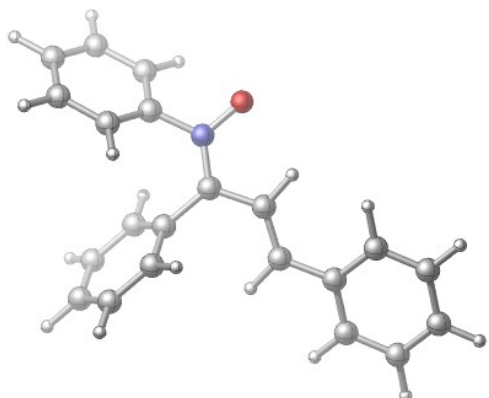


Supplementary Information

**Mechanism of Nitrones and Allenates Cascade Reactions for the Catalytic
Synthesis of Dihydro[1,2-a]indoles**

Wes Lee, †,^a Mingbin Yuan, †,^a Chris Acha, †,^a Ashley Onwu, and Osvaldo Gutierrez ^a

Figure 1.
1'

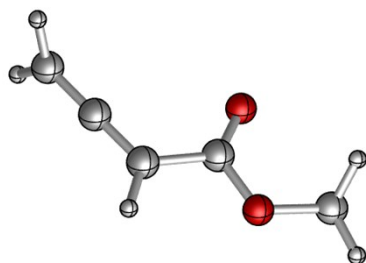


Zero-point correction=	0.325458 (Hartree/Particle)
Thermal correction to Energy=	0.343973
Thermal correction to Enthalpy=	0.344917
Thermal correction to Gibbs Free Energy=	0.276324
Sum of electronic and zero-point Energies=	-939.670262
Sum of electronic and thermal Energies=	-939.651748
Sum of electronic and thermal Enthalpies=	-939.650804
Sum of electronic and thermal Free Energies=	-939.719397

C	-6.92243000	1.78807900	1.04532700
H	-6.01983200	0.09655100	2.03837500
C	-5.97488900	0.78025100	1.19794000
C	-6.85098300	2.66340800	-0.03642100
C	-4.96071800	0.66523300	0.25304900
O	-2.72722600	0.13594100	0.22287600
N	-3.91085200	-0.32939800	0.38650200
C	-5.81755000	2.54344800	-0.96426600
H	-2.07969800	-1.88996700	1.10017000
C	-4.15568100	-1.59955500	0.66366200
C	-4.85713700	1.54909800	-0.81545700
C	-3.00445100	-2.43608900	0.94773100
H	-5.75432800	3.22936000	-1.80217100
C	-3.04474500	-3.78078400	0.99898700
H	-4.02792500	1.44550000	-1.50527200
C	-1.91338300	-4.66161400	1.30745600
H	-3.98225200	-4.28883000	0.77915900
C	-5.53389100	-2.14829800	0.63615300
C	-6.33987000	-2.00314200	-0.49812500
C	-6.02912100	-2.84839700	1.74196900
C	-7.62792000	-2.52704900	-0.51544900
C	-8.12150100	-3.20782700	0.59580100

C	-7.31876700	-3.37028200	1.72288000
H	-9.12734500	-3.61471700	0.58104700
H	-7.69710000	-3.90128900	2.59027700
H	-5.40125100	-2.96945200	2.61992700
H	-5.95355000	-1.47240100	-1.36348100
H	-8.24532700	-2.40791900	-1.39982700
C	-2.07339400	-6.04417600	1.13789300
C	-0.67569500	-4.18480400	1.76803600
C	-1.02997900	-6.92455500	1.40435900
C	0.19487300	-6.43681100	1.85240600
C	0.36567400	-5.06373700	2.03471400
H	-3.02817000	-6.42628500	0.78685700
H	-1.17419900	-7.99085300	1.26287900
H	-0.52887600	-3.12154600	1.92860100
H	1.01087000	-7.12026500	2.06351400
H	1.31510800	-4.67806000	2.39199100
H	-7.71379300	1.89176400	1.77975400
H	-7.59545800	3.44398400	-0.15162100

2

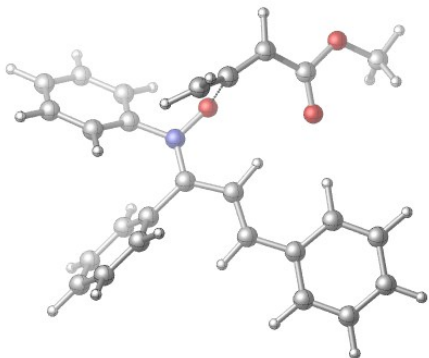


Zero-point correction=	0.100668 (Hartree/Particle)
Thermal correction to Energy=	0.108188
Thermal correction to Enthalpy=	0.109132
Thermal correction to Gibbs Free Energy=	0.068740
Sum of electronic and zero-point Energies=	-344.294924
Sum of electronic and thermal Energies=	-344.287403
Sum of electronic and thermal Enthalpies=	-344.286459
Sum of electronic and thermal Free Energies=	-344.326852

C	-4.205129000	4.089884000	0.364819000
C	-3.973312000	2.847642000	0.058998000
C	-3.742152000	1.593356000	-0.249606000
H	-4.125504000	4.435628000	1.391033000
H	-4.487664000	4.808153000	-0.399028000
C	-4.845775000	0.601840000	-0.235601000
H	-2.749731000	1.249835000	-0.522946000
O	-6.001097000	0.828161000	0.043127000

O	-4.390488000	-0.611586000	-0.581574000
C	-5.378425000	-1.644406000	-0.602564000
H	-4.854677000	-2.550937000	-0.898355000
H	-6.164038000	-1.403264000	-1.321255000
H	-5.823678000	-1.763965000	0.386823000

TS1'+2

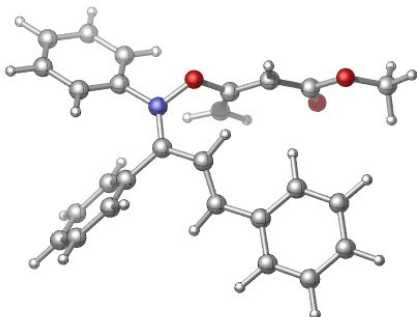


Zero-point correction=	0.427382 (Hartree/Particle)
Thermal correction to Energy=	0.453989
Thermal correction to Enthalpy=	0.454934
Thermal correction to Gibbs Free Energy=	0.367576
Sum of electronic and zero-point Energies=	-1283.952895
Sum of electronic and thermal Energies=	-1283.926287
Sum of electronic and thermal Enthalpies=	-1283.925343
Sum of electronic and thermal Free Energies=	-1284.012701

H	-7.88838900	2.07537300	0.80457800
H	-6.02972200	0.56890400	1.42799500
C	-7.00511800	2.02662500	0.17727700
C	-5.96198100	1.17875800	0.53369700
C	-6.91291900	2.81248800	-0.96925000
C	-2.52295300	-1.60109600	0.88255900
H	-1.63438200	-0.97633700	0.91844100
C	-4.82922400	1.12576500	-0.27590300
C	-3.74988300	-0.95045100	0.47960500
N	-3.69191200	0.29948700	0.06404400
O	-2.52860000	0.92610100	-0.03937600
C	-2.47901700	-2.92402200	1.15927900
C	-5.76572900	2.76112900	-1.75898300
C	-4.71214200	1.92302300	-1.41039700
H	-3.38846000	-3.51534200	1.07066500
H	-5.68731800	3.37850700	-2.64728500
H	-3.80082100	1.88047900	-1.99509600
C	-2.82739600	1.59214200	2.43946500

H	-3.86763500	1.38658000	2.22135800
H	-2.55523800	1.77392400	3.47320800
C	-1.87650400	1.66567900	1.52698200
C	-0.61635600	2.10817100	1.24792300
H	-0.39978100	3.16871100	1.27780800
C	0.40361400	1.20545600	0.80602100
O	0.32209500	-0.01600600	0.69862200
O	1.56382400	1.84977200	0.50575200
C	2.63030000	1.00710600	0.08761000
H	2.36950700	0.47296400	-0.82933100
H	3.48118300	1.66391400	-0.08916100
H	2.87373500	0.27303700	0.85986000
H	-7.73104400	3.47038000	-1.24213300
C	-5.04679000	-1.67419800	0.46058300
C	-5.55748200	-2.21978700	1.64218100
C	-5.74843100	-1.82776300	-0.73850200
C	-6.77382100	-2.89546700	1.62598300
H	-5.00768600	-2.09759000	2.57080900
C	-6.95780600	-2.51353200	-0.75097300
H	-5.34549800	-1.40717900	-1.65514700
C	-7.47395200	-3.04317600	0.43060100
H	-7.17309700	-3.30614100	2.54716500
H	-7.49709400	-2.63437100	-1.68439500
H	-8.42020600	-3.57388400	0.41853400
C	-1.29591600	-3.67245100	1.57936300
C	-1.43889900	-5.03928000	1.86126400
C	-0.02913000	-3.07848200	1.71420900
C	-0.35001100	-5.79977100	2.27185000
H	-2.41619400	-5.50288100	1.75620400
C	1.05515300	-3.84280600	2.12463400
H	0.10964600	-2.02498200	1.48960300
C	0.90102900	-5.20146300	2.40502000
H	-0.47705000	-6.85575000	2.48652000
H	2.03033400	-3.37708100	2.22557400
H	1.75471800	-5.79107800	2.72354800

A'

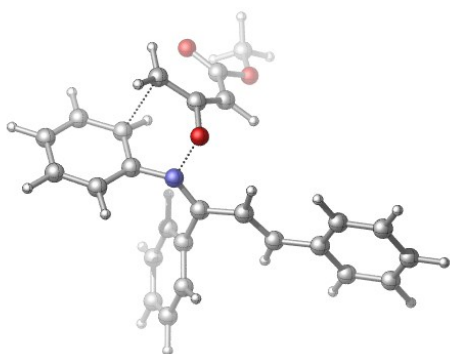


Zero-point correction= 0.429713 (Hartree/Particle)
 Thermal correction to Energy= 0.456105
 Thermal correction to Enthalpy= 0.457049
 Thermal correction to Gibbs Free Energy= 0.371038
 Sum of electronic and zero-point Energies= -1283.961594
 Sum of electronic and thermal Energies= -1283.935201
 Sum of electronic and thermal Enthalpies= -1283.934257
 Sum of electronic and thermal Free Energies= -1284.020268

C	-2.18375600	0.68098500	-4.77702200
C	-1.32425900	1.50981000	-4.05961400
C	-0.81962800	1.10153000	-2.83003900
C	-2.55359000	-0.55922800	-4.25914500
C	-2.06134500	-0.98303700	-3.03018900
C	-1.18024600	-0.15189100	-2.34081200
N	-0.66402500	-0.54114800	-1.06071700
O	-0.72127900	0.47039700	-0.13605300
C	0.56532500	0.89693100	0.37859400
C	1.64463800	0.83650700	-0.43036300
H	1.58459800	0.47452900	-1.44871000
H	2.59546600	1.14975200	-0.02796400
C	0.37521400	1.29511900	1.72414700
C	-0.23743300	-1.72412500	-0.66563000
H	-0.15301700	1.73195700	-2.25098100
H	-1.04424000	2.48033300	-4.45399400
H	-3.23947700	-1.19668200	-4.80604800
H	-2.35977000	-1.93788400	-2.61186600
C	1.44380100	1.76034200	2.51444400
H	-0.60683200	1.18618700	2.16448700
O	2.61689600	1.96346900	2.18405000
O	1.05676000	1.97457700	3.82778200
C	2.09175100	2.42989900	4.68003600
H	1.63808700	2.57189600	5.66182700
H	2.51450800	3.37430000	4.32598000
H	2.90327700	1.69900100	4.74901000

C	0.01953800	-1.92012000	0.73567100
C	0.81417700	-2.91114700	1.20126600
H	-0.37133300	-1.17025000	1.41229800
H	1.21220100	-3.65314700	0.51145100
C	1.21573100	-3.03901800	2.59748300
C	0.02030400	-2.77855500	-1.66790800
C	1.74092500	-4.26115400	3.04366300
C	1.12080100	-1.96124100	3.49621600
C	1.51967300	-2.12253300	4.81565400
C	2.12825700	-4.41952000	4.36849600
C	2.01618800	-3.35068200	5.25598400
H	0.77794900	-0.98714000	3.15263300
H	1.45615000	-1.28312900	5.50025800
H	2.52382900	-5.37074400	4.70805900
H	2.32951500	-3.46920800	6.28821400
H	1.83338600	-5.08792700	2.34498600
C	-0.50209100	-4.06126600	-1.47265900
C	-0.24920700	-5.05729600	-2.41032100
C	0.54076900	-4.78195500	-3.52391100
C	1.07874300	-3.50788200	-3.70660500
C	0.81474100	-2.50208400	-2.78659600
H	-1.11606100	-4.26678900	-0.60143100
H	-0.66782800	-6.04753500	-2.26844900
H	0.74064600	-5.56209300	-4.25083000
H	1.70403700	-3.29738500	-4.56719200
H	1.23014500	-1.50848700	-2.92497600
H	-2.57488400	1.00573900	-5.73515400

TS_{[3+3]-A'}



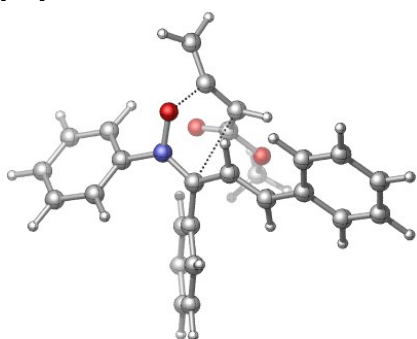
Zero-point correction=	0.427210 (Hartree/Particle)
Thermal correction to Energy=	0.453707
Thermal correction to Enthalpy=	0.454651
Thermal correction to Gibbs Free Energy=	0.366229
Sum of electronic and zero-point Energies=	-1283.933051

Sum of electronic and thermal Energies= -1283.906554
Sum of electronic and thermal Enthalpies= -1283.905610
Sum of electronic and thermal Free Energies= -1283.994032

C	-5.22576200	1.38570800	1.97486100
C	-6.09181400	0.96815400	0.99286900
C	-5.69427000	-0.00612800	0.04476500
C	-3.93036200	0.82572900	2.08164200
C	-3.52241600	-0.14623300	1.20112400
C	-4.42023700	-0.60592100	0.20775000
H	-7.08671200	1.39296600	0.91414000
H	-3.25895100	1.16281900	2.86378400
H	-2.53149400	-0.58546300	1.25656600
N	-3.96396900	-1.45144400	-0.76374700
C	-3.74073000	-2.71867000	-0.85094500
C	-3.09895500	-3.27531600	-2.02949800
C	-3.09034500	-4.60177400	-2.27332000
H	-2.68719800	-2.55629000	-2.72445800
H	-3.56763100	-5.27004700	-1.55920700
C	-5.18136500	1.12765100	-1.98494800
C	-4.95888300	-0.13713300	-2.52484900
C	-5.89637900	-1.03402200	-3.07924400
C	-7.27761500	-0.74045400	-3.12418000
O	-8.00718800	-1.74349000	-3.72523600
O	-3.72902900	-0.60207600	-2.22975700
O	-7.86089800	0.25798300	-2.68174200
C	-9.40706400	-1.52512800	-3.75627300
H	-9.83938700	-2.39520100	-4.25153000
H	-9.65693500	-0.61764600	-4.31282400
H	-9.81788900	-1.42962200	-2.74710200
H	-5.53951600	-1.97704900	-3.47321900
H	-4.33634700	1.64565400	-1.54787800
H	-6.09857700	1.66448200	-2.18968100
H	-6.42918100	-0.46863000	-0.60693000
H	-5.53721300	2.14624000	2.68359800
C	-4.15865100	-3.58018100	0.28852800
C	-3.23142800	-4.41947700	0.91070100
C	-5.48489600	-3.54096100	0.72894000
C	-3.63196100	-5.20954100	1.98451400
H	-2.20373500	-4.44303900	0.56213000
C	-5.88086500	-4.34689600	1.78902900
H	-6.19879200	-2.89637100	0.22462200
C	-4.95389800	-5.17541500	2.42116600
H	-2.91044200	-5.85270700	2.47661300

H	-6.91274200	-4.32835500	2.12239700
H	-5.26423900	-5.79708200	3.25439200
C	-2.50694800	-5.25753200	-3.44285000
C	-2.62989000	-6.65002500	-3.55096400
C	-1.83527300	-4.55526700	-4.45660900
C	-2.09978800	-7.32784400	-4.64292900
H	-3.14879800	-7.19847400	-2.76980000
C	-1.30616400	-5.23298000	-5.54532500
H	-1.72535300	-3.47760400	-4.39598000
C	-1.43696900	-6.61968200	-5.64197700
H	-2.20404700	-8.40524600	-4.71433800
H	-0.78974500	-4.68168500	-6.32386900
H	-1.02133700	-7.14423600	-6.49617900

TS_[3+2](anti)

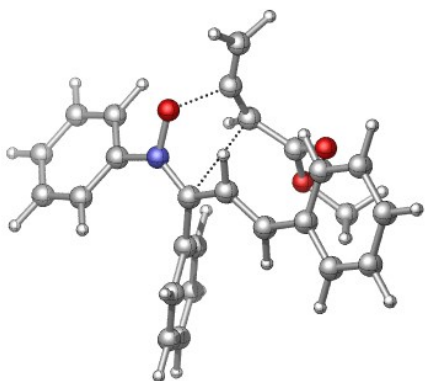


Zero-point correction=	0.427215 (Hartree/Particle)
Thermal correction to Energy=	0.453722
Thermal correction to Enthalpy=	0.454666
Thermal correction to Gibbs Free Energy=	0.367197
Sum of electronic and zero-point Energies=	-1283.960987
Sum of electronic and thermal Energies=	-1283.934481
Sum of electronic and thermal Enthalpies=	-1283.933536
Sum of electronic and thermal Free Energies=	-1284.021005

C	-6.26631400	-0.04618400	-3.31764500
C	-5.38614000	0.81893000	-2.66936600
C	-4.94619800	0.54151700	-1.37935600
C	-6.71492700	-1.19813700	-2.67490000
C	-6.28235100	-1.49161100	-1.38585300
C	-5.39169500	-0.62304600	-0.76261500
N	-4.97443100	-0.88782400	0.59294200
O	-5.12387600	0.12983500	1.41751500
C	-3.55988600	0.91878300	1.76160400
C	-3.92388600	2.16992700	1.95812400

H	-4.95080900	2.49456800	1.83899200
H	-3.17352300	2.89610300	2.25022200
C	-2.49351100	0.04367900	1.75292600
C	-4.42860200	-2.01228900	1.02195600
H	-4.23748600	1.18011700	-0.86436800
H	-5.03676600	1.71524100	-3.17069100
H	-7.40987600	-1.86684800	-3.17120300
H	-6.62872700	-2.37998400	-0.86793400
C	-1.75614700	-0.18580800	0.55000100
H	-2.23079600	-0.51901200	2.63966500
O	-1.93942400	0.33112600	-0.55148200
O	-0.76445000	-1.10560400	0.73148300
C	0.06953700	-1.33102000	-0.39757300
H	0.85950900	-2.00031100	-0.05816100
H	0.49728800	-0.39418300	-0.76151200
H	-0.48738900	-1.80095000	-1.21318500
C	-4.35798300	-2.23813200	2.45469400
C	-3.68226400	-3.26011700	3.01398900
H	-4.87941000	-1.50187100	3.05677900
H	-3.11019700	-3.92587900	2.37080800
H	-6.60543400	0.17961700	-4.32317600
C	-4.03503000	-3.05681900	0.04376300
C	-3.20228900	-2.73557100	-1.03498200
C	-4.49456900	-4.36907200	0.20082200
C	-2.83102100	-3.72405100	-1.93900000
H	-2.85462700	-1.71341300	-1.16474000
C	-4.13041800	-5.34946200	-0.71642500
H	-5.14837000	-4.61446900	1.03166200
C	-3.29472800	-5.02973500	-1.78387000
H	-2.18139400	-3.47221100	-2.77104200
H	-4.50088200	-6.36185500	-0.59630800
H	-3.00679000	-5.79618900	-2.49611000
C	-3.60186000	-3.55320300	4.44660700
C	-2.73173200	-4.56721000	4.87165500
C	-4.35790900	-2.86941500	5.41218500
C	-2.60839200	-4.88434900	6.21990700
H	-2.14535100	-5.10522200	4.13184300
C	-4.23560000	-3.18768500	6.75773800
H	-5.05097300	-2.09033200	5.11120700
C	-3.36020800	-4.19458700	7.16744300
H	-1.92757000	-5.67015200	6.53029900
H	-4.82720900	-2.65136500	7.49246500
H	-3.26877100	-4.44016800	8.22042300

TS_[3+2](syn)

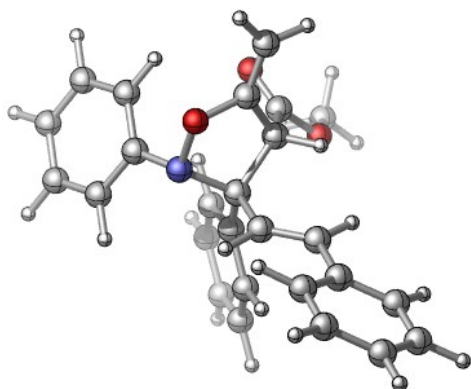


Zero-point correction= 0.427678 (Hartree/Particle)
 Thermal correction to Energy= 0.453933
 Thermal correction to Enthalpy= 0.454878
 Thermal correction to Gibbs Free Energy= 0.369833
 Sum of electronic and zero-point Energies= -1283.961144
 Sum of electronic and thermal Energies= -1283.934889
 Sum of electronic and thermal Enthalpies= -1283.933944
 Sum of electronic and thermal Free Energies= -1284.018989

C	-5.76717900	-0.11175700	-3.41510400
C	-5.30022600	0.87740300	-2.55258100
C	-5.12055200	0.60191900	-1.20097800
C	-6.06503100	-1.38111100	-2.92258500
C	-5.88421600	-1.67338400	-1.57521800
C	-5.39263000	-0.68022700	-0.73063600
N	-5.21014400	-0.92629000	0.67515200
O	-5.53477600	0.08633800	1.44943100
C	-4.03634900	0.89932100	2.11889500
C	-4.56555900	1.71843400	3.00523600
H	-5.61477300	1.66567800	3.27293200
H	-3.93755700	2.46618800	3.47614700
C	-2.89190300	0.39382800	1.56156900
C	-4.57280200	-1.96374900	1.19651700
H	-4.78655000	1.36582700	-0.50806600
H	-5.08101600	1.87080900	-2.92895900
H	-6.44947000	-2.14737400	-3.58693800
H	-6.12335100	-2.65560400	-1.18353200
C	-1.97994500	-0.40423000	2.33932800
O	-2.01918000	-0.63978600	3.53706100
O	-0.99370700	-0.92643300	1.55041900
C	-0.06550200	-1.76118200	2.23053300
H	0.62501900	-2.12686700	1.47124100

H	-0.57691900	-2.59893300	2.71145200
H	0.47757900	-1.20087000	2.99580900
C	-4.57702600	-2.10950600	2.63355000
C	-3.84046200	-3.03253200	3.28428800
H	-5.17265500	-1.39006500	3.18309000
H	-3.25501000	-3.75269700	2.71512500
H	-5.91147700	0.10856400	-4.46741400
H	-2.66891100	0.54277800	0.50961200
C	-3.93287800	-2.97928300	0.32217700
C	-4.36509400	-4.30868500	0.36473200
C	-2.87567900	-2.61593300	-0.51679100
C	-3.76301900	-5.26126700	-0.45144000
H	-5.18004900	-4.58667300	1.02653100
C	-2.27062900	-3.57474900	-1.32204600
H	-2.52491800	-1.58922000	-0.51802800
C	-2.71744000	-4.89456700	-1.29626500
H	-4.10971400	-6.28886000	-0.42604000
H	-1.44612700	-3.29091400	-1.96740700
H	-2.24624600	-5.63910800	-1.92964500
C	-3.78052700	-3.15483500	4.74211400
C	-3.43938100	-4.38735100	5.31415300
C	-4.05198700	-2.06598700	5.58457600
C	-3.40948300	-4.54287500	6.69612300
H	-3.20827400	-5.22908400	4.66682900
C	-4.01847300	-2.22280500	6.96389300
H	-4.23469700	-1.08966800	5.14679700
C	-3.70498000	-3.46203700	7.52383900
H	-3.15248800	-5.50523100	7.12678700
H	-4.22272400	-1.37298700	7.60721000
H	-3.67631600	-3.57951900	8.60231900

A''(anti)



Zero-point correction=

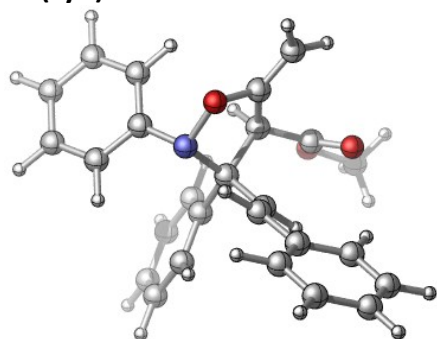
0.432012 (Hartree/Particle)

Thermal correction to Energy=	0.457382
Thermal correction to Enthalpy=	0.458326
Thermal correction to Gibbs Free Energy=	0.375066
Sum of electronic and zero-point Energies=	-1284.016198
Sum of electronic and thermal Energies=	-1283.990829
Sum of electronic and thermal Enthalpies=	-1283.989885
Sum of electronic and thermal Free Energies=	-1284.073144

H	-8.61681200	0.42352900	0.27874400
H	-6.61511800	-0.78919200	1.12101000
C	-7.68971800	0.96082100	0.45013300
C	-6.57563100	0.27701100	0.92120600
C	-7.62088700	2.33377700	0.21766300
C	-2.76292600	-1.65241600	1.54847200
H	-3.41798400	-1.96037000	2.36016100
C	-5.37372900	0.95803500	1.12748900
C	-3.38324600	-0.57960700	0.66108800
N	-4.27166300	0.17874300	1.60740700
O	-3.36898100	1.00783700	2.32501300
C	-1.57280200	-2.23388300	1.38874800
C	-6.43108500	3.01464800	0.46240800
C	-5.30322600	2.33567200	0.91840500
H	-0.94685800	-1.97472500	0.53493600
H	-6.37426700	4.08550600	0.29534900
H	-4.37518200	2.86775500	1.09029300
C	-1.44044300	2.29366100	1.89542400
H	-1.59072000	2.85294900	2.81056200
H	-0.57795500	2.51191100	1.27951300
C	-2.29911000	1.35183500	1.52631100
C	-2.27309400	0.47408200	0.30357300
C	-2.44767700	1.24698000	-0.99205600
O	-2.92885100	2.34831300	-1.10968900
O	-1.97714200	0.52952800	-2.01625200
C	-2.19090100	1.10142700	-3.31049100
H	-1.71604600	2.08153400	-3.37612000
H	-1.74571300	0.40713600	-4.01946200
H	-3.26299100	1.20362400	-3.49678200
H	-8.49320200	2.87121000	-0.13948800
C	-1.02870500	-3.28575600	2.26856100
C	-4.14564700	-1.18146900	-0.52530500
H	-1.31104100	-0.03152400	0.21968000
C	-4.79676800	-0.36972700	-1.46794200
C	-4.21340500	-2.56582500	-0.69665400
C	-5.47078400	-0.92583900	-2.54817400

C	-5.52360400	-2.30921100	-2.70917600
C	-4.89623100	-3.12529200	-1.77662100
H	-4.93033800	-4.20460700	-1.88335400
H	-3.72320700	-3.22256100	0.01159800
H	-4.80177700	0.71018400	-1.35960300
H	-5.96211500	-0.27173500	-3.26153000
H	-6.05076700	-2.74350600	-3.55249500
C	-0.03539000	-4.14303400	1.77990200
C	-1.47314500	-3.45717000	3.58670800
C	-0.95881100	-4.47523400	4.38009900
C	0.01614800	-5.33580000	3.87585400
C	0.47896000	-5.16383700	2.57381500
H	-2.21036600	-2.77546800	3.99936900
H	-1.31224100	-4.59189200	5.39957800
H	0.32819600	-4.01115500	0.76433100
H	0.41856500	-6.12806600	4.49865000
H	1.24286200	-5.82389900	2.17557900

A''(syn)



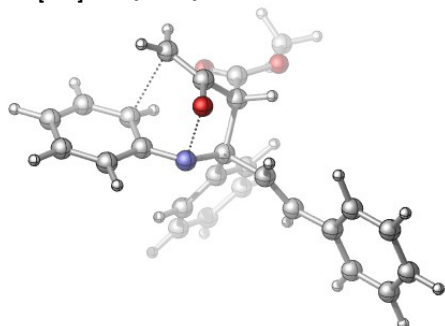
Zero-point correction=	0.432391 (Hartree/Particle)
Thermal correction to Energy=	0.457900
Thermal correction to Enthalpy=	0.458844
Thermal correction to Gibbs Free Energy=	0.374711
Sum of electronic and zero-point Energies=	-1284.024798
Sum of electronic and thermal Energies=	-1283.999289
Sum of electronic and thermal Enthalpies=	-1283.998345
Sum of electronic and thermal Free Energies=	-1284.082477

H	-8.34970300	-0.15575700	-0.50985500
H	-6.47339500	-1.21886900	0.71333600
C	-7.50232700	0.44452300	-0.19495400
C	-6.45318500	-0.15836400	0.48773800
C	-7.47950900	1.81506900	-0.45098700
C	-2.42637300	-1.68671800	1.54857300
H	-1.59938900	-2.14962200	1.01422900

C	-5.35170500	0.60173500	0.88939600
C	-3.23380400	-0.71166800	0.71753700
N	-4.29274400	-0.09075400	1.57847200
O	-3.57309800	0.84153300	2.38396100
C	-2.66655700	-2.00293900	2.82168700
C	-6.39882200	2.57577000	-0.01638800
C	-5.33168800	1.97698200	0.65149300
H	-3.52682900	-1.55923300	3.31855100
H	-6.37919500	3.64590500	-0.19556200
H	-4.50146400	2.58256300	0.99857200
C	-1.57348300	2.09444300	2.29287300
H	-1.77430100	2.51688900	3.26957100
H	-0.65945500	2.35948500	1.77929200
C	-2.41901200	1.23823000	1.73630500
C	-2.36020100	0.54409500	0.40506100
H	-2.87374900	1.15711200	-0.34154000
C	-0.96905200	0.23343900	-0.09801200
O	-0.02357700	-0.07194900	0.58864200
O	-0.92450600	0.30629700	-1.43196900
C	0.33609100	-0.03430400	-2.02126600
H	0.60248300	-1.06240400	-1.77029200
H	0.20000600	0.07652300	-3.09454800
H	1.11404800	0.63948600	-1.65885500
C	-1.85247700	-2.94269400	3.61361700
C	-3.83584000	-1.42121600	-0.48787300
C	-3.92272200	-0.83475500	-1.75175000
C	-4.37925500	-2.69645100	-0.29731400
C	-4.55024100	-1.50624200	-2.79905800
C	-5.01180500	-3.36393100	-1.34055300
C	-5.10056200	-2.76822100	-2.59664900
H	-4.31284500	-3.15909000	0.68275500
H	-5.43454000	-4.34908700	-1.17222200
H	-4.60937200	-1.03655000	-3.77547800
H	-5.59192400	-3.28650300	-3.41368200
H	-3.49999900	0.14505100	-1.94139800
C	-2.42904700	-3.59227400	4.71151200
C	-0.50980400	-3.20425200	3.30716000
C	-1.69733800	-4.50529000	5.46480300
C	-0.37020600	-4.77357700	5.13799100
C	0.22157600	-4.11599200	4.05974500
H	-3.46426200	-3.38229700	4.96680500
H	-2.16305300	-5.00478700	6.30835300
H	-0.03203900	-2.66756700	2.49224100
H	0.20485700	-5.48118100	5.72645500

H	1.26145200	-4.30591100	3.81312600
H	-8.30520800	2.28792600	-0.97209000

TS_[3+3]-A''(anti)

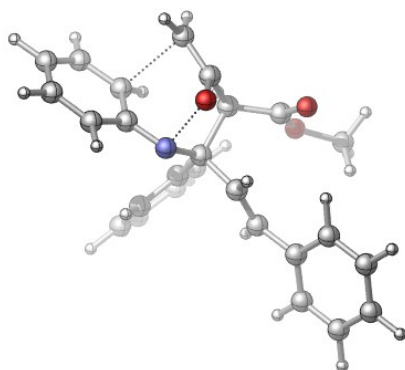


Zero-point correction=	0.430217 (Hartree/Particle)
Thermal correction to Energy=	0.455262
Thermal correction to Enthalpy=	0.456206
Thermal correction to Gibbs Free Energy=	0.372813
Sum of electronic and zero-point Energies=	-1283.974542
Sum of electronic and thermal Energies=	-1283.949497
Sum of electronic and thermal Enthalpies=	-1283.948553
Sum of electronic and thermal Free Energies=	-1284.031946

C	-3.35808600	1.21254700	0.69831900
C	-4.43669600	0.82820900	1.45351200
H	-4.26021600	0.57665600	2.49393400
H	-5.45529300	0.97621300	1.11565000
C	-4.28266500	-3.00532200	2.37194300
C	-2.87893100	-2.92800700	2.55166500
C	-2.12421000	-2.13545400	1.72855400
C	-2.73349600	-1.38189100	0.68162000
C	-4.14810700	-1.42298000	0.54495100
C	-4.90145300	-2.28035300	1.38168900
H	-4.86870200	-3.65280700	3.01652800
H	-2.40555200	-3.50257300	3.34071300
H	-1.04860400	-2.05049100	1.84401400
H	-4.62369000	-0.99183100	-0.32740600
H	-5.97434100	-2.34841300	1.23601600
N	-1.90642900	-0.54597600	0.00473100
O	-2.15216900	1.01690500	1.10477800
C	-3.36156000	1.37069200	-0.80331700
C	-2.33938300	0.16909500	-1.22187200
C	-4.72202800	1.42438600	-1.45808600
O	-5.62480100	0.63076400	-1.30960300
O	-4.82889700	2.49803200	-2.25020100

C	-6.07040700	2.61351100	-2.95498600
H	-5.99236000	3.52322600	-3.54570200
H	-6.21398700	1.74365800	-3.60032700
H	-6.90039500	2.67961200	-2.24984000
C	-1.06245900	0.87049900	-1.66556200
H	-0.62372200	1.44320600	-0.85038000
C	-0.47015100	0.82490400	-2.86008400
H	-0.89264000	0.21051800	-3.65261600
H	-2.84572400	2.29732500	-1.06206500
C	-2.85607900	-0.75900600	-2.31855600
C	-3.44477600	-0.20053600	-3.46051400
C	-2.63432700	-2.13869000	-2.29914200
C	-3.85671800	-0.99998100	-4.52141400
H	-3.56167800	0.87696400	-3.53814900
C	-3.04819900	-2.94107700	-3.36103800
H	-2.13278700	-2.59935500	-1.45655700
C	-3.66985900	-2.37921400	-4.47099500
H	-4.31774500	-0.54035100	-5.38970900
H	-2.87407700	-4.01132000	-3.31724200
H	-3.99257700	-3.00644300	-5.29541500
C	0.77251900	1.54425600	-3.20382700
C	1.49380000	1.16088400	-4.34160100
C	1.26289200	2.60830300	-2.43361800
C	2.68067100	1.80147400	-4.68688900
H	1.12075300	0.34535700	-4.95561000
C	2.44803900	3.24714800	-2.77576300
H	0.70488700	2.95031400	-1.56763500
C	3.16485700	2.84496900	-3.90257400
H	3.22667400	1.48539700	-5.57019300
H	2.80951900	4.06938800	-2.16631800
H	4.08823400	3.34813100	-4.17048300

TS_{[3+3]-A''(syn)}



Zero-point correction=

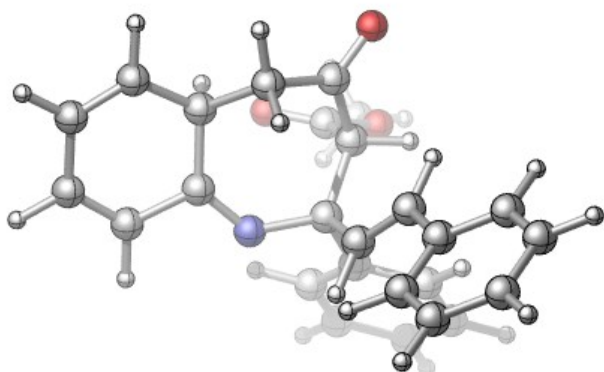
0.430151 (Hartree/Particle)

Thermal correction to Energy=	0.455197
Thermal correction to Enthalpy=	0.456141
Thermal correction to Gibbs Free Energy=	0.374916
Sum of electronic and zero-point Energies=	-1283.979931
Sum of electronic and thermal Energies=	-1283.954885
Sum of electronic and thermal Enthalpies=	-1283.953941
Sum of electronic and thermal Free Energies=	-1284.035166

C	-3.02853200	1.26677600	0.82259900
C	-4.16440300	0.98182900	1.54233000
H	-4.06058500	0.61115600	2.55695000
H	-5.13663300	1.34192600	1.22205000
C	-4.71882800	-2.87050400	1.99067300
C	-3.32811600	-3.06858100	2.18278600
C	-2.42319700	-2.33790300	1.46064300
C	-2.85769000	-1.37114600	0.50532700
C	-4.25679100	-1.13697900	0.36883500
C	-5.17407200	-1.93791500	1.09057000
H	-5.42591200	-3.47348100	2.55141800
H	-2.98467000	-3.80741700	2.89890200
H	-1.35311300	-2.46563300	1.58766100
H	-4.62462300	-0.55894000	-0.47119900
H	-6.23757300	-1.79646700	0.93100800
N	-1.88191400	-0.62342500	-0.06343000
O	-1.87267400	0.84542400	1.19184400
C	-3.08210700	1.51443400	-0.65986000
H	-4.10168800	1.46720300	-1.04788700
C	-2.18539600	0.28651000	-1.20227800
C	-2.47368400	2.83852200	-1.07427700
O	-1.72829200	3.50905400	-0.40158500
O	-2.85128000	3.16853300	-2.31507400
C	-2.19648900	4.31765700	-2.86508200
H	-2.60359900	4.44016100	-3.86627000
H	-2.40050600	5.19883600	-2.25495600
H	-1.11848900	4.14177400	-2.90558400
C	-0.82903500	0.84037600	-1.60129100
H	-0.22146500	1.12339700	-0.74421600
C	-0.40098000	1.06565600	-2.84507100
H	-1.00195200	0.74325900	-3.69424700
C	-2.83286100	-0.46820200	-2.36187900
C	-2.47616900	-1.80125500	-2.60018000
C	-3.69721300	0.16425300	-3.25903100
C	-3.00594200	-2.49540800	-3.68212500
H	-1.78048800	-2.29670100	-1.93077300

C	-4.22258200	-0.53155100	-4.34751100
H	-3.94738200	1.21186400	-3.13042200
C	-3.88742800	-1.86454200	-4.55803700
H	-2.72651800	-3.53172600	-3.84279200
H	-4.89523900	-0.02326800	-5.03101700
H	-4.30229800	-2.40619400	-5.40192900
C	0.86994700	1.74872100	-3.15604600
C	1.55502300	1.45847700	-4.34223600
C	1.40270700	2.71491400	-2.29044500
C	2.75807600	2.09096900	-4.64064200
H	1.14222300	0.72422500	-5.02881600
C	2.60418400	3.34793800	-2.58990800
H	0.84961900	2.98920300	-1.39586800
C	3.28876500	3.03479700	-3.76324100
H	3.28110200	1.84924100	-5.56048300
H	3.00130000	4.09636800	-1.91154800
H	4.22398100	3.53266900	-3.99807800

4'(anti)



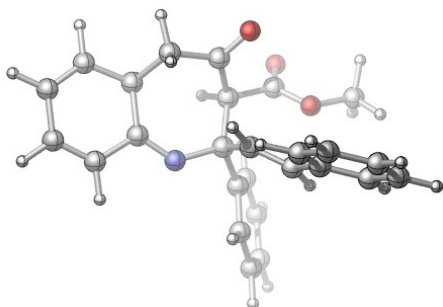
Zero-point correction=	0.432954 (Hartree/Particle)
Thermal correction to Energy=	0.458579
Thermal correction to Enthalpy=	0.459523
Thermal correction to Gibbs Free Energy=	0.375881
Sum of electronic and zero-point Energies=	-1284.057218
Sum of electronic and thermal Energies=	-1284.031593
Sum of electronic and thermal Enthalpies=	-1284.030649
Sum of electronic and thermal Free Energies=	-1284.114291

C	-5.03831900	2.73321100	-0.09185500
C	-3.91151600	2.67043900	0.83410300
C	-5.65904800	1.61862600	-0.51175400
C	-3.42372600	1.48719500	1.21824900
C	-3.94667600	0.17123300	0.70270800

C	-5.26784700	0.27422700	-0.05218500
N	-6.08602200	-0.65538900	-0.37576400
C	-6.06320800	-2.07410500	-0.03801300
C	-4.69022100	-2.77837900	0.17989100
C	-3.89746600	-2.75427800	-1.11848100
O	-3.85970100	-3.95668100	-1.68826100
O	-3.39295800	-1.76673000	-1.60437400
C	-3.26030000	-3.99318100	-2.98922100
H	-3.29805000	-5.03397100	-3.30220400
H	-2.22983000	-3.63822600	-2.94238300
H	-3.83384600	-3.36328700	-3.67287700
C	-6.96627500	-2.21231100	1.17469300
C	-6.75618700	-2.94742800	2.27100700
C	-7.68222700	-3.02814300	3.41783800
H	-7.88424300	-1.63753100	1.06993100
H	-5.85796500	-3.55808200	2.36224000
H	-5.38664900	3.70581500	-0.42574000
H	-3.47799500	3.59502200	1.20016000
H	-6.52519900	1.65527500	-1.16391700
H	-2.57557600	1.43055500	1.89564000
C	-3.96908500	-0.86859500	1.83784500
C	-3.82587000	-2.28603300	1.34556300
O	-3.03898200	-3.05923300	1.84768600
H	-3.14781100	-0.69586500	2.53714000
H	-4.90926800	-0.78541100	2.39501800
H	-3.22204200	-0.16561800	-0.05646900
C	-6.71139000	-2.81967300	-1.22774100
H	-4.89373000	-3.83108800	0.39185200
C	-7.27651800	-4.08365100	-1.04774300
C	-6.64419400	-2.28339300	-2.51486900
C	-7.76907600	-4.79943200	-2.13535500
C	-7.69705400	-4.26174800	-3.41823200
C	-7.13252300	-3.00220900	-3.60408400
H	-6.20779500	-1.30019300	-2.65571800
H	-8.08054700	-4.81923500	-4.26678900
H	-7.07262300	-2.57352000	-4.59971800
H	-7.33660000	-4.50962800	-0.05004200
H	-8.21097000	-5.77841200	-1.97908300
C	-8.66944500	-2.06025300	3.65003200
C	-7.57495400	-4.10037000	4.31174300
C	-8.44507300	-4.21905700	5.39174800
C	-9.43323200	-3.26040800	5.60091500
C	-9.53879700	-2.17865400	4.72716900
H	-10.29560500	-1.41844100	4.89198100

H	-8.74589900	-1.19781700	2.99525700
H	-6.80581000	-4.85114600	4.15149300
H	-8.34971100	-5.06017700	6.07091600
H	-10.11097700	-3.34884600	6.44367400

4'(syn)

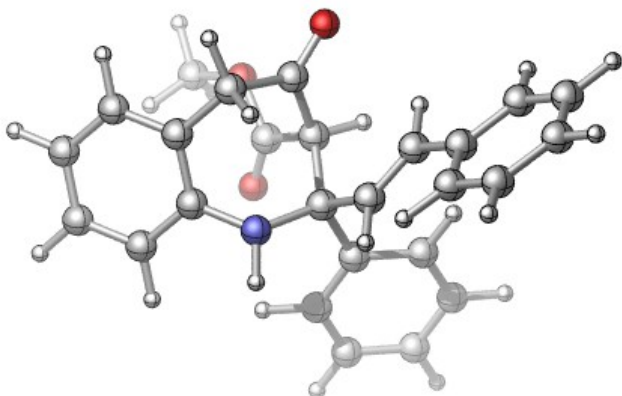


Zero-point correction=	0.432705 (Hartree/Particle)
Thermal correction to Energy=	0.458255
Thermal correction to Enthalpy=	0.459199
Thermal correction to Gibbs Free Energy=	0.374791
Sum of electronic and zero-point Energies=	-1284.049463
Sum of electronic and thermal Energies=	-1284.023913
Sum of electronic and thermal Enthalpies=	-1284.022969
Sum of electronic and thermal Free Energies=	-1284.107377

C	-4.37992100	2.45256400	-0.80554100
C	-3.08577300	2.28474000	-0.14847000
C	-5.25079800	1.43615200	-0.90064400
C	-2.73020900	1.09790200	0.34937300
C	-3.59353000	-0.13596200	0.26829000
C	-4.97922000	0.09751500	-0.34747200
N	-5.96159900	-0.71932400	-0.43409000
C	-6.06845700	-2.11238700	0.01282400
C	-4.71614500	-2.81056400	0.39450400
C	-4.74277900	-4.32184300	0.57274500
O	-5.87518200	-4.78392800	1.08738600
O	-3.80089100	-5.02084400	0.27662300
C	-5.94492500	-6.20479900	1.24307900
H	-6.92059500	-6.40363100	1.68185700
H	-5.14648000	-6.55281900	1.90005300
H	-5.85286700	-6.69060300	0.26942200
H	-4.63459700	3.42552500	-1.21434400
H	-6.22264700	1.55519300	-1.36753400
H	-1.76405800	0.96304400	0.82920700
C	-3.69371300	-0.77739900	1.65991000
C	-4.14481200	-2.22283000	1.67999500

O	-4.05461200	-2.88700000	2.68855800
H	-2.72392500	-0.75209000	2.16778100
H	-4.38326400	-0.20065500	2.28862500
H	-3.04841000	-0.82782700	-0.39050200
H	-4.00008400	-2.63447400	-0.41444800
C	-6.96128700	-2.03753100	1.25001700
H	-6.64628400	-1.27018200	1.95684300
C	-8.01703100	-2.80259600	1.52689100
H	-8.29500100	-3.58541300	0.82364400
C	-8.84018300	-2.72539000	2.74663000
C	-6.73563600	-2.82178500	-1.18180100
C	-9.68524200	-3.79859900	3.05512400
C	-8.81607600	-1.62444200	3.61463700
C	-9.59706100	-1.61142200	4.76388500
C	-10.42387200	-2.69350500	5.06669500
C	-10.46762200	-3.78697200	4.20606600
H	-8.19573100	-0.76441100	3.38156200
H	-9.56796000	-0.74950600	5.42283100
H	-9.72039100	-4.65338100	2.38485800
H	-11.03459900	-2.67921600	5.96348800
H	-11.11186800	-4.63132800	4.42954600
C	-8.01895000	-2.40853700	-1.56371200
C	-8.65321300	-2.96658700	-2.66605700
C	-8.01042500	-3.94429100	-3.42553000
C	-6.72734700	-4.34224900	-3.07401300
C	-6.09224100	-3.77981200	-1.96511400
H	-8.51509400	-1.63564000	-0.98636800
H	-9.65037700	-2.63429300	-2.93686000
H	-8.50429300	-4.38327500	-4.28633400
H	-6.20542100	-5.09032900	-3.66193300
H	-5.08320300	-4.10837500	-1.74250100
H	-2.41811300	3.13682700	-0.07755700

4''(anti)

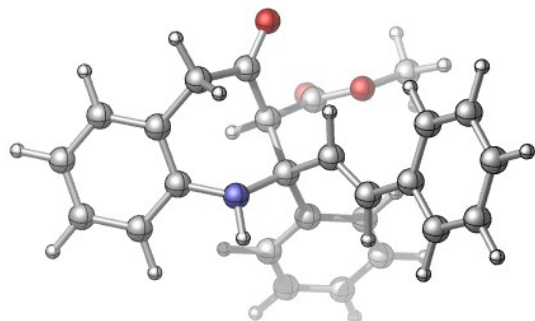


Zero-point correction= 0.434100 (Hartree/Particle)
 Thermal correction to Energy= 0.459285
 Thermal correction to Enthalpy= 0.460229
 Thermal correction to Gibbs Free Energy= 0.378056
 Sum of electronic and zero-point Energies= -1284.105610
 Sum of electronic and thermal Energies= -1284.080425
 Sum of electronic and thermal Enthalpies= -1284.079481
 Sum of electronic and thermal Free Energies= -1284.161654

C	-3.16221600	1.75373000	-0.43267200
C	-2.10631700	1.04238700	0.13466400
C	-4.46082000	1.26781400	-0.34432500
C	-2.37392400	-0.13793200	0.82221200
C	-3.67613500	-0.61997700	0.95300100
C	-4.73093100	0.07106100	0.33021100
N	-6.04675600	-0.40195200	0.45579200
C	-6.50889900	-1.74527100	0.04468000
C	-5.32423800	-2.70122900	-0.26212100
C	-4.40477900	-2.22071600	-1.38622200
O	-3.18499500	-2.75197500	-1.23334000
O	-4.70285900	-1.49118900	-2.29667500
C	-2.19602600	-2.28136300	-2.15599600
H	-1.28008200	-2.81006500	-1.90187700
H	-2.06763600	-1.20324700	-2.02998900
H	-2.49759500	-2.49982300	-3.18124100
H	-2.97394100	2.68313900	-0.96050000
H	-1.08902200	1.40985300	0.05506100
H	-5.27891800	1.81252200	-0.80857400
H	-1.56405800	-0.68800600	1.29422100
C	-3.97898300	-1.84326200	1.77681500
C	-4.47066500	-3.02716900	0.97160100
O	-4.23244500	-4.17103100	1.28233100
H	-3.11987500	-2.16495000	2.36827500

H	-4.80373100	-1.60728100	2.46727700
C	-7.34308300	-2.26542900	1.20891900
H	-8.00563100	-1.49940500	1.60927600
C	-7.36581000	-3.49723900	1.72652100
H	-6.73591000	-4.27955300	1.30704100
C	-8.22106300	-3.92907100	2.84932700
C	-7.43789800	-1.66400600	-1.19109000
H	-6.73522200	0.30174900	0.22101400
H	-5.74237000	-3.65473300	-0.60385600
C	-8.82179100	-3.02530700	3.73667700
C	-8.44099600	-5.29850500	3.04132600
C	-9.63687100	-3.48009400	4.76626100
C	-9.25747100	-5.75482000	4.07165500
C	-9.86194100	-4.84606200	4.93616600
H	-7.97071900	-6.01007700	2.36783200
H	-9.41939700	-6.82028500	4.20009900
H	-8.63571000	-1.96065500	3.63349300
H	-10.09060100	-2.76628400	5.44651700
H	-10.49646000	-5.19757000	5.74320400
C	-7.45402500	-0.55029000	-2.03216600
C	-8.28918300	-2.73313800	-1.48530500
C	-8.31038200	-0.49777900	-3.12860200
C	-9.15850000	-1.56491700	-3.41003600
C	-9.13846800	-2.68803800	-2.58739700
H	-9.79078400	-3.52989200	-2.79638100
H	-8.29965200	-3.60702800	-0.84099900
H	-6.76430400	0.26852200	-1.86069500
H	-8.30508700	0.37840300	-3.76895100
H	-9.82548500	-1.52407400	-4.26498100

4''(syn)



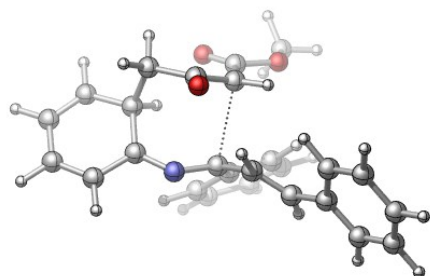
Zero-point correction=	0.433544 (Hartree/Particle)
Thermal correction to Energy=	0.458978
Thermal correction to Enthalpy=	0.459922
Thermal correction to Gibbs Free Energy=	0.376363

Sum of electronic and zero-point Energies= -1284.104779
Sum of electronic and thermal Energies= -1284.079346
Sum of electronic and thermal Enthalpies= -1284.078401
Sum of electronic and thermal Free Energies= -1284.161961

C	-4.21042200	2.11088900	-0.91813300
C	-2.96258200	1.94380600	-0.32495900
C	-5.23871700	1.21159200	-0.65197700
C	-2.76579000	0.89091700	0.56605100
C	-3.79412000	0.00244200	0.86837800
C	-5.03843900	0.14078600	0.22608100
N	-6.08934200	-0.73054500	0.56855400
C	-6.08655700	-2.20133700	0.36169800
C	-4.62005100	-2.70799900	0.18409000
C	-4.55529200	-4.16830400	-0.22355100
O	-5.20367300	-4.95839400	0.63458900
O	-3.98224800	-4.56897000	-1.20669800
C	-5.22671200	-6.34633200	0.28640600
H	-5.80027500	-6.83852800	1.06881100
H	-4.21054800	-6.74160500	0.24543600
H	-5.70669300	-6.47806200	-0.68609700
H	-4.38612700	2.93614000	-1.60062600
H	-6.21067900	1.33889300	-1.12177500
H	-1.80598400	0.77015900	1.06086700
C	-3.63469200	-1.06013100	1.92147100
C	-3.72246000	-2.47853000	1.40002300
O	-3.10977400	-3.38927900	1.91107100
H	-2.69398700	-0.96341800	2.46701000
H	-4.46000900	-0.95873800	2.64341600
H	-4.18054100	-2.14793500	-0.64908900
C	-6.71934200	-2.78503600	1.61739600
H	-6.02437600	-3.04509000	2.41439700
C	-8.03426800	-2.87327700	1.82848900
H	-8.71738200	-2.57750700	1.03220400
C	-8.67697500	-3.33504700	3.07208300
C	-6.82581800	-2.58236300	-0.93587300
H	-7.00093600	-0.35753700	0.32854300
C	-7.98926500	-4.07037500	4.04778600
C	-8.63051200	-4.47410400	5.21277200
C	-9.97348900	-4.16109200	5.42245600
C	-10.67221000	-3.44603000	4.45335900
C	-10.02923000	-3.04177200	3.28727500
H	-6.95158200	-4.34599500	3.88448600
H	-8.08367100	-5.04432200	5.95699600

H	-10.47275900	-4.48091700	6.33134200
H	-11.71965500	-3.20465700	4.60365600
H	-10.57676400	-2.48478000	2.53163200
C	-7.50190500	-3.80080000	-1.07344500
C	-6.73444200	-1.74327800	-2.05043100
C	-8.08449900	-4.15700400	-2.28704800
C	-8.00063700	-3.30615700	-3.38548100
C	-7.31977600	-2.09822100	-3.26296600
H	-7.57568500	-4.47332600	-0.22641500
H	-8.60819500	-5.10412600	-2.36947200
H	-8.45801300	-3.58391200	-4.32950800
H	-7.23878700	-1.42844200	-4.11306100
H	-6.18973400	-0.80753500	-1.97953300
H	-2.15413100	2.63409500	-0.53957000

TS-4'(anti)

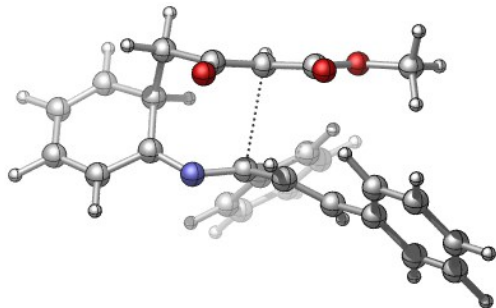


Zero-point correction=	0.430370 (Hartree/Particle)
Thermal correction to Energy=	0.455758
Thermal correction to Enthalpy=	0.456702
Thermal correction to Gibbs Free Energy=	0.373993
Sum of electronic and zero-point Energies=	-1284.024076
Sum of electronic and thermal Energies=	-1283.998688
Sum of electronic and thermal Enthalpies=	-1283.997744
Sum of electronic and thermal Free Energies=	-1284.080452

C	-6.14535900	3.14705400	0.99416000
C	-4.73035400	3.43733400	0.84147600
C	-6.62639700	1.88358700	1.01997100
C	-3.84686800	2.43116100	0.76589400
C	-4.24121100	0.99481600	0.86460800
C	-5.72833000	0.75875600	0.86443500
N	-6.23811300	-0.42397100	0.77388000
C	-5.80900400	-1.60492500	0.33086400
C	-3.57372300	-2.03573700	1.41093900
C	-2.56741500	-1.85084500	0.39858400
O	-2.18843300	-3.04072600	-0.14201800

O	-2.07953000	-0.80052400	-0.01154400
C	-1.25996000	-2.94507900	-1.21622800
H	-1.08728400	-3.96617100	-1.55481100
H	-0.32323800	-2.49362700	-0.88097500
H	-1.67316600	-2.34139000	-2.02883500
H	-6.83743900	3.97924600	1.08250700
H	-4.40872300	4.47173700	0.80054300
H	-7.68492100	1.67128600	1.11631900
H	-2.78056300	2.62391500	0.68030800
C	-3.57447300	0.40354500	2.14962300
C	-3.95475500	-1.05289800	2.37612000
O	-4.67225800	-1.32491100	3.34929500
H	-2.49522900	0.50982800	2.01606500
H	-3.90219700	0.96882500	3.02492800
H	-3.80002400	0.43986700	0.02575600
H	-3.80272500	-3.06452800	1.66444400
C	-6.28347200	-2.75028100	1.11622700
H	-6.24486700	-2.56949500	2.18865400
C	-6.78967200	-3.88503200	0.61008500
H	-6.89764100	-3.99638700	-0.46730200
C	-5.38880000	-1.72980000	-1.08989300
C	-4.76712600	-2.90185000	-1.54553700
C	-5.60855500	-0.67964600	-1.99137200
C	-4.36900500	-3.01390700	-2.87129600
H	-4.55429600	-3.70050000	-0.84476300
C	-5.20523900	-0.79572900	-3.31689300
H	-6.11674800	0.22113500	-1.66267800
C	-4.58437600	-1.96102600	-3.76000000
H	-3.87730900	-3.92095800	-3.20759900
H	-5.38347600	0.02294000	-4.00576000
H	-4.26911700	-2.04948700	-4.79450900
C	-7.25869400	-5.01081200	1.42871200
C	-8.11018100	-5.96646300	0.85946300
C	-6.86603000	-5.16742600	2.76667900
C	-8.58000500	-7.03771700	1.61221100
H	-8.40917700	-5.85976100	-0.17976500
C	-7.33360800	-6.23887300	3.51629100
H	-6.17461300	-4.45841200	3.21333500
C	-8.19486800	-7.17547700	2.94352400
H	-9.24441300	-7.76637200	1.15914400
H	-7.01813300	-6.35085900	4.54849700
H	-8.55508400	-8.01353400	3.53131900

TS-4'(syn)

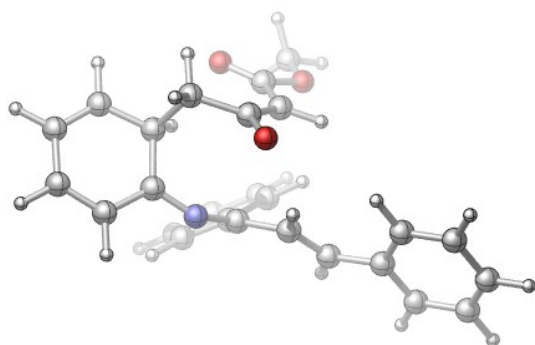


Zero-point correction= 0.430082 (Hartree/Particle)
 Thermal correction to Energy= 0.455603
 Thermal correction to Enthalpy= 0.456548
 Thermal correction to Gibbs Free Energy= 0.373930
 Sum of electronic and zero-point Energies= -1284.020004
 Sum of electronic and thermal Energies= -1283.994483
 Sum of electronic and thermal Enthalpies= -1283.993538
 Sum of electronic and thermal Free Energies= -1284.076156

C	-5.70599300	3.07821600	0.68650000
C	-4.34145500	3.19626700	0.20731300
C	-6.26912300	1.88245100	0.98091500
C	-3.57160600	2.10203600	0.10249300
C	-4.04407700	0.74784600	0.52034900
C	-5.52307700	0.66217300	0.78567800
N	-6.14345500	-0.46897900	0.93418500
C	-5.82623500	-1.68809700	0.48564500
C	-3.47232800	-2.10362700	1.57426600
C	-3.63499500	-3.45132400	2.05486400
O	-3.19897800	-4.36637600	1.13327100
O	-4.11592600	-3.82433500	3.11310700
C	-3.36993600	-5.72744200	1.51564600
H	-3.02799400	-6.32210900	0.66923700
H	-4.41985300	-5.94124500	1.73288400
H	-2.77559800	-5.95882300	2.40296000
H	-6.29425500	3.98416500	0.79800900
H	-3.95930600	4.17713700	-0.05120100
H	-7.29777800	1.79482500	1.31097500
H	-2.53610000	2.17240100	-0.21899800
C	-3.27052400	0.37084600	1.83552100
C	-3.75006400	-0.97060700	2.39242600
O	-4.41546900	-0.95524700	3.43296600
H	-2.20463600	0.35086300	1.59027200
H	-3.45589900	1.13831000	2.59049000
H	-3.77464600	0.00109900	-0.23498500

H	-2.86669500	-1.97473300	0.68362600
C	-6.29550900	-2.80272300	1.29305900
H	-6.30780000	-2.60269500	2.36220000
C	-6.72202400	-3.97283000	0.77985000
H	-6.75235300	-4.09394600	-0.30137600
C	-5.49047600	-1.84850900	-0.95714300
C	-4.70940800	-2.92465100	-1.40177500
C	-5.97697800	-0.92087000	-1.88849500
C	-4.41505400	-3.05737700	-2.75333200
H	-4.30529600	-3.62636000	-0.67868300
C	-5.68500900	-1.06530100	-3.24062000
H	-6.60401100	-0.09947500	-1.55690600
C	-4.90221800	-2.13143800	-3.67560600
H	-3.79533500	-3.88323900	-3.08641000
H	-6.07482600	-0.34672200	-3.95358600
H	-4.67120800	-2.24166900	-4.73012100
C	-7.23030200	-5.10463600	1.55921100
C	-7.99889000	-6.08039600	0.90902800
C	-6.97205000	-5.24564200	2.93256000
C	-8.52385400	-7.15746400	1.61448500
H	-8.19100900	-5.98246300	-0.15608100
C	-7.49588400	-6.32479000	3.63298900
H	-6.32417800	-4.53078600	3.43011500
C	-8.27659900	-7.27955300	2.97997100
H	-9.12201700	-7.90197000	1.09933800
H	-7.28670400	-6.42922500	4.69272900
H	-8.68135700	-8.12145000	3.53258000

B'



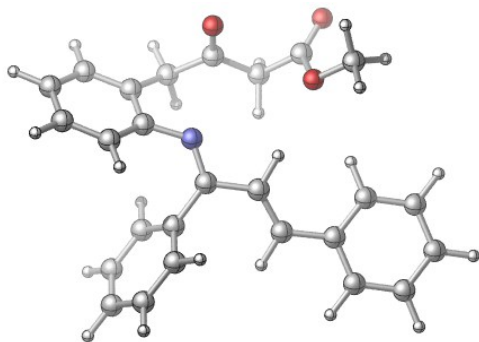
Zero-point correction=	0.430359 (Hartree/Particle)
Thermal correction to Energy=	0.456629
Thermal correction to Enthalpy=	0.457573
Thermal correction to Gibbs Free Energy=	0.372268
Sum of electronic and zero-point Energies=	-1284.027178
Sum of electronic and thermal Energies=	-1284.000907

Sum of electronic and thermal Enthalpies= -1283.999963
Sum of electronic and thermal Free Energies= -1284.085268

C	-5.85990000	3.27108200	0.81968100
C	-4.41604400	3.37514900	0.76753000
C	-6.50791900	2.08035600	0.83867000
C	-3.66703100	2.26075100	0.78205400
C	-4.24810100	0.89298000	0.89041200
C	-5.74811700	0.85865800	0.78305300
N	-6.35430800	-0.27633500	0.69394800
C	-6.22521000	-1.45996000	0.18776400
C	-3.62719600	-2.19830000	1.61307800
C	-2.62833300	-2.01314600	0.61763500
O	-2.29953400	-3.20024400	0.00865000
O	-2.07429700	-0.97181200	0.24924400
C	-1.35106300	-3.09064200	-1.04163400
H	-1.22300700	-4.09749800	-1.43964000
H	-0.39548600	-2.70887400	-0.67302800
H	-1.71316400	-2.41985900	-1.82610400
H	-6.44398100	4.18653700	0.83207200
H	-3.96261000	4.35849600	0.72521300
H	-7.58912500	2.01190300	0.85427900
H	-2.58149900	2.31041400	0.77165400
C	-3.73833600	0.26589600	2.23252000
C	-4.17528400	-1.18807600	2.43038100
O	-5.04672100	-1.39731900	3.30281600
H	-2.64918100	0.33935300	2.19969400
H	-4.12984700	0.84588300	3.07177200
H	-3.83064800	0.25251800	0.09940700
H	-3.96259500	-3.21415300	1.79087400
C	-6.62059800	-2.59865300	0.99814000
H	-6.55111000	-2.41805400	2.06823600
C	-7.04603100	-3.76851900	0.48776100
H	-7.16791400	-3.87602200	-0.58901600
C	-5.76057900	-1.59367700	-1.21450200
C	-4.97239400	-2.69222700	-1.58481000
C	-6.04623700	-0.59130300	-2.14971500
C	-4.48003000	-2.78015600	-2.88238600
H	-4.69963700	-3.43445700	-0.84267100
C	-5.56161500	-0.69441600	-3.44770400
H	-6.66435900	0.25375600	-1.86149900
C	-4.77749300	-1.78788200	-3.81434500
H	-3.85554400	-3.62248400	-3.16112800
H	-5.79502800	0.07696800	-4.17356600

H	-4.39396200	-1.86320300	-4.82657800
C	-7.38212600	-4.93888400	1.30078500
C	-8.13196300	-5.97661300	0.73218900
C	-6.95116700	-5.05801600	2.63203900
C	-8.46827500	-7.09930900	1.48070300
H	-8.45633100	-5.89369900	-0.30148200
C	-7.28238100	-6.18368500	3.37442400
H	-6.33804900	-4.27733000	3.07498400
C	-8.04499100	-7.20391900	2.80368800
H	-9.05495400	-7.89348300	1.03087000
H	-6.93886400	-6.27145700	4.39981500
H	-8.30078400	-8.08180000	3.38795500

B''

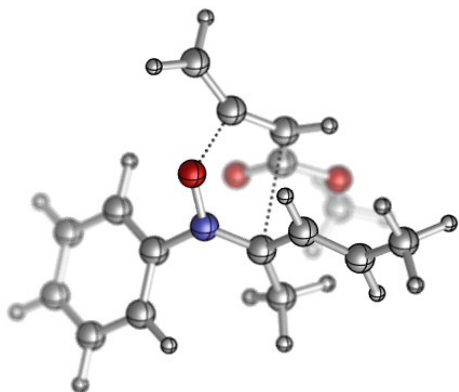


Zero-point correction=	0.431484 (Hartree/Particle)
Thermal correction to Energy=	0.458088
Thermal correction to Enthalpy=	0.459033
Thermal correction to Gibbs Free Energy=	0.371690
Sum of electronic and zero-point Energies=	-1284.106843
Sum of electronic and thermal Energies=	-1284.080239
Sum of electronic and thermal Enthalpies=	-1284.079295
Sum of electronic and thermal Free Energies=	-1284.166638

H	3.73189600	0.29648000	0.95319600
H	2.75209700	1.05707900	2.23215100
O	2.40553600	2.26352800	-0.11199200
C	2.80150300	0.23110600	1.52058000
H	2.73301700	-0.72506300	2.03639100
O	-0.71718600	2.36512300	0.91402200
H	0.23327400	-1.58291000	0.36357200
C	1.59078500	1.37467300	-0.13111100
O	1.67746800	0.27625500	0.63498100
C	-0.49074600	-2.28110500	-0.05045800
C	-0.10418700	-3.46449100	-0.55339700
H	-4.15352800	-1.35405700	1.71380100

C	-1.86653800	-1.76588800	-0.02988700
N	-1.98461000	-0.53189000	0.31363900
C	-4.25525900	-0.37175100	1.26317400
C	-0.84128900	1.90679800	-0.19797600
C	0.34501300	1.35261900	-0.97724800
C	-3.21376100	0.12979000	0.47664700
C	-5.39877600	0.39142300	1.47442200
H	-6.19934200	-0.00226900	2.09241600
C	-3.31495300	1.41470300	-0.08706700
C	-5.51382100	1.65511600	0.90061400
H	0.10164100	0.33357300	-1.29246000
H	0.50277300	1.97003300	-1.86687300
C	-2.17540700	1.91643800	-0.93855200
C	-4.47225300	2.15814900	0.12253800
H	-4.55496700	3.14627800	-0.32158400
H	-2.36169700	2.95274900	-1.24256300
H	-2.08487300	1.32073700	-1.85372200
H	-6.40501800	2.25139900	1.06567200
C	-2.99985600	-2.64924900	-0.44435800
C	1.28606800	-3.93765900	-0.60190800
H	-0.85220600	-4.14868700	-0.95024800
C	-3.85423500	-2.23753400	-1.47123100
C	-3.22307000	-3.87538900	0.18816800
C	-4.91763600	-3.04326800	-1.86234200
C	-5.14443100	-4.25996500	-1.22040300
C	-4.29892100	-4.67329400	-0.19379900
H	-4.47418500	-5.61857700	0.30922100
H	-2.56069600	-4.19534500	0.98740300
H	-3.68211500	-1.28153000	-1.95803300
H	-5.57234100	-2.72057800	-2.66513500
H	-5.97948000	-4.88442700	-1.52071700
C	2.37832100	-3.07664400	-0.41197500
C	1.53432900	-5.29381800	-0.84857900
C	3.67666000	-3.56892800	-0.44440000
C	3.91030400	-4.92570600	-0.67381900
C	2.83532900	-5.78645000	-0.87929900
H	2.20813600	-2.01435700	-0.25928900
H	4.51135600	-2.89043200	-0.29833200
H	0.69582600	-5.96610500	-1.00930900
H	3.00949200	-6.84117000	-1.06578900
H	4.92619800	-5.30618600	-0.70029300

Scheme 3.
TS_[3+2]-A-anti

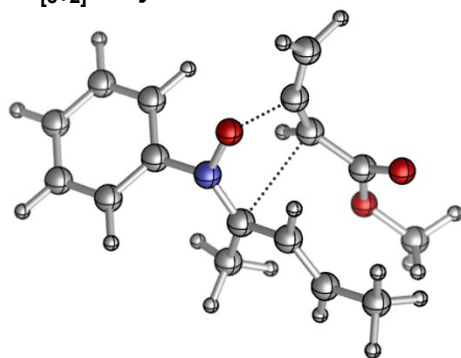


Zero-point correction= 0.427215 (Hartree/Particle)
 Thermal correction to Energy= 0.453722
 Thermal correction to Enthalpy= 0.454666
 Thermal correction to Gibbs Free Energy= 0.367197
 Sum of electronic and zero-point Energies= -1283.960987
 Sum of electronic and thermal Energies= -1283.934481
 Sum of electronic and thermal Enthalpies= -1283.933536
 Sum of electronic and thermal Free Energies= -1284.021005

C	-6.26631400	-0.04618400	-3.31764500
C	-5.38614000	0.81893000	-2.66936600
C	-4.94619800	0.54151700	-1.37935600
C	-6.71492700	-1.19813700	-2.67490000
C	-6.28235100	-1.49161100	-1.38585300
C	-5.39169500	-0.62304600	-0.76261500
N	-4.97443100	-0.88782400	0.59294200
O	-5.12387600	0.12983500	1.41751500
C	-3.55988600	0.91878300	1.76160400
C	-3.92388600	2.16992700	1.95812400
H	-4.95080900	2.49456800	1.83899200
H	-3.17352300	2.89610300	2.25022200
C	-2.49351100	0.04367900	1.75292600
C	-4.42860200	-2.01228900	1.02195600
H	-4.23748600	1.18011700	-0.86436800
H	-5.03676600	1.71524100	-3.17069100
H	-7.40987600	-1.86684800	-3.17120300
H	-6.62872700	-2.37998400	-0.86793400
C	-1.75614700	-0.18580800	0.55000100
H	-2.23079600	-0.51901200	2.63966500
O	-1.93942400	0.33112600	-0.55148200
O	-0.76445000	-1.10560400	0.73148300
C	0.06953700	-1.33102000	-0.39757300
H	0.85950900	-2.00031100	-0.05816100
H	0.49728800	-0.39418300	-0.76151200

H	-0.48738900	-1.80095000	-1.21318500
C	-4.35798300	-2.23813200	2.45469400
C	-3.68226400	-3.26011700	3.01398900
H	-4.87941000	-1.50187100	3.05677900
H	-3.11019700	-3.92587900	2.37080800
H	-6.60543400	0.17961700	-4.32317600
C	-4.03503000	-3.05681900	0.04376300
C	-3.20228900	-2.73557100	-1.03498200
C	-4.49456900	-4.36907200	0.20082200
C	-2.83102100	-3.72405100	-1.93900000
H	-2.85462700	-1.71341300	-1.16474000
C	-4.13041800	-5.34946200	-0.71642500
H	-5.14837000	-4.61446900	1.03166200
C	-3.29472800	-5.02973500	-1.78387000
H	-2.18139400	-3.47221100	-2.77104200
H	-4.50088200	-6.36185500	-0.59630800
H	-3.00679000	-5.79618900	-2.49611000
C	-3.60186000	-3.55320300	4.44660700
C	-2.73173200	-4.56721000	4.87165500
C	-4.35790900	-2.86941500	5.41218500
C	-2.60839200	-4.88434900	6.21990700
H	-2.14535100	-5.10522200	4.13184300
C	-4.23560000	-3.18768500	6.75773800
H	-5.05097300	-2.09033200	5.11120700
C	-3.36020800	-4.19458700	7.16744300
H	-1.92757000	-5.67015200	6.53029900
H	-4.82720900	-2.65136500	7.49246500
H	-3.26877100	-4.44016800	8.22042300

TS_[3+2]-A-syn



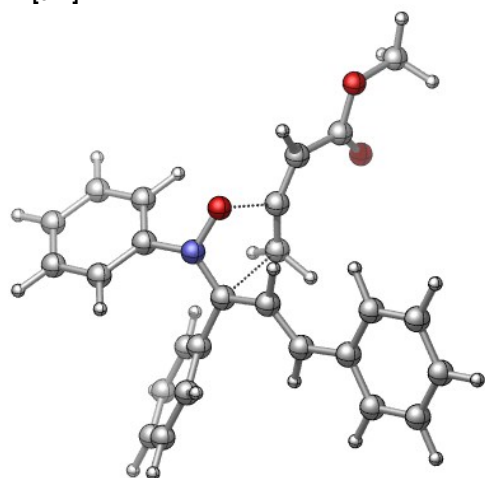
Zero-point correction=	0.427678 (Hartree/Particle)
Thermal correction to Energy=	0.453933
Thermal correction to Enthalpy=	0.454878
Thermal correction to Gibbs Free Energy=	0.369833
Sum of electronic and zero-point Energies=	-1283.961144

Sum of electronic and thermal Energies= -1283.934889
Sum of electronic and thermal Enthalpies= -1283.933944
Sum of electronic and thermal Free Energies= -1284.018989

C	-5.76717900	-0.11175700	-3.41510400
C	-5.30022600	0.87740300	-2.55258100
C	-5.12055200	0.60191900	-1.20097800
C	-6.06503100	-1.38111100	-2.92258500
C	-5.88421600	-1.67338400	-1.57521800
C	-5.39263000	-0.68022700	-0.73063600
N	-5.21014400	-0.92629000	0.67515200
O	-5.53477600	0.08633800	1.44943100
C	-4.03634900	0.89932100	2.11889500
C	-4.56555900	1.71843400	3.00523600
H	-5.61477300	1.66567800	3.27293200
H	-3.93755700	2.46618800	3.47614700
C	-2.89190300	0.39382800	1.56156900
C	-4.57280200	-1.96374900	1.19651700
H	-4.78655000	1.36582700	-0.50806600
H	-5.08101600	1.87080900	-2.92895900
H	-6.44947000	-2.14737400	-3.58693800
H	-6.12335100	-2.65560400	-1.18353200
C	-1.97994500	-0.40423000	2.33932800
O	-2.01918000	-0.63978600	3.53706100
O	-0.99370700	-0.92643300	1.55041900
C	-0.06550200	-1.76118200	2.23053300
H	0.62501900	-2.12686700	1.47124100
H	-0.57691900	-2.59893300	2.71145200
H	0.47757900	-1.20087000	2.99580900
C	-4.57702600	-2.10950600	2.63355000
C	-3.84046200	-3.03253200	3.28428800
H	-5.17265500	-1.39006500	3.18309000
H	-3.25501000	-3.75269700	2.71512500
H	-5.91147700	0.10856400	-4.46741400
H	-2.66891100	0.54277800	0.50961200
C	-3.93287800	-2.97928300	0.32217700
C	-4.36509400	-4.30868500	0.36473200
C	-2.87567900	-2.61593300	-0.51679100
C	-3.76301900	-5.26126700	-0.45144000
H	-5.18004900	-4.58667300	1.02653100
C	-2.27062900	-3.57474900	-1.32204600
H	-2.52491800	-1.58922000	-0.51802800
C	-2.71744000	-4.89456700	-1.29626500
H	-4.10971400	-6.28886000	-0.42604000

H	-1.44612700	-3.29091400	-1.96740700
H	-2.24624600	-5.63910800	-1.92964500
C	-3.78052700	-3.15483500	4.74211400
C	-3.43938100	-4.38735100	5.31415300
C	-4.05198700	-2.06598700	5.58457600
C	-3.40948300	-4.54287500	6.69612300
H	-3.20827400	-5.22908400	4.66682900
C	-4.01847300	-2.22280500	6.96389300
H	-4.23469700	-1.08966800	5.14679700
C	-3.70498000	-3.46203700	7.52383900
H	-3.15248800	-5.50523100	7.12678700
H	-4.22272400	-1.37298700	7.60721000
H	-3.67631600	-3.57951900	8.60231900

TS_[3+2]-B-anti

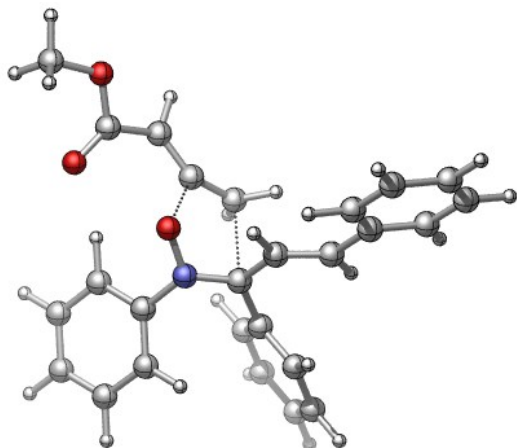


Zero-point correction=	0.426463 (Hartree/Particle)
Thermal correction to Energy=	0.453237
Thermal correction to Enthalpy=	0.454181
Thermal correction to Gibbs Free Energy=	0.364628
Sum of electronic and zero-point Energies=	-1283.945330
Sum of electronic and thermal Energies=	-1283.918555
Sum of electronic and thermal Enthalpies=	-1283.917611
Sum of electronic and thermal Free Energies=	-1284.007164

C	-5.96220700	0.04018000	-3.37174800
C	-5.20995200	0.93534100	-2.61545400
C	-4.89922900	0.64753100	-1.28925000
C	-6.41523500	-1.14659800	-2.79670800
C	-6.10824700	-1.44874100	-1.47471900
C	-5.33449800	-0.55468600	-0.73776100
N	-5.00528800	-0.83458000	0.63454400
O	-4.96728800	0.20563700	1.41526600
C	-3.10101600	0.60303000	1.59532200
C	-2.40017300	-0.41625900	1.04228400
H	-1.80178100	-1.06730900	1.66859800
H	-2.15320900	-0.37335700	-0.01441100

C	-3.15955900	1.75413700	2.24571000
C	-4.25502900	-1.88959900	1.02111500
H	-4.33487700	1.34280000	-0.67763400
H	-4.86510700	1.86566200	-3.05442000
H	-7.01706900	-1.83814800	-3.37664800
H	-6.45758400	-2.36861400	-1.01811000
C	-1.92344100	2.51630000	2.53017600
H	-4.10206800	2.17250000	2.58176200
O	-0.79180900	2.19614400	2.24088700
O	-2.21753300	3.65930600	3.17704600
C	-1.09301500	4.47740700	3.50106000
H	-1.49621800	5.35467700	4.00312900
H	-0.55814400	4.76717300	2.59436700
H	-0.40819600	3.94007700	4.16044100
C	-4.18147500	-2.12232200	2.46912900
C	-3.52025300	-3.13894400	3.04402100
H	-4.68907200	-1.37286200	3.06774300
H	-3.01771700	-3.86957900	2.41214000
H	-6.20514100	0.27043000	-4.40371900
C	-4.02187200	-3.02101600	0.07238400
C	-4.62201600	-4.26105700	0.32320300
C	-3.25530000	-2.86138700	-1.08545200
C	-4.46249700	-5.31590200	-0.57058000
H	-5.22585100	-4.39151600	1.21572700
C	-3.09076100	-3.91798400	-1.97425300
H	-2.80216700	-1.90040000	-1.30071500
C	-3.69500200	-5.14733400	-1.72013100
H	-4.94089500	-6.26854600	-0.36839900
H	-2.49163800	-3.77885900	-2.86807200
H	-3.56801000	-5.96989200	-2.41636500
C	-3.40848200	-3.37263600	4.49025300
C	-2.94943500	-4.61924800	4.93722400
C	-3.73394600	-2.39861700	5.44629800
C	-2.83732000	-4.89568100	6.29586800
H	-2.68404200	-5.37833000	4.20608900
C	-3.62131800	-2.67432700	6.80306300
H	-4.05663800	-1.41243200	5.12740700
C	-3.17610800	-3.92442400	7.23420800
H	-2.48332100	-5.86840300	6.62172800
H	-3.87247400	-1.90770200	7.52918000
H	-3.08601800	-4.13445300	8.29499900

TS_[3+2]-B-syn

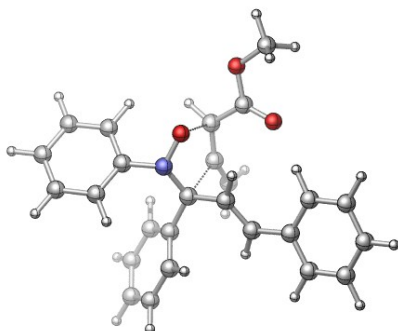


Zero-point correction= 0.427901 (Hartree/Particle)
 Thermal correction to Energy= 0.454158
 Thermal correction to Enthalpy= 0.455102
 Thermal correction to Gibbs Free Energy= 0.369254
 Sum of electronic and zero-point Energies= -1283.936927
 Sum of electronic and thermal Energies= -1283.910670
 Sum of electronic and thermal Enthalpies= -1283.909726
 Sum of electronic and thermal Free Energies= -1283.995574

C	-6.38650100	-0.04908200	-3.18061800
C	-5.72601300	0.95183100	-2.47324000
C	-5.24907500	0.71364900	-1.18641100
C	-6.58725700	-1.29746200	-2.59128100
C	-6.11489300	-1.55278700	-1.31028100
C	-5.42561500	-0.55001700	-0.62747100
N	-4.94883500	-0.77475600	0.70949700
O	-4.91048700	0.27477300	1.47051600
C	-3.04712300	0.79658100	1.45950600
C	-2.32315800	-0.32154700	1.19670600
H	-1.94851500	-0.95038600	1.99380200
H	-1.83754500	-0.40906200	0.22990300
C	-3.02310300	2.08525800	1.76535100
C	-4.17926900	-1.81457000	1.09554300
H	-4.78192800	1.49520500	-0.59760100
H	-5.58753200	1.93146600	-2.91884100
H	-7.12280000	-2.07452500	-3.12624600
H	-6.27733600	-2.51791000	-0.84379400
C	-4.16412300	3.03143500	1.83385100
H	-2.06109300	2.52869300	2.00970100
O	-5.17878300	3.02318300	1.17525400
O	-3.89047100	3.99985800	2.72931100
C	-4.88455600	5.01901100	2.84173000
H	-4.50076400	5.73181500	3.56879400
H	-5.82966400	4.59400200	3.18564600
H	-5.04366800	5.50356700	1.87636000
C	-4.15072700	-2.05986700	2.54350200
C	-3.44445900	-3.03264500	3.14092900
H	-4.74403400	-1.35905100	3.12300400
H	-2.80505400	-3.66915700	2.53058100
H	-6.75965900	0.14528000	-4.18070000
C	-3.86466100	-2.91567600	0.13709800

C	-4.31407800	-4.21772000	0.38580700
C	-3.15229100	-2.65948700	-1.03961100
C	-4.05933600	-5.23860200	-0.52609400
H	-4.87876600	-4.42665000	1.28837100
C	-2.89465100	-3.67989900	-1.94701600
H	-2.81731600	-1.64958400	-1.25002300
C	-3.34754000	-4.97327300	-1.69271800
H	-4.42233400	-6.24101200	-0.32425000
H	-2.33992000	-3.46404100	-2.85405400
H	-3.14747600	-5.76979500	-2.40198100
C	-3.42535200	-3.32013800	4.58125800
C	-2.47061000	-4.22003100	5.07453800
C	-4.32729700	-2.74123400	5.48753400
C	-2.40342400	-4.52142500	6.43102200
H	-1.77169900	-4.68101700	4.38171300
C	-4.26069500	-3.04248700	6.84162800
H	-5.09415300	-2.06074400	5.13108400
C	-3.29775800	-3.93174200	7.32037600
H	-1.65440400	-5.21840400	6.79288200
H	-4.96783100	-2.58793800	7.52812100
H	-3.25142900	-4.16680100	8.37869600

TS_[3+2]-A'-anti

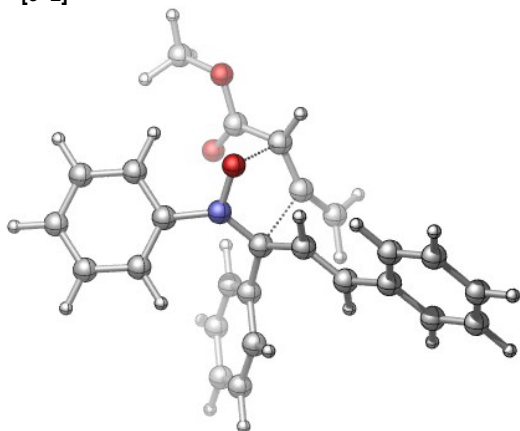


Zero-point correction=	0.428862 (Hartree/Particle)
Thermal correction to Energy=	0.454732
Thermal correction to Enthalpy=	0.455676
Thermal correction to Gibbs Free Energy=	0.371762
Sum of electronic and zero-point Energies=	-1283.941421
Sum of electronic and thermal Energies=	-1283.915551
Sum of electronic and thermal Enthalpies=	-1283.914607
Sum of electronic and thermal Free Energies=	-1283.998521

C	-6.42364400	-0.36325000	-3.46888700
C	-5.76349100	0.67891800	-2.82410800
C	-5.30018200	0.51936600	-1.52116000
C	-6.63302200	-1.56809400	-2.79898500
C	-6.17132900	-1.74218500	-1.50000100
C	-5.48211500	-0.70136500	-0.87584700
N	-5.03222600	-0.83047400	0.48696200
O	-5.03125400	0.25662700	1.17276500
C	-2.47868300	-0.55813800	0.97939100
C	-1.38654100	-1.28928500	0.90384100
H	-1.41889000	-2.36882500	0.77793500
H	-0.40421300	-0.82968900	0.97987300
C	-3.00541600	0.69525900	1.16280200

C	-4.19810000	-1.81802900	0.94952700
H	-4.82195700	1.33593100	-0.99541200
H	-5.61331800	1.62681600	-3.32995200
H	-7.16752900	-2.37689200	-3.28574500
H	-6.34371800	-2.67508300	-0.97589600
C	-3.12904400	1.26633500	2.52007800
H	-3.08958600	1.39393900	0.33760900
O	-2.94746400	0.67227200	3.56145800
O	-3.50206900	2.55382800	2.46425600
C	-3.69015600	3.18705300	3.73120000
H	-3.97416700	4.21428900	3.51176300
H	-2.76625700	3.16111200	4.31210500
H	-4.47928500	2.68332000	4.29288200
C	-4.21277700	-1.98911900	2.41622500
C	-3.62580500	-2.98986300	3.08787900
H	-4.72006200	-1.19367000	2.95161300
H	-3.11492700	-3.78262300	2.54412300
H	-6.78837900	-0.23400600	-4.48229100
C	-3.95822900	-3.00303700	0.06446800
C	-4.51924000	-4.24412000	0.38656800
C	-3.25269100	-2.87058600	-1.13682900
C	-4.38105000	-5.32734400	-0.47652600
H	-5.08713100	-4.35189400	1.30468800
C	-3.11147500	-3.95402300	-1.99623900
H	-2.82556500	-1.90771800	-1.39735500
C	-3.67597800	-5.18518600	-1.66888400
H	-4.83113400	-6.28033300	-0.21846700
H	-2.56419100	-3.83501700	-2.92550600
H	-3.56832400	-6.02947200	-2.34216400
C	-3.62297100	-3.11217500	4.55332300
C	-3.41131300	-4.36917100	5.13595200
C	-3.81618500	-2.00490900	5.39325900
C	-3.42379900	-4.52614800	6.51809800
H	-3.24358700	-5.22992500	4.49360800
C	-3.82831200	-2.16427100	6.77412100
H	-3.91578200	-1.01472500	4.95858000
C	-3.63781000	-3.42384000	7.34245100
H	-3.26532300	-5.50846100	6.95183600
H	-3.97360200	-1.29850700	7.41283400
H	-3.64441700	-3.54253100	8.42116500

TS_[3+2]-A'-syn

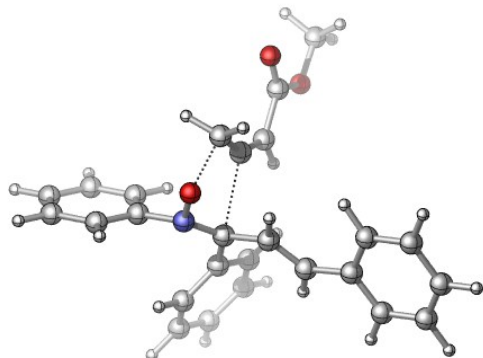


Zero-point correction= 0.428415 (Hartree/Particle)
 Thermal correction to Energy= 0.454301
 Thermal correction to Enthalpy= 0.455245
 Thermal correction to Gibbs Free Energy= 0.370072
 Sum of electronic and zero-point Energies= -1283.940925
 Sum of electronic and thermal Energies= -1283.915040
 Sum of electronic and thermal Enthalpies= -1283.914096
 Sum of electronic and thermal Free Energies= -1283.999268

C	-6.88709700	-0.17562600	-3.06653800
C	-6.23517000	0.91093200	-2.48736000
C	-5.50975800	0.75355400	-1.31329100
C	-6.82518800	-1.41879200	-2.44399100
C	-6.10231400	-1.59134900	-1.26750900
C	-5.41097100	-0.50768100	-0.72236500
N	-4.72046100	-0.60259800	0.54140100
O	-4.53108500	0.50713400	1.16012200
C	-2.13327800	-0.66100700	1.09641400
C	-1.17216400	-1.55110100	1.20623400
H	-1.37748100	-2.61667600	1.27864000
H	-0.12905400	-1.24589200	1.22028400
C	-2.47030900	0.66592700	1.00687000
C	-4.01257100	-1.66565800	1.05086900
H	-5.03175300	1.60025900	-0.83698900
H	-6.29699200	1.89304300	-2.94504600
H	-7.35308300	-2.26755000	-2.86594100
H	-6.08899000	-2.55964000	-0.78492300
C	-2.50026400	1.25707000	-0.34321500
H	-2.45145400	1.33299200	1.86035200
O	-2.40126800	0.62136600	-1.37444600
O	-2.66593500	2.58942400	-0.31717400
C	-2.68017700	3.21751100	-1.60132400
H	-2.85138700	4.27537700	-1.41357900
H	-3.47861900	2.80186200	-2.22075800
H	-1.72455300	3.06669100	-2.10757400
C	-4.08770600	-1.78020700	2.52221600
C	-3.61464100	-2.80160500	3.25151400
H	-4.55823200	-0.92482700	2.99793800
H	-3.10206700	-3.62002800	2.74950100
H	-7.45233400	-0.05029800	-3.98387600
C	-3.85728000	-2.88162300	0.19582200
C	-4.44259100	-4.10083400	0.55259200
C	-3.17930300	-2.77754000	-1.02543900
C	-4.35973900	-5.19664800	-0.30280800
H	-4.99244400	-4.18209700	1.48405500
C	-3.09863800	-3.87339500	-1.87605900
H	-2.73356100	-1.82456900	-1.29921500
C	-3.68854100	-5.08508600	-1.51754800
H	-4.82743100	-6.13438400	-0.02116300
H	-2.57636800	-3.78204100	-2.82283300
H	-3.62605800	-5.93924900	-2.18417100
C	-3.70064700	-2.92984300	4.71321700
C	-3.05617500	-4.01261200	5.32733900
C	-4.40190900	-2.02619500	5.52641900
C	-3.10019200	-4.18697400	6.70691700
H	-2.51157100	-4.72211300	4.70997100

C	-4.44617100	-2.19981100	6.90375400
H	-4.92301400	-1.18441400	5.08141900
C	-3.79554700	-3.27996700	7.50152400
H	-2.59229100	-5.03201200	7.16062400
H	-4.99539100	-1.49128400	7.51565700
H	-3.83461300	-3.41284400	8.57773500

TS_[3+2]-B'-anti

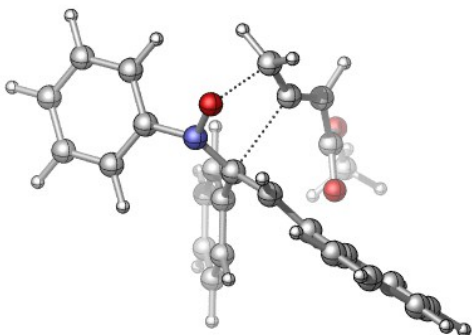


Zero-point correction=	0.427523 (Hartree/Particle)
Thermal correction to Energy=	0.454027
Thermal correction to Enthalpy=	0.454972
Thermal correction to Gibbs Free Energy=	0.365585
Sum of electronic and zero-point Energies=	-1283.936463
Sum of electronic and thermal Energies=	-1283.909959
Sum of electronic and thermal Enthalpies=	-1283.909014
Sum of electronic and thermal Free Energies=	-1283.998401

C	-5.81357600	-0.14278000	-3.55183100
C	-4.57473300	-0.66086000	-3.18230700
C	-4.33222800	-1.03683800	-1.86356700
C	-6.81768000	0.01261900	-2.59691600
C	-6.58679400	-0.35660900	-1.27672400
C	-5.35132700	-0.89269600	-0.92517000
N	-5.14774800	-1.19964900	0.47095500
O	-5.23926100	-0.15190100	1.23911500
C	-2.62821100	-0.58389500	0.97612100
C	-3.40019000	0.49966000	1.27236100
H	-3.59103200	1.24157700	0.50179700
H	-3.48017800	0.85247200	2.29662100
C	-1.38560800	-0.99072600	0.76699100
C	-4.36131200	-2.20091200	0.90948700
H	-3.36733800	-1.43180900	-1.56434500
H	-3.78759800	-0.76993000	-3.92071000
H	-7.78131700	0.42245400	-2.88017900
H	-7.34635000	-0.23404200	-0.51232500
C	-0.26179800	-0.02807300	0.89332700
H	-1.10727600	-2.00463100	0.49825900
O	-0.35018400	1.14545200	1.18149000
O	0.91595700	-0.63098400	0.64311100
C	2.06187400	0.21345300	0.75086700
H	2.92049500	-0.41421300	0.52020100
H	2.14417100	0.61785600	1.76181700
H	1.99318600	1.04187200	0.04274800

C	-4.22679600	-2.34464500	2.36588800
C	-3.91534000	-3.48617300	3.00103300
H	-4.43403300	-1.44160000	2.92757900
H	-3.77531400	-4.40285600	2.43257900
H	-5.99551000	0.14510500	-4.58195400
C	-4.18631200	-3.40277200	0.04670200
C	-2.95916400	-4.07064500	0.00896400
C	-5.26344000	-3.91753900	-0.68481400
C	-2.79781800	-5.20582500	-0.78051400
H	-2.13463200	-3.71031200	0.61367800
C	-5.10150100	-5.05406500	-1.46834600
H	-6.22980500	-3.42505800	-0.63770600
C	-3.86590800	-5.69604700	-1.52651700
H	-1.83650500	-5.70809800	-0.80748200
H	-5.94476300	-5.44173600	-2.03046600
H	-3.74066800	-6.58138500	-2.14131400
C	-3.76710700	-3.61388500	4.45742200
C	-3.80486900	-4.89038100	5.03503700
C	-3.58060400	-2.50620800	5.29806500
C	-3.68693000	-5.05665400	6.41100400
H	-3.93634600	-5.75776300	4.39354900
C	-3.46240900	-2.67205300	6.67210900
H	-3.50463200	-1.51050900	4.87210800
C	-3.51842200	-3.94697700	7.23544400
H	-3.72509100	-6.05332900	6.83887700
H	-3.31474100	-1.80413000	7.30693400
H	-3.42158700	-4.07365200	8.30884400

TS_[3+2]-B'-syn

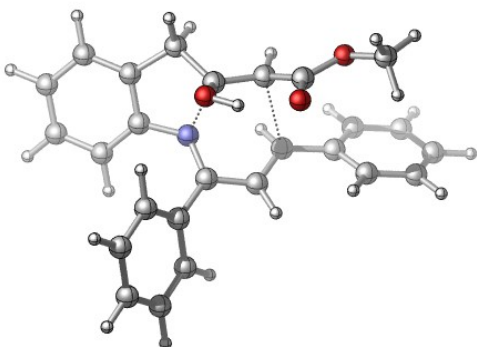


Zero-point correction= 0.427499 (Hartree/Particle)
 Thermal correction to Energy= 0.453720
 Thermal correction to Enthalpy= 0.454664
 Thermal correction to Gibbs Free Energy= 0.368832
 Sum of electronic and zero-point Energies= -1283.935271
 Sum of electronic and thermal Energies= -1283.909051
 Sum of electronic and thermal Enthalpies= -1283.908106
 Sum of electronic and thermal Free Energies= -1283.993939

C	-6.71739300	-0.36855000	-3.28615600
C	-5.92980900	0.61433600	-2.69372100
C	-5.40575200	0.42295600	-1.41817500
C	-6.99270700	-1.54563300	-2.59097800
C	-6.47236000	-1.75030500	-1.31917400
C	-5.65726700	-0.77171000	-0.74867200

N	-5.14820200	-0.93791100	0.58503400
O	-5.02740300	0.15187500	1.28095200
C	-2.50105800	-0.72470200	1.08537300
C	-3.09165000	0.48584500	1.28151600
H	-3.18303100	1.19063900	0.46076800
H	-3.11458300	0.91940900	2.27724500
C	-1.34120200	-1.32669000	0.86732500
C	-4.49407300	-2.02261400	1.05737400
H	-4.82583600	1.19696800	-0.93215300
H	-5.72617200	1.54129500	-3.21934400
H	-7.62667600	-2.30579000	-3.03490500
H	-6.69377100	-2.65962500	-0.77228900
C	-1.11951200	-2.78600200	0.69406000
H	-0.42740500	-0.73784100	0.77871600
O	-1.64207900	-3.68585400	1.31257200
O	-0.18747700	-3.00882500	-0.25080000
C	0.10968200	-4.38559400	-0.48838100
H	0.86425400	-4.39810300	-1.27272700
H	-0.79138200	-4.91336100	-0.81109800
H	0.49285400	-4.85594100	0.41961700
C	-4.52532100	-2.15982800	2.52052500
C	-3.99862600	-3.16962400	3.23057600
H	-5.04242000	-1.34293100	3.01509700
H	-3.40417900	-3.92049600	2.71807300
H	-7.12905400	-0.21382800	-4.27779700
C	-4.28829800	-3.18907500	0.15270200
C	-4.79272200	-4.44969900	0.47965900
C	-3.58856200	-3.02674800	-1.04948000
C	-4.59522700	-5.53027800	-0.37714500
H	-5.34986400	-4.58268900	1.40083400
C	-3.38871700	-4.10495200	-1.90097800
H	-3.19070700	-2.04808300	-1.30264600
C	-3.89000800	-5.36333400	-1.56513300
H	-4.99581600	-6.50372400	-0.11345800
H	-2.83773100	-3.96572700	-2.82572300
H	-3.73186400	-6.20701000	-2.22926600
C	-4.10955200	-3.31921400	4.68805700
C	-3.28347800	-4.25021600	5.33272400
C	-5.01350800	-2.58070700	5.46765600
C	-3.34062700	-4.42678400	6.71162800
H	-2.58562400	-4.83433700	4.73872300
C	-5.07089800	-2.75634600	6.84436200
H	-5.68906000	-1.87536400	4.99378500
C	-4.23415700	-3.67822500	7.47371300
H	-2.68849600	-5.15075400	7.18981700
H	-5.77804900	-2.17757800	7.43018200
H	-4.28492800	-3.81597200	8.54890500

Scheme 4.
cis-endo

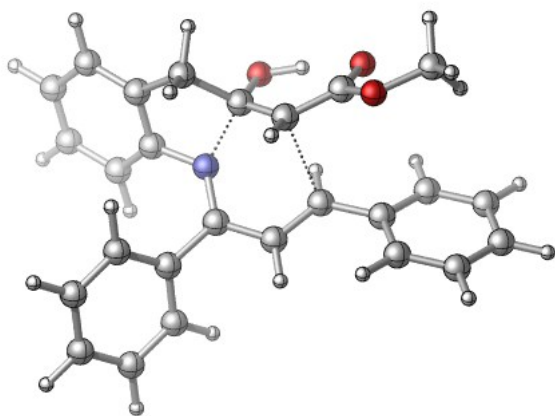


Zero-point correction= 0.324568 (Hartree/Particle)
 Thermal correction to Energy= 0.342866
 Thermal correction to Enthalpy= 0.343811
 Thermal correction to Gibbs Free Energy= 0.279534
 Sum of electronic and zero-point Energies= -900.842748
 Sum of electronic and thermal Energies= -900.824449
 Sum of electronic and thermal Enthalpies= -900.823505
 Sum of electronic and thermal Free Energies= -900.887782

H	-4.96631600	3.22613200	-1.42196100
H	-2.79637000	2.99476800	0.31471200
C	-4.93932500	2.13969500	-1.40421900
C	-5.99531400	1.39881700	-1.94837100
C	-2.59516200	2.10282000	-0.28649000
C	-3.85184700	1.48128700	-0.84237500
H	-1.92734000	2.40190400	-1.10331600
O	-0.13223300	0.62072000	2.88251600
C	-5.94125100	0.00242900	-1.93688300
C	-3.81128200	0.07592100	-0.80695100
H	-6.75248400	-0.57372600	-2.37280600
C	-1.88270100	1.08339900	0.60125500
C	-0.43405900	0.99288000	0.54984600
C	-4.85553800	-0.67046300	-1.37197600
C	0.31726200	0.97374900	1.77615900
N	-2.60899200	-0.40755900	-0.28566300
C	-2.41547600	-1.55538000	0.38638400
O	-2.46104200	1.00045400	1.83262000
H	-4.81693600	-1.75383400	-1.37733100
C	-0.05950500	-1.21900500	-0.07817600
C	-1.07466700	-1.91215600	0.59116100
O	1.60306300	1.35836200	1.62618600
H	3.39234700	1.69988200	2.50444600
H	-1.75428900	0.71190100	2.46850600
H	2.49232000	0.32485900	3.21165200
C	2.41227500	1.33881100	2.81461600
H	-0.83978800	-2.65777500	1.34226500
H	-0.33902500	-0.78533900	-1.03246700

H	1.99129600	1.99449200	3.58028100
H	-6.85002400	1.90831800	-2.38244500
H	0.05860900	1.41355700	-0.31687400
C	-3.49945600	-2.35370200	1.02233100
C	-3.48403600	-3.75409000	0.92617000
C	-4.51728800	-1.73197100	1.76520900
C	-4.47115200	-4.51829000	1.54950200
H	-2.70280700	-4.23947000	0.34861400
C	-5.49630500	-2.49853000	2.39384500
H	-4.51384100	-0.65212900	1.86609100
C	-5.47987800	-3.89231200	2.28424400
H	-4.45245400	-5.60040000	1.45995600
H	-6.27174000	-2.00844000	2.97521500
H	-6.24795200	-4.48592000	2.77107100
C	1.37089700	-1.49437800	0.10751100
C	2.26942600	-1.19850700	-0.93361300
C	1.88029300	-2.06288700	1.29068000
C	3.62825500	-1.47919600	-0.80779400
H	1.89134100	-0.75288600	-1.84981100
C	3.23902500	-2.34239500	1.41648100
H	1.21116600	-2.27282400	2.11884200
C	4.11761900	-2.05431000	0.36754800
H	4.30507200	-1.25041800	-1.62549100
H	3.61498900	-2.78328400	2.33491300
H	5.17632300	-2.27367600	0.46783600

cis-exo

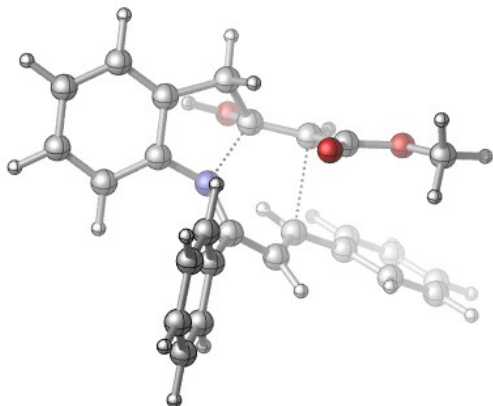


Zero-point correction=	0.324606 (Hartree/Particle)
Thermal correction to Energy=	0.343018
Thermal correction to Enthalpy=	0.343962
Thermal correction to Gibbs Free Energy=	0.279346
Sum of electronic and zero-point Energies=	-900.840707
Sum of electronic and thermal Energies=	-900.822295
Sum of electronic and thermal Enthalpies=	-900.821351
Sum of electronic and thermal Free Energies=	-900.885967

H	-3.28909800	2.94189600	-0.37999500
C	-3.28830900	1.85692100	-0.32248900
C	-4.49458900	1.14680400	-0.31205600
C	-2.08777300	1.15941700	-0.25283400
H	1.84529400	0.60931000	0.50785400
O	2.45538400	0.58139700	-2.74374300
C	-4.48732000	-0.25056100	-0.24892500
C	-2.08779600	-0.24140800	-0.18652400
H	-5.42662600	-0.79565900	-0.25529300
C	0.18123100	0.57362500	-0.90259400
C	1.57976800	0.46043500	-0.53103700
C	-3.28611900	-0.96125700	-0.19312900
C	2.60526200	0.65571500	-1.50493000
N	-0.78289200	-0.77002800	-0.22449900
C	-0.32727300	-1.73769100	0.58743800
O	-0.07910600	0.52448700	-2.24523000
H	-3.28154800	-2.04533400	-0.16320500
C	1.67183300	-1.96505000	-0.79037200
C	0.94312400	-2.28783600	0.34724600
O	3.82039900	0.91255700	-0.96178300
H	5.07092500	0.18548800	-2.47258600
H	0.79894500	0.45552900	-2.70812100
H	5.77601000	1.31558700	-1.27745300
C	4.90203800	1.09344100	-1.88970500
H	1.39570500	-2.87017600	1.14155300
H	1.11310800	-1.67086600	-1.67364700
H	4.69747300	1.92414500	-2.56956300
H	-5.43806800	1.68176500	-0.35999900
C	-0.67469900	1.67026700	-0.23343600
H	-0.32572700	1.82702200	0.79419300
H	-0.53888700	2.60306600	-0.78712700
C	-1.06712000	-2.18355700	1.80457400
C	-1.16153500	-3.55488900	2.08994700
C	-1.62260700	-1.26397900	2.70999900
C	-1.80208300	-3.99791800	3.24754300
H	-0.74145600	-4.27320300	1.39244300
C	-2.25236000	-1.70792300	3.87072300
H	-1.54812500	-0.19998400	2.51208600
C	-2.34854600	-3.07586500	4.14164600
H	-1.87463100	-5.06253100	3.44870700
H	-2.66633000	-0.98474800	4.56697900
H	-2.84545400	-3.41897700	5.04407300
C	3.04900200	-2.40295900	-1.03151100
C	3.50905300	-2.52011300	-2.35716700
C	3.93353800	-2.72670300	0.01630300

C	4.80048600	-2.96929100	-2.62791100
H	2.84377700	-2.25701300	-3.17299100
C	5.22334200	-3.17253700	-0.25554700
H	3.61283100	-2.61205900	1.04683200
C	5.66095100	-3.29897500	-1.57831000
H	5.13455600	-3.06293200	-3.65682300
H	5.89292600	-3.41623700	0.56379700
H	6.66799500	-3.64711800	-1.78747800

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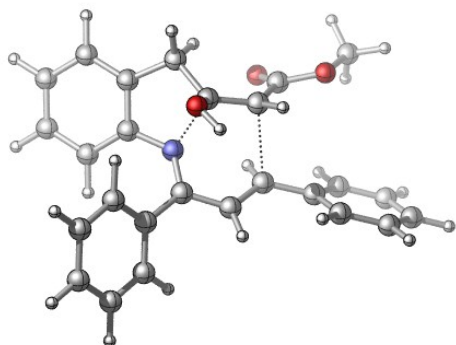


Zero-point correction=	0.323951 (Hartree/Particle)
Thermal correction to Energy=	0.342884
Thermal correction to Enthalpy=	0.343828
Thermal correction to Gibbs Free Energy=	0.277686
Sum of electronic and zero-point Energies=	-900.838310
Sum of electronic and thermal Energies=	-900.819377
Sum of electronic and thermal Enthalpies=	-900.818433
Sum of electronic and thermal Free Energies=	-900.884575

H	-5.43592100	2.98545100	-0.36063700
H	-2.86891800	1.74090200	1.42962600
C	-5.19276300	1.98271400	-0.70130700
C	-6.12708700	1.23423500	-1.42435400
C	-2.80870100	2.01843500	0.37401000
C	-3.94966100	1.42838400	-0.40838800
H	-2.75209700	3.10924500	0.30029600
O	-1.32830100	0.36015700	2.53841000
C	-5.80365300	-0.05472900	-1.86299100
C	-3.62799200	0.13487400	-0.85545800
H	-6.52896400	-0.62777200	-2.43324200
C	-1.51584500	1.42155200	-0.20483800
C	-0.32664600	1.27302100	0.57801300
C	-4.55380800	-0.61393900	-1.59281200
C	-0.36705700	0.86412300	1.95340700
N	-2.29486100	-0.21135000	-0.58657500

C	-1.88502500	-1.38251000	-0.08096600
O	-1.19442100	1.91869900	-1.45136700
H	-4.29856600	-1.60515200	-1.95111200
C	0.41854100	-0.73364600	-0.52506800
C	-0.50274700	-1.62971300	0.00149600
O	0.84019900	1.03727000	2.57201800
H	0.19941100	1.16847100	4.55866000
H	-2.01152700	2.04452100	-1.95754000
H	1.92392300	0.79352800	4.26192100
C	0.90057800	0.60504500	3.93664100
H	-0.17823000	-2.45476100	0.62556800
H	0.09456300	-0.12521500	-1.36390500
H	0.66776400	-0.45953500	4.02374800
H	-7.10202100	1.65521900	-1.64947700
H	0.57354700	1.73771700	0.20138200
C	-2.82663600	-2.39073700	0.48862700
C	-2.69338600	-3.74125700	0.13191700
C	-3.81666500	-2.02708100	1.41576000
C	-3.53872800	-4.70721400	0.68021500
H	-1.93145400	-4.02940200	-0.58637200
C	-4.65426300	-2.99402600	1.96759700
H	-3.90604000	-0.99089600	1.72211200
C	-4.52181100	-4.33608300	1.59879100
H	-3.42892800	-5.74741800	0.38818900
H	-5.40783400	-2.70119300	2.69271700
H	-5.17920500	-5.08650300	2.02769400
C	1.86980600	-0.82730400	-0.33675400
C	2.45216100	-1.52113500	0.74138900
C	2.72218500	-0.20134300	-1.26604800
C	3.83619500	-1.60336700	0.86885900
H	1.81796200	-1.98650400	1.48889600
C	4.10695700	-0.28294700	-1.13736700
H	2.28710900	0.34629800	-2.09780500
C	4.66932300	-0.98717100	-0.06997800
H	4.26808300	-2.14318200	1.70635800
H	4.74691600	0.20189700	-1.86849300
H	5.74830500	-1.05077600	0.03405000

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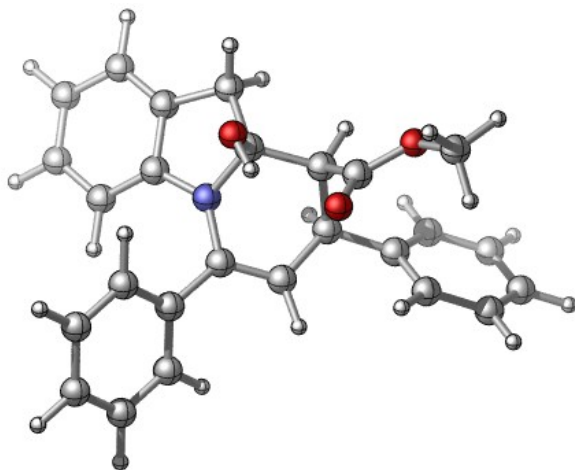


Zero-point correction= 0.324352 (Hartree/Particle)
 Thermal correction to Energy= 0.343213
 Thermal correction to Enthalpy= 0.344157
 Thermal correction to Gibbs Free Energy= 0.277926
 Sum of electronic and zero-point Energies= -900.832355
 Sum of electronic and thermal Energies= -900.813495
 Sum of electronic and thermal Enthalpies= -900.812551
 Sum of electronic and thermal Free Energies= -900.878782

H	-5.35549400	3.48399900	-0.52860800
H	-2.86039000	3.08921000	0.67956500
C	-5.33988600	2.40010100	-0.60806300
C	-6.50591800	1.70192200	-0.94221400
C	-2.80463300	2.30682700	-0.08460400
C	-4.15709300	1.70499400	-0.37905300
H	-2.38287900	2.74663400	-0.99128300
H	0.25279600	1.03054200	0.80575800
O	-0.64167400	1.89199100	-2.25147400
C	-6.47222100	0.30972500	-1.05954200
C	-4.13144300	0.30323500	-0.47328900
H	-7.37235400	-0.23275800	-1.33419900
C	-1.85432400	1.23288600	0.43203100
C	-0.48269900	1.12976800	0.01543600
C	-5.29185300	-0.39944400	-0.82953600
C	0.00387200	1.70808600	-1.22178600
N	-2.85134300	-0.23047300	-0.30214200
C	-2.53833300	-1.38987400	0.29480400
O	-2.05302700	1.04718500	1.78430700
H	-5.26821100	-1.47848800	-0.93349100
C	-0.34272600	-1.10070200	-0.69893000
C	-1.19027900	-1.77523100	0.18474300
O	1.33413100	1.99433100	-1.14186700
H	1.44140000	3.47846900	-2.61003500
H	-1.38979300	0.42588100	2.12038400
H	1.84097400	1.83713000	-3.16584600
C	1.92393100	2.53809100	-2.33192400
H	-0.80329100	-2.53226700	0.85835700

H	-0.82476100	-0.65259600	-1.56249600
H	2.97230000	2.70990700	-2.08864900
H	-7.43173200	2.24191300	-1.11512700
C	-3.46233100	-2.17907700	1.15767800
C	-3.49645300	-3.57789700	1.04497800
C	-4.26851700	-1.55402600	2.12389900
C	-4.32602500	-4.33623100	1.87206500
H	-2.88021500	-4.06680400	0.29617800
C	-5.08931500	-2.31447900	2.95424100
H	-4.22624600	-0.47592000	2.23358200
C	-5.12462000	-3.70638600	2.82834600
H	-4.34872600	-5.41694700	1.76803500
H	-5.69991500	-1.82091200	3.70454700
H	-5.76951100	-4.29542700	3.47363000
C	1.08948400	-1.40073600	-0.83122300
C	1.71755600	-1.22287600	-2.07752900
C	1.86011100	-1.87891600	0.24516500
C	3.06572600	-1.53187100	-2.24946500
H	1.13503200	-0.85144600	-2.91604300
C	3.20823200	-2.18259500	0.07417900
H	1.40305000	-1.99881300	1.22277100
C	3.81555200	-2.01348200	-1.17408200
H	3.53059900	-1.39677800	-3.22142800
H	3.78896800	-2.54799900	0.91587300
H	4.86687600	-2.25140200	-1.30499100

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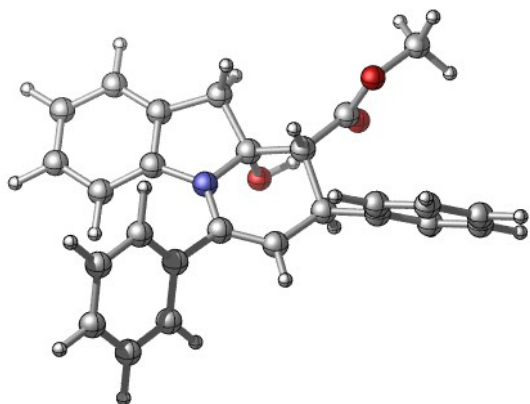
<i>Zero-point correction=</i>	<i>0.328840 (Hartree/Particle)</i>
<i>Thermal correction to Energy=</i>	<i>0.346836</i>
<i>Thermal correction to Enthalpy=</i>	<i>0.347780</i>
<i>Thermal correction to Gibbs Free Energy=</i>	<i>0.283329</i>
<i>Sum of electronic and zero-point Energies=</i>	<i>-900.896765</i>
<i>Sum of electronic and thermal Energies=</i>	<i>-900.878769</i>

Sum of electronic and thermal Enthalpies= -900.877825
Sum of electronic and thermal Free Energies= -900.942276

H	-4.44529100	3.62422700	-1.18486200
H	-2.24607200	2.95406900	0.70035600
C	-4.60445200	2.55271800	-1.09599000
C	-5.77703600	1.96595900	-1.59550600
C	-2.27183900	2.09399100	0.02723300
C	-3.64470700	1.75106900	-0.49738600
H	-1.58321700	2.29480900	-0.80237200
O	-0.01307800	-0.41669100	2.87794200
C	-5.95511800	0.58444700	-1.50190500
C	-3.84373300	0.36250300	-0.38323600
H	-6.85760500	0.13016800	-1.90128300
C	-1.84603300	0.82378500	0.80217800
C	-0.33350600	0.42792800	0.61730300
C	-4.99486600	-0.23859300	-0.90001100
C	0.39226800	0.25416100	1.93949500
N	-2.73873100	-0.22247100	0.24303800
C	-2.44948000	-1.58137200	0.46222500
O	-2.17782400	1.06488500	2.16065900
H	-5.14768700	-1.30893300	-0.83885400
C	-0.20810800	-0.89056200	-0.24665600
C	-1.16110300	-1.93577100	0.27919900
O	1.56272600	0.90157500	1.95262700
H	1.80551500	1.06576400	4.02335900
H	-1.80248200	0.33811300	2.68857600
H	3.23990200	1.37047700	2.98969500
C	2.36437600	0.74220800	3.14352800
H	-0.80709100	-2.92213600	0.55204900
H	-0.57442100	-0.57999400	-1.23539800
H	2.65821600	-0.30264600	3.26135100
H	-6.53837400	2.58382200	-2.06122900
H	0.17582200	1.22794700	0.07647200
C	-3.49926200	-2.48792600	0.98554200
C	-3.54928600	-3.83438700	0.59070900
C	-4.43655100	-2.02016300	1.92263500
C	-4.50340400	-4.69633000	1.13123700
H	-2.84617000	-4.19694700	-0.15307200
C	-5.39002700	-2.88308100	2.45955200
H	-4.39687800	-0.98114300	2.23484600
C	-5.42695500	-4.22387500	2.06664500
H	-4.53206800	-5.73461200	0.81393900
H	-6.10364800	-2.50977100	3.18822200
H	-6.17365600	-4.89375600	2.48247900
C	1.22866400	-1.35691200	-0.41667800

C	1.96180100	-0.94909000	-1.53934600
C	1.85939900	-2.18080100	0.52785700
C	3.28721300	-1.34870100	-1.71673600
H	1.48685500	-0.31660600	-2.28535200
C	3.18461200	-2.58380000	0.35253000
H	1.31554400	-2.50738800	1.40916900
C	3.90357700	-2.16926500	-0.77016700
H	3.83471800	-1.02413100	-2.59681700
H	3.65325400	-3.22495300	1.09351300
H	4.93314300	-2.48587400	-0.90792700

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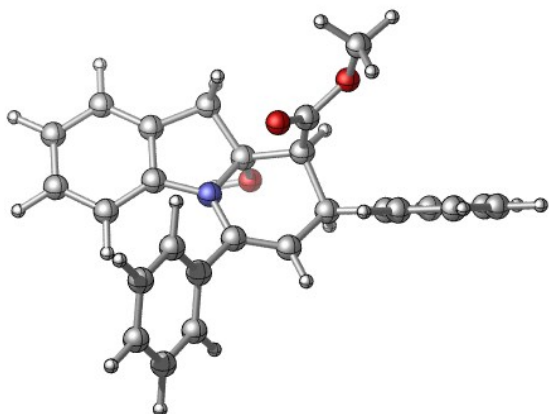


Zero-point correction=	0.329600 (Hartree/Particle)
Thermal correction to Energy=	0.347607
Thermal correction to Enthalpy=	0.348551
Thermal correction to Gibbs Free Energy=	0.283832
Sum of electronic and zero-point Energies=	-900.907546
Sum of electronic and thermal Energies=	-900.889540
Sum of electronic and thermal Enthalpies=	-900.888596
Sum of electronic and thermal Free Energies=	-900.953315

H	-2.49174600	3.35969900	-0.03665100
C	-2.70730900	2.29896000	0.05918800
C	-4.02886900	1.85239700	0.20790200
C	-1.67756900	1.37233700	0.03048500
H	1.76355500	-0.17185000	0.98126700
O	2.74607600	0.95496200	-1.92060500
C	-4.29011700	0.48575400	0.30609400
C	-1.94542800	-0.00554400	0.14917100
H	-5.31520200	0.13883700	0.40038000
C	0.27328400	0.15379900	-0.55647200
C	1.69222900	-0.25434900	-0.10582500
C	-3.25968600	-0.46330000	0.26975600
C	2.72892100	0.65437900	-0.73355800
N	-0.72931800	-0.71766600	0.06554000

C	-0.42869200	-2.05841000	0.31871600
O	0.14178800	-0.00790600	-1.96675600
H	-3.49082400	-1.51820100	0.32020900
C	1.93388000	-1.74366100	-0.52120700
C	0.79453500	-2.56221900	0.03461500
O	3.63884800	1.08118700	0.14504400
H	4.28170900	2.80974100	-0.84223600
H	0.93843000	0.39819900	-2.35867200
H	5.27118400	1.35441200	-1.13080300
C	4.69777200	1.90965500	-0.38626000
H	0.99064100	-3.59532900	0.29534200
H	1.91193200	-1.76391300	-1.61875200
H	5.32220400	2.16379300	0.46820300
H	-4.84513000	2.56750100	0.23321300
C	-0.18931100	1.56785800	-0.12713000
H	0.27497600	1.85935200	0.82402000
H	0.08310000	2.30838900	-0.88257900
C	-1.42473800	-2.91023600	1.03154100
C	-1.87772800	-2.56050400	2.31430100
C	-1.86453000	-4.11290600	0.46168900
C	-2.75302400	-3.39516400	3.00677300
H	-1.53731200	-1.63509800	2.76869800
C	-2.74235300	-4.94803100	1.15668500
H	-1.52043100	-4.38594800	-0.53097900
C	-3.18985500	-4.59102300	2.42942300
H	-3.09101400	-3.11484900	4.00008000
H	-3.07746100	-5.87488900	0.70056700
H	-3.87347400	-5.23921700	2.96953400
C	3.29972500	-2.24444700	-0.07353400
C	4.33972100	-2.38073300	-1.00226200
C	3.55569800	-2.55849600	1.26933900
C	5.60555600	-2.81536800	-0.60206700
H	4.15520600	-2.14785500	-2.04794700
C	4.81844800	-2.99305500	1.67238200
H	2.75677200	-2.46821000	2.00033200
C	5.84888800	-3.12229900	0.73738500
H	6.39763300	-2.91839500	-1.33817600
H	4.99775600	-3.23354500	2.71640700
H	6.83118800	-3.46350200	1.05060600

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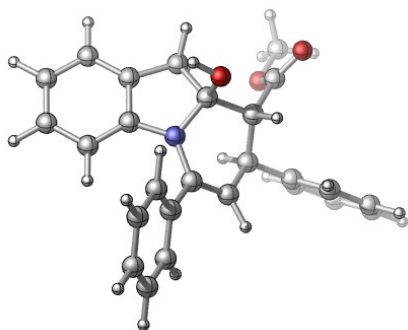


Zero-point correction= 0.329521 (Hartree/Particle)
 Thermal correction to Energy= 0.347535
 Thermal correction to Enthalpy= 0.348479
 Thermal correction to Gibbs Free Energy= 0.282321
 Sum of electronic and zero-point Energies= -900.902438
 Sum of electronic and thermal Energies= -900.884424
 Sum of electronic and thermal Enthalpies= -900.883480
 Sum of electronic and thermal Free Energies= -900.949639

H	-5.27974700	2.98401600	0.13034600
H	-2.66808200	1.54208200	1.44057300
C	-5.15875200	2.01488000	-0.34601400
C	-6.22967600	1.41727800	-1.02584700
C	-2.63970700	1.75948100	0.36700000
C	-3.93989600	1.35677800	-0.28798200
H	-2.37230500	2.81052000	0.23628900
O	-1.45942400	-0.82860100	2.15089200
C	-6.04998500	0.18104600	-1.64793700
C	-3.76735400	0.09991900	-0.90386000
H	-6.87439400	-0.27302400	-2.19035700
C	-1.61987600	0.85159300	-0.35869300
C	-0.34279100	0.46594700	0.40552100
C	-4.82163700	-0.49061000	-1.60772800
C	-0.61827900	-0.01539500	1.81957700
N	-2.43420500	-0.32204000	-0.72646100
C	-1.82869400	-1.55720300	-0.96830100
O	-1.12384600	1.49852900	-1.53304700
H	-4.70175400	-1.43451000	-2.12118600
C	0.44234600	-0.59576000	-0.44881500
C	-0.48999300	-1.70522000	-0.86011500
O	0.21899500	0.57784100	2.69341200
H	0.32521000	-0.91333600	4.15164200
H	-1.88463800	1.72432000	-2.08872100
H	-0.91235500	0.33625900	4.43579700
C	0.09783400	0.15134000	4.06472100

H	-0.07776200	-2.69658900	-1.00467400
H	0.76206100	-0.03501500	-1.33621100
H	0.82425500	0.74266700	4.62008500
H	-7.19027000	1.92000600	-1.07733100
H	0.27138900	1.36519200	0.47681500
C	-2.68754500	-2.75430800	-1.19810800
C	-3.58953000	-3.17629000	-0.20748400
C	-2.55519600	-3.51650100	-2.36647800
C	-4.34629500	-4.33240700	-0.38922200
H	-3.68159400	-2.59966300	0.70766400
C	-3.31496600	-4.67490100	-2.54690800
H	-1.85918500	-3.19396400	-3.13475800
C	-4.21379100	-5.08396000	-1.56080000
H	-5.03598100	-4.65155300	0.38674700
H	-3.20486600	-5.25414800	-3.45899500
H	-4.80606000	-5.98329700	-1.70126300
C	1.70307400	-1.08610300	0.25086200
C	2.92590000	-0.44424100	0.01263300
C	1.67769500	-2.16023200	1.15267800
C	4.09216800	-0.85807400	0.65807700
H	2.96396800	0.38541800	-0.68930200
C	2.84252900	-2.57740700	1.79959200
H	0.73956300	-2.67096300	1.34857200
C	4.05409200	-1.92763700	1.55506100
H	5.03028900	-0.34928800	0.45559000
H	2.80303800	-3.41333700	2.49224500
H	4.96100900	-2.25477300	2.05503800

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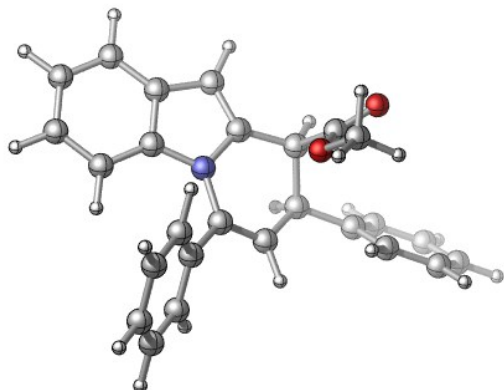


Zero-point correction=	0.328359 (Hartree/Particle)
Thermal correction to Energy=	0.346649
Thermal correction to Enthalpy=	0.347593
Thermal correction to Gibbs Free Energy=	0.282262
Sum of electronic and zero-point Energies=	-900.895122
Sum of electronic and thermal Energies=	-900.876832
Sum of electronic and thermal Enthalpies=	-900.875888
Sum of electronic and thermal Free Energies=	-900.941219

H	-4.71833900	2.95745200	-2.36427700
H	-2.36430500	3.00734000	-0.56851800
C	-4.80660300	1.95987400	-1.94217300
C	-5.95906300	1.19285400	-2.16725700
C	-2.39341600	1.96414900	-0.89473600
C	-3.77189400	1.42526200	-1.18908900
H	-1.76273500	1.87933300	-1.78581300
H	-0.08182800	0.60859100	1.29054300
O	1.01323300	2.66831500	0.34489100
C	-6.04239100	-0.10116000	-1.64970500
C	-3.87697600	0.13268300	-0.64312500
H	-6.92922500	-0.69961500	-1.83835400
C	-1.87312300	1.03888200	0.23722300
C	-0.35685300	0.67076600	0.23531800
C	-5.00768300	-0.65272900	-0.88367200
C	0.50415500	1.79559300	-0.32780800
N	-2.72029400	-0.16638900	0.09239900
C	-2.27417400	-1.42441700	0.54333000
O	-2.08285100	1.63528500	1.51703200
H	-5.09067700	-1.65826900	-0.49146600
C	-0.10158300	-0.72566700	-0.40955100
C	-0.97695900	-1.71826100	0.32780200
O	0.63941400	1.72053800	-1.66732200
H	2.46416300	2.71723600	-1.86938200
H	-2.99852700	1.95087100	1.54858500
H	1.01762300	3.73267200	-2.09204100
C	1.45086400	2.74716700	-2.27451500
H	-0.53364300	-2.61034100	0.75495900
H	-0.42606400	-0.66902600	-1.45726900
H	1.45725300	2.52271200	-3.33988800
H	-6.77796400	1.60037900	-2.75160900
C	-3.20040800	-2.29139800	1.31195800
C	-4.10166100	-1.72587900	2.22963800
C	-3.16383300	-3.68799800	1.17231300
C	-4.93497300	-2.53805400	2.99642800
H	-4.12640200	-0.64698500	2.34681200
C	-3.99778400	-4.49917600	1.94192000
H	-2.48989800	-4.13237500	0.44621000
C	-4.88621500	-3.92776800	2.85575500
H	-5.62069100	-2.08660700	3.70743700
H	-3.96073700	-5.57772900	1.81993600
H	-5.53937900	-4.55975000	3.44999900
C	1.37074100	-1.10779000	-0.38667100
C	2.08758900	-1.25735100	-1.58049600
C	2.04186600	-1.32233800	0.82669200

C	3.43810000	-1.61183100	-1.56657000
H	1.58285100	-1.09368000	-2.52849200
C	3.39205600	-1.67439700	0.84473500
H	1.50486200	-1.21869200	1.76589400
C	4.09542900	-1.82091000	-0.35306400
H	3.97474000	-1.72529100	-2.50412900
H	3.89359400	-1.83574600	1.79454700
H	5.14577000	-2.09653700	-0.33999300

3-cis

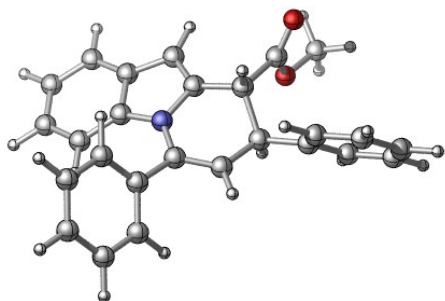


Zero-point correction=	0.301391 (Hartree/Particle)
Thermal correction to Energy=	0.318014
Thermal correction to Enthalpy=	0.318958
Thermal correction to Gibbs Free Energy=	0.257253
Sum of electronic and zero-point Energies=	-824.529104
Sum of electronic and thermal Energies=	-824.512480
Sum of electronic and thermal Enthalpies=	-824.511536
Sum of electronic and thermal Free Energies=	-824.573242

H	-4.87153800	3.38562800	-1.80283300
C	-4.95848400	2.34681300	-1.49724800
C	-6.15555900	1.65805600	-1.64960700
C	-2.48603100	2.06155600	-0.72687300
C	-3.85043300	1.67628800	-0.95439400
O	0.81002000	1.99732600	1.88377600
C	-6.25602200	0.30382300	-1.27809800
C	-3.97646100	0.31617400	-0.55313700
H	-7.19531700	-0.22157300	-1.42300000
C	-1.83464000	0.97779100	-0.20939200
C	-0.38855300	0.79501200	0.15323000
C	-5.17590800	-0.38546300	-0.73281700
C	-0.07714500	1.22203900	1.59003200
N	-2.72918100	-0.09056400	-0.06340300
C	-2.30316400	-1.35801100	0.40579700
H	-5.27011300	-1.42985000	-0.46737100

C	0.03630800	-0.68323300	-0.17862900
C	-0.98983400	-1.64880000	0.36574100
O	-0.89764500	0.65394600	2.49228800
H	-0.80175800	2.10604200	3.99270400
H	0.33500800	0.74757800	4.17941900
C	-0.67271200	1.02906400	3.86708300
H	-0.65331600	-2.58698900	0.79014200
H	0.00358800	-0.72906500	-1.27689600
H	-1.41848700	0.48415900	4.44364600
H	-7.02037300	2.16300200	-2.06958800
H	-2.03768700	3.02202600	-0.94028200
H	0.21308000	1.46669900	-0.46231000
C	-3.28903000	-2.26410600	1.04709300
C	-4.15374100	-1.78956300	2.04834800
C	-3.31818000	-3.62709200	0.71602600
C	-5.02324400	-2.66091300	2.70139800
H	-4.13370100	-0.73819000	2.31742600
C	-4.18940000	-4.49773200	1.37241100
H	-2.66306200	-3.99760800	-0.06629900
C	-5.04488600	-4.01765600	2.36557600
H	-5.68178700	-2.28151300	3.47709000
H	-4.20401100	-5.54921500	1.10146300
H	-5.72567700	-4.69414700	2.87344300
C	1.46447400	-0.99400300	0.24184800
C	2.51102400	-0.83092600	-0.67580200
C	1.77498700	-1.42108300	1.54113300
C	3.83294300	-1.08638600	-0.30890700
H	2.28693600	-0.50559200	-1.68874900
C	3.09625000	-1.67851400	1.91095300
H	0.97897200	-1.55527100	2.26764700
C	4.12981100	-1.51214800	0.98737700
H	4.62876700	-0.95812400	-1.03677500
H	3.31664500	-2.01091800	2.92121300
H	5.15723700	-1.71541800	1.27427800

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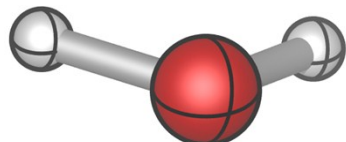
Zero-point correction= 0.301283 (Hartree/Particle)

Thermal correction to Energy=	0.318051
Thermal correction to Enthalpy=	0.318995
Thermal correction to Gibbs Free Energy=	0.256737
Sum of electronic and zero-point Energies=	-824.529761
Sum of electronic and thermal Energies=	-824.512993
Sum of electronic and thermal Enthalpies=	-824.512048
Sum of electronic and thermal Free Energies=	-824.574307

H	-4.87229500	3.20855700	-1.96445000
C	-4.94910500	2.18373500	-1.61251200
C	-6.14641000	1.48526300	-1.71138800
C	-2.46206900	1.94228500	-0.87512900
C	-3.82854800	1.54080400	-1.06259900
H	-0.24584200	0.82685200	1.14797400
O	1.09931300	2.63033200	0.04323100
C	-6.23511700	0.14838800	-1.27950300
C	-3.94263900	0.19978400	-0.60065800
H	-7.17510700	-0.38543700	-1.38300000
C	-1.79605300	0.88415000	-0.32584100
C	-0.35654500	0.69119700	0.06535900
C	-5.14195200	-0.51313800	-0.72550000
C	0.54384200	1.74290100	-0.57067800
N	-2.68423800	-0.18005300	-0.11720200
C	-2.24103200	-1.41969400	0.40661600
H	-5.22609900	-1.54518700	-0.41247200
C	0.08005600	-0.77085300	-0.28715400
C	-0.92796000	-1.71232200	0.33386700
O	0.65748100	1.56868000	-1.89953000
H	2.52282500	2.46311100	-2.19657900
H	1.11958800	3.52788200	-2.46334800
C	1.50406000	2.51329300	-2.58612500
H	-0.57200900	-2.62550100	0.79598000
H	0.03387000	-0.85819200	-1.38069500
H	1.47955000	2.21947500	-3.63425600
H	-7.02097100	1.96912900	-2.13597600
H	-2.02925600	2.89785700	-1.13569000
C	-3.20614800	-2.29667100	1.11729500
C	-4.06610800	-1.77502100	2.09892900
C	-3.21984800	-3.67763300	0.86894500
C	-4.91335000	-2.61774600	2.81579500
H	-4.06222900	-0.70904600	2.30352100
C	-4.06913500	-4.51923300	1.58858400
H	-2.57066300	-4.08556800	0.10047000
C	-4.91828200	-3.99246400	2.56332500

H	-5.56770800	-2.20120900	3.57573300
H	-4.07169500	-5.58513600	1.38114700
H	-5.58172900	-4.64676500	3.12074600
C	1.50911800	-1.05381100	0.14890600
C	2.53569900	-1.13944800	-0.80033900
C	1.83450700	-1.21099500	1.50451500
C	3.85485000	-1.37717700	-0.40800200
H	2.29882600	-1.02068800	-1.85402600
C	3.15149000	-1.44769600	1.89938000
H	1.05159700	-1.15350000	2.25603100
C	4.16678600	-1.53181000	0.94346800
H	4.63634100	-1.44432400	-1.15930600
H	3.38426500	-1.56829500	2.95337800
H	5.19166100	-1.71833600	1.25023000

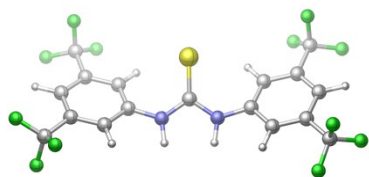
H₂O



Zero-point correction=	0.021335 (Hartree/Particle)
Thermal correction to Energy=	0.024170
Thermal correction to Enthalpy=	0.025114
Thermal correction to Gibbs Free Energy=	0.003020
Sum of electronic and zero-point Energies=	-76.403924
Sum of electronic and thermal Energies=	-76.401089
Sum of electronic and thermal Enthalpies=	-76.400145
Sum of electronic and thermal Free Energies=	-76.422239

O	-0.18806000	-0.46052300	0.00000000
H	0.77650600	-0.40771200	0.00000000
H	-0.46026300	0.46635200	0.00000000

Figure 2
cat A

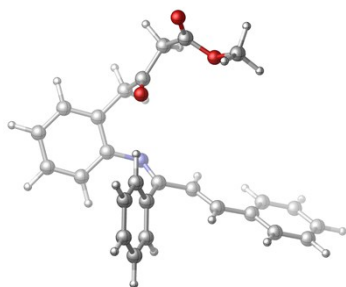


Zero-point correction= 0.240926 (Hartree/Particle)
 Thermal correction to Energy= 0.269474
 Thermal correction to Enthalpy= 0.270418
 Thermal correction to Gibbs Free Energy= 0.173558
 Sum of electronic and zero-point Energies= -2358.237816
 Sum of electronic and thermal Energies= -2358.209268
 Sum of electronic and thermal Enthalpies= -2358.208324
 Sum of electronic and thermal Free Energies= -2358.305184

C	-0.70321600	-2.77177200	12.30979500
S	-1.83455800	-2.73909300	13.55424600
N	-0.48380800	-1.72828800	11.44632100
H	0.07542400	-1.92215900	10.62407600
N	0.08848000	-3.85009200	12.00888800
H	0.63179500	-3.78924600	11.15588000
C	-1.08972600	-0.44957200	11.43435900
C	-1.48161900	0.07609200	10.19999300
C	-1.23090100	0.32062800	12.59460700
C	-2.01859400	1.36218800	10.12799100
H	-1.37737700	-0.52042600	9.29997600
C	-1.78643200	1.59548500	12.50680800
H	-0.90431600	-0.06852800	13.54829800
C	-2.18389600	2.12849100	11.27927600
H	-2.60758500	3.12321800	11.22193300
C	0.14118600	-5.12511800	12.61867400
C	0.32330100	-6.23177900	11.78127200
C	0.10466200	-5.30498400	14.00579400
C	0.45905100	-7.50678700	12.32747600
H	0.36322500	-6.09743400	10.70569900
C	0.22330500	-6.59073600	14.53344300
H	-0.00394000	-4.45327600	14.66126300
C	0.40158500	-7.69976100	13.70707000
H	0.51142000	-8.69021800	14.13055600
C	0.60673500	-8.69534800	11.41432300
C	0.12408600	-6.78223900	16.02490200

C	-2.37405800	1.93788400	8.78262800
C	-1.99504500	2.39888100	13.76431200
F	-0.59299700	-9.24518000	11.11336100
F	1.35355800	-9.66924700	11.97771000
F	1.19002300	-8.36091300	10.24192600
F	-1.89113400	3.72619500	13.53275600
F	-3.22310300	2.18795400	14.29227300
F	-1.09577600	2.08131300	14.72046000
F	-1.29821200	2.50141100	8.18322000
F	-2.83764600	0.98966500	7.93822000
F	-3.31904200	2.89650700	8.87741400
F	-1.16117400	-6.93262500	16.42112800
F	0.79335700	-7.88117300	16.43638400
F	0.62227900	-5.72537300	16.70282800

B'''

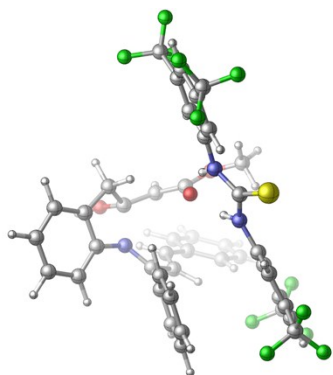


Zero-point correction=	0.426219 (Hartree/Particle)
Thermal correction to Energy=	0.453440
Thermal correction to Enthalpy=	0.454384
Thermal correction to Gibbs Free Energy=	0.362871
Sum of electronic and zero-point Energies=	-1284.654887
Sum of electronic and thermal Energies=	-1284.627666
Sum of electronic and thermal Enthalpies=	-1284.626722
Sum of electronic and thermal Free Energies=	-1284.718235

H	3.74480800	4.84655500	-0.70686500
H	2.99354900	4.53207500	0.87733200
O	1.19829500	5.58271900	-0.80865400
C	3.27971400	4.08509700	-0.07709000
H	3.96213300	3.25145000	0.08119200
O	-0.74451500	3.17935500	0.57423900
H	0.14217800	-1.74663600	-0.03310100
C	1.14348800	4.39132600	-1.03135300
O	2.12624700	3.52299200	-0.73394900
C	0.16628000	-1.48691300	1.02187100

C	1.17848100	-1.90092100	1.81444300
H	-3.77813100	-0.72687500	2.11625400
C	-0.95155100	-0.62961400	1.43028800
N	-1.70329100	-0.20105000	0.46606200
C	-3.91527600	0.15186300	1.49572100
C	-0.91778100	2.99498800	-0.61569100
C	-0.03353600	3.67980100	-1.66293100
C	-2.87604800	0.55014700	0.63416900
C	-5.11339800	0.85976900	1.54017900
H	-5.90526200	0.53152600	2.20733600
C	-3.07260400	1.66670900	-0.21227400
C	-5.29698700	1.98169100	0.72898800
H	0.30748200	2.93501000	-2.38948600
H	-0.64211000	4.41461500	-2.19945600
C	-1.99938400	2.08376200	-1.18404400
C	-4.27711600	2.37265200	-0.13886800
H	-4.42013500	3.23558100	-0.78449300
H	-2.43364300	2.57577200	-2.06214000
H	-1.46937700	1.19396700	-1.55256700
H	-6.22852600	2.53820300	0.76160300
H	1.17973300	-1.58748800	2.85553100
C	-1.11734800	-0.27721500	2.88058700
C	-1.11416700	1.06754000	3.28275400
C	-1.26997100	-1.28096000	3.84971900
C	-1.25710000	1.39629000	4.63062900
H	-1.00010700	1.84840100	2.53749200
C	-1.42902800	-0.94640300	5.19547700
H	-1.27622700	-2.32373700	3.54718500
C	-1.41843100	0.39289400	5.58937600
H	-1.24474300	2.43949600	4.93252700
H	-1.55765200	-1.73212700	5.93401400
H	-1.53486400	0.65349400	6.63718400
C	2.31664800	-2.73516500	1.42119100
C	3.32318300	-2.98988000	2.37227800
C	2.45804300	-3.30048100	0.13755300
C	4.43256900	-3.77192600	2.05597400
H	3.22883500	-2.56449200	3.36786000
C	3.56507700	-4.08199900	-0.17733900
H	1.69623400	-3.13208900	-0.61675000
C	4.55827300	-4.32112900	0.77883100
H	5.19682500	-3.95306100	2.80581700
H	3.65508200	-4.50944000	-1.17158900
H	5.42017900	-4.93224500	0.52862300

trans-endo-cat

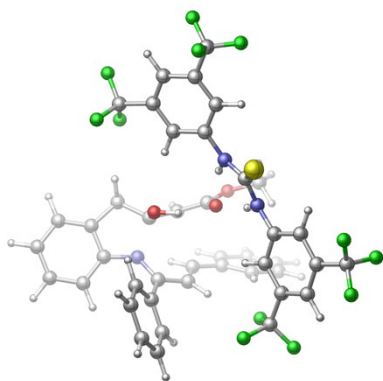


Zero-point correction=	0.669723 (Hartree/Particle)		
Thermal correction to Energy=	0.725301		
Thermal correction to Enthalpy=	0.726245		
Thermal correction to Gibbs Free Energy=	0.568636		
Sum of electronic and zero-point Energies=	-3642.865627		
Sum of electronic and thermal Energies=	-3642.810048		
Sum of electronic and thermal Enthalpies=	-3642.809104		
Sum of electronic and thermal Free Energies=	-3642.966713		
C	-3.85689800	-1.12935100	4.71800400
S	-4.63919300	-1.82252700	6.04318400
N	-4.39972600	-0.18583100	3.88222200
H	-3.74078400	0.21824300	3.21045100
N	-2.56121900	-1.39292200	4.35535400
H	-2.17952200	-0.78197400	3.62559100
C	-5.66784900	0.41928600	3.86227000
C	-5.74409500	1.68056800	3.24784700
C	-6.84295700	-0.17256400	4.34494200
C	-6.96458700	2.33909500	3.13480600
H	-4.84389500	2.14783600	2.86362300
C	-8.05513900	0.51069800	4.23285100
H	-6.80775500	-1.15128500	4.79923100
C	-8.13462500	1.76644200	3.63455700
H	-9.08209700	2.28381100	3.55569700
C	-1.63997500	-2.33180300	4.84739800
C	-0.28432100	-2.00680600	4.70434600
C	-1.98674100	-3.58442700	5.37341800
C	0.70528200	-2.91537600	5.07329500
H	-0.00565300	-1.04055700	4.29889400
C	-0.98225300	-4.47440000	5.75024700
H	-3.02602300	-3.85713800	5.48073200
C	0.36966400	-4.15712000	5.60823900
H	1.13815200	-4.85842600	5.90704700

C	2.14246800	-2.55412400	4.82015300
C	-1.36740500	-5.85069900	6.22480600
C	-7.02837300	3.66012500	2.41584400
C	-9.29380200	-0.11606600	4.81834900
F	2.39494600	-1.25319100	5.10312000
F	2.47208100	-2.72428700	3.50960300
F	2.99957100	-3.30216900	5.53961700
F	-9.39452500	0.12429900	6.14706700
F	-10.42093600	0.36193000	4.24658100
F	-9.30002100	-1.45877600	4.66431300
F	-8.02224000	4.44336000	2.88822500
F	-5.87421700	4.35433600	2.52963700
F	-7.25586900	3.49613200	1.09022700
F	-1.45538900	-6.72303700	5.18816900
F	-0.45891800	-6.36134000	7.08482600
F	-2.56561500	-5.86060500	6.84489200
H	-5.19631100	-0.20067900	-2.55886300
H	-3.50182700	0.56361400	0.25677200
C	-4.36157200	-0.88282400	-2.42605100
C	-4.33404400	-2.11008100	-3.09537200
C	-3.08687900	0.68256900	-0.74785900
C	-3.30930500	-0.54719600	-1.57906900
H	-3.48983500	1.59788000	-1.18959000
O	-2.11844000	0.46935600	2.24500900
C	-3.24780600	-2.97820300	-2.93237000
C	-2.22790700	-1.42565300	-1.41613400
H	-3.22657400	-3.92111000	-3.47020100
C	-1.54916300	0.82062100	-0.62928400
C	-0.99654400	1.57947200	0.47533700
C	-2.17783700	-2.64446000	-2.10116100
C	-1.38843400	1.40100200	1.81090100
N	-1.21273400	-0.85555000	-0.61627100
C	-0.45294300	-1.52714500	0.26269200
O	-0.97519000	1.29958200	-1.80581400
H	-1.32881400	-3.30961900	-1.99399700
C	1.25778300	0.22253300	0.25933000
C	0.72560900	-0.93702600	0.77843900
O	-0.86297800	2.33667000	2.65429300
H	-0.84576300	1.31579900	4.48553900
H	-1.39343600	0.85741300	-2.56025600
H	-2.28966000	2.31301400	4.18802900
C	-1.20867500	2.24534100	4.03843600
H	1.15652100	-1.39880200	1.65894400
H	0.93486600	0.52567000	-0.73100500

H	-0.71972500	3.09274000	4.51907000
H	-5.15344200	-2.38708900	-3.75111000
H	-0.36209200	2.41752900	0.22611800
C	2.38359800	0.97383700	0.80248500
C	2.93846800	2.00596100	0.01846600
C	2.94739900	0.71802400	2.06977300
C	4.02161100	2.75098000	0.47584600
H	2.50868900	2.21697100	-0.95683700
C	4.03165500	1.46210100	2.52325300
H	2.54339300	-0.06292400	2.70362400
C	4.57263700	2.48020100	1.73071100
H	4.43547800	3.54068600	-0.14347200
H	4.45552200	1.25099200	3.50022700
H	5.41682400	3.05972100	2.09169000
C	-0.85070400	-2.86472500	0.78121000
C	0.12510400	-3.85996600	0.95429900
C	-2.17497000	-3.13721200	1.16653500
C	-0.21399400	-5.09809900	1.49996100
H	1.14886400	-3.66350500	0.65155900
C	-2.50796600	-4.37147900	1.71805200
H	-2.93368100	-2.36985200	1.06199500
C	-1.52969200	-5.35598700	1.88811700
H	0.55104800	-5.85820200	1.62492000
H	-3.53066100	-4.56163900	2.02879100
H	-1.78931100	-6.31015100	2.33546100

cis-endo-cat



Zero-point correction= 0.670204 (Hartree/Particle)
 Thermal correction to Energy= 0.725556
 Thermal correction to Enthalpy= 0.726501
 Thermal correction to Gibbs Free Energy= 0.567961
 Sum of electronic and zero-point Energies= -3642.871064

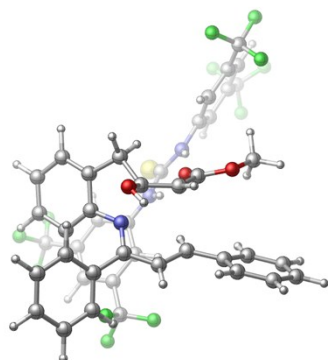
Sum of electronic and thermal Energies= -3642.815712
Sum of electronic and thermal Enthalpies= -3642.814768
Sum of electronic and thermal Free Energies= -3642.973308

H	-4.48060200	2.09276600	-2.56614500
H	-2.68929900	2.16290100	-0.31492400
C	-4.41159100	1.02238200	-2.39289200
C	-5.29520100	0.14395500	-3.03022300
C	-2.34440600	1.25698400	-0.82019500
C	-3.44059300	0.51560300	-1.53724700
H	-1.55612900	1.54952200	-1.52375300
O	-0.41117900	0.10295900	2.82194400
C	-5.18256800	-1.23370900	-2.81952200
C	-3.35024000	-0.86547800	-1.30632300
H	-5.85747600	-1.91501700	-3.32912000
C	-1.77323500	0.30433800	0.24108600
C	-0.32253000	0.37199100	0.46641500
C	-4.21062800	-1.75448900	-1.96281900
C	0.22560900	0.40273200	1.76383200
N	-2.25510800	-1.18303900	-0.48633200
C	-2.10089700	-2.30650000	0.25454100
O	-2.55500800	0.36758800	1.38504400
H	-4.12403300	-2.82453100	-1.81561000
C	0.29063100	-1.99977400	0.00856900
C	-0.78576100	-2.62914200	0.62769800
O	1.52637600	0.75564400	1.82094900
H	1.66857200	1.48527300	3.77874600
H	-1.97518200	0.09945600	2.13683000
H	3.18361600	1.05755800	2.93452500
C	2.15042900	0.76311600	3.11494600
H	-0.63452200	-3.33376900	1.43704900
H	0.09140800	-1.56179500	-0.96303700
H	2.12005500	-0.22929000	3.56987800
H	-6.06185500	0.53170000	-3.69364100
H	0.30018600	0.72126400	-0.34573400
C	-1.65788300	0.66689100	5.96912700
S	-2.56658400	0.78523800	7.38293500
N	-1.57167000	1.64503800	5.01083800
H	-1.13625000	1.35144400	4.13498500
N	-0.92322200	-0.42914600	5.59312000
H	-0.52991700	-0.37848200	4.65185400
C	-2.23902500	2.88336100	4.92524200
C	-2.70640300	3.26144500	3.66000200
C	-2.37708300	3.76319600	6.00546800

C	-3.30422700	4.50729400	3.47853900
H	-2.60820000	2.57600100	2.82387100
C	-2.99437600	4.99833800	5.80748200
H	-1.99714200	3.49047100	6.97940000
C	-3.46059400	5.38514800	4.55011200
H	-3.92087000	6.35446400	4.40697300
C	-0.90009600	-1.73157100	6.12641700
C	-0.82227300	-2.77724000	5.19629600
C	-0.88768600	-2.02639500	7.49512400
C	-0.73936100	-4.09879200	5.62618300
H	-0.83706400	-2.54577800	4.13678100
C	-0.81637500	-3.35822800	7.90676500
H	-0.93773500	-1.22844300	8.22153300
C	-0.74188300	-4.40461400	6.98687400
H	-0.68570700	-5.43216200	7.32284200
C	-0.72568000	-5.20024000	4.60136500
C	-0.73765000	-3.66314400	9.38022300
C	-3.83801200	4.86973800	2.11838700
C	-3.18926200	5.91812100	6.98432800
F	-1.97181200	-5.51975000	4.18516100
F	-0.16234700	-6.32978900	5.07418400
F	-0.03112500	-4.84129300	3.48701400
F	-3.20919100	7.21692000	6.61017300
F	-4.36085400	5.67540900	7.61808100
F	-2.21020900	5.77664800	7.90464000
F	-3.04993500	4.38830100	1.12536500
F	-5.07454500	4.36070800	1.91166900
F	-3.92734600	6.20561600	1.94790300
F	0.54210300	-3.63847600	9.82495900
F	-1.42531400	-2.76720900	10.11962800
F	-1.22711800	-4.88955600	9.66774900
C	1.69712100	-2.18595100	0.34803100
C	2.67562700	-1.76273900	-0.57348300
C	2.12239100	-2.78418400	1.55217300
C	4.03084000	-1.93926200	-0.31034100
H	2.36080500	-1.29620800	-1.50280400
C	3.47812700	-2.96066000	1.81247400
H	1.39576900	-3.11906500	2.28389600
C	4.43627400	-2.53931800	0.88458600
H	4.76999900	-1.61054600	-1.03418100
H	3.79088400	-3.42753400	2.74135200
H	5.49266300	-2.67823800	1.09318000
C	-3.23376000	-3.10822600	0.77664800
C	-3.12713100	-4.50699300	0.85845600

C	-4.39469400	-2.48078400	1.26394700
C	-4.16106600	-5.26377200	1.40805200
H	-2.23837700	-4.99888200	0.47519100
C	-5.42120100	-3.24026300	1.81889200
H	-4.46497100	-1.39914900	1.23328300
C	-5.31028400	-4.63252100	1.88834100
H	-4.06976600	-6.34428800	1.45941200
H	-6.30742500	-2.74573100	2.20473900
H	-6.11509900	-5.22121200	2.31805900

trans-exo-cat



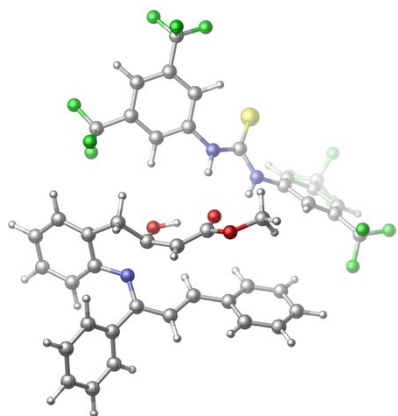
Zero-point correction=	0.669018 (Hartree/Particle)
Thermal correction to Energy=	0.724910
Thermal correction to Enthalpy=	0.725854
Thermal correction to Gibbs Free Energy=	0.565986
Sum of electronic and zero-point Energies=	-3642.860449
Sum of electronic and thermal Energies=	-3642.804557
Sum of electronic and thermal Enthalpies=	-3642.803612
Sum of electronic and thermal Free Energies=	-3642.963481

H	-4.57993400	3.44485600	-0.42419800
H	-3.18765700	1.51313000	1.24418000
C	-4.56479700	2.60194600	-1.10976900
C	-5.37583100	2.60396200	-2.24883400
C	-2.73776800	1.36034400	0.25846800
C	-3.73144400	1.51549000	-0.86057300
H	-1.92063700	2.07599300	0.14611100
O	0.11403100	1.44387100	-0.94441500
C	-5.33370100	1.52606700	-3.13997500
C	-3.71345500	0.42655100	-1.74215100
H	-5.93233700	1.55040300	-4.04481900
C	-2.18008900	-0.07079900	0.24110400

C	-0.75884700	-0.30680700	0.41652000
C	-4.50585000	0.42955500	-2.89831500
C	0.24931700	0.57821500	-0.05074800
N	-2.74911900	-0.53109700	-1.39380600
C	-2.84169000	-1.85729500	-1.60531500
O	-2.96231100	-0.85768200	1.07653300
H	-4.45064700	-0.39012700	-3.60474300
C	-0.41632500	-1.95086200	-1.45679200
C	-1.64875200	-2.59314100	-1.45764200
O	1.45001700	0.35577400	0.54346300
H	-2.54736300	-1.72827400	1.16839400
H	-1.71748800	-3.66326300	-1.29443800
H	-0.38325700	-0.98037200	-1.93958500
H	-6.02822400	3.44828000	-2.44845600
H	-0.46752200	-0.99824000	1.19787100
C	0.04414400	3.80495200	-3.45278600
S	0.04567800	4.98078100	-4.66485900
N	-0.62790900	2.61225800	-3.53858000
H	-0.48137400	1.95724800	-2.76914300
N	0.70697900	3.89826500	-2.25905900
H	0.56383900	3.11118500	-1.62006700
C	-1.43562200	2.11641900	-4.58306000
C	-1.33457100	0.75250300	-4.88017700
C	-2.37429300	2.90128900	-5.26520300
C	-2.15828100	0.18218800	-5.85010700
H	-0.60590800	0.14063100	-4.36074200
C	-3.17602000	2.31824800	-6.24496500
H	-2.47615200	3.95027800	-5.02928400
C	-3.07759100	0.96004200	-6.55040100
H	-3.70343200	0.51953000	-7.31662300
C	1.52762000	4.90261200	-1.71932000
C	1.62732100	4.92095600	-0.32031800
C	2.29041300	5.81222600	-2.46644500
C	2.48503300	5.81295400	0.31832700
H	1.03091200	4.22956600	0.26609600
C	3.12170000	6.71683100	-1.80576200
H	2.23662400	5.80380800	-3.54470000
C	3.23741700	6.72752000	-0.41514200
H	3.90138400	7.42272700	0.08147200
C	2.60331800	5.73242100	1.81586100
C	3.88460800	7.73021600	-2.61882000
C	-2.09908100	-1.30106500	-6.08897100
C	-4.23638000	3.14366300	-6.92445300
F	1.39351400	5.79552400	2.41799500

F	3.36386200	6.71989000	2.32830400
F	3.16075300	4.55544700	2.20063700
F	-3.93467200	4.45812000	-6.93357400
F	-4.42684000	2.75913000	-8.20619200
F	-5.43658300	3.02010700	-6.30145600
F	-2.45243100	-1.62944300	-7.34878100
F	-0.86745300	-1.80658000	-5.86400600
F	-2.94870000	-1.96777500	-5.26001600
F	3.15216700	8.84872100	-2.83415500
F	5.02131700	8.12056100	-2.00001600
F	4.22959300	7.24936200	-3.83321100
C	0.86671900	-2.60914900	-1.22278100
C	2.03845600	-2.03213300	-1.74963700
C	0.97719300	-3.81323300	-0.49905700
C	3.27658300	-2.64674500	-1.57849700
H	1.96692700	-1.10333400	-2.30835500
C	2.21532300	-4.42330000	-0.32457800
H	0.09186700	-4.26194200	-0.05969600
C	3.36837100	-3.84440400	-0.86557700
H	4.16826000	-2.19294700	-1.99977400
H	2.28527600	-5.34925300	0.23789200
H	4.33292400	-4.32321500	-0.72728600
C	2.56144600	1.16691800	0.13658300
H	2.53373000	2.13716300	0.64159300
H	3.45407600	0.62333800	0.44584200
H	2.56669000	1.31839900	-0.94400500
C	-4.12244600	-2.57472900	-1.83413000
C	-4.18548600	-3.60889800	-2.78184300
C	-5.26209800	-2.27841700	-1.06631600
C	-5.36711600	-4.32672300	-2.96553200
H	-3.31481200	-3.82599100	-3.39191000
C	-6.43658200	-3.00507500	-1.24545600
H	-5.20870300	-1.49953600	-0.31361000
C	-6.49415300	-4.02750400	-2.19751100
H	-5.40777200	-5.11680400	-3.70915000
H	-7.30766600	-2.77727500	-0.63859700
H	-7.41346900	-4.58782400	-2.33866500

cis-exo-cat



Zero-point correction= 0.670754 (Hartree/Particle)
 Thermal correction to Energy= 0.725623
 Thermal correction to Enthalpy= 0.726567
 Thermal correction to Gibbs Free Energy= 0.571456
 Sum of electronic and zero-point Energies= -3642.870578
 Sum of electronic and thermal Energies= -3642.815709
 Sum of electronic and thermal Enthalpies= -3642.814765
 Sum of electronic and thermal Free Energies= -3642.969875

H	-4.41505500	0.29518400	-1.88557800
C	-3.90864500	-0.61279600	-1.57623100
C	-4.54566200	-1.85566900	-1.66809600
C	-2.60837900	-0.55869400	-1.08814500
H	0.68347000	0.96114200	0.69644600
O	2.13324500	1.24355500	-2.26768900
C	-3.87471200	-3.02570100	-1.29532700
C	-1.94658200	-1.73400200	-0.71586400
H	-4.37321800	-3.98576500	-1.38775400
C	-0.26128400	-0.00852200	-1.02837400
C	0.82096200	0.71377700	-0.34847700
C	-2.56083300	-2.98274600	-0.82279800
C	1.84665100	1.37918000	-1.03240100
N	-0.60251100	-1.46348600	-0.35296800
C	0.06150300	-2.08557600	0.64263500
O	-0.01581300	-0.26525400	-2.37671800
H	-2.03476900	-3.89244200	-0.55693800
C	2.23176700	-1.44845900	-0.27528700
C	1.46114200	-1.97744300	0.74334000
O	2.58182800	2.20389800	-0.24527700
H	3.39277400	3.47410600	-1.69960300
H	0.85671400	0.14451300	-2.59038300
H	4.45952600	2.14502400	-1.15519100

C	3.70071100	2.86800400	-0.84376100
H	1.91085400	-2.24265000	1.69324000
H	1.80886600	-1.45149100	-1.27443800
H	4.10717700	3.51272600	-0.06471900
H	-5.56355300	-1.91378200	-2.04089800
C	-1.68286000	0.60376800	-0.87471600
H	-1.79252600	1.01278700	0.13670700
H	-1.81177800	1.41882800	-1.58772500
C	2.61166400	2.66286100	-5.37896900
S	2.78875900	3.28890400	-6.93748300
N	1.46006300	2.72440700	-4.64266800
H	1.47710800	2.21938400	-3.75244900
N	3.60885700	2.02881900	-4.68228500
H	3.39078700	1.77920700	-3.71554300
C	0.20193600	3.25640600	-4.99508500
C	-0.93245300	2.54227500	-4.59178500
C	0.04809600	4.47881900	-5.66363100
C	-2.20661100	3.04339500	-4.86622600
H	-0.81746000	1.59296200	-4.07711300
C	-1.23162400	4.95254100	-5.94384300
H	0.91797200	5.04405700	-5.96369600
C	-2.36953000	4.24407200	-5.55192700
H	-3.35946200	4.61740600	-5.78237000
C	4.91585000	1.70882400	-5.10799500
C	5.95528700	1.84493700	-4.18036800
C	5.19606900	1.19629700	-6.38153900
C	7.25672100	1.47652700	-4.52298900
H	5.74957600	2.25043300	-3.19695900
C	6.50578700	0.85448300	-6.71518000
H	4.39864500	1.06040700	-7.09723700
C	7.54673800	0.98801600	-5.79554100
H	8.55898300	0.71154100	-6.06329500
C	8.34782600	1.55441700	-3.48969300
C	6.80933000	0.36629500	-8.10768400
C	-3.40890300	2.27818600	-4.38418500
C	-1.40338700	6.28691800	-6.62114800
F	8.11233000	2.51446200	-2.57054600
F	9.55302500	1.80279400	-4.04248800
F	8.47016300	0.38367700	-2.80561800
F	-0.30344000	6.65748100	-7.30860000
F	-2.44129200	6.27583000	-7.48820700
F	-1.65903400	7.27017600	-5.72412200
F	-4.53729700	2.63071100	-5.03137500
F	-3.25197100	0.94469800	-4.52892300

F	-3.63420300	2.49455700	-3.05752700
F	5.74651100	-0.24573800	-8.67280700
F	7.15921400	1.38503900	-8.92766300
F	7.83654300	-0.51280000	-8.11755300
C	3.65990700	-1.17220400	-0.20341400
C	4.38933400	-1.07689800	-1.40555600
C	4.34384300	-0.99284600	1.01691900
C	5.75907200	-0.82841500	-1.39000400
H	3.87117800	-1.20434700	-2.35070400
C	5.71110000	-0.73774000	1.02926500
H	3.79691000	-1.03213200	1.95346200
C	6.42277500	-0.65396600	-0.17320500
H	6.31189800	-0.76423600	-2.31994600
H	6.22408200	-0.59455100	1.97526400
H	7.48812800	-0.44538100	-0.16590700
C	-0.66305200	-2.81299900	1.71995800
C	-0.16868700	-4.04432000	2.17966500
C	-1.79365900	-2.25782000	2.34414000
C	-0.79571100	-4.71110600	3.23224300
H	0.69940400	-4.48393300	1.69823900
C	-2.40986600	-2.92009500	3.40250700
H	-2.17844300	-1.29942600	2.01197400
C	-1.91661700	-4.15055100	3.84676500
H	-0.40867700	-5.66753000	3.56996500
H	-3.27430800	-2.47402800	3.88460800
H	-2.40347300	-4.66712500	4.66827400