0,3.3233949368,3.7986042522,4.2351899505
H,0,3.4371983182,-0.4467426942,4.9271014413
C,0,3.3018254265,1.7005971737,4.7231862776
H,0,2.8796437438,1.852818248,5.7119485606
H,0,4.844092318,1.1708665537,1.2105742653
C,0,4.4383126297,-1.2074223414,2.6160107337
O,0,4.5184639195,-2.096873254,3.484547654
C,0,4.5340153537,-1.5411268868,1.2296321924
H,0,4.7978967649,-0.8426114048,0.4440754716
S,0,5.1094128382,-3.1798331829,1.0165437873
C,0,5.348792624,-3.2378764312,-0.7650675023
H,0,4.3667798752,-3.1480225102,-1.2297836701
H,0,6.0040077178,-2.4275316945,-1.0894342432
H,0,5.7815994676,-4.2072936974,-1.0152649674
C,0,6.8249068533,-3.1989737722,1.596868827
H,0,6.7723896144,-3.0112965,2.6695292231
H,0,7.2360733213,-4.1922704015,1.4062604017
H,0,7.4020650854,-2.4255983681,1.0887150008
C,0,1.9352808257,-3.013052886,1.0148856989
C,0,1.8001073979,-4.0055909263,0.0275486945
C,0,1.7980764179,-3.38314509,2.364263305
C,0,1.5393717535,-5.3218226717,0.3817621089
C,0,1.5332100412,-4.7006301657,2.713998123
C,0,1.4048266965,-5.6731440777,1.7250673305
H,0,1.8806122831,-3.7511827352,-1.0251056013
H,0,1.9043946571,-2.6290083954,3.1371796409
H,0,1.4310216491,-6.0763566346,-0.3911145841
H,0,1.4256541968,-4.9688873076,3.7601642436
H,0,1.1953245935,-6.7028900774,1.9980231092
N,0,1.7270521729,0.9905582985,-1.8520308701
C,0,1.7565873872,2.4783706575,-1.9012166279
C,0,1.5554716892,0.3808052386,-3.1619347517
C,0,0.5560744364,3.079290291,-1.1749807823
C,0,3.0759619326,3.0075329799,-1.3414105528
N,0,1.6845634209,2.6987937436,-3.339595928
H,0,2.4154521661,-0.2609793353,-3.3933407316
C,0,1.5833195795,1.5806896036,-4.091288242
C,0,0.2579474289,-0.4298160307,-3.3662478078
H,0,0.5768929943,2.8052470813,-0.1166107324
H,0,0.5920890941,4.170449992,-1.2305386175
H,0,-0.3784774221,2.726111351,-1.6151826278
H,0,3.1538929049,2.8113674169,-0.2691323822
H,0,3.9224734509,2.5472917961,-1.857116846

TS-3 10 and 2 (SS), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -1899.37341691 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.556033 a.u.
1 imaginary frequency = 234.3536 i cm⁻¹

1;
1;
C,0,1.9273338521,0.2748607817,-0.6988904208
C,0,2.0241808922,-1.1033682149,-0.5687460516
C,0,2.1752051327,-1.6546894828,0.7066786882
H,0,2.0091988886,0.8835651522,0.2010570016
H,0,2.0055075533,-1.7350237939,-1.4465521578
H,0,2.0454046835,-0.9754311944,1.5441103406
C,0,4.3195866766,1.3078056294,2.0602484733
C,0,3.9195104987,2.5987988883,2.393681388
C,0,3.9817941403,0.2339145488,2.8886672076
H,0,4.2130061268,3.4346194201,1.7690212098
C,0,3.160241823,2.8223723581,3.5385868611
C,0,3.2360516652,0.4681516836,4.0460790802
H,0,2.8477812585,3.8280040226,3.7936264859
H,0,2.9941686961,-0.3712308398,4.6875290772
C,0,2.8163384194,1.7541357406,4.3635141123
H,0,2.2305488153,1.9265149116,5.2584421859
H,0,4.9256378855,1.1512373422,1.1743236411
C,0,4.3785210677,-1.1828774972,2.5882966098
O,0,4.470237946,-2.010638552,3.5036423145
C,0,4.5051681986,-1.5603017749,1.2191204466
H,0,4.7520239079,-0.8779601324,0.4181126788
S,0,5.0970614732,-3.2005664243,1.0257715513
C,0,5.305519772,-3.2552709462,-0.7640451171
H,0,4.3149983031,-3.1563364062,-1.2042193069
H,0,5.9562708172,-2.4407723394,-1.0792302246
H,0,5.7328796953,-4.2223915838,-1.0218520627
C,0,6.8267730089,-3.1639519676,1.5703751856
H,0,6.7958245621,-2.9587658842,2.6387469091
H,0,7.254034868,-4.1483492208,1.3828449328
H,0,7.3585500063,-2.3837759683,1.0297115832
C,0,1.9938954519,-3.0717786353,1.0232171992
C,0,1.9159383218,-4.0614608206,0.0318418607
C,0,1.922129886,-3.453340173,2.3703872299
C,0,1.7841881555,-5.3971834148,0.3833778873
C,0,1.7895103003,-4.7906134729,2.7184214257
C,0,1.7254690978,-5.7648160784,1.7267167216
H,0,1.9425665036,-3.7955935123,-1.0186475026
H,0,1.9832990504,-2.6964678686,3.1436127467
H,0,1.7183020187,-6.1531985857,-0.389607446
H,0,1.7381106289,-5.0722149354,3.7629387979
H,0,1.6220796625,-6.8087743743,1.9971053851
N,0,1.7456755731,0.9424417167,-1.8228483264
C,0,1.7789660176,2.4323262308,-1.883333594
C,0,1.5621662152,0.3210102899,-3.1309649486
C,0,0.6073111901,3.0541547432,-1.1283943467
C,0,3.1207208928,2.94290338,-1.3615271131
N,0,1.6679762062,2.64212252,-3.3240107329
H,0,2.409774211,-0.3298476214,-3.3668758206
C,0,1.5777029613,1.5204377448,-4.0671475337
C,0,0.2362664791,-0.4560527865,-3.2913448156
H,0,0.6233986434,2.7340075678,-0.0843075966
H,0,0.6977750872,4.1419036733,-1.1424249663
H,0,-0.3431467103,2.7642219609,-1.5775393872
H,0,3.218794587,2.725552681,-0.2969859383
H,0,3.941910722,2.4744374395,-1.9064642063

H,0,3.128314473,4.0908715101,-1.4735947809
C,0,1.6734985772,4.0177995844,-3.9275147111
O,0,1.4959616765,1.5196729113,-5.3066059234
H,0,0.2462875625,-0.680196207,-4.4323238682
H,0,0.3214672439,-1.3714487998,-2.8152960504
C,0,-0.9964346869,0.3058570925,-2.9766496549
H,0,2.5990335762,4.559289625,-3.7122408874
H,0,1.5842637291,3.882919564,-5.0058880347
H,0,0.8213631668,4.6018968328,-3.5688817907
C,0,-1.584642175,1.2328742364,-3.8447151872
C,0,-1.5822428219,0.0908453023,-1.7255669066
C,0,-2.7222666996,1.9382612589,-3.4620997246
H,0,-1.1455291042,1.400407445,-4.8247781387
C,0,-2.7220968436,0.7934696236,-1.3425221919
H,0,-1.1418991554,-0.6365393133,-1.047240806
C,0,-3.292345979,1.7229043845,-2.2088416095
H,0,-3.1692980503,2.6521360114,-4.1479210454
H,0,-3.1667116097,0.6119111065,-0.3682485518
H,0,-4.1824751238,2.2702497777,-1.9130007686

H,0,3.1807583531,4.0251564099,-1.482619858
C,0,1.5743729485,3.9716509279,-3.8982376624
O,0,1.4795010548,1.4469802668,-5.2756890771
H,0,0.1648352396,-0.7077954719,-4.3521228566
H,0,0.2819965161,-1.3905649232,-2.7315834322
C,0,-0.9551128641,0.3537097273,-2.8468668302
H,0,1.5408225298,3.8578711968,-4.9797864559
H,0,0.6632136241,4.4701016699,-3.5608443046
H,0,2.4429421247,4.5744177299,-3.6284842699
C,0,-1.5207788247,1.3119895429,-3.692068785
C,0,-1.4728453608,0.1973745183,-1.560016423
C,0,-2.5733532921,2.1084418384,-3.2517684901
H,0,-1.1335229002,1.4325375066,-4.6989105628
C,0,-2.5298687073,0.9893203686,-1.1195459383
H,0,-1.0440956265,-0.5503572425,-0.899005753
C,0,-3.0775775713,1.9515035633,-1.9628193203
H,0,-3.0041154848,2.846689287,-3.9180334427
H,0,-2.9254248637,0.8550804615,-0.1195486123
H,0,-3.8999286821,2.5693186981,-1.6222535279

TS-3 12 and 2 (SR), optimization in solv. CHCl₃
PBE1PBE/6-311G(d,p), E = -1495.05561226 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.409512 a.u.
1 imaginary frequency = 265.0858 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1495.4874374 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1495.5131333 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1496.261943 a.u.

1; 1
C,0,2.6637594355,0.1834299337,-0.8788730702
C,0,2.5927986415,-1.2000681028,-0.9399693436
C,0,2.4750885222,-1.945356964,0.2434846834
H,0,2.6205266631,0.65320232,0.101560049
H,0,2.6712538067,-1.7089404525,-1.8929872088
H,0,2.223977228,-1.390944042,1.1448589382
C,0,3.9761228349,-0.5179716369,3.4960520496
C,0,3.6606889186,0.3244143693,4.5568859953
C,0,4.5066967237,0.0064736099,2.3104964997
H,0,3.2519962735,-0.0919737257,5.4724829013
C,0,3.8717081313,1.6972961227,4.4475626381
C,0,4.7173934893,1.3878231071,2.2124578112
H,0,3.6267839516,2.3518951019,5.2786499259
H,0,5.1373692037,1.7771157905,1.2903724911
C,0,4.4019080873,2.2279565043,3.2725995099
H,0,4.5721631086,3.296974412,3.1864407297
H,0,3.8113742258,-1.5850712529,3.6088593702
C,0,4.865313914,-0.8242721429,1.1234977654
O,0,5.3398469472,-0.2870503172,0.1041785369
C,0,4.5351591886,-2.2145143364,1.095314828
H,0,4.4000498153,-2.8159467024,1.9883077535
S,0,5.3456904879,-3.0564420147,-0.2253750393
C,0,7.1170720049,-2.7682949173,0.0023547964
H,0,7.2747868427,-1.7031989884,-0.1630029286
H,0,7.411957304,-3.0593559946,1.011338463
H,0,7.6444056868,-3.3570427215,-0.750534323
C,0,5.2331758918,-4.7747061223,0.3064462005
H,0,4.179643322,-5.054705536,0.320764816
H,0,5.76374504,-5.3773470092,-0.4325478455
H,0,5.6848730321,-4.8909366146,1.2929035417
C,0,2.0225483964,-3.3487603665,0.2614605519
C,0,1.9794142222,-4.1466820831,-0.8916398352
C,0,1.6014033306,-3.9089593193,1.4773929155
C,0,1.542476635,-5.4661404587,-0.8235093519
C,0,1.1627341323,-5.2247699337,1.5441628737
C,0,1.1361497777,-6.010933481,0.3926902002
H,0,2.2839463774,-3.7431445007,-1.8519869904
H,0,1.6180576824,-3.2993209358,2.3773555253
H,0,1.5142285711,-6.068903175,-1.7261395182
H,0,0.8371610144,-5.6378343848,2.4940100567
H,0,0.7932919267,-7.0397926002,0.4420839498
N,0,2.7379110486,1.0480662476,-1.883587774
C,0,2.8441544293,0.6680988309,-3.2858709974
C,0,2.9415526762,2.4718423922,-1.6365065857
C,0,1.9726863585,1.5881355003,-4.1318725444
H,0,2.5214144215,-0.3648541827,-3.4184788873
H,0,3.8932307617,0.7507732828,-3.5975056075
H,0,2.7185003828,2.6912925771,-0.589691251
H,0,3.9951754839,2.7153909893,-1.8270809011
C,0,2.0556120351,3.2909948425,-2.5618093393
H,0,2.1442934229,1.3845772297,-5.1914611299
H,0,0.9114146623,1.4005840093,-3.904877468
O,0,2.2888234465,2.9447622991,-3.9102763745
H,0,2.2874411814,4.3532669725,-2.4549625803
H,0,0.9971079004,3.132418571,-2.3031651931

TS-3 12 and 2 (SR), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1496.26386499 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.409056 a.u.
Thermal correction to Gibbs Free Energy at 20 °C = 0.410460 a.u.
1 imaginary frequency = 312.7035 i cm⁻¹

1; 1
C,0,2.5711581054,0.1757203913,-0.7777895642
C,0,2.5012721355,-1.2076378066,-0.8864876609
C,0,2.4127577145,-1.9724029979,0.2831076133
H,0,2.5207618981,0.607894395,0.219860983
H,0,2.5922568642,-1.6888801669,-1.8492797763
H,0,2.1462441097,-1.4468063139,1.195820638
C,0,3.8799063835,-0.4121560483,3.3318342388
C,0,3.554013904,0.4759240238,4.3507294974
C,0,4.4797434176,0.0509663017,2.1571808468
H,0,3.0904775455,0.107168421,5.257674392
C,0,3.8240884257,1.8337191834,4.2065946466
C,0,4.7473765486,1.4164523611,2.0210420373
H,0,3.5709744189,2.5235643582,5.0027844238
H,0,5.2164777905,1.7646758663,1.1084908197
C,0,4.4227110721,2.3029196241,3.0398150576
H,0,4.6388166489,3.3586000285,2.9271248024
H,0,3.6618484048,-1.4644357722,3.4690493271
C,0,4.824911823,-0.8427820043,1.0030707724
O,0,5.2549144769,-0.355621123,-0.0498757517
C,0,4.4826385202,-2.226998474,1.0745639974
H,0,4.3912605502,-2.7650401579,2.0092039158
S,0,5.1927865985,-3.1948943014,-0.226098314
C,0,6.978678381,-2.8911886361,-0.1452901372
H,0,7.1298408524,-1.8617489187,-0.4591253007
H,0,7.3226810891,-3.0526820712,0.8746346383
H,0,7.449140699,-3.5839922797,-0.8423751898
C,0,5.1294378971,-4.846979881,0.504827437
H,0,4.0837546132,-5.1042839293,0.6643323663
H,0,5.5789404293,-5.5317714122,-0.2119074999
H,0,5.6827567155,-4.8425712508,1.4426175891
C,0,2.0333501966,-3.40263839,0.2719361512
C,0,2.0590436451,-4.1743440982,-0.8954361944
C,0,1.6555657328,-4.0127847799,1.4749693973
C,0,1.7332483486,-5.5266002215,-0.8536883877
C,0,1.3275242584,-5.3608627925,1.5153955762
C,0,1.3726163937,-6.1247137077,0.3496329411
H,0,2.3348315731,-3.7299575026,-1.8436516758
H,0,1.6221173371,-3.4219720906,2.3852222784
H,0,1.7583598901,-6.1121073227,-1.7648192365
H,0,1.0347360698,-5.8172459669,2.4532125632
H,0,1.1191341559,-7.1775132148,0.3791765218
N,0,2.6697189123,1.0695885255,-1.747041746
C,0,2.8302721903,0.7177877381,-3.1568764134
C,0,2.9457457981,2.4761766052,-1.4425472394
C,0,2.0686751643,1.715657636,-4.0213845489
H,0,2.4411199173,-0.2825656534,-3.3343605965
H,0,3.8981071764,0.73709023,-3.4016500481
H,0,2.670727801,2.6774491597,-0.4068734144
H,0,4.0206620869,2.6510599118,-1.5668069479
C,0,2.1677860387,3.3742032883,-2.392228791
H,0,2.2859282013,1.5328259316,-5.072917223
H,0,0.9896767164,1.6007093626,-3.8531384599
O,0,2.4585297866,3.0439844243,-3.7367212801
H,0,2.4572639267,4.413717003,-2.2439413366
H,0,1.0906906496,3.2708745158,-2.2082737354

TS-3 12 and 2 (SS), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1495.05026051 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.408332 a.u.
1 imaginary frequency = 220.9998 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1495.4818226 a.u.
1; 1
C,0,1.8217825551,0.3333132378,-0.4492583382
C,0,1.9793038168,-1.0425187618,-0.4512422191
C,0,2.1910517861,-1.7061639812,0.7682903967
H,0,1.8897609278,0.8486853925,0.5066146853
H,0,1.9469348347,-1.6039067753,-1.3779489682
H,0,2.0959482438,-1.0929177511,1.6602172471
C,0,4.4849430763,1.2692115187,1.4923104208
C,0,4.2882047577,2.6358070762,1.6716003396
C,0,4.2945058765,0.3818646721,2.5592380572
H,0,4.4543493418,3.3180419001,0.8430626271
C,0,3.8940286395,3.128049284,2.9139793551
C,0,3.9126683064,0.888858981,3.807040045
H,0,3.7420567697,4.194408712,3.0522088876
H,0,3.7846441047,0.1900433679,4.6274634666
C,0,3.7072809817,2.251303779,3.982208544
H,0,3.4053834941,2.6332221075,4.9527771464
H,0,4.813332742,0.9061649844,0.523297952
C,0,4.4918061153,-1.094602364,2.4446652048
O,0,4.585792915,-1.7957546558,3.4680407392
C,0,4.4751379073,-1.7043812484,1.1449937955
H,0,4.7571109418,-1.1800553534,0.2389598466
S,0,5.0322308823,-3.3680224693,1.2332662182
C,0,5.2440123448,-3.7669271415,-0.5081075284
H,0,4.2533243112,-3.7947470522,-0.9618363807
H,0,5.8780198941,-3.0247607312,-0.9970938522
H,0,5.6972184157,-4.7573689642,-0.5660350417
C,0,6.7591850571,-3.3045571686,1.7751185545
H,0,6.7366228383,-2.9219431521,2.7955446669
H,0,7.1485657231,-4.324579808,1.760900199
H,0,7.3368320148,-2.6506682742,1.1208384065
C,0,1.8987735078,-3.1258876933,0.9934765892
C,0,1.6569855086,-4.0290712586,-0.0543935985
C,0,1.818822715,-3.5945797195,2.3156627734
C,0,1.3498239844,-5.3572573959,0.2140820566
C,0,1.5069723537,-4.9218319086,2.5809161036
C,0,1.2725537892,-5.8074739044,1.5313062286
H,0,1.6868658764,-3.6939155001,-1.0868958581
H,0,2.0149372739,-2.909337697,3.1354881604
H,0,1.1584672482,-6.0414152319,-0.6069483775
H,0,1.445524702,-5.2654804303,3.6087921451
H,0,1.025184461,-6.8443085224,1.7377346102
N,0,1.5838363038,1.1409828458,-1.4769087242
C,0,1.4311844009,0.7048803521,-2.858985212
C,0,1.4874198706,2.5868931022,-1.3039076199
C,0,0.1659350252,1.3199132991,-3.4478952119
H,0,1.3733167427,-0.3823622907,-2.9076105898
H,0,2.3066595591,1.0358126954,-3.4314772557
H,0,1.5030694319,2.8269868846,-0.2384173524
H,0,2.3570352118,3.05593213,-1.781802977
C,0,0.2150198899,3.1014268244,-1.9615429124
H,0,0.1081810083,1.0917672309,-4.5147911473
H,0,-0.7173020294,0.8934178032,-2.9475824368
O,0,0.1731243825,2.7244000072,-3.3211158547
H,0,0.1925582284,4.1931862772,-1.9271433916
H,0,-0.6650570614,2.7122058225,-1.4265326208

TS-3 12 and 2 (SS), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1496.26323763 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.410644 a.u.
1 imaginary frequency = 292.5324 i cm⁻¹
1; 1
C,0,1.5927688293,0.3395429648,0.4643440531
C,0,1.9002073665,-0.9112847604,-0.062013688
C,0,2.1901987693,-1.9608151207,0.8148826511
H,0,1.5361574705,0.4274583046,1.5479634652
H,0,1.9402359777,-1.0801514196,-1.1293507684
H,0,1.9407820674,-1.8097748619,1.8640704945
C,0,4.7194918827,0.4540626747,-0.2135024126
C,0,4.7962959016,1.600465639,-0.9955134969
C,0,4.5041823435,0.5537958289,1.1643448073
H,0,4.9582118784,1.5150013004,-2.063663202
C,0,4.6565979803,2.8556602994,-0.4088631287
C,0,4.3712780248,1.8177994811,1.7462745253
H,0,4.7109319598,3.7488120527,-1.0210020712
H,0,4.1976883214,1.880728414,2.8137440794
C,0,4.4495442153,2.9632407379,0.9648990474
H,0,4.3454786373,3.9397590765,1.4233834431
H,0,4.8052041225,-0.5133350325,-0.6932632757
C,0,4.3097733012,-0.6413872115,2.0421287832
O,0,3.9932132619,-0.497442447,3.2304368756
C,0,4.3557232931,-1.9385809982,1.4375883099
H,0,4.9279649486,-2.1492507987,0.5439197519
S,0,4.4216973144,-3.2378015235,2.6389933352
C,0,5.0534809967,-4.6156061725,1.6562264598
H,0,4.285175396,-4.9072611367,0.9435435898
H,0,5.9674230591,-4.3064118746,1.1509458581
H,0,5.2491592782,-5.4318801601,2.3496315161
C,0,5.8903237637,-2.88562316,3.6452768885
H,0,5.6756021685,-1.9693664495,4.1892243276
H,0,6.0167836913,-3.7221320814,4.3312371888
H,0,6.7508449482,-2.7704808854,2.9888134884
C,0,2.1537530414,-3.3651245736,0.3576751347
C,0,2.6386235097,-3.7409426232,-0.9007943106
C,0,1.6204115306,-4.3432142625,1.2025060444
C,0,2.591903036,-5.068822669,-1.3015881668
C,0,1.5701213991,-5.6744278991,0.7967241975
C,0,2.0579685831,-6.0399356974,-0.4532292737
H,0,3.0763472897,-2.9957813556,-1.5569803223
H,0,1.2377367623,-4.058007081,2.1766401553
H,0,2.9755896078,-5.352222763,-2.2742533679
H,0,1.1501000908,-6.4224293345,1.4582245703
H,0,2.0234803056,-7.0755423231,-0.769179312
N,0,1.3601284954,1.4673421996,-0.1813526976
C,0,1.3398321071,1.6097404803,-1.6370621835
C,0,0.897845982,2.6750483392,0.5062042401
C,0,-0.0721214039,1.9965897287,-2.0677456593
H,0,1.6620588553,0.6887381136,-2.1163770654
H,0,2.0380264856,2.4076697254,-1.9036543017
H,0,0.8845171161,2.4983315095,1.5817261203
H,0,1.5992441514,3.4840034992,0.2834247479
C,0,-0.4930159366,3.0323445985,-0.0097598802
H,0,-0.0983685172,2.1935221376,-3.1387041893
H,0,-0.7688431806,1.1809718116,-1.8334355943
O,0,-0.4797279665,3.1849653724,-1.4166349266
H,0,-0.8198021818,3.9819815261,0.4123092095
H,0,-1.2062963317,2.2474653738,0.2752399352

TS-3 13 and 2 (SR), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1419.92832159 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.405103 a.u.
1 imaginary frequency = 271.9141 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1420.3140256 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1420.339224 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1421.0552309 a.u.
1; 1
C,0,2.8263191419,1.9533740665,-4.0330892466
N,0,2.7503258497,1.0726222817,-1.8520386318
C,0,2.6703037824,0.2447290608,-0.8261118136
C,0,2.5933323646,-1.1398085808,-0.8973081923
C,0,2.4837238157,-1.906077268,0.273105248
H,0,2.6325995764,0.7265277158,0.1490516684
H,0,2.6397626726,-1.6228758024,-1.8668814584
H,0,2.2553784125,-1.3623826814,1.1871929611
C,0,4.057546015,-0.5769220714,3.5221168437
C,0,3.7803214848,0.2556240204,4.6012094504
C,0,4.5939370542,-0.048306984,2.3409327182
H,0,3.3665548862,-0.1638006058,5.5131482328
C,0,4.0362250743,1.6225149155,4.5148557748
C,0,4.8510605918,1.3265977697,2.2664831202
H,0,3.8208843404,2.2693650635,5.3601012802
H,0,5.2792495928,1.7182978022,1.3491952157
C,0,4.5739529223,2.1568239765,3.3450184472
H,0,4.7799342413,3.220849025,3.2770958809
H,0,3.8592133331,-1.6401774874,3.6173733697
C,0,4.9122981354,-0.8683308379,1.1355760133
O,0,5.39692922,-0.3303112297,0.1222001154
C,0,4.5325328135,-2.2464436855,1.0862256609
H,0,4.3888468719,-2.8590290887,1.9702522677
S,0,5.3059891402,-3.0923496684,-0.254702412
C,0,7.0871467765,-2.8534052662,-0.0458712527
H,0,7.2719034006,-1.7923322625,-0.208336379
H,0,7.3852219398,-3.1568609756,0.9584725923
H,0,7.5900995158,-3.4535318576,-0.8063465552
C,0,5.15772228,-4.8136708119,0.2589256378
H,0,4.0973870596,-5.064362823,0.2947714354
H,0,5.6536334311,-5.4215004346,-0.4997607058
H,0,5.6286489372,-4.9552951168,1.2330952497
C,0,1.990354375,-3.2967606918,0.2700571224
C,0,1.9193767188,-4.0740366866,-0.8956069726
C,0,1.556989467,-3.863833822,1.4781616721
C,0,1.4441079748,-5.3811448926,-0.8469825378
C,0,1.0798414061,-5.167251592,1.5255836069
C,0,1.0261894116,-5.9336152027,0.3618577438
H,0,2.2319906846,-3.6632712392,-1.8503203035
H,0,1.5930371927,-3.2684604639,2.3871757005
H,0,1.3947043469,-5.9679721419,-1.7592007884
H,0,0.7450538485,-5.5856824563,2.4699062727
H,0,0.6531757535,-6.95257825,0.395978386
H,0,1.7929772684,2.2210195685,-4.2767122173
H,0,3.3848701374,1.8814955063,-4.9683526246
C,0,2.8296242628,2.5306241752,-1.7174855176
H,0,1.8241202661,2.9446169868,-1.5706128778
H,0,3.4447966226,2.7961882911,-0.8536865972
C,0,3.4169955048,2.9689843951,-3.0535085627
H,0,4.5082921492,2.88381095,-3.0276800194
H,0,3.16019088,4.0015761985,-3.2981484104
C,0,2.8540541835,0.6436393446,-3.2472759137
H,0,2.0289095898,-0.0289054609,-3.5026905212
H,0,3.7964492825,0.098287326,-3.3851111765

TS-3 13 and 2 (SR), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1421.05745503 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.405153 a.u.
Thermal correction to Gibbs Free Energy at 20 °C = 0.406512 a.u.
1 imaginary frequency = 323.9818 i cm⁻¹
1; 1
C,0,3.1578136226,2.196221435,-3.4812065628
N,0,2.5625463214,1.1292690854,-1.4640303311
C,0,2.396073843,0.2109421428,-0.5373808982
C,0,2.4067512954,-1.1648462802,-0.7413743673
C,0,2.4036466234,-2.0175284747,0.3706554436
H,0,2.233784938,0.5946682914,0.4684220782
H,0,2.5053665969,-1.5556179256,-1.7454368739
H,0,2.1810085335,-1.5534807031,1.3283614187
C,0,3.9660903222,-0.2613610941,3.0625633319
C,0,3.6559680826,0.7405590701,3.9756308176
C,0,4.6088010522,0.0539115329,1.861849927
H,0,3.1538617628,0.488560668,4.9016953053
C,0,3.9875656346,2.0639663876,3.699112148
C,0,4.9384534527,1.3858131603,1.5923209688
H,0,3.7459253759,2.8431272839,4.4121911617
H,0,5.434295892,1.6169256405,0.6566913873
C,0,4.6324675626,2.3851476293,2.5068248569
H,0,4.8949434061,3.4144572555,2.2920383036
H,0,3.6935280531,-1.2842562491,3.2965826506
C,0,4.9071855763,-0.9602472181,0.8015221714
O,0,5.3468151554,-0.5961508296,-0.2936670039
C,0,4.4950246153,-2.3175750638,1.0045509606
H,0,4.4459287986,-2.7771311493,1.9842770751
S,0,5.138900464,-3.3921031274,-0.2515137024
C,0,6.9390559254,-3.1780063112,-0.1887737458
H,0,7.1481024845,-2.1916139932,-0.5933629686
H,0,7.2706823268,-3.2648751384,0.8443977543
H,0,7.3729721207,-3.9562996554,-0.8152835667
C,0,5.0086545492,-5.0092479908,0.5422172079
H,0,3.9549299737,-5.2293456043,0.6981870341
H,0,5.4432639341,-5.7321681446,-0.1459728299
H,0,5.5535464994,-4.9912139809,1.484901512
C,0,2.0121284161,-3.4424356279,0.2897821522
C,0,1.9982839808,-4.1466933619,-0.9188637336
C,0,1.6512281343,-4.111288571,1.4660896936
C,0,1.6456810505,-5.4925712381,-0.9449657925
C,0,1.2910792969,-5.4521178858,1.4383612927
C,0,1.2939500294,-6.1489622969,0.2310215944
H,0,2.263008764,-3.6519600821,-1.8452574206
H,0,1.6586760017,-3.57125417,2.407843595
H,0,1.6405468048,-6.0274677258,-1.8869339114
H,0,1.009155233,-5.9548379449,2.3555698465
H,0,1.0165792987,-7.1959261921,0.2073324361
H,0,2.2170100359,2.5303449837,-3.924707039
H,0,3.9185913163,2.1829497986,-4.2599614534
C,0,2.6029593639,2.5740427832,-1.1917760404
H,0,1.5976171487,2.9949079491,-1.2867978502
H,0,2.9705027123,2.7478508656,-0.179215028
C,0,3.5233979931,3.0937627708,-2.2930635235
H,0,4.5665362301,2.9349324168,-2.0081289384
H,0,3.3713518516,4.1532572795,-2.4932194554
C,0,2.9738213626,0.8184794711,-2.8396947668
H,0,2.217948219,0.2084790607,-3.3381322022
H,0,3.9110769618,0.2522900686,-2.7909751188

TS-3 13 and 2 (SS), optimization in solv. CHCl₃
PBE1PBE/6-311G(d,p), E= -1419.92314775 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.404663 a.u.
1 imaginary frequency = 220.2903 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1420.308666 a.u.
1; 1
C,0,1.1953134007,1.8872791175,-3.6281572907
N,0,1.6262159965,1.1349209884,-1.4380055893
C,0,1.8305193263,0.3633971211,-0.3837516671
C,0,2.0199919196,-1.0100183695,-0.3968771693
C,0,2.2162398594,-1.696182663,0.8116586391
H,0,1.8345078961,0.8854299206,0.5712113655
H,0,2.0147546728,-1.5436218349,-1.3411846264
H,0,2.1019271276,-1.0995832205,1.7129614836
C,0,4.4833761169,1.2732878932,1.6061220758
C,0,4.2971151454,2.6377417476,1.8110533472
C,0,4.3046731435,0.3693907243,2.6610929389
H,0,4.4579936008,3.3335470682,0.9927138418
C,0,3.9225343384,3.1111874794,3.0666347448
C,0,3.9418422618,0.8574639096,3.92205822
H,0,3.7782100471,4.17585039,3.2246212641
H,0,3.8220658074,0.1457120797,4.7325505138
C,0,3.7450457585,2.2176230777,4.1223371081
H,0,3.4578030919,2.5847840489,5.1030024987
H,0,4.7951405654,0.9248829813,0.6264363168
C,0,4.5005511392,-1.1048428774,2.5211008344
O,0,4.5947843048,-1.823588017,3.5321898206
C,0,4.4874896912,-1.6919278184,1.2104372714
H,0,4.7745399269,-1.1497756578,0.3166612658
S,0,5.054457204,-3.3535714744,1.2704272165
C,0,5.2643532761,-3.7227792951,-0.4779370224
H,0,4.2725417731,-3.7499620491,-0.9294032956
H,0,5.8922545619,-2.968713398,-0.9564403441
H,0,5.7241481425,-4.7089772832,-0.5531538116
C,0,6.7820972521,-3.286140825,1.8092607904
H,0,6.7587565691,-2.9266293911,2.8380575993
H,0,7.1813613498,-4.3016738894,1.7712908037
H,0,7.35156254,-2.6119698301,1.1685440535
C,0,1.9231428147,-3.1217161158,1.0046402147
C,0,1.6708448022,-3.9963764064,-0.0645809488
C,0,1.8491918778,-3.6244982021,2.3145648061
C,0,1.362162312,-5.330633717,0.1710031577
C,0,1.5362668104,-4.9577149279,2.546987482
C,0,1.2932439184,-5.8153329963,1.476240397
H,0,1.6904847733,-3.632978418,-1.0877035962
H,0,2.0523336118,-2.9618003969,3.1511154973
H,0,1.1623580304,-5.9921204568,-0.6664784614
H,0,1.480432994,-5.3278320908,3.5659993294
H,0,1.0447766572,-6.856657607,1.6572628328
H,0,0.1055771071,1.9293794757,-3.7231590426
H,0,1.6204223768,1.8760625026,-4.6335331326
C,0,1.6939489313,3.054523674,-2.7742260802
H,0,2.7721467739,3.1930684561,-2.9073469962
H,0,1.197203331,3.9986324925,-3.0057424403
C,0,1.3999321704,2.5819188408,-1.3563312887
H,0,2.0488556986,3.0218946533,-0.5945902642
H,0,0.356192217,2.7784803584,-1.0809136117
C,0,1.6001583351,0.6541742379,-2.8210249927
H,0,0.8942600903,-0.1764101015,-2.9229533488
H,0,2.5982975596,0.2898540914,-3.0959027104

TS-3 13 and 2 (SS), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E= -1421.05766858 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.406395 a.u.
1 imaginary frequency = 312.3902 i cm⁻¹
1; 1
C,0,0.6025122931,2.7955060403,-1.8488648973
N,0,1.2545809013,1.354796293,-0.1006310508
C,0,1.5738582569,0.2788691886,0.5831696332
C,0,1.8606481227,-0.9746739532,0.0503796991
C,0,2.2150008705,-2.022221295,0.9082105754
H,0,1.6097295433,0.4096281396,1.6637521482
H,0,1.8409284267,-1.1292415034,-1.021146569
H,0,1.9967564346,-1.8820426113,1.9658586072
C,0,4.7199471016,0.4211188396,-0.2153009254
C,0,4.828461356,1.5653714805,-0.9971791977
C,0,4.5392997371,0.5265241588,1.1671926374
H,0,4.9680501586,1.4756033113,-2.0681536113
C,0,4.7533780763,2.8233770683,-0.4060917908
C,0,4.4655853263,1.7941475177,1.7526961577
H,0,4.8393468459,3.7148598506,-1.0169469846
H,0,4.3170241648,1.8624492103,2.8237315432
C,0,4.5734510477,2.9368184464,0.9712483885
H,0,4.5158244696,3.9159704552,1.4324128103
H,0,4.7583742117,-0.5479790195,-0.6972678431
C,0,4.3414702356,-0.6622623074,2.0517207169
O,0,4.0426284209,-0.5113029273,3.2431048656
C,0,4.3711293129,-1.9649963192,1.4537150897
H,0,4.9290935735,-2.1789736554,0.5517351579
S,0,4.474334011,-3.2575315224,2.6621141611
C,0,5.1146357267,-4.628989223,1.6758496956
H,0,4.3426937495,-4.9330540627,0.9723523972
H,0,6.0181601009,-4.3074755155,1.159748792
H,0,5.3300383542,-5.4405514589,2.3688464339
C,0,5.9493752358,-2.8818666954,3.6496622909
H,0,5.7280251998,-1.9697089874,4.1976568935
H,0,6.0957057063,-3.7175638514,4.3328752329
H,0,6.8004119673,-2.7535956632,2.9835076559
C,0,2.1768733896,-3.4252622556,0.4421452171
C,0,2.6367029811,-3.787618524,-0.8294175225
C,0,1.6752322153,-4.41495557,1.2925238407
C,0,2.598900373,-5.1139397685,-1.2368295176
C,0,1.6331711059,-5.7445670762,0.8801063542
C,0,2.0980542401,-6.0970461112,-0.3822357389
H,0,3.0478489655,-3.0327611943,-1.4917693242
H,0,1.3110116747,-4.1405163449,2.2767393505
H,0,2.9639610249,-5.3863884114,-2.2197615612
H,0,1.2375493309,-6.5016021235,1.5463889769
H,0,2.0708041614,-7.1313985372,-0.7030122233
H,0,-0.4895630887,2.7730939854,-1.8509049418
H,0,0.9384775214,3.1762284353,-2.8121134521
C,0,1.1086467734,3.6252207329,-0.6627411775
H,0,2.1622575678,3.8785565962,-0.8012207523
H,0,0.5441672404,4.5441715491,-0.5123724468
C,0,0.9635712972,2.6622760105,0.5116062921
H,0,1.6631539968,2.8484683806,1.3275327053
H,0,-0.0582158577,2.6623934974,0.9025329265
C,0,1.1493968966,1.3938876915,-1.5660283113
H,0,0.4898909444,0.596391951,-1.914513149
H,0,2.1440483067,1.2408176586,-1.9957732581

TS-3 12 and 2 (SR) counterion CCl_3COO^- ,optimization in solv. CHCl_3

M06-2X/6-311+G(d,p), E= -3103.68433913 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.417679 a.u.

Thermal correction to Gibbs Free Energy at 20 °C = 0.419391 a.u.

1 imaginary frequency = 294.7588 i cm^{-1}

0; 1

C,0,2.6168877143,0.3868149527,-0.9109450524
C,0,2.5885222311,-0.9953497178,-1.0484978061
C,0,2.4900620376,-1.7722871376,0.1122830618
H,0,2.6983909256,-1.4770987467,-2.0112868227
H,0,2.1802329968,-1.2487040904,1.0122633869
C,0,5.6761889649,0.3757105801,-0.2823184715
C,0,5.9524929319,1.4831233274,-1.0770888692
C,0,5.6998158122,-0.9094378628,-0.8283636827
H,0,5.9355653854,2.4728714582,-0.635287116
C,0,6.2383376131,1.3161079799,-2.4285031512
C,0,6.0014077982,-1.071581123,-2.1827943444
H,0,6.4477225774,2.1792020048,-3.0508281799
H,0,6.0229123905,-2.0737111308,-2.5953387178
C,0,6.260838434,0.0356498765,-2.9809222684
H,0,6.4833437763,-0.0969971044,-4.0334704498
H,0,5.4538846153,0.5313698022,0.7659277569
C,0,5.3848911236,-2.1294250645,-0.0158148851
O,0,5.8062121884,-3.2425659134,-0.3579794661
C,0,4.5042428986,-1.9425966975,1.0921362915
H,0,4.3962142862,-0.9992577368,1.6079743889
S,0,4.4462492756,-3.3317114924,2.1716844742
C,0,6.1051328245,-3.4014286461,2.9028772747
H,0,6.7801022337,-3.665278326,2.091029668
H,0,6.3473301542,-2.4259875429,3.3211646469
H,0,6.1015809049,-4.1773732002,3.6676437193
C,0,3.5249568438,-2.6149672992,3.5501830956
H,0,2.5113318393,-2.4264575075,3.2040726086
H,0,3.524524741,-3.3451612995,4.3574776431
H,0,3.990413715,-1.6747909581,3.8445124123
C,0,2.1647353001,-3.2097776658,0.0474205753
C,0,2.7272422676,-4.046548233,-0.9230580589
C,0,1.2863760665,-3.7561590665,0.9892480098
C,0,2.4228208827,-5.4013504559,-0.9405385911
C,0,0.9738953035,-5.1111220739,0.963456859
C,0,1.5467717045,-5.937444461,0.0018608939
H,0,3.4302314861,-3.6423380978,-1.6427551056
H,0,0.8268680154,-3.108499939,1.729150631
H,0,2.8740896393,-6.0440389531,-1.6870956514
H,0,0.2828380722,-5.5194677442,1.6914569978
H,0,1.311697083,-6.9950783552,-0.015745391
N,0,2.6738161293,1.2976588964,-1.8680528134
C,0,2.654510063,1.0142665853,-3.2994750311
C,0,2.7270240067,2.7269626604,-1.5616649882
C,0,1.5056138686,1.7900251161,-3.9376223811
H,0,2.534829626,-0.0523453764,-3.4749681361
H,0,3.6068164477,1.3411074492,-3.7281613396
H,0,2.6907639202,2.859693444,-0.4797717894
H,0,3.679423021,3.1191453184,-1.9357256499
C,0,1.5764040008,3.4295944403,-2.2694565992
H,0,1.5311145638,1.674469141,-5.020900531
H,0,0.5480809825,1.4090422694,-3.5580247754
O,0,1.6150604567,3.1738610061,-3.6645141928
H,0,1.6537766252,4.5087242156,-2.140912985
H,0,0.6192353407,3.0851834759,-1.8562932854
H,0,2.6036257475,0.7972879085,0.0989321753
O,0,2.8681799867,0.3470704824,2.485623047

TS-3 13 and 2 (SR) counterion CCl_3COO^- ,optimization in solv. CHCl_3

M06-2X/6-311+G(d,p), E= -3028.47738493 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.412887 a.u.

Thermal correction to Gibbs Free Energy at 20 °C = 0.414568 a.u.

1 imaginary frequency = 286.1324 i cm^{-1}

0; 1

C,0,2.4860125889,2.3295148334,-3.628944043
N,0,2.1564651512,1.2097205227,-1.5791252667
C,0,2.0629539482,0.2682355364,-0.6665561128
C,0,2.1862629381,-1.0962094725,-0.9176005553
C,0,2.1005665589,-1.996176765,0.1459914995
H,0,2.3953784426,-1.4524705137,-1.9190991491
H,0,1.7348376212,-1.5885143545,1.0850288567
C,0,5.1713419633,0.1924443156,-0.2694841381
C,0,5.5551500707,1.2908432509,-1.0316954735
C,0,5.4054778347,-1.1052288409,-0.7316365892
H,0,5.3821273257,2.2888503286,-0.6446478433
C,0,6.1601548016,1.1042507476,-2.2715254781
C,0,6.0137509376,-1.2846961726,-1.9776789245
H,0,6.457952354,1.9611958735,-2.8658402744
H,0,6.1949872246,-2.2951672334,-2.3244169444
C,0,6.3838991585,-0.1877203271,-2.7464709691
H,0,6.8522243055,-0.3373188635,-3.7124060829
H,0,4.697328754,0.3718608905,0.6874887108
C,0,5.0487912165,-2.3249160716,0.0675651978
O,0,5.5109932596,-3.4319208726,-0.2450367232
C,0,4.1236803424,-2.1611245899,1.1430232357
H,0,3.9909306828,-1.2321161935,1.6772902814
S,0,4.0545527552,-3.5756030223,2.1877847316
C,0,5.6780995949,-3.6275666071,2.9967329614
H,0,6.400887885,-3.8191228366,2.2061168726
H,0,5.861178424,-2.6709268963,3.4826488441
H,0,5.6677336699,-4.4474272588,3.7140078871
C,0,3.051458579,-2.9214130708,3.5394133949
H,0,3.0708516444,-3.6544069767,4.3440889126
H,0,3.448650316,-1.9556421314,3.8510124612
H,0,2.0377306659,-2.7970896237,3.1649946529
C,0,1.8760574127,-3.4377002432,-0.0747709871
C,0,2.5139934099,-4.1280759534,-1.1119135416
C,0,1.0098963306,-4.1356008208,0.7730107266
C,0,2.293875341,-5.4874498384,-1.2878707787
C,0,0.7804126179,-5.494915995,0.5875052864
C,0,1.4267165437,-6.1744577494,-0.440420751
H,0,3.2059166137,-3.6049924825,-1.7621342312
H,0,0.494683554,-3.6040025126,1.5668320739
H,0,2.803836259,-6.0149537763,-2.085309083
H,0,0.0979155842,-6.0215803246,1.2439392234
H,0,1.2557540563,-7.2349706275,-0.5824722848
H,0,1.4876020427,2.5507180808,-4.0137936704
H,0,3.192991968,2.3981713026,-4.454984983
C,0,2.07883243,2.6508720011,-1.2883319919
H,0,1.0291742911,2.9618264187,-1.2809428168
H,0,2.5192386941,2.8442881383,-0.3096924464
C,0,2.8227950104,3.2739335025,-2.4678041904
H,0,3.897817309,3.2639701653,-2.2774494177
H,0,2.5131502785,4.3020266945,-2.6517355784
C,0,2.498207311,0.9426593693,-2.9811440555
H,0,1.7737559614,0.2551599836,-3.4236734105
H,0,3.489762381,0.4760809004,-3.013226738
H,0,1.8964682516,0.6086427718,0.3541228519
O,0,3.1598161152,2.1075089917,1.8341422457
C,0,3.0994258604,1.1848841945,2.646128358

C,0,3.4414026559,1.4451328006,2.5056426705
O,0,3.4808075951,2.3554266885,1.6786598659
C,0,4.3454184923,1.6582992973,3.8115564328
Cl,0,4.8344670147,3.3445437381,4.0455877056
Cl,0,3.5023438364,1.0847065348,5.272145876
Cl,0,5.8264127948,0.6571202096,3.5784749906

O,0,2.4854185073,0.1091472302,2.6172442813
C,0,4.0414244536,1.3414660207,3.9326420734
Cl,0,3.2311475512,0.736717357,5.3996022128
Cl,0,5.4956624715,0.3250258926,3.6195956622
Cl,0,4.5648617243,3.0120009434,4.2054568281

TS-3 15 and 2 (SR), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1572.18578382 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.425296 a.u.
1 imaginary frequency = 250.8496 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1572.6323719 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1572.6586628 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1573.4648831 a.u.
1; 1
C,0,3.3898957301,4.554204804,-1.3499694501
C,0,3.4961869038,5.0185153795,-2.6610375876
C,0,3.4154234659,4.1299804474,-3.7339954028
C,0,3.2281455018,2.7797135703,-3.4791623354
C,0,3.0943038347,1.6261135998,-4.4340115041
C,0,3.2016079847,3.2007287083,-1.0782036492
C,0,3.1238739371,2.3323728013,-2.1622887006
N,0,2.9431868127,0.9362400262,-2.146690814
C,0,3.0012922969,0.395717727,-3.5144518467
C,0,2.8034554883,0.1783173259,-1.0657354673
C,0,2.6398880009,-1.1975735535,-1.0626730179
C,0,2.4596969559,-1.8892841572,0.1427160817
H,0,3.4564966422,5.254552484,-0.52318463
H,0,3.6436580182,6.0775628125,-2.847174747
H,0,3.4980244529,4.4901331613,-4.7552724245
H,0,3.1311958936,2.8549383047,-0.0521878464
H,0,2.1077671049,-0.2054326145,-3.702849679
H,0,2.7872575058,0.7150562929,-0.1215222287
H,0,2.6721115632,-1.7378973466,-2.0015626191
H,0,2.2578168964,-1.2900732707,1.0273679709
C,0,4.0377672025,-0.2305110215,3.165892661
C,0,3.8010097948,0.7569153767,4.1163508394
C,0,4.7124785814,0.0779872257,1.977714159
H,0,3.2760448114,0.5075908267,5.0334158598
C,0,4.2364708419,2.0615865011,3.8935777375
C,0,5.145225206,1.3928642005,1.7632831975
H,0,4.0526666932,2.8296575737,4.6388965092
H,0,5.6680725885,1.6160167101,0.8387546342
C,0,4.9103312962,2.3779004804,2.7148569589
H,0,5.2552796468,3.3926532538,2.5399532332
H,0,3.6905635818,-1.2403025548,3.3621868018
C,0,4.9913607131,-0.9181940982,0.9014279265
O,0,5.5175262714,-0.5518532876,-0.1674635153
C,0,4.5395330698,-2.2637891433,1.0415678629
H,0,4.347442804,-2.7391741476,1.9975368659
S,0,5.2342607989,-3.3301083465,-0.1751496681
C,0,7.0308241837,-3.1965036322,-0.0077191136
H,0,7.2862099015,-2.1805669179,-0.3067816042
H,0,7.3230083898,-3.3894457859,1.0253066698
H,0,7.47679264,-3.9234793024,-0.6890576583
C,0,4.9670024393,-4.9524965424,0.5623091066
H,0,3.8928407176,-5.133819098,0.6016827908
H,0,5.4407435236,-5.6864982707,-0.0910722412
H,0,5.4078821882,-4.9867331068,1.5599702137
C,0,1.9333547418,-3.2613177251,0.2045225821
C,0,1.8781711626,-4.1021445626,-0.9182039796
C,0,1.4572971842,-3.7519236593,1.431011505
C,0,1.3721784211,-5.3935369313,-0.8111135569
C,0,0.9497309933,-5.0401945202,1.5359527966
C,0,0.909141933,-5.8682282676,0.4142901154
H,0,2.2291329999,-3.7544198641,-1.884433961
H,0,1.4877649672,-3.1111319074,2.308711438
H,0,1.3357456004,-6.0299493621,-1.6899911033
H,0,0.5822845149,-5.3995877111,2.4922707847
H,0,0.5127498684,-6.875724558,0.4941100471

TS-3 15 and 2 (SR), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1573.46685408 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.423517 a.u.
Thermal correction to Gibbs Free Energy at 20 °C = 0.424995 a.u.
1 imaginary frequency = 286.5199 i cm⁻¹
1; 1
C,0,3.1929680727,4.5565939351,-1.0866025082
C,0,3.5715708416,5.0361961543,-2.3393276569
C,0,3.6942685798,4.1662887362,-3.42278933
C,0,3.4387110323,2.8173781497,-3.2354775302
C,0,3.4773341161,1.6786554742,-4.2238363861
C,0,2.9321646201,3.2031682851,-0.8844555175
C,0,3.0694326997,2.3560022324,-1.9759009281
N,0,2.8816738084,0.9551764221,-2.0167554363
C,0,3.1786724585,0.4326061019,-3.3651647382
C,0,2.6488406782,0.1769010812,-0.9753167262
C,0,2.5213891783,-1.2051914129,-1.0121832378
C,0,2.3939279943,-1.9034071917,0.190809822
H,0,3.0960647956,5.2433774772,-0.2545273783
H,0,3.7687796438,6.0926621814,-2.472606571
H,0,3.9851551301,4.5386868102,-4.3982046194
H,0,2.6356618901,2.84354076,0.0929435999
H,0,2.3214707279,-0.1343602013,-3.7303647442
H,0,2.5430505625,0.688523197,-0.0224035942
H,0,2.5929143654,-1.7277712273,-1.9567455397
H,0,2.2066122327,-1.3107933125,1.0825784652
C,0,4.0943182866,-0.135779727,2.9406355098
C,0,3.8310415485,0.9105585689,3.8168615173
C,0,4.6900537462,0.116674465,1.700541592
H,0,3.3703830521,0.7076223881,4.7760969178
C,0,4.1576038368,2.2176477283,3.4628040171
C,0,5.0097223304,1.4319021375,1.3508887136
H,0,3.9522561454,3.0309768507,4.1486376645
H,0,5.4591244806,1.6167106861,0.3817870239
C,0,4.7465474448,2.4770433209,2.2282890797
H,0,4.9975763648,3.4933819695,1.9470992313
H,0,3.8281013523,-1.1443737222,3.2356704571
C,0,4.958388905,-0.9541211899,0.6867813505
O,0,5.4123887262,-0.6525868636,-0.4250383006
C,0,4.5137241205,-2.2817381135,0.9507425198
H,0,4.3889274051,-2.6958317001,1.9424500948
S,0,5.0792219109,-3.4447117747,-0.2537242429
C,0,6.88889763,-3.3281546248,-0.2291221405
H,0,7.13981186,-2.3531117721,-0.6381281327
H,0,7.2368811982,-3.434395731,0.7964493008
H,0,7.2672513158,-4.1266874666,-0.8656313937
C,0,4.8685465377,-5.0081450221,0.6279718394
H,0,3.8062605467,-5.1550815558,0.8118233507
H,0,5.2470583106,-5.7933381069,-0.024768984
H,0,5.4293724354,-4.9702948768,1.5607343389
C,0,1.9243194122,-3.2991992076,0.2742935796
C,0,1.8638397143,-4.1391914723,-0.8438657517
C,0,1.5316216549,-3.8033344292,1.52109363
C,0,1.4342782705,-5.4558588602,-0.7112835786
C,0,1.0975720674,-5.1152626471,1.6510936312
C,0,1.0536580713,-5.948227451,0.5336058273
H,0,2.1509710743,-3.774781751,-1.8226156106
H,0,1.572084296,-3.1562114626,2.3919950463
H,0,1.3939404951,-6.0963977765,-1.5840586131
H,0,0.7920863865,-5.4895173253,2.6206152733
H,0,0.7167590357,-6.9728761223,0.6329289469

H,0,2.1975444857,1.7283250297,-5.0532926168
H,0,3.9492304508,1.5545245102,-5.1119650303
H,0,3.878256501,-0.2543461666,-3.5971943503

H,0,2.7230856925,1.8138192596,-5.0007049111
H,0,4.448889676,1.6004123205,-4.7124213267
H,0,4.0379812349,-0.2378465955,-3.2839719119

TS-3 15 and 2 (SS), optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1572.18068107 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.423468 a.u.
1 imaginary frequency = 196.8666 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1572.6267585 a.u.
1; 1
C,0,1.3604186914,4.7814130458,-0.8036328105
C,0,1.1698870782,5.2255576482,-2.1124741106
C,0,1.1657413586,4.319100619,-3.173040497
C,0,1.3531385382,2.9704976588,-2.9085003784
C,0,1.3943314472,1.8000087307,-3.8507273566
C,0,1.5490283603,3.4302192569,-0.5220678126
C,0,1.5414972887,2.5435921206,-1.5943814191
N,0,1.7124245402,1.1456860529,-1.5672455096
C,0,1.6243530659,0.5897219974,-2.9281687458
C,0,1.9020252747,0.400257815,-0.4831985393
C,0,2.0372884994,-0.9768154747,-0.4656819971
C,0,2.2005813886,-1.6438178636,0.7571403696
H,0,1.3605407181,5.4962343256,0.0132834393
H,0,1.0234657348,6.2833433148,-2.3061399086
H,0,1.0170695287,4.6636820878,-4.1921292555
H,0,1.6987546551,3.102288519,0.501185798
H,0,0.7991325907,-0.1275556197,-2.96526994
H,0,1.9361381381,0.945296223,0.4560053865
H,0,2.0033451671,-1.5328943746,-1.3961804382
H,0,2.1138196606,-1.0287722861,1.6483146966
C,0,4.5014714071,1.2958216201,1.7195075422
C,0,4.3125461449,2.6512515508,1.9760032882
C,0,4.2993340859,0.349715334,2.732158058
H,0,4.4866066717,3.3785468626,1.1885961404
C,0,3.9122208924,3.0734103929,3.2421905049
C,0,3.9102097673,0.7862338915,4.0040203575
H,0,3.7668451571,4.1311119134,3.4409844426
H,0,3.7725869612,0.0417699511,4.7815855836
C,0,3.7113948873,2.1374852844,4.2561618617
H,0,3.4045796415,2.4645095797,5.2451057956
H,0,4.8346081942,0.9872642914,0.7334738426
C,0,4.4973778175,-1.1184846144,2.5365715404
O,0,4.5574925256,-1.8774640496,3.5223581471
C,0,4.5332619113,-1.6545139237,1.2087512632
H,0,4.8294098363,-1.0873688524,0.3340592741
S,0,5.063205041,-3.3249733298,1.2326841426
C,0,5.2986129603,-3.660269413,-0.5188434694
H,0,4.3137341775,-3.6721907988,-0.9856580328
H,0,5.9389803719,-2.9027858392,-0.9744241487
H,0,5.7521599256,-4.6485838339,-0.605106239
C,0,6.7808379033,-3.3062539173,1.8075240681
H,0,6.7408515394,-2.9795710451,2.8467350135
H,0,7.1654700175,-4.3260288771,1.7448979481
H,0,7.3740138079,-2.6204724178,1.2015943423
C,0,1.9077048346,-3.0602544667,0.97154197
C,0,1.6824905497,-3.9598568745,-0.0845632454
C,0,1.8103115386,-3.5348526056,2.2912811382
C,0,1.3729349104,-5.2887299961,0.1740549975
C,0,1.4968939027,-4.8635459267,2.5457661011
C,0,1.2779250074,-5.7443294616,1.4887133269
H,0,1.72667625,-3.6204094094,-1.115198632
H,0,1.9951282165,-2.853273386,3.1165073704
H,0,1.1935969995,-5.9699245455,-0.6520792816
H,0,1.4221718909,-5.212424559,3.570939146
H,0,1.0287941258,-6.7823114122,1.6870940935
H,0,0.4599955069,1.7012415573,-4.4108311886
H,0,2.2005644193,1.9025504072,-4.5831702382

TS-3 15 and 2 (SS), optimization in solv. CHCl₃
M06-2X/6-311+G(d,p), E = -1573.46841229 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.425303 a.u.
1 imaginary frequency = 287.4153 i cm⁻¹
1; 1
C,0,0.863016128,4.5457542915,1.2417760374
C,0,0.9175085178,5.3924844596,0.1359006938
C,0,1.1095494196,4.8736700898,-1.1451690012
C,0,1.2466580136,3.5042257139,-1.3015982672
C,0,1.5165119234,2.6940374118,-2.5442430948
C,0,1.0006006387,3.1670652353,1.0981649703
C,0,1.1950027389,2.6763065299,-0.1850491179
N,0,1.4088070761,1.3341031949,-0.5797149544
C,0,1.4497304523,1.2356742661,-2.0528279569
C,0,1.5947715271,0.3083273575,0.2313808478
C,0,1.8223599008,-1.0033852435,-0.1650059755
C,0,2.118503605,-1.9657356652,0.8022804015
H,0,0.7094098417,4.961787383,2.2300017979
H,0,0.8060086533,6.4610193685,0.2730846305
H,0,1.153774444,5.5318186944,-2.005347865
H,0,0.9586044129,2.51888565,1.9646575213
H,0,0.5463349227,0.7244707884,-2.3933186231
H,0,1.5781821882,0.5396720937,1.2934926786
H,0,1.8074472732,-1.2702107461,-1.2141799612
H,0,1.922458254,-1.7006174723,1.8400190086
C,0,4.76524708,0.3721392203,-0.4999488704
C,0,4.8584948176,1.4511989965,-1.372203839
C,0,4.4966018769,0.5863297102,0.8561169474
H,0,5.0640079464,1.2781928642,-2.4225364314
C,0,4.6814837138,2.7503494531,-0.900984209
C,0,4.3277907008,1.8949584271,1.3206668924
H,0,4.7493144257,3.5895516523,-1.5841501449
H,0,4.1100542628,2.0471509923,2.3710556736
C,0,4.4208520043,2.9712825242,0.4490398466
H,0,4.2717447384,3.980108871,0.8163850418
H,0,4.8850200512,-0.6303752126,-0.892771235
C,0,4.2917734885,-0.5256795808,1.83718973
O,0,3.9676006592,-0.2696861565,3.0059611725
C,0,4.3447623001,-1.8741443178,1.3667057535
H,0,4.8908043826,-2.1781764974,0.4835964632
S,0,4.4172754653,-3.0416442661,2.6925130191
C,0,5.0186965755,-4.5217638862,1.850833867
H,0,4.2554919394,-4.8458165485,1.1461751133
H,0,5.9538184537,-4.2916106148,1.3427916034
H,0,5.1668352056,-5.2812979063,2.6168675396
C,0,5.904331036,-2.5930283986,3.6298114748
H,0,5.6925241721,-1.6353667453,4.0988979728
H,0,6.0587194201,-3.3662001688,4.3810306073
H,0,6.746252286,-2.524599144,2.943517067
C,0,2.0712637401,-3.4070161289,0.4976330571
C,0,2.5061993824,-3.9127111792,-0.7337902106
C,0,1.5854298002,-4.2920422227,1.4659109646
C,0,2.4597092492,-5.2762362902,-0.9865358507
C,0,1.5321426069,-5.6589794422,1.2070194573
C,0,1.9725689494,-6.1533604219,-0.0161217026
H,0,2.9074083027,-3.2387607814,-1.4830072271
H,0,1.2385455496,-3.9059309784,2.418463563
H,0,2.8081248395,-5.6600303368,-1.937882028
H,0,1.1472127918,-6.3353088849,1.9605326002
H,0,1.9377961024,-7.2172942085,-0.2164824223
H,0,0.7862144518,2.8856563306,-3.3302675712
H,0,2.508056698,2.9263025727,-2.9413749061

H,0,2.5518909976,0.0569632622,-3.1575950758

H,0,2.3224656028,0.650533303,-2.3444795496

Pre-complex: Int-2a cis and 2, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -1760.11004024 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.415383 a.u.
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6722727 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1760.6982859 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1761.5809662 a.u.

0; 1
C,0,-3.7595677824,-4.7101993907,-2.0449660735
C,0,-3.3741216524,-5.6165366108,-1.0538377194
C,0,-3.0596009446,-5.1786144871,0.2312067141
C,0,-3.1386930577,-3.8220117349,0.5177248565
C,0,-2.8817537012,-3.0777723311,1.7918567511
C,0,-3.8400813407,-3.34801914,-1.7754856506
C,0,-3.5275859313,-2.9356215789,-0.4847862995
N,0,-3.534274751,-1.6172142446,0.0353348512
C,0,-2.8825116232,-1.610813368,1.3540256135
C,0,-1.4285898628,-0.9784440393,1.2658768403
C,0,-3.9932382023,-0.5654186521,-0.5882391311
C,0,-4.0215999827,0.7574052832,-0.082180456
C,0,-4.6321132264,1.7280310563,-0.8125637186
O,0,-1.2806448091,-0.1129877066,0.3825453829
O,0,-0.6482744965,-1.3995244124,2.1374133807
H,0,-3.989373331,-5.0684335556,-3.0431915791
H,0,-3.3122668761,-6.6738621681,-1.2916622124
H,0,-2.7546722078,-5.8852953827,0.9968801942
H,0,-4.1194162108,-2.6512899061,-2.5587356009
H,0,-3.4602764046,-0.9715842725,2.0269245962
H,0,-4.4269006175,-0.7490025998,-1.5676649762
H,0,-3.5246424275,0.9711905981,0.8551731378
H,0,-5.0727156605,1.4398021548,-1.7670884808
C,0,6.9643542839,1.8509196993,-0.3992839872
C,0,8.2358084119,2.4095680075,-0.498869384
C,0,6.793952131,0.4625350599,-0.3979578523
H,0,8.3515316902,3.4900564282,-0.508185025
C,0,9.3566098709,1.5874275394,-0.595474723
C,0,7.9245925086,-0.3515469488,-0.5129206581
H,0,10.3487039389,2.0240236211,-0.6711707196
H,0,7.7719658577,-1.4263060397,-0.5330058165
C,0,9.1966712816,0.2027105487,-0.6037679983
H,0,10.0660477346,-0.4444818458,-0.6840903478
H,0,6.0967039302,2.5023807973,-0.3493152679
C,0,5.4485235573,-0.2212050843,-0.3067547297
O,0,5.3611136371,-1.3984657406,-0.7153266674
C,0,4.3969550183,0.5309777486,0.255711904
H,0,4.5190932153,1.4934137423,0.7377953609
S,0,2.858766471,-0.2005043485,0.3406968353
C,0,2.4268618764,-0.4248684779,2.0855507023
H,0,3.0878033794,-1.2015247144,2.4734237347
H,0,2.5939430305,0.5111664687,2.6240895306
H,0,1.3759573516,-0.7404751292,2.1453690817
C,0,1.6802870051,1.1038240699,-0.0654248062
H,0,1.8242858801,1.3429333244,-1.120007935
H,0,0.6653808076,0.7233534911,0.1134169532
H,0,1.8861450463,1.9845524744,0.547958358
C,0,-4.7672470505,3.1283338244,-0.4707985871
C,0,-4.2485345682,3.682713862,0.7142017676
C,0,-5.448053249,3.970966347,-1.3669499536
C,0,-4.41003982,5.0319240035,0.9864684873
C,0,-5.6086606535,5.3220066671,-1.0911456609
C,0,-5.0899274319,5.8553086611,0.0865858535
H,0,-3.714489576,3.0573572994,1.4224623125

H,0,-5.8500340534,3.5530712844,-2.2861982749
H,0,-4.0039195922,5.4486234717,1.9029562296
H,0,-6.1362944406,5.9595707304,-1.793572775
H,0,-5.2124485888,6.9118261561,0.3051720501
H,0,-3.6662428598,-3.285379809,2.5284692657
H,0,-1.91571977,-3.3069547009,2.2478923218

TS(SR)v, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1836.46377785 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.440930 a.u.
1 imaginary frequency = 312.2707 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0705974 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0974931 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1838.0188459 a.u.

0; 1
C,0,3.8286620747,-1.9922267396,-2.8513135636
C,0,3.5510028352,-2.7567908982,-1.7096017291
C,0,3.1238227686,-2.1564022306,-0.5129615548
H,0,3.6645237962,-0.9024344735,-2.7611102846
H,0,3.6860488062,-3.8325144469,-1.7684486352
H,0,2.8398256284,-1.1064027879,-0.5891349607
C,0,3.5876670142,-1.6199151739,3.4585079395
C,0,2.9877813639,-1.5655111486,4.7119801488
C,0,3.7657832602,-0.4508511398,2.7091112575
H,0,2.8512339482,-2.4789969143,5.2829122371
C,0,2.5593492408,-0.3459704164,5.2312803643
C,0,3.3302611758,0.7696770069,3.2400169765
H,0,2.0920602866,-0.3068130547,6.2111125128
H,0,3.4775603624,1.6659666254,2.6461836286
C,0,2.7302036938,0.8232702193,4.4910098005
H,0,2.3956912983,1.7756802218,4.8918221788
H,0,3.8991328759,-2.5827136912,3.0666504173
C,0,4.4265857563,-0.4158858648,1.371337259
O,0,4.605244642,0.6731572996,0.7941417629
C,0,4.8120611608,-1.6423441704,0.721249141
H,0,5.0045947825,-2.5551156551,1.2758588579
S,0,6.0067557696,-1.3233811902,-0.5403239275
C,0,7.3800167745,-0.4895102688,0.288261485
H,0,6.9885980625,0.4628187417,0.6445247744
H,0,7.7498640512,-1.1000864299,1.1129720286
H,0,8.1596581512,-0.3249495203,-0.4581549733
C,0,6.7404725489,-2.9454951176,-0.800788159
H,0,6.0231296613,-3.5817626924,-1.3246277054
H,0,7.6168095199,-2.7968340398,-1.4346543843
H,0,7.0354462382,-3.3771669757,0.1578173414
C,0,2.3479066644,-2.9337695104,0.4783550915
C,0,2.6453357635,-4.2746945791,0.7607948316
C,0,1.2649829324,-2.3353446195,1.1312321456
C,0,1.8791556775,-4.9919818483,1.6714418398
C,0,0.4894479233,-3.0580067576,2.0334107154
C,0,0.7954976138,-4.3871196326,2.3089379867
H,0,3.4846173665,-4.7572420287,0.2665558061
H,0,1.0269151825,-1.2951461336,0.9254261119
H,0,2.1242611108,-6.0290935503,1.8819430934
H,0,-0.3511444641,-2.5777170284,2.5254959044
H,0,0.1946769182,-4.9512859851,3.0162352136
O,0,4.2188725605,-2.420528972,-3.9687406441
H,0,4.4612597686,-3.8481787767,-4.1902893984
O,0,4.5976270741,-4.8201298803,-4.5478938501
C,0,5.1016960624,-5.6473360573,-3.6698443548
C,0,5.2757829378,-7.0416431458,-4.2514635455
O,0,5.3825998718,-5.3781702979,-2.5099527816
N,0,6.0195155762,-6.9979766491,-5.5145080964
C,0,6.0860476252,-8.011220782,-3.3781049857
H,0,4.2609653546,-7.4443254183,-4.4122341882
C,0,6.7090115726,-8.197569334,-5.6459188021
H,0,5.5089931148,-6.6526976091,-6.3145972017
C,0,6.79033733,-8.8553880613,-4.4079764465

TS(SR)g, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1836.46018061 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.440918 a.u.
1 imaginary frequency = 343.9272 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0663915 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0933419 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1838.0153201 a.u.

0; 1
C,0,1.542214487,2.7861531011,-0.2674546829
C,0,1.532551464,2.7028031108,1.1267870035
C,0,1.820611774,1.4861779377,1.7818446172
H,0,1.81861075,1.8771681511,-0.82707122
H,0,1.2588279939,3.5942786188,1.6842484278
H,0,2.2563361325,0.7191587439,1.1407811114
C,0,0.7892125281,-2.2791801597,0.773893161
C,0,1.3906371748,-3.3643503971,0.1450906846
C,0,0.4816956134,-1.1238972977,0.0448574229
H,0,1.6130573275,-4.2628948648,0.7129767536
C,0,1.7037042735,-3.2985447174,-1.2113663953
C,0,0.788651194,-1.0682070138,-1.3202050922
H,0,2.1804775727,-4.1438580374,-1.6992133349
H,0,0.5682933793,-0.1625060401,-1.8765805447
C,0,1.4059480809,-2.1481034439,-1.9399433312
H,0,1.6590922749,-2.0876637914,-2.9941906507
H,0,0.5329769651,-2.3493423767,1.8272038337
C,0,-0.1736926445,0.0649542125,0.65738982
O,0,-0.8257119534,0.8621941538,-0.0317372471
C,0,0.1066735785,0.3808863319,2.0392845366
H,0,0.3496731927,-0.3950805995,2.7599806895
S,0,-1.0632734897,1.5667943477,2.6452924908
C,0,-2.6920121297,0.8201931877,2.4119637236
H,0,-2.7231377227,-0.1670586542,2.8748234391
H,0,-3.4280922845,1.4893505455,2.8616439789
H,0,-2.8451045823,0.7574888868,1.3350560871
C,0,-0.8802112529,1.3981233595,4.4293586125
H,0,0.1208910267,1.7413047163,4.6937544734
H,0,-1.6265089026,2.0442146057,4.894189127
H,0,-1.0267603155,0.3600460712,4.7328451347
C,0,2.3921037282,1.447155417,3.1585923677
C,0,2.4704370051,2.5844088734,3.9722041646
C,0,2.9048254109,0.2406603029,3.6558096136
C,0,3.0202863633,2.5089545015,5.2502518906
C,0,3.4604500906,0.16524044,4.9272056413
C,0,3.5139526792,1.3004738664,5.7344448661
H,0,2.1187188514,3.5417800783,3.6012692429
H,0,2.8698274256,-0.6475743801,3.0287060304
H,0,3.074163931,3.4037729795,5.8636702682
H,0,3.8574740296,-0.7794188792,5.287508824
H,0,3.9482699647,1.245578047,6.7282073385
O,0,1.2939727498,3.8351021992,-0.928697444
H,0,1.3915753405,3.6969105921,-2.3052913659
O,0,1.4415887805,3.7057389339,-3.3771608357
C,0,1.5914911642,2.5154134071,-3.8894120788
C,0,1.6173739104,2.5512322912,-5.4104542554
O,0,1.6775065641,1.469931052,-3.2592192011
N,0,2.5704452692,3.5491127178,-5.9071635561
C,0,2.0699384899,1.2471083472,-6.0840942185
H,0,0.5926611898,2.8002739998,-5.736946044
C,0,3.0332678901,3.121422881,-7.1440828283
H,0,2.2934064049,4.5147417709,-5.8060294384
C,0,2.7706377017,1.7520934997,-7.3183024035

H,0,6.7992353856,-7.4450171564,-2.7656763554
H,0,5.450392472,-8.5792891266,-2.6947065637
C,0,7.3067774342,-8.7335929232,-6.783707267
C,0,7.476685989,-10.051813159,-4.2976910688
C,0,7.9887110633,-9.9461194012,-6.6591608007
H,0,7.2402284767,-8.2275514054,-7.742604986
C,0,8.0781072226,-10.6048220872,-5.4347953618
H,0,7.5406032634,-10.5631530679,-3.3402437754
H,0,8.4531111713,-10.3829768725,-7.5392205577
H,0,8.6099024361,-11.5487062167,-5.3630699428

H,0,2.7600372824,0.7127291648,-5.4188143431
H,0,1.232051823,0.5765880062,-6.2894745068
C,0,3.7082825123,3.8513157995,-8.1195715769
C,0,3.1878598889,1.1030626375,-8.4666955479
C,0,4.1157121571,3.1842087038,-9.2772849084
H,0,3.9077025356,4.9110494901,-7.9879112166
C,0,3.8628188272,1.8262727699,-9.4580840425
H,0,2.9857764442,0.0434060106,-8.6035771486
H,0,4.6357537312,3.7415619354,-10.0519676052
H,0,4.1852813572,1.3296038553,-10.368215312

TS(RS)v, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1836.46366758 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.440768 a.u.
1 imaginary frequency = 310.3746 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0704849 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.097368 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1838.0186695 a.u.

0; 1
C,0,-2.765517453,0.4602655985,-0.5859895367
C,0,-3.6172445117,-0.6181184059,-0.8807546497
H,0,-1.7867779278,0.2867015975,-0.1489264719
H,0,-4.6423336592,-0.3497584946,-1.13783117
C,0,-3.4810929153,-1.9003877527,-0.156076511
C,0,-2.2263141562,-2.4391117255,0.1620202305
C,0,-4.6291500238,-2.5829105964,0.2605440759
C,0,-2.1275842475,-3.6265797059,0.8768098746
C,0,-4.5299471225,-3.7649469492,0.9890752997
C,0,-3.2794932087,-4.2922337102,1.2968502316
H,0,-1.3223829668,-1.9264734162,-0.1563216067
H,0,-5.6079930244,-2.1788358944,0.0160967876
H,0,-1.1481492595,-4.0323868055,1.113321521
H,0,-5.4324985092,-4.2762754088,1.3105757637
H,0,-3.1996328624,-5.2168690916,1.8609362138
C,0,-3.1519799854,1.7823611135,-0.8480839357
H,0,-4.1623283029,1.918457395,-1.2761637507
O,0,-2.4818748318,2.8239047224,-0.6243342894
H,0,-1.1431253957,2.7463459223,-0.0407642887
O,0,-0.2238982782,2.8795206989,0.4377856568
C,0,0.6701858621,1.9773875298,0.1272917448
C,0,1.9914455933,2.2333142789,0.8348662007
O,0,0.5082304831,1.0459993005,-0.6487985143
N,0,1.7941287496,2.4096242047,2.27682455
C,0,3.0115725759,1.0890929885,0.7395136316
H,0,2.416689509,3.1480834367,0.3868133374
C,0,2.9518864394,1.9882057149,2.9196442558
H,0,1.3822793482,3.2865801082,2.5618681481
C,0,3.7271624388,1.1919134015,2.0611628983
H,0,2.4823401037,0.1327425546,0.6415354472
H,0,3.6644523688,1.19035876,-0.1306844148
C,0,3.3533830393,2.2302478451,4.2308715502
C,0,4.9070070627,0.6258988503,2.5108415946
C,0,4.5508909834,1.6595393555,4.6682759982
H,0,2.7566094745,2.8499201674,4.8940666314
C,0,5.3254465456,0.8655809323,3.825389693
H,0,5.5090682488,0.0091594885,1.8479253908
H,0,4.8833270311,1.8459969917,5.6859771172
H,0,6.2551196891,0.4359784657,4.1860108267
C,0,-3.2756197583,-1.3306144575,-2.8859039689
H,0,-2.4582516623,-2.0353763266,-2.7719482802
C,0,-4.5758235617,-1.7366134582,-3.3549457973
O,0,-5.3476760523,-0.8918012496,-3.8465322223
C,0,-5.0160275039,-3.15564234,-3.2129504029
C,0,-4.2039678944,-4.1749576783,-2.7015025832
C,0,-6.3083988784,-3.4714552591,-3.6500007858
C,0,-4.6766372148,-5.4811091628,-2.6327259609
H,0,-3.2051207554,-3.9577925539,-2.3370489356
C,0,-6.7798494278,-4.7756859802,-3.5810226904
H,0,-6.9238277895,-2.6694437363,-4.0445135693
C,0,-5.9627553142,-5.7850649941,-3.0733528901
H,0,-4.0394531051,-6.2629361648,-2.2304181625
H,0,-7.7839564679,-5.0081265356,-3.92361812

TS(RS)g, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1836.46005417 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.441023 a.u.
1 imaginary frequency = 345.7699 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0662632 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0931991 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1838.0149689 a.u.

0; 1
C,0,0.6900010978,-1.7605757177,-0.5861496427
C,0,2.0812571625,-1.75985975,-0.4660946681
C,0,2.8263769195,-0.5833715972,-0.7019302683
H,0,0.2094442505,-0.824081328,-0.9139540816
H,0,2.5626212724,-2.678657219,-0.142558861
H,0,2.2707558304,0.210190651,-1.2025142292
C,0,1.9811232275,3.24142268,0.1361211241
C,0,1.4887572628,4.3515900446,-0.541963628
C,0,1.1411829263,2.1561035663,0.4147834048
H,0,2.1417343067,5.1958836476,-0.7422908411
C,0,0.1595217678,4.3807793722,-0.9596185229
C,0,-0.1957312262,2.1957922373,0.0001436373
H,0,-0.2215254026,5.2457275033,-1.4948566695
H,0,-0.8355256417,1.342068889,0.2001359747
C,0,-0.6788975481,3.2998970188,-0.6915175906
H,0,-1.7120662231,3.313801088,-1.0254591758
H,0,3.0146376808,3.2387982511,0.4710129452
C,0,1.6022116914,0.9443965995,1.1477766892
O,0,0.7971735524,0.2110189219,1.7389576351
C,0,2.9801905383,0.5266897517,1.016755341
H,0,3.7771993582,1.245783371,0.8493960092
S,0,3.3655945708,-0.6795281063,2.25863985
C,0,5.1667385273,-0.6569152266,2.2555856554
H,0,5.5368443891,0.3574445007,2.4139644925
H,0,5.500947253,-1.3177265252,3.056797858
H,0,5.5018927361,-1.0443391709,1.2926380283
C,0,3.0330666127,0.117875641,3.8452866337
H,0,3.3548491656,-0.5686502484,4.6308233572
H,0,3.566380957,1.0671823884,3.9094357675
H,0,1.9546608384,0.2658971909,3.8904830542
C,0,4.2489668294,-0.6272619492,-1.1478794005
C,0,5.0058087386,-1.8055230408,-1.1298231181
C,0,4.8527624033,0.5397105527,-1.636790415
C,0,6.3301305193,-1.8087099568,-1.5624122673
C,0,6.1712090266,0.5366077899,-2.076265996
C,0,6.9194146182,-0.6386668527,-2.034012827
H,0,4.5550192888,-2.7330923044,-0.7917474505
H,0,4.2730166695,1.4593634114,-1.6776763362
H,0,6.8979734541,-2.734452017,-1.5418665474
H,0,6.6148216088,1.4518959087,-2.4574647464
H,0,7.9496432234,-0.6444028458,-2.3772214843
O,0,-0.0524254161,-2.764812441,-0.3837118635
H,0,-1.4079610587,-2.5223399421,-0.539777884
O,0,-2.475708253,-2.4428784696,-0.6247665308
C,0,-2.8731599329,-1.2459911838,-0.9587444952
C,0,-4.3900789823,-1.1631168621,-1.0595426173
O,0,-2.1470483517,-0.2897858769,-1.1958159626
N,0,-5.0277242165,-1.6305709367,0.1762979203
C,0,-4.9518100941,0.2534841835,-1.2470316326
H,0,-4.6877982175,-1.7984447304,-1.9112972517
C,0,-6.2341542679,-0.9588500925,0.3181594097
H,0,-5.0119555611,-2.627921851,0.3328420376
C,0,-6.2595652744,0.1810171674,-0.5029326769

H,0,-6.3281692138,-6.8066094538,-3.0199780489
S,0,-2.7916424953,0.1890765483,-3.6459890129
C,0,-2.8590139815,-0.112098491,-5.4278086062
H,0,-2.5201943713,0.7982732139,-5.9264570847
H,0,-2.2277322956,-0.9614286428,-5.6915293926
H,0,-3.9047070574,-0.3067064904,-5.6639194685
C,0,-1.0102370649,0.2026107821,-3.3956841777
H,0,-0.6136893012,1.018835911,-4.0023621765
H,0,-0.7996340387,0.4067824232,-2.3431120576
H,0,-0.5817866687,-0.7494366697,-3.7156760769

H,0,-4.2670413395,0.979059056,-0.7896011842
H,0,-5.0525192267,0.5212523901,-2.3016274698
C,0,-7.305616109,-1.2633600157,1.1544938996
C,0,-7.3543191973,1.0267019206,-0.4878077896
C,0,-8.4072934129,-0.4044735376,1.1529458228
H,0,-7.2890694506,-2.1469684846,1.7862732907
C,0,-8.4408378343,0.7293845486,0.3443727947
H,0,-7.3760717128,1.9091977725,-1.1228021659
H,0,-9.2552621783,-0.6330691712,1.79319519
H,0,-9.3099781463,1.3801464357,0.3562434688

TS(SS)v, optimization in solv. CHCl₃

PBE1PBE/6-31G(d,p), E = -1836.46221321 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.441984 a.u.

1 imaginary frequency = 319.6130 i cm⁻¹

SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0679792 a.u.

SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0948031 a.u.

SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1838.0155863 a.u.

0; 1
C,0,1.9340621923,-2.1362335625,-0.9108561297
C,0,2.231584722,-1.9707122833,0.4576005777
H,0,1.8640404207,-3.1233571345,-1.3559841553
H,0,2.0596130278,-0.9691252384,0.8520774398
C,0,3.7292299696,1.0819319853,1.715919238
C,0,3.3954817002,2.3314647481,2.2286161922
C,0,4.1422072252,0.0525895463,2.5716376702
H,0,3.0776826444,3.1222514202,1.5558898924
C,0,3.4691962021,2.5668833945,3.5994644369
C,0,4.2147190051,0.3016105869,3.9478061963
H,0,3.2077353401,3.5429938864,3.9974875807
H,0,4.5373169055,-0.50677515,4.5959331692
C,0,3.8798471831,1.5484188327,4.4589173008
H,0,3.9379063993,1.729115541,5.5282232822
H,0,3.6683921712,0.9226468475,0.6435162829
C,0,4.5157220736,-1.3153625256,2.1016631091
O,0,4.9292214481,-2.1615786002,2.9105224601
C,0,4.3034274275,-1.6630567484,0.7145920022
H,0,4.4389897712,-0.9185259569,-0.0646503127
S,0,5.1074844782,-3.1955236945,0.3450462089
C,0,5.1118796009,-3.2178028657,-1.45514942
H,0,4.0957364079,-3.3777276826,-1.8214393162
H,0,5.5213372525,-2.2825606474,-1.8414142711
H,0,5.7388294513,-4.0596629429,-1.7546511267
C,0,6.8674297571,-2.9159046999,0.6613536442
H,0,6.9639519038,-2.7694411782,1.736505022
H,0,7.4061760136,-3.8122013218,0.3470765491
H,0,7.2101320446,-2.0388486972,0.109936072
C,0,1.9476973964,-3.0444114789,1.4373912095
C,0,1.9198730287,-4.3982003974,1.0728272222
C,0,1.6662262015,-2.7065381666,2.7674115539
C,0,1.6181542961,-5.3787817355,2.0107955903
C,0,1.3553607034,-3.6866631917,3.7037510861
C,0,1.3318865916,-5.0271989814,3.3286649668
H,0,2.1265474918,-4.6908825916,0.0474389747
H,0,1.6839047824,-1.6616056503,3.06638673
H,0,1.5999760731,-6.4222117538,1.7097355136
H,0,1.1314767208,-3.4021004808,4.7276578241
H,0,1.0906824541,-5.7947866501,4.0581550796
C,0,1.7884379591,-1.0321353809,-1.7499560035
O,0,1.562991709,-1.0374959301,-2.9912487717
H,0,1.8686284489,-0.0381446496,-1.2673065281
H,0,1.4743932189,-2.2742439608,-3.7424656802
O,0,1.3185971193,-3.0375210436,-4.4466267971
C,0,1.9348238951,-4.1583881871,-4.1822857255
C,0,1.6829995097,-5.2011302888,-5.2615169631
O,0,2.6179299314,-4.3882712652,-3.1932149652
N,0,2.0210014501,-4.6720803339,-6.5875861968
C,0,2.534858883,-6.4737673922,-5.1427888008
H,0,0.6120770309,-5.4606909421,-5.2088597487
C,0,2.432702705,-5.7358852555,-7.3813980905
H,0,1.3633784111,-4.0130684541,-6.9790405194
C,0,2.7588354978,-6.8455650733,-6.5851664967

TS(SS)g, optimization in solv. CHCl₃

PBE1PBE/6-31G(d,p), E = -1836.46173883 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.441651 a.u.

1 imaginary frequency = 325.5641 i cm⁻¹

SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0669192 a.u.

SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0939647 a.u.

SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1838.0157518 a.u.

0; 1
C,0,3.5919945858,-1.7030315417,0.2241341795
C,0,3.5013347904,-0.4178876712,0.7550432534
C,0,2.9584889648,-0.2256708977,2.0456108593
H,0,3.2574524784,-2.5313989749,0.8722301101
H,0,3.8286837026,0.4146266291,0.1384233726
H,0,2.8721982388,-1.1403142793,2.6311721871
C,0,0.7664076437,-3.0077522799,2.6439286936
C,0,0.7881117957,-4.3452350622,3.0257170424
C,0,0.3645554178,-2.017942855,3.5500509105
H,0,1.1133066452,-5.0880217163,2.3040673652
C,0,0.4033532608,-4.7078463469,4.3142496746
C,0,-0.0221753162,-2.3945780203,4.8428851806
H,0,0.4200552098,-5.7522342188,4.6126468762
H,0,-0.3329315881,-1.6167709384,5.5329909239
C,0,-0.0032139105,-3.7297655407,5.2225131236
H,0,-0.3032658636,-4.0110686227,6.2277317301
H,0,1.0676725244,-2.7628025261,1.6306305032
C,0,0.3262465709,-0.5669712839,3.2136287891
O,0,-0.0959517611,0.261885375,4.0363225265
C,0,0.8672301418,-0.1210302817,1.941865792
H,0,0.7346394614,-0.732619974,1.0541686887
S,0,0.4034336066,1.5664835687,1.6878873815
C,0,0.8640788761,1.81720297,-0.0331254289
H,0,1.9494940709,1.7605857467,-0.1024434295
H,0,0.4064022598,1.0565454448,-0.6677849113
H,0,0.5267133886,2.8143717403,-0.3194778193
C,0,-1.3999460404,1.571455896,1.5385134772
H,0,-1.7085768165,2.58229117,1.2644453885
H,0,-1.7168949625,0.8469794958,0.7868768492
H,0,-1.7850194627,1.3116582543,2.5241375903
C,0,3.2802826056,0.9612743865,2.874640565
C,0,3.7854803146,2.1475707159,2.3243111354
C,0,3.0949279208,0.8993676561,4.2631047098
C,0,4.0833635953,3.2382005184,3.1346269888
C,0,3.399601154,1.9863802877,5.0740550674
C,0,3.8904237423,3.1625481263,4.5119575628
H,0,3.9718760344,2.217911831,1.2570217603
H,0,2.7147817973,-0.0149844906,4.7096301666
H,0,4.4781414151,4.1465811988,2.6888809618
H,0,3.2548736604,1.9138184992,6.1478565878
H,0,4.1284951253,4.0127406733,5.144315551
O,0,4.0214886804,-1.9971381641,-0.9286684004
H,0,3.9533388168,-3.3730095568,-1.1848422364
O,0,3.9401393383,-4.4072847403,-1.4466994744
C,0,3.0461432517,-5.0894451375,-0.7829445772
C,0,2.9879395447,-6.5404305463,-1.2308749841
O,0,2.2969398782,-4.6404696599,0.0748726522
N,0,4.323440907,-7.1254795494,-1.3745920335
C,0,2.2750982575,-7.496570077,-0.2629427714
H,0,2.4585146434,-6.5432660729,-2.2004745282
C,0,4.2115206841,-8.4941883118,-1.1662751616
H,0,4.8651227222,-6.8031987532,-2.1634293308
C,0,3.0084782391,-8.7904911567,-0.5036790337

H,0,3.4788197301,-6.2353528322,-4.6365026188
H,0,2.037623276,-7.2490755656,-4.5548923489
C,0,2.5768924522,-5.7795015115,-8.7658743282
C,0,3.2383212532,-8.0053860879,-7.1679803481
C,0,3.0537197486,-6.9596912018,-9.3409743814
H,0,2.3204626727,-4.9231663072,-9.38309831
C,0,3.3830981051,-8.0649326081,-8.5593779603
H,0,3.4910683257,-8.8660228023,-6.5534013712
H,0,3.1633244401,-7.0135327619,-10.4208429249
H,0,3.7478637483,-8.9733869453,-9.0289884667

H,0,2.4131564288,-7.1474596596,0.7687371548
H,0,1.2000371187,-7.5486222123,-0.4490267887
C,0,5.1179603755,-9.5008920824,-1.4894115977
C,0,2.7074437136,-10.0945796248,-0.1533765544
C,0,4.7964163231,-10.8138896461,-1.1372868941
H,0,6.0463407872,-9.274216521,-2.0059735886
C,0,3.6075139344,-11.1172591408,-0.4776019655
H,0,1.7769811657,-10.3255266862,0.3597000237
H,0,5.4889254217,-11.6123453311,-1.3902759571
H,0,3.3770454899,-12.1460900317,-0.2181518895

TS(RR)v, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1836.46198002 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.441293 a.u.
1 imaginary frequency = 317.5026 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0680942 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0949023 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1838.0155440 a.u.

0; 1
C,0,1.4453995842,-1.3274822671,-0.1758618371
C,0,1.9086423373,-0.0196417745,-0.3132830568
C,0,2.8533805543,0.5142175043,0.5876849707
H,0,1.834564271,-1.8947512207,0.6920632184
H,0,1.5540936059,0.559047433,-1.1598071502
H,0,2.9728738166,-0.041502664,1.517909372
C,0,5.0639098838,-1.6275632726,2.5793075934
C,0,5.1433703596,-2.2769429558,3.8071272521
C,0,5.7207051598,-0.4064300967,2.3801331857
H,0,4.6321100879,-3.2242135266,3.9493235188
C,0,5.8766912346,-1.714602023,4.8493079213
C,0,6.4565827604,0.1483708884,3.4345742665
H,0,5.9369726057,-2.2233417987,5.8069583275
H,0,6.9603595578,1.0940504485,3.2629462263
C,0,6.5332929068,-0.4989456336,4.6604565586
H,0,7.1053814622,-0.0577430075,5.4713103773
H,0,4.4915751728,-2.0879632594,1.7797249552
C,0,5.6904120315,0.3511514113,1.0928301202
O,0,6.3624410172,1.3868523716,0.9629132876
C,0,4.8025450897,-0.0871866433,0.0403089759
H,0,4.5971060176,-1.1438007049,-0.1032825961
S,0,5.1935477073,0.7425702654,-1.473719368
C,0,4.3434569335,-0.2658085719,-2.6991935303
H,0,4.6626421381,0.0952209124,-3.6784766497
H,0,4.6162083692,-1.3155304901,-2.5738602509
H,0,3.2646000249,-0.1281444365,-2.6000910896
C,0,6.9109651112,0.311061095,-1.8442336535
H,0,7.1514627834,0.7312944846,-2.8228739971
H,0,7.5165270794,0.7777453223,-1.0682170957
H,0,7.0307451495,-0.7733784344,-1.8420158408
C,0,3.0087489953,1.977846085,0.7519589617
C,0,2.7013847661,2.8805940994,-0.2762371567
C,0,3.4451546815,2.4909058836,1.9802528741
C,0,2.8270730799,4.2505673233,-0.0779417845
C,0,3.5613296863,3.8619119694,2.1820687976
C,0,3.2542704347,4.7468980736,1.1522510438
H,0,2.352532677,2.5146230588,-1.2373813262
H,0,3.6871593606,1.8049410021,2.7879799882
H,0,2.5823606605,4.9344090153,-0.8854558621
H,0,3.8926397176,4.2384926823,3.1453559059
H,0,3.3450475697,5.8180798421,1.3067895026
O,0,0.6243273472,-1.9313719847,-0.920127784
H,0,0.029779134,-1.2465732231,-2.0453384141
O,0,-0.5550680593,-0.875381498,-2.8366872083
C,0,0.0852381012,-0.069984854,-3.6417049416
C,0,-0.809983568,0.420789915,-4.7699798575
O,0,1.259968961,0.2577243612,-3.5435850746
N,0,-2.0296813105,1.0391219369,-4.2383378327
C,0,-0.1963064651,1.5169002711,-5.6528549571
H,0,-1.0587918788,-0.4604920446,-5.3854340722
C,0,-2.4461017145,2.008464236,-5.1432986852
H,0,-2.722331048,0.4020034588,-3.8716994181
C,0,-1.4007875775,2.3437067776,-6.0188925116

TS(RR)g, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1836.46201371 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.442235 a.u.
1 imaginary frequency = 327.3585 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0670316 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0940412 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1838.0157344 a.u.

0; 1
C,0,0.9143225486,-0.3243635328,-1.1528261331
C,0,1.7297784455,0.7772270337,-1.4031866614
C,0,2.7775824632,1.0921732908,-0.5076139633
H,0,1.1173483441,-0.8888400012,-0.2263867327
H,0,1.5515167161,1.35596367,-2.3050937649
H,0,2.7028930214,0.5918287219,0.4571692056
C,0,3.6566400853,-1.9417233342,1.2071301888
C,0,3.2424504646,-2.7530810181,2.2583866359
C,0,4.7548728844,-1.0857708799,1.3613394868
H,0,2.3824435511,-3.3987240491,2.1110167801
C,0,3.9244050246,-2.72108749,3.4724829153
C,0,5.4338695072,-1.0629278296,2.586530982
H,0,3.6021379351,-3.354874332,4.293791698
H,0,6.2835881292,-0.3957578912,2.6904439129
C,0,5.0218954193,-1.8748075774,3.6345963126
H,0,5.5540955809,-1.8488912094,4.5810257046
H,0,3.1046653588,-1.9959521176,0.2744775356
C,0,5.2475646281,-0.1834386699,0.2821169288
O,0,6.2634886702,0.5098042504,0.4510802697
C,0,4.4738518194,-0.0604176542,-0.9392932628
H,0,3.9630031972,-0.9291053287,-1.3443930727
S,0,5.4294057024,0.8010013966,-2.1528005652
C,0,4.4634828631,0.4914713778,-3.6397477335
H,0,4.9764606253,0.9683404375,-4.4758493081
H,0,4.3614952473,-0.5821260795,-3.8086627988
H,0,3.4810960721,0.9410861099,-3.4985572632
C,0,6.8805771261,-0.2266092215,-2.4886487235
H,0,7.4308151805,0.236412423,-3.3104743964
H,0,7.4771038905,-0.2126198459,-1.5770156305
H,0,6.5715633473,-1.2408666911,-2.7447728295
C,0,3.3496889905,2.4562947871,-0.4083440161
C,0,3.2449695476,3.3920997232,-1.4472374244
C,0,4.0068371229,2.8415790947,0.7686875996
C,0,3.7867291692,4.6661303337,-1.3148555588
C,0,4.5421996108,4.1173345992,0.9041049391
C,0,4.4380156911,5.0335874829,-0.1395692584
H,0,2.7202045547,3.1361363265,-2.3628741838
H,0,4.0907760029,2.1333785354,1.5881691791
H,0,3.6913149844,5.3776445924,-2.1299416365
H,0,5.0407891437,4.3963836911,1.8275815847
H,0,4.8561101284,6.0304747291,-0.0356172527
O,0,-0.0286831853,-0.7314360619,-1.8911008281
H,0,-0.6187751948,-1.9011405501,-1.3960228249
O,0,-1.1225391411,-2.7865886812,-1.0778723567
C,0,-0.399322631,-3.5323522574,-0.2868407253
C,0,-1.126721375,-4.8062619836,0.1130544073
O,0,0.7172926666,-3.255903408,0.1324372618
N,0,-1.7094240065,-5.4824572315,-1.0496434905
C,0,-0.2443519856,-5.8851564905,0.7591314068
H,0,-1.9177088766,-4.504938594,0.822081333
C,0,-1.7651585208,-6.8416526893,-0.7694924463
H,0,-2.5232229555,-5.042916657,-1.4548219947
C,0,-0.9110054479,-7.1561322689,0.3005842837

H,0,0.5262968625,2.0967342902,-5.0647511704
H,0,0.3388246763,1.1036909544,-6.5113494578
C,0,-3.6814861206,2.6461386629,-5.2244987086
C,0,-1.5815423093,3.3238760325,-6.9786265806
C,0,-3.8523485636,3.6273827752,-6.2038565683
H,0,-4.4920043039,2.3847813811,-4.5501849834
C,0,-2.8205771456,3.9687506463,-7.0754339011
H,0,-0.773342999,3.5846893926,-7.6576506769
H,0,-4.8132831762,4.1281469803,-6.2867386948
H,0,-2.9780622545,4.7318874017,-7.8315747969

H,0,0.778437036,-5.8054996903,0.3689705749
H,0,-0.1880307365,-5.7768436454,1.8448452767
C,0,-2.4930211347,-7.8342995232,-1.4209869093
C,0,-0.7733350452,-8.4669330413,0.7212399154
C,0,-2.3504435784,-9.1518951835,-0.9796921632
H,0,-3.1582424974,-7.5915951922,-2.2447865698
C,0,-1.503228744,-9.4743037676,0.0781229676
H,0,-0.1125201352,-8.7123470888,1.5491486029
H,0,-2.918321392,-9.9372611279,-1.471467599
H,0,-1.4119879145,-10.5051447198,0.4066812887

Int(SR)v, optimization in solv. CHCl₃

PBE1PBE/6-31G(d,p), E= -1836.48749769 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.445701 a.u.

SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0938334 a.u.SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.1221412 a.u.SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1838.046948 a.u.

0; 1
 C,0,-0.1814598002,-1.9944641547,2.379569007
 C,0,-0.5336882214,-0.9609366258,1.5855764542
 C,0,-1.9627760411,-0.633752677,1.2922126346
 H,0,-0.9516940965,-2.6076640974,2.8559612633
 H,0,0.2464747426,-0.3698795351,1.110441989
 H,0,-2.6114987725,-1.2914295939,1.8850733718
 C,0,-3.940695633,1.2461133278,-1.5469208395
 C,0,-4.7004165436,2.2282951511,-2.1714937435
 C,0,-4.5563975916,0.0830174014,-1.0654049685
 H,0,-4.2191881514,3.1301358302,-2.5360901839
 C,0,-6.0738959194,2.0566011584,-2.3257996128
 C,0,-5.9421649377,-0.0775334827,-1.2199457945
 H,0,-6.6631192154,2.8253647363,-2.8169000641
 H,0,-6.4038653418,-0.982135503,-0.8381498809
 C,0,-6.6950906404,0.901543517,-1.8486744616
 H,0,-7.7660261412,0.7699438729,-1.9675843017
 H,0,-2.8763080677,1.4098493933,-1.4198401873
 C,0,-3.823841367,-1.0127286297,-0.3958597431
 O,0,-4.396830404,-1.9985131323,0.0482750015
 C,0,-2.3112236572,-0.9413367404,-0.2038516387
 H,0,-1.8074304166,-0.2404233244,-0.8733162958
 S,0,-1.6025316085,-2.6040409541,-0.5728512203
 C,0,-2.5463107932,-3.1849462215,-2.0035895549
 H,0,-3.5303302367,-3.4934227841,-1.6552303869
 H,0,-2.6224102857,-2.4072010002,-2.764887228
 H,0,-2.0015411174,-4.0457150865,-2.3956739426
 C,0,-0.0479615111,-2.2060322937,-1.3945861318
 H,0,0.5887292142,-1.6032532595,-0.7317693919
 H,0,0.4351473527,-3.1622944324,-1.6075995939
 H,0,-0.2548664622,-1.6711071908,-2.3241071208
 C,0,-2.3377494005,0.8079227432,1.5854554289
 C,0,-1.5351569919,1.8629322608,1.1369735108
 C,0,-3.5004896802,1.1035815281,2.2995970041
 C,0,-1.8931460104,3.1822823248,1.3959246082
 C,0,-3.8577990398,2.4240141323,2.5626732363
 C,0,-3.0562537723,3.4671330964,2.1091103079
 H,0,-0.6163385784,1.6543865671,0.5937753191
 H,0,-4.1294530637,0.2923985446,2.6586403725
 H,0,-1.2573874674,3.9905444007,1.0460350639
 H,0,-4.762791638,2.6353555651,3.1249016899
 H,0,-3.3319251307,4.4973031499,2.3146060685
 O,0,1.0440932585,-2.3858573948,2.6781208299
 H,0,1.7583609077,-1.8065930325,2.2048904309
 O,0,2.9239342052,-1.0393649685,1.6840252825
 C,0,2.9222518162,-0.3444309229,0.6255828941
 C,0,4.2080048274,0.4581001007,0.4041458788
 O,0,1.9971981166,-0.2138945374,-0.204630418
 N,0,5.4049882143,-0.335840302,0.6972126943
 C,0,4.4675396449,0.9651663499,-1.022076841
 H,0,4.1535558657,1.325998656,1.0868515393
 C,0,6.4599033175,0.1854351634,-0.0298807634
 H,0,5.5436400071,-0.5934840351,1.6627844714
 C,0,5.9735941402,0.9812949326,-1.0847148717
 H,0,4.0443275598,0.2555843237,-1.7454470398

Int(SR)g, optimization in solv. CHCl₃

PBE1PBE/6-31G(d,p), E= -1836.48601401 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.444596 a.u.

SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0919674 a.u.SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.1202753 a.u.SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1838.0461462 a.u.

0; 1
 C,0,-0.4115078393,0.0260125654,2.0342526982
 C,0,-1.7349604126,-0.2320095459,1.9533809626
 C,0,-2.2492916539,-1.3667007474,1.1217196388
 H,0,0.2899466173,-0.5920161827,1.4652601857
 H,0,-2.4414744523,0.3838320817,2.5058914516
 H,0,-1.4012457625,-1.8447545143,0.6154426381
 C,0,-5.9792100538,-2.0174151335,-0.3269325393
 C,0,-7.2593957981,-2.5197713821,-0.5306025044
 C,0,-4.9282591405,-2.4082732234,-1.1677976689
 H,0,-8.0667888723,-2.2187181556,0.1291905026
 C,0,-7.5038164152,-3.4081549365,-1.5746503069
 C,0,-5.1839075371,-3.3131601633,-2.2101016795
 H,0,-8.5062510033,-3.7947269986,-1.7325912846
 H,0,-4.3591743529,-3.6127950112,-2.8482168093
 C,0,-6.4630071796,-3.8057328126,-2.4148823999
 H,0,-6.6530096956,-4.5010829418,-3.2264842022
 H,0,-5.8124355461,-1.3444442191,0.5069383665
 C,0,-3.5356961953,-1.9253725831,-1.0251753504
 O,0,-2.6317061728,-2.372985924,-1.7161128335
 C,0,-3.1898966364,-0.8455166562,0.0027167359
 H,0,-4.0776346376,-0.3996441354,0.4595767776
 S,0,-2.412894584,0.6334795852,-0.7745244456
 C,0,-0.8245790835,0.115422728,-1.4528463122
 H,0,-0.9153237103,-0.8976387536,-1.8445432564
 H,0,-0.6115794308,0.8255767433,-2.2551178935
 H,0,-0.0525078724,0.2106382458,-0.6812071066
 C,0,-3.3881434797,0.8149125134,-2.2852459547
 H,0,-4.4340267967,0.9445822559,-2.0018412304
 H,0,-3.0331018526,1.7205579631,-2.7795871012
 H,0,-3.2628100492,-0.0514208981,-2.9358407544
 C,0,-2.9987130263,-2.4508505479,1.8834254674
 C,0,-3.962815178,-2.1272178537,2.8433069376
 C,0,-2.747173439,-3.7979760505,1.6123486022
 C,0,-4.658576031,-3.1276785428,3.5148779528
 C,0,-3.439918195,-4.801045567,2.2861939975
 C,0,-4.3992777931,-4.4686331236,3.2378788308
 H,0,-4.1619777125,-1.085636899,3.0821883512
 H,0,-1.9992938865,-4.0636273054,0.8691524715
 H,0,-5.400134939,-2.8595178471,4.2619695256
 H,0,-3.2259491992,-5.8432176029,2.0675664936
 H,0,-4.939171537,-5.2493393473,3.7655100501
 O,0,0.1268935779,1.0001835834,2.7343866707
 H,0,1.1465618384,1.0431968529,2.4766343266
 O,0,2.5164037659,1.0774829838,2.0906129713
 C,0,2.7441629998,0.8666084361,0.8557200587
 C,0,4.1986294356,1.1147890276,0.4484572284
 O,0,1.9270997882,0.5240200275,-0.0171945401
 N,0,5.138223642,0.5109382594,1.3988107294
 C,0,4.6423636063,0.5298039604,-0.899934525
 H,0,4.3355027637,2.2114485947,0.4268306575
 C,0,6.3217541197,0.2495008114,0.7316741073
 H,0,5.1667829322,0.9225189291,2.3196560387
 C,0,6.1027062957,0.2450287159,-0.6590538929
 H,0,4.0804657829,-0.3921565833,-1.0990177701

H,0,4.0013864449,1.9353817797,-1.209560284
C,0,7.8286713378,-0.0161929726,0.1394890739
C,0,6.8524634288,1.5732740293,-1.9732504614
C,0,8.7031828838,0.5947516539,-0.7629648692
H,0,8.2073921381,-0.6255001522,0.9554541941
C,0,8.2313264135,1.3834416019,-1.8095877817
H,0,6.4781831647,2.1891309156,-2.7879412565
H,0,9.7736986076,0.4541022429,-0.6370326723
H,0,8.9303131384,1.8534493768,-2.4949670749

H,0,4.4509291249,1.2119438887,-1.7318374023
C,0,7.5835787137,-0.0241667759,1.256572004
C,0,7.1420961546,-0.0356014563,-1.5269470435
C,0,8.6242103465,-0.2990947011,0.3656236779
H,0,7.7567091006,-0.016566599,2.3291426686
C,0,8.4171519215,-0.3056611371,-1.0117743251
H,0,6.9745367964,-0.0384093228,-2.6016343527
H,0,9.6158553741,-0.5048456558,0.7605073789
H,0,9.2425246353,-0.5162789355,-1.6852998198

Int(RS)v, optimization in solv. CHCl₃

PBE1PBE/6-31G(d,p), E= -1836.48741723 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.445322 a.u.

SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0939364 a.u.SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.1222330 a.u.SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1838.0471143 a.u.

O; 1
C,0,0.4080016731,-1.7794679899,0.1702749176
C,0,1.8131358089,-1.2694478254,0.1909351193
H,0,-0.4044396976,-1.0910634885,0.3906213745
H,0,2.4985376277,-2.1015011482,-0.0161274472
C,0,2.2255718721,-0.6252497325,1.5031580558
C,0,1.4018084832,0.3117331974,2.1361202597
C,0,3.4490641418,-0.9512573733,2.0924621733
C,0,1.7975970449,0.9104178087,3.3281131104
C,0,3.844919281,-0.3553204726,3.2875787688
C,0,3.021073514,0.5794173893,3.9073927575
H,0,0.4372835696,0.5681012645,1.7050285737
H,0,4.0961980428,-1.6826360122,1.6139577076
H,0,1.1439812498,1.6316108641,3.8102635137
H,0,4.7973082602,-0.6253874373,3.7345880617
H,0,3.3265368996,1.0437695206,4.8404079453
C,0,0.1170280127,-3.0584068698,-0.1522958984
H,0,0.9248838382,-3.7563622218,-0.3911432308
O,0,-1.0781990521,-3.612777344,-0.2212722385
H,0,-1.8328709532,-2.9433356832,0.0274623262
O,0,-3.0136744453,-2.1692966063,0.4484164004
C,0,-3.1329109284,-0.9258655242,0.2341021157
C,0,-4.4350676706,-0.3253732979,0.7732399077
O,0,-2.34258474,-0.1756890734,-0.3746467777
N,0,-4.7250318629,-0.7961465052,2.1306025114
C,0,-4.4779879655,1.202966152,0.9174119954
H,0,-5.2372225628,-0.643874481,0.0826993339
C,0,-5.4992365147,0.1556364629,2.7676878993
H,0,-4.9520955769,-1.7742631124,2.2268155277
C,0,-5.4013811844,1.3885528839,2.0946649208
H,0,-3.4690308081,1.5763287298,1.1367018985
H,0,-4.8148007972,1.6975835058,0.0031424986
C,0,-6.2621855823,0.0342727711,3.9279529303
C,0,-6.0599722438,2.5024731715,2.5823240533
C,0,-6.9268190564,1.1677379308,4.4029254059
H,0,-6.3440158693,-0.9168949605,4.4465969164
C,0,-6.8346962257,2.3920163342,3.7450366799
H,0,-5.9853039199,3.4555417194,2.0634668632
H,0,-7.5326702944,1.0855356242,5.3017365838
H,0,-7.3650074536,3.2580098869,4.1298036165
C,0,2.0503826996,-0.2388334011,-0.9630130755
H,0,1.4758366076,0.6746176043,-0.7936732135
C,0,3.5447849786,-0.009935143,-1.1733489089
O,0,4.1789759873,-0.9147494117,-1.6992572284
C,0,4.191235612,1.2414331775,-0.7244506804
C,0,3.4989346205,2.2969573035,-0.1158856241
C,0,5.5738329968,1.3567147177,-0.9372794542
C,0,4.1798993972,3.4456056123,0.2699429489
H,0,2.4351257257,2.2293167624,0.0818295403
C,0,6.2485514639,2.5049107656,-0.5538870392
H,0,6.0956255419,0.5289768762,-1.4061112253
C,0,5.5509890533,3.5519138759,0.0502046633
H,0,3.6392577225,4.2576282358,0.7454713731
H,0,7.317725567,2.5880142881,-0.7221523743
H,0,6.0788497009,4.451619248,0.3522690198

Int(RS)g, optimization in solv. CHCl₃

PBE1PBE/6-31G(d,p), E= -1836.48618003 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.445685 a.u.

SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0920181 a.u.SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.1203211 a.u.SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1838.0459064 a.u.

O; 1
C,0,1.002003548,1.6582566041,-1.0980489139
C,0,1.9155029938,0.9739097775,-0.1277983684
H,0,1.3951818344,1.9862167897,-2.0579368788
H,0,1.3363323841,0.6937421256,0.7608677627
C,0,3.110764024,1.7912133458,0.3406718532
C,0,3.8830570565,2.5283565715,-0.5626328433
C,0,3.4713110002,1.793985331,1.6903049176
C,0,4.9892374492,3.2502767487,-0.1252207648
C,0,4.5763283322,2.5186771406,2.1307448221
C,0,5.3396669731,3.2472426463,1.2235415294
H,0,3.6114191657,2.5528077034,-1.614818495
H,0,2.8788209579,1.2260471384,2.4034693405
H,0,5.5752243729,3.822702217,-0.8385984487
H,0,4.8375315089,2.5147521687,3.1849962978
H,0,6.2005623985,3.8144447469,1.5649370638
C,0,-0.2979685129,1.8628503648,-0.7941450729
H,0,-0.6871043264,1.5108125623,0.1661120214
O,0,-1.1802581573,2.4333177353,-1.586896538
H,0,-2.1250864759,2.2959183298,-1.1512955294
O,0,-3.4019895501,2.0724660136,-0.5380479341
C,0,-3.5251623068,1.0060460801,0.1450162025
C,0,-4.948220233,0.768425755,0.658937922
O,0,-2.6319895662,0.1955158096,0.4529660371
N,0,-5.939203629,0.9433273889,-0.4090489065
C,0,-5.2558372866,-0.6366415327,1.1965949911
H,0,-5.1217662658,1.5087461837,1.4604585163
C,0,-7.0482857044,0.1742558834,-0.1047919919
H,0,-6.0665881071,1.8854396891,-0.7471814182
C,0,-6.714525934,-0.800316587,0.8545898374
H,0,-4.6331809308,-1.3709342582,0.6690556928
H,0,-5.0340033612,-0.7311424653,2.2623844001
C,0,-8.3339644271,0.2392833584,-0.6392437185
C,0,-7.6624472249,-1.713867046,1.2784128472
C,0,-9.2814816445,-0.686483735,-0.194911422
H,0,-8.5959989609,0.9937897387,-1.3758124769
C,0,-8.9603017016,-1.6552127404,0.7530304941
H,0,-7.4062166733,-2.4666278426,2.020509884
H,0,-10.2909084846,-0.6414781555,-0.5957811649
H,0,-9.7150148018,-2.3607996537,1.0874000494
C,0,2.4599117874,-0.3508847038,-0.7268516286
H,0,3.1012129879,-0.1225089135,-1.5829843458
C,0,3.1591596025,-1.2253603552,0.3160935941
O,0,2.4861407242,-1.680261208,1.2297238139
C,0,4.6103359931,-1.5028994128,0.2130697818
C,0,5.4536938075,-0.9006206069,-0.7304909434
C,0,5.1488093523,-2.4204662608,1.1287508773
C,0,6.8072924498,-1.2164831894,-0.7579218753
H,0,5.077619472,-0.1620778012,-1.4298594037
C,0,6.4971518478,-2.7389434859,1.0929283344
H,0,4.4851773464,-2.8726693668,1.8583723674
C,0,7.3286028555,-2.1372209216,0.147507063
H,0,7.4563910958,-0.740314001,-1.4857857401
H,0,6.9047752594,-3.4539493985,1.8007104045
H,0,8.3856677193,-2.3843970056,0.1194879889

S,0,1.3626839456,-1.0062582475,-2.4937864045
C,0,2.2055600955,-0.144570266,-3.8434448788
H,0,1.6614134732,-0.4038514205,-4.7534834339
H,0,2.1913038903,0.9359822275,-3.6904872161
H,0,3.2253307266,-0.521274496,-3.8987308772
C,0,-0.2642037402,-0.2459803891,-2.637445438
H,0,-0.7147770317,-0.6671925364,-3.5389016117
H,0,-0.8781583838,-0.4925141193,-1.7601204397
H,0,-0.1530249648,0.8355247179,-2.7394963628

S,0,1.0759567272,-1.2320468229,-1.5623658226
C,0,-0.1737744938,-1.6120293295,-0.3204916572
H,0,-0.7542777465,-2.4335159526,-0.7468387616
H,0,0.3168131432,-1.9151008799,0.6042757045
H,0,-0.8320475742,-0.7469156305,-0.1836578256
C,0,1.7977961076,-2.8679645155,-1.8292423703
H,0,1.0671321681,-3.4457595051,-2.397206386
H,0,2.7033248787,-2.7439380448,-2.425569291
H,0,2.018789756,-3.3576966193,-0.8798984748

Int(SS)v, optimization in solv. CHCl₃

PBE1PBE/6-31G(d,p), E= -1836.48271389 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.447468 a.u.

SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0899163 a.u.SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.1186519 a.u.SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1838.0446673 a.u.

0; 1

C,0,1.1598910073,-0.6854318265,-1.5247972168
 C,0,2.3441472259,-0.044467142,-0.8663258671
 H,0,0.2117816756,-0.1573554543,-1.4192472887
 H,0,3.2497883993,-0.6427733212,-1.0275356714
 C,0,-0.436820079,-1.7417657129,1.3671480748
 C,0,-1.5456248126,-2.4527752159,1.816030988
 C,0,0.8529330159,-2.198208413,1.6715906106
 H,0,-2.5400175719,-2.1140422035,1.5357268011
 C,0,-1.3745354445,-3.5991842194,2.5880979889
 C,0,1.0167566743,-3.3656457958,2.4345537362
 H,0,-2.2428602975,-4.1476185843,2.9421855618
 H,0,2.0226393988,-3.7117811261,2.6496374401
 C,0,-0.0917466323,-4.0541219178,2.9011858783
 H,0,0.0381823995,-4.9500744055,3.5006292607
 H,0,-0.6048404779,-0.8699330025,0.7382728504
 C,0,2.0779968576,-1.5316842292,1.1877069217
 O,0,3.172185562,-2.0773695418,1.23100555
 C,0,2.0145238309,-0.094721452,0.6464949198
 H,0,1.0380154252,0.3699164096,0.8142981458
 S,0,3.1088536868,1.028670668,1.6330312757
 C,0,2.8151041881,0.506134743,3.3327048326
 H,0,1.751992341,0.6402622867,3.5389482822
 H,0,3.1134658456,-0.5334596668,3.4732250419
 H,0,3.3970318232,1.1677967908,3.9762557661
 C,0,4.7971737905,0.4659563056,1.3609318799
 H,0,5.083829311,0.785541499,0.3588112974
 H,0,5.4162035231,0.9817582887,2.0975219396
 H,0,4.8448028888,-0.6173675408,1.4658719919
 C,0,2.5826036509,1.3724311404,-1.3564164686
 C,0,1.5638886774,2.3323559785,-1.2917233493
 C,0,3.8146072311,1.7343894095,-1.9070094767
 C,0,1.7873090033,3.6263144074,-1.7495928187
 C,0,4.0368398831,3.0304569286,-2.3693434195
 C,0,3.0248542928,3.9812127574,-2.2856020984
 H,0,0.5820697103,2.0581906757,-0.9101800488
 H,0,4.600951171,0.9878500718,-1.9987964311
 H,0,0.9877171472,4.3595514645,-1.6973384461
 H,0,4.9989467818,3.2919522545,-2.8003663159
 H,0,3.1938189582,4.9917497159,-2.645726714
 C,0,1.1593573157,-1.8929837369,-2.1122935895
 O,0,0.0811270809,-2.4984053212,-2.6039571834
 H,0,2.0732720256,-2.478687981,-2.2339782467
 H,0,-0.7489011419,-1.9746359647,-2.3411710652
 O,0,-2.1292084912,-1.3364689441,-1.938242098
 C,0,-2.4230335869,-0.3471382132,-1.2080908505
 C,0,-3.9341241785,-0.2090512331,-0.9560157133
 O,0,-1.6504166622,0.4828851628,-0.6788987174
 N,0,-4.431316474,-1.3992413748,-0.2442920703
 C,0,-4.3845445247,0.9453219305,-0.0536784382
 H,0,-4.4272406073,-0.1293018614,-1.9390692946
 C,0,-5.5589893552,-1.0285749703,0.4753947574
 H,0,-4.4634580918,-2.2480344492,-0.7910228613
 C,0,-5.5958968397,0.3688255721,0.6323250905
 H,0,-3.5806403416,1.1667143656,0.6605018577

Int(SS)g, optimization in solv. CHCl₃

PBE1PBE/6-31G(d,p), E= -1836.48376672 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.445480 a.u.

SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0902544 a.u.SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.1185064 a.u.SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1838.0449009 a.u.

0; 1

C,0,0.2182528252,1.1761525239,-1.2626910629
 C,0,-1.0880876959,0.8316396563,-1.2685096084
 C,0,-1.8001080555,0.6144654045,0.0304250899
 H,0,0.7371053648,1.2847421256,-0.3049476804
 H,0,-1.6177013141,0.686561362,-2.206180706
 H,0,-1.0617150452,0.7312654295,0.8340435803
 C,0,-5.1476600582,-0.8809034809,1.2212240448
 C,0,-6.4576689636,-0.8640007276,1.6851468372
 C,0,-4.8844143727,-1.1292523926,-0.1321547651
 H,0,-6.6546090021,-0.6687752003,2.7344689885
 C,0,-7.5132663215,-1.0939202418,0.8063309916
 C,0,-5.9547854564,-1.3622863585,-1.0088753637
 H,0,-8.535459639,-1.0787279105,1.1727217952
 H,0,-5.7350222755,-1.555270155,-2.0536746233
 C,0,-7.260205798,-1.3427098968,-0.5430530184
 H,0,-8.0830522889,-1.5206243491,-1.2283461134
 H,0,-4.3437853186,-0.684828789,1.9218241828
 C,0,-3.5211387764,-1.1945198496,-0.7061199182
 O,0,-3.3304821449,-1.5231381634,-1.8687424886
 C,0,-2.3017610736,-0.8677930262,0.1565367161
 H,0,-2.4574456021,-1.1362830876,1.2057182615
 S,0,-0.9609507442,-1.9469394396,-0.4861944047
 C,0,0.35217449,-1.7209563552,0.7277345109
 H,0,0.9851333843,-0.875785316,0.4313424905
 H,0,-0.0657957845,-1.5919889735,1.7280155014
 H,0,0.9529859932,-2.6322097948,0.6913263319
 C,0,-1.576947721,-3.5744650641,0.0074620267
 H,0,-0.7929803386,-4.2939736143,-0.2342122765
 H,0,-1.8089431676,-3.6061726615,1.0733410517
 H,0,-2.4594742772,-3.7900963056,-0.5954075558
 C,0,-2.9340131446,1.5782630933,0.344513791
 C,0,-3.7752369502,2.0696474872,-0.6568625581
 C,0,-3.1465534222,1.9908752913,1.6623916011
 C,0,-4.8136519657,2.9416349462,-0.3436556367
 C,0,-4.183553759,2.864739565,1.9784774776
 C,0,-5.0233716952,3.3395759745,0.9746508718
 H,0,-3.6127697015,1.7785898379,-1.6904945839
 H,0,-2.4863688878,1.6311094012,2.4492407561
 H,0,-5.4576381279,3.316016701,-1.1341109716
 H,0,-4.3290298603,3.1808268548,3.0074871304
 H,0,-5.83083827,4.0243543926,1.2165329277
 O,0,0.9647305945,1.3655980572,-2.3292757931
 H,0,1.9506401311,1.4625371242,-1.9879561003
 O,0,3.2792983186,1.5816090554,-1.4552116096
 C,0,3.5564599613,0.9264338531,-0.4009120974
 C,0,5.0329385232,0.9971015465,-0.0037823434
 O,0,2.7860178377,0.2355958401,0.2918016236
 N,0,5.569656628,2.3534851428,-0.1427953802
 C,0,5.3720786718,0.6359454827,1.4501416329
 H,0,5.571330471,0.3060850027,-0.6783064216
 C,0,6.635646805,2.491716069,0.7267443956
 H,0,5.6379996865,2.7140925893,-1.0824321259
 C,0,6.5845304265,1.4915278652,1.7166382289
 H,0,4.5335805418,0.915554709,2.101560468

H,0,-4.5835842248,1.8606972095,-0.6170506219
C,0,-6.5408798528,-1.8394893695,1.040105828
C,0,-6.6147407185,0.9595372625,1.3583484662
C,0,-7.5672562118,-1.2266762145,1.7635304143
H,0,-6.5167094248,-2.9184216788,0.9137845929
C,0,-7.6124499491,0.156001213,1.9259630538
H,0,-6.6476613641,2.039868246,1.479663159
H,0,-8.3473063646,-1.8448413813,2.2004290964
H,0,-8.4228672387,0.6113658576,2.4874003599

H,0,5.5429786113,-0.4349496219,1.5832420847
C,0,7.6388338208,3.4593311678,0.7409318017
C,0,7.5310185062,1.4597032046,2.7242935717
C,0,8.5915852064,3.4080248643,1.7616568898
H,0,7.6843289125,4.2291231225,-0.0243999994
C,0,8.5482607285,2.4236421942,2.7461417741
H,0,7.4926747028,0.6877075066,3.4895516312
H,0,9.385048285,4.1508153508,1.779806706
H,0,9.3029312618,2.400565711,3.5266164819

Int(RR)v, optimization in solv. CHCl₃

PBE1PBE/6-31G(d,p), E = -1836.48133521 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.446879 a.u.

SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0887846 a.u.

SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.1172655 a.u.

SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1838.0426339 a.u.

0; 1
C,0,1.2406848069,-0.1242445436,2.8473847715
C,0,1.2283732401,0.3951702753,1.6077900681
C,0,2.4120750288,1.0086225768,0.9215521134
H,0,2.12349399,-0.0594701853,3.4875551952
H,0,0.3340464865,0.26936501,0.9999775605
H,0,3.253920388,1.1064721635,1.6182833507
C,0,1.42776821,-2.7521269216,-0.0092437699
C,0,0.8879932025,-4.0289782545,-0.1280267412
C,0,2.7739199735,-2.6051178242,0.3531614291
H,0,-0.1597055714,-4.137941892,-0.3904765196
C,0,1.6770247507,-5.1538744948,0.0977281415
C,0,3.558901006,-3.7418705298,0.6044543035
H,0,1.2484640464,-6.1467098428,-0.0049833949
H,0,4.5943303858,-3.6062841373,0.9003639588
C,0,3.0158185457,-5.0095405997,0.4665048602
H,0,3.6291850798,-5.8865115164,0.6494565047
H,0,0.7621182099,-1.8983764543,-0.1389466472
C,0,3.4251077975,-1.2890141011,0.5132609444
O,0,4.483225946,-1.1578690488,1.1124451188
C,0,2.8129866599,-0.0407841433,-0.1421567422
H,0,1.9433080898,-0.2814449824,-0.7612112436
S,0,3.9691174945,0.662570885,-1.4094874416
C,0,4.6168972095,-0.7931031265,-2.2518861179
H,0,5.2870159242,-0.4342659205,-3.0345017045
H,0,5.1497979582,-1.4388349071,-1.5529562108
H,0,3.7748745139,-1.3174091013,-2.7063266706
C,0,5.4173920329,1.2336437392,-0.5058628235
H,0,6.1812684363,1.4502723559,-1.2551509328
H,0,5.1343547756,2.1563417201,0.0010639477
H,0,5.7385013955,0.4698055586,0.2020518256
C,0,2.0997897956,2.3662753494,0.3187567722
C,0,1.0547631678,2.5197030276,-0.6013595867
C,0,2.8320016363,3.4947004098,0.6975047602
C,0,0.7660235387,3.7692855562,-1.1389041622
C,0,2.5411003873,4.7477987454,0.1610504769
C,0,1.510411239,4.886632361,-0.7630062033
H,0,0.44419781,1.6630031375,-0.8785049299
H,0,3.6226907125,3.3971554883,1.4388988494
H,0,-0.0505781794,3.8733147285,-1.8473528519
H,0,3.1167841383,5.6145941306,0.4724743149
H,0,1.2797477628,5.8617781823,-1.1815969253
O,0,0.2218880458,-0.7520197529,3.4235913063
H,0,-0.5469375905,-0.8412450966,2.7584389993
O,0,-1.8142270944,-1.0046394199,1.8831091097
C,0,-1.9584143027,-0.9581957457,0.6278048753
C,0,-3.4031436398,-1.1625238809,0.1555587023
O,0,-1.0782612657,-0.814273558,-0.2505766964
N,0,-4.368590261,-0.4740902712,1.0150540374
C,0,-3.7512899655,-0.6364866201,-1.2452528791
H,0,-3.5861795954,-2.2531715949,0.180002534
C,0,-5.5031012694,-0.2063242666,0.274245375
H,0,-4.4488752658,-0.8093714519,1.9628071
C,0,-5.2106710168,-0.2865147569,-1.1015149277
H,0,-3.1464537443,0.2542140239,-1.4615983421

Int(RR)g, optimization in solv. CHCl₃

PBE1PBE/6-31G(d,p), E = -1836.48388166 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.446039 a.u.

SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0903813 a.u.

SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.118647 a.u.

SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1838.0449117 a.u.

0; 1
C,0,-0.1333604021,1.2871306947,-0.9486762748
C,0,1.1544922121,0.8811758254,-0.9759142659
C,0,1.8567538903,0.5733115917,0.3097769981
H,0,-0.6476023577,1.3783901566,0.0133712209
H,0,1.6723774904,0.7468871289,-1.9217496621
H,0,1.1295829592,0.7043787719,1.1216012112
C,0,5.1498167511,-1.122597156,1.3392672947
C,0,6.4734231007,-1.1989329959,1.7562020825
C,0,4.822339152,-1.3453207301,-0.0044084277
H,0,6.7205157004,-1.0220896025,2.7981493089
C,0,7.4785363257,-1.4986759309,0.839829138
C,0,5.8420234427,-1.6477759265,-0.9196020008
H,0,8.5115404987,-1.5574211119,1.169678785
H,0,5.5726001258,-1.8209061161,-1.9562186856
C,0,7.1612099379,-1.7220046149,-0.5003962472
H,0,7.9448733736,-1.9540793858,-1.2147827724
H,0,4.3860470137,-0.8708345053,2.0662069328
C,0,3.4378085695,-1.3196508352,-0.5286546115
O,0,3.1867515773,-1.6188345952,-1.6877396627
C,0,2.2696713919,-0.9390613695,0.3824000363
H,0,2.4427262293,-1.2432755324,1.4190615732
S,0,0.8471586451,-1.9206816897,-0.2430363588
C,0,-0.4214838248,-1.6442077734,1.0069946146
H,0,-1.097122099,-2.4996994209,0.9397627386
H,0,0.0200699369,-1.5969070496,2.0042813126
H,0,-0.98793292,-0.7382516062,0.761187383
C,0,1.3787987467,-3.5918519258,0.198144909
H,0,0.5503040858,-4.2618874038,-0.0373749588
H,0,2.2319882276,-3.8416194873,-0.4330486712
H,0,1.6372618033,-3.6603940084,1.2561272203
C,0,3.0466035258,1.4558435552,0.6542892426
C,0,3.9010976273,1.9516433667,-0.3333578512
C,0,3.2987852261,1.7874616264,1.9881557823
C,0,4.9914022121,2.7466559049,0.0080400564
C,0,4.3876487639,2.5841430131,2.3325993552
C,0,5.2406453453,3.0624159168,1.3414862919
H,0,3.7088967486,1.7257393128,-1.3780565044
H,0,2.6294657334,1.4248800269,2.7659196008
H,0,5.6452413451,3.125164239,-0.7722941782
H,0,4.5635671469,2.8379958545,3.3740228694
H,0,6.0890072824,3.6869322705,1.6054741128
O,0,-0.8727197563,1.5580755812,-2.0042700212
H,0,-1.8526276451,1.6654215876,-1.6601498057
O,0,-3.1965931463,1.7706647256,-1.1310504041
C,0,-3.4731600045,1.1445430505,-0.0600992569
C,0,-4.9552804389,1.2032782996,0.3199175218
O,0,-2.6855774697,0.5503257413,0.70127572
N,0,-5.8194338516,0.9538123559,-0.8378013979
C,0,-5.4425660214,0.1711839256,1.3475020165
H,0,-5.1375447154,2.2187223579,0.7164029551
C,0,-7.0215275677,0.4436540255,-0.3833575244
H,0,-5.8153158245,1.658873859,-1.5594504634
C,0,-6.8737339251,-0.0482915048,0.9275850969
H,0,-4.8503483568,-0.74818743,1.2490090519

H,0,-3.5415536386,-1.368598849,-2.0286123379
C,0,-6.7795098081,0.1437468152,0.7124465519
C,0,-6.189313514,-0.0131599931,-2.0391423298
C,0,-7.7582424376,0.4101011949,-0.2486914901
H,0,-7.0104525898,0.2018467701,1.7725155875
C,0,-7.4781445407,0.3340007312,-1.6109049739
H,0,-5.9640543024,-0.0745776498,-3.1015459769
H,0,-8.7601577174,0.6754822672,0.0792263207
H,0,-8.2567820878,0.5398728314,-2.339334503

H,0,-5.3270496534,0.522263487,2.3757387633
C,0,-8.2406910596,0.3407548204,-1.0512444927
C,0,-7.9407489964,-0.6486758922,1.5706128604
C,0,-9.3103803153,-0.2620140736,-0.3844119356
H,0,-8.35951197,0.7247286044,-2.0606232636
C,0,-9.173305365,-0.7534109428,0.9116229515
H,0,-7.8281990617,-1.0287558561,2.5835209346
H,0,-10.2696118233,-0.3406914894,-0.8897360447
H,0,-10.0204960432,-1.2127210155,1.4121531608

TS(RRR)v, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1836.46402310 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.442776 a.u.
1 imaginary frequency = 280.8921 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.070156 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.097435 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1838.0200931 a.u.
0; 1
C,0,-1.0326210732,0.0475836517,2.9930944829
C,0,-1.3183039546,0.7267013934,1.8203097149
C,0,-2.7148819223,0.7586621663,1.2725676728
H,0,-1.9065294209,-0.3513947607,3.547632616
H,0,-0.507909303,1.1980085217,1.271446271
H,0,-3.4290086882,0.4838581294,2.0586332264
C,0,-0.1664372787,-2.4327390424,0.4970744269
C,0,0.7642655381,-3.4615158699,0.4028132215
C,0,-0.3929409595,-1.5875838438,-0.5961225242
H,0,0.9469398918,-4.1014360437,1.2603378386
C,0,1.4716167063,-3.6598714707,-0.7808153007
C,0,0.3368414241,-1.7831975499,-1.777456817
H,0,2.1959434846,-4.4660612075,-0.8509218203
H,0,0.1631340609,-1.1094580425,-2.6105023552
C,0,1.25782231,-2.8174046302,-1.8722043824
H,0,1.8122461521,-2.9676493602,-2.7936692743
H,0,-0.6732236157,-2.2586167194,1.4400991769
C,0,-1.3597698799,-0.4543770548,-0.5770525873
O,0,-1.2993089403,0.4322326255,-1.4186509725
C,0,-2.5110959842,-0.4681589827,0.4121746849
H,0,-2.5589704007,-1.3734707722,1.0173737375
S,0,-4.2138267977,-0.912508025,-0.7438489728
C,0,-4.2086927919,0.1764615218,-2.1801079108
H,0,-3.2180117555,0.1991738087,-2.6348001054
H,0,-4.9647469276,-0.1922942195,-2.8767371419
H,0,-4.4794387761,1.172172133,-1.8274880513
C,0,-3.7556320446,-2.4891938789,-1.4915767536
H,0,-4.5726497847,-2.8159869112,-2.1372703431
H,0,-2.8332387544,-2.3941745452,-2.0672643774
H,0,-3.6202192314,-3.2123926981,-0.6856207158
C,0,-3.2155057412,2.027707687,0.6205639576
C,0,-2.3710401985,2.9359605459,-0.0237207268
C,0,-4.5852787918,2.3101118856,0.6718272382
C,0,-2.8892046245,4.0821547685,-0.6191384456
C,0,-5.1073018683,3.4543328141,0.0718021093
C,0,-4.2574790364,4.3436204709,-0.5800012372
H,0,-1.3043434519,2.7459458974,-0.0689195548
H,0,-5.2516910697,1.6283119628,1.1966621023
H,0,-2.2179274324,4.7770158899,-1.1156317045
H,0,-6.173555911,3.654972023,0.1259518465
H,0,-4.6561365818,5.2406997525,-1.0448079612
O,0,0.1079108807,-0.1681840588,3.5083717972
H,0,1.273408636,-0.0962508512,2.6677938471
O,0,2.1702996259,-0.2732229327,2.1433974736
C,0,2.3907989855,0.5605131844,1.1595657813
C,0,3.6087474018,0.1644843521,0.34573523
O,0,1.6988933298,1.5202654709,0.8571099753
N,0,4.1037036246,1.2584471437,-0.4812460037
C,0,4.8520624677,-0.2668116229,1.1493915606
H,0,3.2861738044,-0.6891569815,-0.2785094659
C,0,5.4516901331,1.0393351194,-0.7202312228
H,0,3.5145034539,1.5538451037,-1.2453895455
C,0,5.9706368643,0.1334398388,0.2215867985

TS(RRR)g, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E = -1836.46859519 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.439927 a.u.
1 imaginary frequency = 351.8320 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.071854 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0989189 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1838.0221989 a.u.
0; 1
C,0,0.0400500284,-0.6110820718,-2.4007661146
C,0,1.4103893021,-0.5238074264,-2.2393544067
C,0,2.0903091421,-1.2515685731,-1.1140882713
H,0,-0.4931517626,-1.2779653959,-1.6994113825
H,0,1.9877684102,0.1395243681,-2.874836801
H,0,1.4885855653,-2.115701141,-0.8119933616
C,0,-0.0590984071,2.2556053357,-0.2132366932
C,0,-0.8665455738,3.3724083608,-0.022877665
C,0,1.334850543,2.3975512698,-0.2267025948
H,0,-1.9453147624,3.2507677298,-0.0273327593
C,0,-0.2979190047,4.6301898454,0.1609292997
C,0,1.8998837151,3.6710271505,-0.0611252295
H,0,-0.9341050441,5.4973068959,0.3134705645
H,0,2.9807517186,3.7663004276,-0.0916330319
C,0,1.0893830669,4.7789607631,0.1398961748
H,0,1.5349301167,5.7597149712,0.2769332766
H,0,-0.5431261719,1.2998046742,-0.3919292099
C,0,2.2747542564,1.2613265509,-0.4298046872
O,0,3.4462707248,1.458233083,-0.7283479784
C,0,1.7953614673,-0.1436473715,-0.1376200204
H,0,0.7674681314,-0.195545984,0.2177509144
S,0,2.665905882,-0.5891143893,1.7930978179
C,0,4.4086338202,-0.1391728206,1.700956654
H,0,4.5268798704,0.8300733794,1.2147743427
H,0,4.8066100516,-0.1294962635,2.7179043791
H,0,4.9070066513,-0.9111543999,1.1134492468
C,0,2.0112445445,0.72312637,2.8448810329
H,0,2.4228699786,0.6011977443,3.8485716722
H,0,2.2646256049,1.7079911215,2.4486892643
H,0,0.9269850539,0.605710553,2.8825745212
C,0,3.5129085537,-1.7280645288,-1.2931981551
C,0,4.4485261785,-1.0709987346,-2.0967376377
C,0,3.9103724578,-2.8896609267,-0.621219416
C,0,5.7490529858,-1.5535071243,-2.2078088862
C,0,5.2138925254,-3.3707714455,-0.7246711579
C,0,6.1394542125,-2.700182599,-1.518956968
H,0,4.1695128312,-0.167724307,-2.6270595442
H,0,3.1870756502,-3.4292572152,-0.0133682864
H,0,6.4624969472,-1.0287698863,-2.8367439823
H,0,5.4995409902,-4.2748017557,-0.1945489906
H,0,7.1556694103,-3.0727768648,-1.6088638363
O,0,-0.6551097593,0.0227124365,-3.2578356012
H,0,-1.9545296649,-0.1195757008,-2.9769523176
O,0,-3.0249128233,-0.2302751424,-2.7685724069
C,0,-3.317422761,-0.0627734751,-1.511340326
C,0,-4.8184198167,-0.1120652402,-1.2628292442
O,0,-2.5167549666,0.1361064665,-0.6034906563
N,0,-5.4211313949,-1.3070709732,-1.8633191509
C,0,-5.2341914467,-0.196788391,0.212700377
H,0,-5.2423141836,0.8016145641,-1.7147603551
C,0,-6.5433926809,-1.6402027767,-1.1160173103
H,0,-5.5000315093,-1.3023217771,-2.8700689496
C,0,-6.4983623314,-1.0127009909,0.1403247801

H,0,4.9082701431,0.294077625,2.0917081943
H,0,4.8295098703,-1.3287322308,1.4015310315
C,0,6.2723127397,1.6096066259,-1.6903901031
C,0,7.3126983066,-0.1998269137,0.2049386163
C,0,7.6243060069,1.2569028232,-1.7000144083
H,0,5.8732810436,2.3057391454,-2.4227505972
C,0,8.1479066523,0.3632932583,-0.7686639936
H,0,7.7147304563,-0.8986701817,0.9346154409
H,0,8.276025075,1.6880203463,-2.4554624485
H,0,9.201061923,0.1007987158,-0.7988892462

H,0,-4.452638079,-0.7152221917,0.7827240776
H,0,-5.3643903693,0.790363402,0.6626291022
C,0,-7.5913623208,-2.4934642778,-1.4533776864
C,0,-7.4983135331,-1.2389688187,1.0691769009
C,0,-8.5980100612,-2.7056054236,-0.5084284077
H,0,-7.6298839776,-2.9754550403,-2.4261546833
C,0,-8.5610447526,-2.0897837666,0.7405866035
H,0,-7.4655390029,-0.7537366137,2.0417426488
H,0,-9.4277350395,-3.3609825875,-0.7598007302
H,0,-9.3573881871,-2.2661960508,1.4573082424

TS(SSS)v, optimization in solv. CHCl₃

PBE1PBE/6-31G(d,p), E = -1836.46402453 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.441287 a.u.

1 imaginary frequency = 293.9900 i cm⁻¹SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0697697 a.u.SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0970026 a.u.SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1838.0193961 a.u.

0; 1
C,0,-1.389959088,-1.0189309684,1.9374988186
C,0,-2.7311591389,-0.954479806,1.2688300263
H,0,-0.5299366144,-1.402080794,1.3958761151
H,0,-3.5167218293,-0.8100020043,2.0204735605
C,0,-3.1565139058,-2.0937906081,0.3703363816
C,0,-2.2468009614,-2.8894794819,-0.3314963564
C,0,-4.5228847542,-2.3673188266,0.2396913296
C,0,-2.6965081736,-3.9148933566,-1.1579953395
C,0,-4.9758243763,-3.3899076459,-0.5915780506
C,0,-4.0602967272,-4.165768549,-1.2969893477
H,0,-1.1820495867,-2.7046687934,-0.2408456179
H,0,-5.241992127,-1.7772383977,0.8044644854
H,0,-1.9751710201,-4.5230355121,-1.6962963434
H,0,-6.0408910471,-3.5862541328,-0.6762515788
H,0,-4.4055089513,-4.968353909,-1.9423084272
C,0,-1.2140520889,-0.5393793599,3.2251000679
H,0,-2.1349879657,-0.223484489,3.7563114122
O,0,-0.1247285106,-0.4241482688,3.8673641847
H,0,1.1110951052,-0.3961658543,3.1342611329
O,0,2.0588179651,-0.1669253794,2.7318716417
C,0,2.3679483553,-0.8347730287,1.6506316734
C,0,3.7070644757,-3.3898670994,1.0838186514
O,0,1.6805326113,-1.6856349516,1.1066267948
N,0,4.7414071499,-0.309774139,2.118822078
C,0,4.3149113802,-1.3311831618,0.033375885
H,0,3.5336142917,0.603105348,0.6319347904
C,0,5.970072762,-0.5347215896,1.513834487
H,0,4.6585712305,0.455946374,2.7715139522
C,0,5.7928591719,-1.1468611726,0.2612012137
H,0,4.0024552821,-2.3629716107,0.2391375027
H,0,3.9838449665,-1.0882917951,-0.9789532885
C,0,7.24518597,-0.2696836474,2.0077319052
C,0,6.8902467896,-1.5044800924,-0.5014222149
C,0,8.3432928076,-0.6284165281,1.2222068532
H,0,7.3834997731,0.2073889608,2.9738816666
C,0,8.1780882457,-1.238762012,-0.0190500021
H,0,6.7550042252,-1.9794014364,-1.4702267465
H,0,9.3448959146,-0.4209419708,1.5896279782
H,0,9.0466658453,-1.5054550632,-0.6135863284
C,0,-2.4598574178,0.395419106,0.646102659
H,0,-2.5787124049,1.1913849307,1.3808838752
C,0,-1.2204922877,0.5365638868,-0.2185011298
O,0,-1.0771394582,-0.1987423857,-1.1861929353
C,0,-0.2562463977,1.6414750238,0.0459666092
C,0,-0.1712885509,2.3265815794,1.2643373149
C,0,0.6229672489,1.9794182489,-0.9928553204
C,0,0.7663372793,3.3395339987,1.4321140806
H,0,-0.8000263255,2.0423985512,2.10130554
C,0,1.5533485675,2.9957553496,-0.8250959845
H,0,0.5573637171,1.4276852241,-1.9250807695
C,0,1.6244988469,3.6795697376,0.3888321285
H,0,0.8354082781,3.8557304276,2.3845448768
H,0,2.2251877979,3.2558507056,-1.6375218797

TS(SSS)g, optimization in solv. CHCl₃

PBE1PBE/6-31G(d,p), E = -1836.46885004 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.442099 a.u.

1 imaginary frequency = 342.8570 i cm⁻¹SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0722669 a.u.SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0994719 a.u.SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1838.0225771 a.u.

0; 1
C,0,1.0149900947,2.891616529,-0.7562272559
C,0,1.8599276372,1.8894147254,-0.0195562645
H,0,1.4618619612,3.4983568345,-1.5370842448
H,0,1.3982181414,1.6452930079,0.9433727122
C,0,3.3162670515,2.1960793866,0.2377352614
C,0,4.1054360228,2.957870819,-0.6281389335
C,0,3.9026631049,1.6924819301,1.4045188045
C,0,5.446889534,3.1922982359,-0.3417467544
C,0,5.2473112203,1.91970525,1.690362157
C,0,6.0251397257,2.67084906,0.8140120614
H,0,3.6785697107,3.3568571753,-1.541118358
H,0,3.2963536885,1.1187044457,2.1022529938
H,0,6.0445575548,3.7860452653,-1.0274482901
H,0,5.680624255,1.5193528935,2.602441994
H,0,7.072553327,2.8566259925,1.033205479
C,0,-0.3506137646,2.9408714884,-0.5388853377
H,0,-0.7465372704,2.263995585,0.2381924439
O,0,-1.1842831042,3.6591134088,-1.1781538654
H,0,-2.451291691,3.2060886426,-1.0338655328
O,0,-3.4834444384,2.8573553,-1.015979101
C,0,-3.5825809136,1.577940471,-0.7964226591
C,0,-5.0066470221,1.0753631596,-1.0124791878
O,0,-2.6630946443,0.828589156,-0.4833562025
N,0,-5.2841500913,1.0427948234,-2.4583879185
C,0,-5.259721102,-0.3687842949,-0.5614558132
H,0,-5.694213713,1.7678509215,-0.5037103909
C,0,-6.1895487308,0.0105406596,-2.6944126291
H,0,-5.4811290639,1.9399922771,-2.8802376951
C,0,-6.2249377644,-0.8702701335,-1.6024681905
H,0,-4.311240933,-0.9200700847,-0.5936007092
H,0,-5.6399869481,-0.4210252847,0.4619363511
C,0,-6.9603803345,-0.2214553482,-3.8302807701
C,0,-7.0302720553,-1.9951716596,-1.6407105253
C,0,-7.7754056064,-1.3557898703,-3.851417277
H,0,-6.9368645448,0.4637105138,-4.6729593574
C,0,-7.8157072891,-2.2379778327,-2.7739675487
H,0,-7.0611011642,-2.6787348274,-0.7957482979
H,0,-8.3922815927,-1.5463436334,-4.7255512315
H,0,-8.4599752415,-3.1112048951,-2.8109989646
C,0,1.489991778,0.7888246201,-0.9806015695
H,0,0.5042648964,0.3878051485,-0.7503597698
C,0,1.7545315117,0.9697800507,-2.460414335
O,0,2.8764894285,1.2796236132,-2.8442307868
C,0,0.6706227118,0.6628223543,-3.4338656529
C,0,-0.680048544,0.5439319791,-3.0799765768
C,0,1.0429212916,0.5164084574,-4.7786582984
C,0,-1.6365467634,0.2808582337,-4.0556483396
H,0,-1.0195001497,0.6891490891,-2.0589929607
C,0,0.0879132222,0.2416949306,-5.7466259087
H,0,2.0907863671,0.6244839334,-5.0400210593
C,0,-1.2552500622,0.1247140741,-5.3859904756
H,0,-2.6828223925,0.2168036592,-3.7688333105
H,0,0.3859997228,0.123905877,-6.7842009096

H,0,2.354557732,4.4722991934,0.5237581103
S,0,-4.0645663396,1.014706276,-0.5817303657
C,0,-3.8823885505,0.2135784876,-2.1861327281
H,0,-4.5977219898,0.6773998761,-2.8689498454
H,0,-2.8587556335,0.311546069,-2.5476268299
H,0,-4.1274493792,-0.8398609672,-2.046269316
C,0,-3.604488887,2.7144652545,-0.9744930065
H,0,-4.3345295829,3.1163068837,-1.6794460268
H,0,-3.6440868976,3.2894009802,-0.047691117
H,0,-2.6011648172,2.7616673161,-1.4021138866

H,0,-2.0044875563,-0.0817504415,-6.1449302882
S,0,2.5335519881,-1.0388905481,-0.4816164049
C,0,4.2063609096,-0.8901917347,-1.1362535874
H,0,4.668198531,-1.8795748304,-1.1088436709
H,0,4.1828567871,-0.4865670842,-2.1490870088
H,0,4.7474766636,-0.2090642497,-0.4783905917
C,0,1.8041046235,-2.228636017,-1.6258280198
H,0,2.2904019877,-3.1952777287,-1.4813386776
H,0,0.7448937427,-2.316531019,-1.3785933236
H,0,1.9183023257,-1.8978834599,-2.659683426

TS(RSR)v, optimization in solv. CHCl₃

PBE1PBE/6-31G(d,p), E= -1836.47190158 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.442138 a.u.

1 imaginary frequency = 323.5348i cm⁻¹

SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0759314 a.u.

SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.1028652 a.u.

SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1838.0250198 a.u.

0; 1
C,0,-1.0960647734,-0.5836499797,2.6040337877
C,0,-1.1397909464,0.3052984453,1.5432129571
C,0,-2.3992346326,0.9929136851,1.0908939112
H,0,-2.036347577,-0.7420261648,3.1606276834
H,0,-0.2426131769,0.4635147982,0.9509262421
H,0,-3.1886463017,0.8782473493,1.8406814972
C,0,-3.2773837989,-3.7574370469,-0.0913645757
C,0,-2.7545030361,-4.9428873478,-0.5876246209
C,0,-2.5014520007,-2.5896608824,-0.0865556527
H,0,-3.3632998652,-5.8419114148,-0.6007198737
C,0,-1.443229961,-4.9774588306,-1.0632327217
C,0,-1.1810946876,-2.6312556462,-0.5515761044
H,0,-1.0302966955,-5.9063512368,-1.4461011266
H,0,-0.5330853732,-1.7616644715,-0.4800537495
C,0,-0.6584755552,-3.8270028903,-1.0336320706
H,0,0.3716971675,-3.8592165394,-1.3748948755
H,0,-4.2904681624,-3.7121034413,0.2964201643
C,0,-3.1200917894,-1.3549479894,0.4558036174
O,0,-4.095179811,-1.4016082164,1.1977120045
C,0,-2.6200558607,-0.0010637378,-0.007675452
H,0,-1.83518663,-0.0213408279,-0.7612711091
S,0,-4.163006126,0.6851118432,-1.3371681106
C,0,-4.786864682,-0.8055955334,-2.1392956259
H,0,-3.9735572353,-1.2323754547,-2.7280395506
H,0,-5.1338514601,-1.5258339547,-1.3964884759
H,0,-5.6060280098,-0.5220289631,-2.802980521
C,0,-5.5065619747,1.0468468561,-0.1934597456
H,0,-6.4244394122,1.1792241249,-0.7695794233
H,0,-5.5987387747,0.2322846098,0.5273937229
H,0,-5.2559483431,1.9813884328,0.3104357083
C,0,-2.2678827594,2.4428072329,0.6940758483
C,0,-1.3941233481,2.8479193089,-0.3211049992
C,0,-3.0130325785,3.4181280741,1.3626528302
C,0,-1.2753502195,4.1917762983,-0.6607497613
C,0,-2.8943831109,4.7646954206,1.02578443
C,0,-2.0261032334,5.1549629027,0.0106414314
H,0,-0.7888825699,2.1126199181,-0.8459106697
H,0,-3.6845525097,3.1197485961,2.1647992157
H,0,-0.5903606691,4.4881206121,-1.4498247076
H,0,-3.4794794572,5.5077437432,1.5600129358
H,0,-1.9308666231,6.2037519528,-0.2545247109
O,0,-0.0831995476,-1.2401684351,3.0028397727
H,0,1.1388428765,-1.0765765671,2.3580632247
O,0,2.1683190817,-1.0137152056,2.0570658295
C,0,2.3776421553,-0.8868166696,0.7776289152
C,0,3.8595571445,-0.8994231376,0.4427487104
O,0,1.5239653491,-0.8059367462,-0.0972658188
N,0,4.1330089734,-0.4278903378,-0.9100750163
C,0,4.7483897248,0.0039271921,1.3236453779
H,0,4.193987002,-1.9442990073,0.5734566527
C,0,5.4243704529,0.0803303459,-0.9340810821
H,0,3.8396582727,-1.0289020766,-1.6659299099
C,0,5.8589007574,0.3658318309,0.371541386

TS(RSR)g, optimization in solv. CHCl₃

PBE1PBE/6-31G(d,p), E= -1836.46923919 a.u.

Thermal correction to Gibbs Free Energy at 25 °C = 0.440783 a.u.

1 imaginary frequency = 343.3434 i cm⁻¹

SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0736927 a.u.

SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.1004308 a.u.

SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1838.0217143 a.u.

0; 1
C,0,0.5489790959,-0.9464217446,-1.2423351258
C,0,1.9342956463,-0.9592959657,-1.3038737153
C,0,2.8128203875,-1.0901978517,-0.0865345715
H,0,0.0840695183,-1.0127798842,-0.2451891299
H,0,2.424729872,-0.8568526838,-2.2686519635
H,0,2.2130414783,-1.4026230161,0.7732670529
C,0,2.2287590785,3.1106541243,-1.1024681221
C,0,1.7641427334,4.275469575,-1.702802057
C,0,1.3992028665,2.3852651467,-0.2379005749
H,0,2.4164516153,4.8395865681,-2.362223455
C,0,0.4622994985,4.7106827671,-1.46565218
C,0,0.0903259542,2.8302736982,-0.0029125435
H,0,0.0977587774,5.6141472887,-1.9456203551
H,0,-0.5544179261,2.2382061216,0.6386059214
C,0,-0.3754016922,3.9818790625,-0.6218067886
H,0,-1.3953969255,4.3121109901,-0.4503076889
H,0,3.2438571276,2.7856261054,-1.308391789
C,0,1.8350576173,1.1586138734,0.473081035
O,0,1.2534802303,0.7655108358,1.4771542372
C,0,3.0443492249,0.3858248347,-0.0081843411
H,0,3.5759791729,0.8005477913,-0.8609434026
S,0,4.5569655672,0.8273334718,1.4777045716
C,0,4.1402470326,2.4597694299,2.1276095855
H,0,4.3205715216,3.1920328928,1.3394670028
H,0,3.0957154812,2.4918880807,2.4429775823
H,0,4.7977487366,2.6690628721,2.9738285834
C,0,3.9933097296,-0.2200724147,2.8306838046
H,0,4.5431687613,0.0559778714,3.7324084539
H,0,2.917382916,-0.0927182868,2.9657008123
H,0,4.2287397513,-1.2507344147,2.5613596056
C,0,4.0156058982,-1.9885159981,-0.2306859944
C,0,5.0937262389,-1.6591735799,-1.0589152825
C,0,4.0462285617,-3.208813481,0.4513591967
C,0,6.1740503101,-2.5262744699,-1.1977615717
C,0,5.1243253538,-4.0786352686,0.3124951276
C,0,6.1932514323,-3.7385997801,-0.5124042187
H,0,5.0937854491,-0.7219971611,-1.610231956
H,0,3.2103372008,-3.4820559825,1.091244381
H,0,7.0024532523,-2.253837813,-1.8453026428
H,0,5.1279491002,-5.02261947,0.8497292342
H,0,7.0363025761,-4.4143043745,-0.6218369522
O,0,-0.214549031,-0.840781017,-2.2528636836
H,0,-1.5471801502,-0.7450349714,-1.9429971396
O,0,-2.6147473185,-0.6655423868,-1.8067843411
C,0,-2.9407835543,-0.1442738989,-0.6558390899
C,0,-4.4429903684,0.0676813316,-0.5356862265
O,0,-2.1631236704,0.1750900515,0.2331023031
N,0,-5.1890191701,-1.1403595462,-0.9032274606
C,0,-4.9457294775,0.3888055659,0.8790503859
H,0,-4.6986726405,0.8992652651,-1.2156368882
C,0,-6.3885400319,-1.1303164745,-0.2045839146
H,0,-5.207735804,-1.3659207383,-1.8872185232
C,0,-6.3157446771,-0.2377531528,0.8784958038

H,0,4.1926258664,0.899204427,1.6327748424
H,0,5.077386239,-0.5054639865,2.2312553601
C,0,6.2372807239,0.3470687272,-2.0328344591
C,0,7.103941248,0.928702304,0.5860328408
C,0,7.4958423176,0.9077854092,-1.8003699577
H,0,5.9064153015,0.1214053299,-3.0427049654
C,0,7.9331596708,1.1983067698,-0.5102983824
H,0,7.4402681636,1.151104897,1.5958141471
H,0,8.1454311917,1.1145726882,-2.6468314432
H,0,8.917415309,1.6291843538,-0.3537878979

H,0,-4.2857919042,-0.0845159738,1.6173042459
H,0,-4.9457997451,1.4619276548,1.0843142476
C,0,-7.5369191892,-1.8838002256,-0.4359766671
C,0,-7.389109433,-0.0979489392,1.7400575646
C,0,-8.6154787215,-1.7255201671,0.4376163795
H,0,-7.5963953711,-2.5704888309,-1.2756842251
C,0,-8.5523204912,-0.8450362112,1.5152664096
H,0,-7.3346739861,0.5923338897,2.5784995622
H,0,-9.5223534984,-2.2992181158,0.2653289425
H,0,-9.4051109891,-0.7353138693,2.178377549

TS(SRS)v, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -1836.47198109 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.441327 a.u.
1 imaginary frequency = 327.9955 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.0756445 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.1025868 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1838.0250035 a.u.
0; 1
C,0,-0.0125603784,-0.2949437686,3.2834010642
C,0,0.1876548842,0.2437765604,2.0238958209
C,0,1.543896128,0.6341014664,1.5012140902
H,0,0.8768258155,-0.3896076401,3.930501757
H,0,-0.6535821023,0.326932803,1.3413158271
H,0,2.273508743,0.6649918256,2.3167143771
C,0,-0.0335524949,-3.1563285089,0.8525901522
C,0,-0.6804544268,-4.3759426817,0.6819818961
C,0,1.2558935001,-3.1251228508,1.3984765953
H,0,-1.6875968096,-4.3927126224,0.2769505417
C,0,-0.0492195339,-5.5639624138,1.0429046872
C,0,1.8745869345,-4.3216545178,1.7875781316
H,0,-0.5577036057,-6.5133973852,0.901835225
H,0,2.863890383,-4.277046711,2.2325653409
C,0,1.2297579439,-5.5358593423,1.6000372716
H,0,1.7180548452,-6.4608288298,1.891634313
H,0,-0.5682428697,-2.2388831575,0.6218625526
C,0,1.9983609563,-1.8602218427,1.6221775619
O,0,2.9203601381,-1.7933280003,2.4276617344
C,0,1.6977655176,-0.6543092778,0.7542183228
H,0,0.9604654502,-0.8138857653,-0.030003534
S,0,3.3917502704,-0.5512969208,-0.5650469856
C,0,3.9084141531,-2.2633109865,-0.8112809143
H,0,4.8075642361,-2.264334149,-1.4306518899
H,0,4.1071741163,-2.7462053895,0.1471875182
H,0,3.1053097175,-2.7819955138,-1.3370033195
C,0,4.6762793493,0.0372114554,0.5520736212
H,0,5.6438943879,-0.0810655786,0.0607851602
H,0,4.485659814,1.0967201494,0.7293913155
H,0,4.6289660429,-0.5250910396,1.4867057958
C,0,1.6092626008,1.9114053836,0.700125435
C,0,0.8937276232,2.0679935452,-0.4920234909
C,0,2.3789919332,2.9825369225,1.1628555541
C,0,0.9517464242,3.2624149066,-1.2033597216
C,0,2.4369259551,4.1800437758,0.4537234442
C,0,1.7243988098,4.3224342998,-0.7334247861
H,0,0.2743685842,1.2571641941,-0.8676432126
H,0,2.9301506433,2.8797592448,2.095065373
H,0,0.3880086819,3.3664837425,-2.1258650429
H,0,3.0383631741,5.001845212,0.8315460179
H,0,1.7677310089,5.254636147,-1.2888091009
O,0,-1.1146166522,-0.6964552437,3.7741634517
H,0,-2.2764247867,-0.584453676,3.0308754549
O,0,-3.2794200231,-0.4893843437,2.6493841467
C,0,-3.4241933948,-0.7160073588,1.3753541205
C,0,-4.8788589082,-0.5833962863,0.945147835
O,0,-2.5391890119,-1.0228660916,0.5853146835
N,0,-5.4563594089,0.682936996,1.4067833227
C,0,-5.1130137808,-0.5587118207,-0.5723208114
H,0,-5.4184130014,-1.4380540056,1.3891288236
C,0,-6.4536236067,1.0496872638,0.5137878799
H,0,-5.6478635774,0.747707966,2.396032759
C,0,-6.3102312594,0.3477660771,-0.6949899757

TS(SRS)g, optimization in solv. CHCl₃
PBE1PBE/6-31G(d,p), E= -1836.46973975 a.u.
Thermal correction to Gibbs Free Energy at 25 °C = 0.439622 a.u.
1 imaginary frequency = 331.7850 i cm⁻¹
SP at B2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.074051 a.u.
SP at mPW2PLYP/6-311+G(d,p) in CHCl₃, E = -1837.1005414 a.u.
SP at M06-2X/6-311+G(d,p) in CHCl₃, E = -1838.0216855 a.u.
0; 1
C,0,0.5358146285,-1.2147412239,0.8278727978
C,0,1.9022220669,-1.0257456326,0.9736365836
C,0,2.8087328655,-0.6999164847,-0.1836229844
H,0,0.1058788512,-1.0986170898,-0.1804751241
H,0,2.3576848102,-1.1486922674,1.953256543
H,0,2.257887001,-0.8015174845,-1.1235149618
C,0,1.4978654677,2.4815133932,2.2514781003
C,0,0.9781496533,3.4167307082,3.1391837645
C,0,1.1163086853,2.50273247,0.9044957398
H,0,1.2693253517,3.3877522367,4.1845297837
C,0,0.0764841606,4.3794533686,2.6908613334
C,0,0.194918718,3.4639914328,0.4664749834
H,0,-0.3269480479,5.1092429435,3.3866412579
H,0,-0.1054686334,3.4560668918,-0.57634062
C,0,-0.3173881813,4.4001759869,1.3530030346
H,0,-1.0271875248,5.1445899274,1.0055242315
H,0,2.1669903542,1.7122950421,2.6222005327
C,0,1.6274395361,1.5369921652,-0.101255452
O,0,1.1055816084,1.4335254532,-1.2051872048
C,0,2.8885433018,0.748215615,0.1804504822
H,0,3.3768722741,0.9468445136,1.1317478494
S,0,4.372350336,1.7374555856,-1.0288935318
C,0,3.853424734,3.4645461069,-1.1012437737
H,0,2.8299213074,3.5402520693,-1.4721152133
H,0,3.9221960702,3.8757317382,-0.0931110396
H,0,4.5371076044,4.0025265156,-1.760889602
C,0,3.9074490259,1.1707852557,-2.6743431346
H,0,4.4507471358,1.7651152176,-3.4114730708
H,0,4.2138938886,0.1265842325,-2.7521967019
H,0,2.8270673112,1.2662579852,-2.8008161991
C,0,4.1033440801,-1.4716462948,-0.2558428541
C,0,5.0958126583,-1.337586351,0.7211660537
C,0,4.315305072,-2.3736720625,-1.3027349069
C,0,6.2692431982,-2.0823008002,0.650152253
C,0,5.4877401977,-3.1218476379,-1.3750296755
C,0,6.4695831942,-2.976863452,-0.3987891269
H,0,4.9535571399,-0.6536778193,1.5546078497
H,0,3.5473058966,-2.4973879945,-2.0630099649
H,0,7.0283507797,-1.9651039507,1.418173452
H,0,5.6321787196,-3.8190339103,-2.1953055368
H,0,7.3851836325,-3.5582454597,-0.453330776
O,0,-0.2528025875,-1.5189793221,1.7773216566
H,0,-1.5685204284,-1.6669198639,1.4035985776
O,0,-2.6200343764,-1.8118559506,1.2166754199
C,0,-2.9187812638,-1.755308453,-0.0523191135
C,0,-4.3963633753,-2.0142185133,-0.3031625794
O,0,-2.1301648937,-1.5616181953,-0.9672993811
N,0,-5.2509717437,-1.2662200648,0.6230503898
C,0,-4.9067184886,-1.5914393439,-1.6890882055
H,0,-4.5477846528,-3.10079699,-0.1744248619
C,0,-6.4649061243,-1.0344325695,-0.0077926167
H,0,-5.2573058441,-1.5879212101,1.5799354531
C,0,-6.3342885462,-1.2084376873,-1.396470584

H,0,-4.2328504837,-0.1329576813,-1.0709591381
H,0,-5.2670471725,-1.5595059308,-0.9829215381
C,0,-7.4647649287,1.9932736528,0.6787835803
C,0,-7.1734145714,0.5902136827,-1.7486830246
C,0,-8.3335941934,2.2211328883,-0.3910162671
H,0,-7.5798422513,2.5328772329,1.6145691177
C,0,-8.1978958279,1.5325823879,-1.5944028813
H,0,-7.0643498885,0.0478530185,-2.6848490202
H,0,-9.133636124,2.9475818576,-0.2752433071
H,0,-8.8881756915,1.7231396747,-2.4105987115

H,0,-4.3261223692,-0.7319025602,-2.0477318449
H,0,-4.7997084961,-2.3873540013,-2.4296114261
C,0,-7.6777563029,-0.6421391272,0.5537886339
C,0,-7.4140106871,-0.9839767007,-2.2316055682
C,0,-8.7611759254,-0.4274655793,-0.3016431277
H,0,-7.7817499692,-0.5127134092,1.6274097871
C,0,-8.640822511,-0.5941810834,-1.6793981721
H,0,-7.3148559646,-1.117898059,-3.3061843758
H,0,-9.7168357914,-0.1299154923,0.1219872191
H,0,-9.4980195876,-0.4262507626,-2.3244084511