Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Electronic Supplementary Information

Exploring the Catalytic Role of TBD in Carboxylative Cyclizations

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A. General Information

Materials.

All reagents and solvents were purchased from Sigma Aldrich and Alfa Aesar and used as received, without further purification unless otherwise noted.

Kinetics study details and methods.

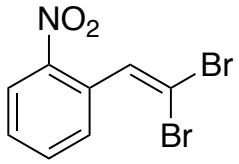
For the collection of the kinetics data, the TBD catalyzed carboxylative cyclization reaction of **1** was performed in an experimental apparatus designed to deliver constant CO_2 pressure. The ^{1}H and ^{13}C NMR spectra of the product (**2**) obtained in this experiment are consistent with those reported in the literature.[1] To monitor the progress of the reaction a chromatographic method was developed using supercritical fluid chromatography-ultra-high-pressure liquid chromatography (SFC-UHPLC). Separation was performed on a 1260 Infinity II HPLC (Agilent, Santa Clara, USA) using a 150 x 4.6 mm Zorbax RX-SIL column (Agilent, Santa Clara, USA). Samples were eluted using a gradient elution method with CO_2 and iPrOH and analyzed for absorbance at 254 nm using a diode array detector (DAD). The mobile phase was pumped for 10 minutes with 95:5 CO_2:iPrOH, and then for 20 minutes with 85:15 CO_2:iPrOH at 0.5 mL/min. HPLC-grade isopropanol was purchased from Sigma-Aldrich (St. Louis, USA) and used as obtained. Naphthalene was used as an internal standard and was recrystallized from ethanol prior to use. A standard curve was created to ensure the response factor of **1** was linear within experimentally relevant concentrations (Figure S1). From the ratio of integrated peak areas of naphthalene and **1**, and the known starting concentration of **1**, the concentration of **1** was calculated for all samples. Kinetics data for the reaction performed in diglyme was averaged based on the results of 2 runs for the experiments at 10 and 20 mol % catalyst loading and 3 runs for the experiments at 40 mol % catalyst loading. Kinetics data was also collected for a single run of the reaction performed in the literature reaction solvent (MeCN) at 40 mol % catalyst loading (Table S8 and Figure S2). In this experiment, similar conversion and rates were observed compared to the reaction performed with the same catalyst loading in diglyme.

Computational details and methods.

All calculations were conducted using Gaussian 09 software.[2] Solvation was included in all calculations using the integral equation formalism variant of the polarizable continuum model (IEFPCM) with acetonitrile as the solvent.[3] All structures were optimized at the M06-2X/def2TZVP level.[4,5] Vibrational analysis was performed at 373.15 K on all optimized geometries, ensuring intermediates and transition states contained zero and one imaginary frequencies, respectively. To estimate the basis set superposition error, counterpoise corrections were performed on the IEFPCM-M06-2X/def2TZVP optimized geometries. All structures were visualized using CYLview 1.0,[6] with the exception of the NCI plot (Figure S3), which was calculated using NCIPlot and visualized using VMD.[7,8]

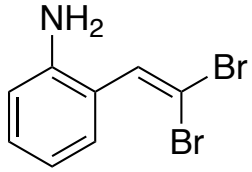
B. Synthetic Procedures

Procedure for the synthesis of o-nitro-gem-dibromovinylbenzene.



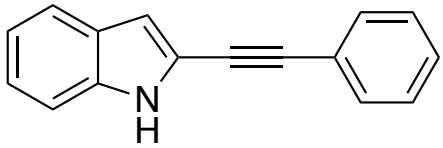
To a solution of ortho-nitrobenzaldehyde (1.51 g, 10 mmol) and carbon tetrabromide (4.98 g, 15 mmol) in 50 mL DCM, is slowly added a solution of triphenylphosphine (7.87 g, 30 mmol) in 40 mL DCM at 0 °C. The mixture is allowed to stir at 0 °C for 30 minutes and then at room temperature for 60 minutes. The mixture is filtered through a silica plug which is washed with a small portion of DCM and then concentrated *in vacuo*. The crude residue is used without further purification. The ^{1}H and ^{13}C NMR spectra are consistent with those reported in the literature.[9]

Procedure for the synthesis of o-gem-dibromovinylaniline.



The crude residue from the synthesis of o-nitro-gem-dibromovinylbenzene is dissolved in a solution of 21 mL anhydrous ethanol and 3.5 mL glacial acetic acid. To the solution is added iron powder (4.0 g, 70 mmol) and iron (III) chloride (0.25 g, 1.5 mmol), and the mixture is refluxed. The progress of the reaction is monitored by TLC (7:1 hexanes:EtOAc). Upon complete conversion of starting material the reaction is filtered through a silica plug which is washed with a small amount of methanol and concentrated *in vacuo*. The crude residue is purified by flash column chromatography (7:1 hexanes:EtOAc) to give the product (1.76 g, 6.35 mmol) as a brown oil in a 63.5% yield over two steps. The ^{1}H and ^{13}C NMR spectra are consistent with those reported in the literature.[9]

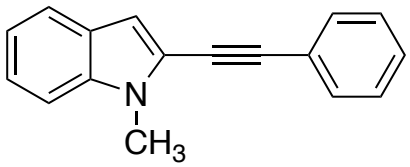
Procedure for the synthesis of 2-phenylethynylindole (1).



To a 100 mL round-bottom flask is added 10 % w/w Pd/C (0.358 g, 0.32 mmol), triphenylphosphine (0.2g, 0.76 mmol), and a stir bar. The flask is equipped with a septum and is purged with argon for 10 minutes. To a second 100 mL pear-shaped flask is added o-gem-dibromovinylaniline (1.76 g, 6.36 mmol) and copper (I) iodide (35 mg, 0.18 mmol), and a stir bar. The flask is equipped with a septum and purged with argon for 10 minutes. After purging, a solution of phenylacetylene (1.04 mL, 9.4 mmol) and diisopropylamine (2.21 mL, 15.6 mmol) in 60 mL dry toluene is added to the flask containing vinylaniline and cuprous iodide via syringe. This mixture is stirred until homogeneity is obtained, and then cannulated to the first flask containing Pd/C and triphenylphosphine. The resulting mixture is heated at 100 °C for 2 hours. The mixture is then diluted with 100 mL Et_2O, filtered, washed with 70 mL H_2O and 50 mL brine, and dried with anhydrous $MgSO_4$. The solvent is concentrated *in vacuo* an the crude residue is purified by flash column chromatography with gradient elution (19:1 to 9:1 hexanes:EtOAc) affording the product

2-phenylethynylindole (0.963g, 4.44 mmol) as a pale-yellow solid in a 67.0% yield. The ^{1}H and ^{13}C NMR spectra are consistent with those reported in the literature.[10]

Procedure for the synthesis of 1-methyl-2-phenylethynylindole (1a).



To a solution of 2-phenylethynylindole (14.5 mg, 0.067 mmol) in 1 mL dry DMF is added 60% w/w NaH in oil (6.0 mg, 0.15 mmol) with stirring. The solution rapidly turns from a straw-yellow colour to a deep red. Upon cessation of gas evolution, methyl iodide (5 μL, 0.080 mmol) is added and the mixture is stirred for 2 hours. The mixture is diluted with 10 mL Et_2O, washed with three portions of sat. $LiCl_{(aq)}$ solution, and dried over anhydrous $MgSO_4$. The solvent in concentrated *in vacuo* and the crude product is purified by flash column chromatography (9:1 v/v hexanes:EtOAc) affording the product 1-methyl-2-phenylethynylindole (13.8 mg, 0.0597 mmol) as a pale-yellow solid in an 89.5% yield. The ^{1}H and ^{13}C NMR spectra are consistent with those reported in the literature.[11]

C. Standard Curve for the Response Factor of 1

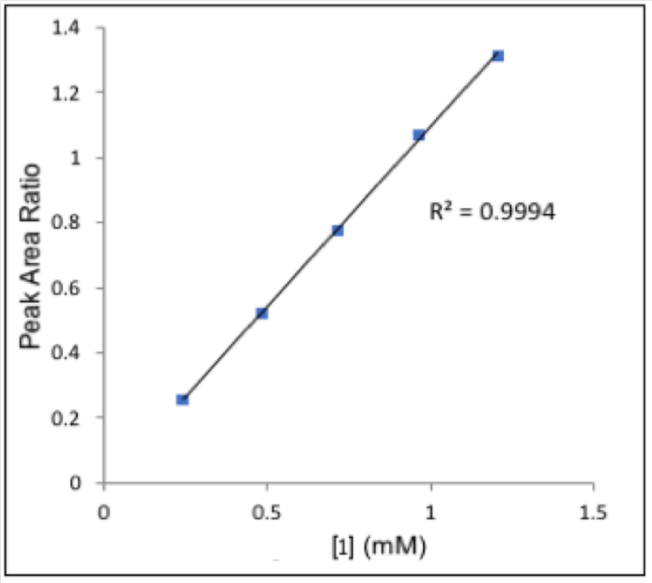


Figure S1. Standard curve showing change in the integrated peak area ratio of naphthalene to **1** as a function of varying **1** concentration.

D. Kinetics Data for the Carboxylative Cyclization Reaction of 1

Table S1. Raw kinetics data for 40 mol% TBD loading in diglyme, run number 1.

Time (h)	Naphthalene Area	**1** Area	**2** Area	Peak Ratio (**1**/Naphthalene)	**1** Concentration (M)
0	6749.1	8516.7	0	1.2619016	0.1815
1	15769.3	17244.5	5055.4	1.0935489	0.1572857
2	9940.4	9383.6	5161.7	0.9439862	0.1357740
3	11028.2	9244.5	7515.5	0.8382601	0.1205674
4	9177.1	7000.0	7104.9	0.7627682	0.1097094
6	12408.6	8179.8	11800.1	0.6592041	0.0948137
8	11064.2	6278.5	11758.1	0.5674608	0.0816182
10	13235.2	6678.5	15752.4	0.5046014	0.0725771
12	15098.3	6714.1	19484.1	0.4446924	0.0639604

Table S2. Raw kinetics data for 40 mol% TBD loading in diglyme, run number 2.

Time (h)	Naphthalene Area	**1** Area	**2** Area	Peak Ratio (**1**/Naphthalene)	**1** Concentration (M)
0	8594.2	13089.7	0	1.5230853	0.1821
1	14997.8	17605.5	5637.2	1.1738722	0.1403481
2	7392.1	7370.7	4100.9	0.9971050	0.1192138
3	10228.4	9366.7	7277.4	0.9157542	0.1094875
4	11040.8	9280.6	9143.9	0.8405731	0.1004989
6	11890.6	8739.2	12023.8	0.7349671	0.0878726
8	13020.9	8330.7	14999.2	0.6397945	0.0764938
10	12336.8	6682.3	15771.3	0.5416559	0.0647603
12	9157.1	4763.9	13078.3	0.5202411	0.0622000

Table S3. Raw kinetics data for 40 mol% TBD loading in diglyme, run number 3.

Time (h)	Naphthalene Area	**1** Area	**2** Area	Peak Ratio (**1**/Naphthalene)	**1** Concentration (M)
0	6937.4	9761.2	0	1.4070401	0.1820
1	13026.2	14536.5	5548.6	1.1159433	0.1443468
2	13091.9	12436.1	8964.5	0.9499080	0.1228702
3	12747.2	10653.1	10836.6	0.8357208	0.1081001
4	15035.4	11400.4	14646.3	0.7582372	0.0980776
6	13571.1	8486.1	15871.6	0.6253067	0.0808831
8	12532.5	6605.4	16631.3	0.5270616	0.0681752
10	15520.3	6785.7	22351.3	0.4372145	0.0565535
12	20304.6	7702.1	32241.3	0.3793278	0.0490659

Table S4. Raw kinetics data for 20 mol% TBD loading in diglyme, run number 1.

Time (h)	Naphthalene Area	**1** Area	**2** Area	Peak Ratio (**1**/Naphthalene)	**1** Concentration (M)
0	5368.4	7642.4	0	1.4235899	0.1818
1	2407.1	2932.2	447.2	1.2181463	0.1555638
2	3799.0	4361.6	1261.5	1.1480916	0.1466174
3	5383.2	5866.4	2387.1	1.0897607	0.1391682
4	4124.6	4200.5	2140.1	1.0184018	0.1300553
6	4410.2	4071.4	2890.0	0.9231781	0.1178948
8	4522.3	3901.1	3460.2	0.8626363	0.1101632
10	6033.4	4979.0	5179.4	0.8252395	0.1053875
12	6331.2	4876.5	5843.5	0.7702331	0.0983629

Table S5. Raw kinetics data for 20 mol% TBD loading in diglyme, run number 2.

Time (h)	Naphthalene Area	**1** Area	**2** Area	Peak Ratio (**1**/Naphthalene)	**1** Concentration (M)
0	2981.0	4330.8	0	1.4528011	0.1819
1	3323.7	4314.1	562.1	1.2979812	0.1625156
2	4192.8	5119.2	1252.5	1.2209502	0.1528708
3	5337.1	6155.0	2147.8	1.1532480	0.1443940
4	4943.2	5350.7	2362.7	1.0824365	0.1355280
6	3952.2	3766.3	2321.7	0.9529629	0.1193171
8	7321.7	6479.7	5335.2	0.8849994	0.1108076
10	4123.8	3185.4	3152.5	0.7724429	0.0967148
12	5792.5	4388.9	5172.8	0.7576867	0.0948672

Table S6. Raw kinetics data for 10 mol% TBD loading in diglyme, run number 1.

Time (h)	Naphthalene Area	**1** Area	**2** Area	Peak Ratio (**1**/Naphthalene)	**1** Concentration (M)
0	3112.1	4346.2	0	1.3965490	0.1817
1	3957.3	5168.7	202.6	1.3061178	0.1699343
2	4812.0	6183.2	459.9	1.2849543	0.1671808
3	5100.6	6495.2	678.2	1.2734188	0.1656800
4	5252.3	6376.6	850.5	1.2140586	0.1579568
6	4601.0	5399.3	968.5	1.1735058	0.1526806
8	7485.6	8468.3	1883.8	1.1312787	0.1471866
10	5589.1	6172.1	1562.1	1.1043102	0.1436779
12	5308.0	5684.1	1658.6	1.0708553	0.1393252

Table S7. Raw kinetics data for 10 mol% TBD loading in diglyme, run number 2.

Time (h)	Naphthalene Area	**1** Area	**2** Area	Peak Ratio (**1**/Naphthalene)	**1** Concentration (M)
0	4416.1	6295.6	0	1.4256018	0.1817
1	9865.7	12459.6	417.8	1.2629210	0.1609655
2	9679.3	12238.2	825.6	1.2643683	0.1611500
3	12917.1	16289.8	1628.9	1.2611035	0.1607339
4	9528.2	11464.5	1406.4	1.2032178	0.1533561
6	11456.7	13680.7	2296.9	1.1941222	0.1521968
8	12351.0	14353.6	2918.2	1.1621407	0.1481206
10	10467.2	11792.5	2729.0	1.1266146	0.1435926
12	10241.3	11442.7	2962.6	1.1173093	0.1424066

Table S8. Raw kinetics data for 40 mol% TBD loading in acetonitrile.

Time (h)	Naphthalene Area	**1** Area	**2** Area	Peak Ratio (**1**/Naphthalene)	**1** Concentration (M)
0	1638.5	16043.0	0	9.7912725	0.1814
1	2667.5	17078.3	5723.5	6.4023618	0.1186147
2	1852.8	10444.2	5247.4	5.6369819	0.1044347
3	1986.4	10385.8	6743.1	5.2284535	0.0968660
4	4519.6	22587.7	18304.2	4.9977210	0.0925913
5	3429.7	16110.6	15194.7	4.6973788	0.0870269
6	4620.3	20772.2	22414.9	4.4958552	0.0832934
8	3625.5	14506.0	19688.4	4.0011033	0.0741273
10	3701.2	12963.9	21284.0	3.5026208	0.0648920
12	11418.1	34938.0	58724.7	3.0598786	0.0566895

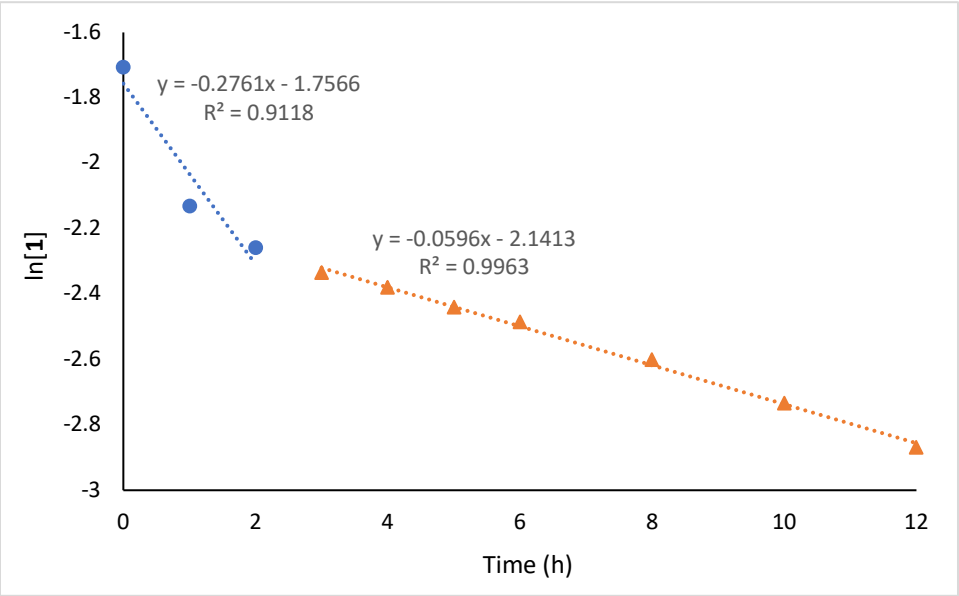
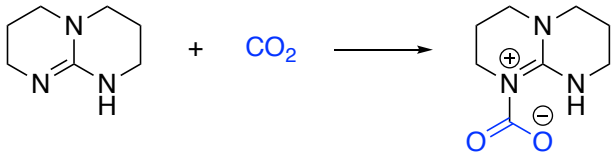


Figure S2. Kinetic profile of TBD catalyzed carboxylative cyclization of **1** in MeCN at 40 mol % catalyst loading. Data separated at the time of one catalyst turnover.

E. Computed Thermal Stability of the TBD:CO_2 Adduct

Table S9. Computational energy values for the thermal stability of the TBD:CO_2 adduct in various solvents.



Solvent	Temperature (K)	ΔG (kcal/mol)
MeCN	298.15	-5.1
MeCN	373.15	-1.8
Et_2O	298.15	-2.2
Et_2O	373.15	0.6

Although diglyme was used for kinetic experiments, Et_2O was chosen for computational modelling as it is a similar solvent available in the Gaussian package, being both aprotic and having a dielectric constant similar to that of diglyme.[12]

F. Non-covalent Interactions of Int3

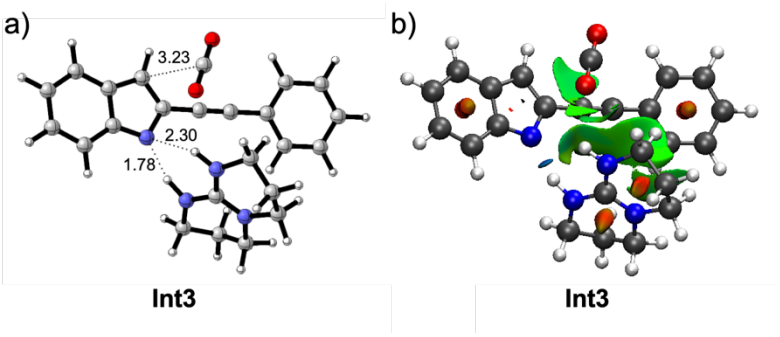
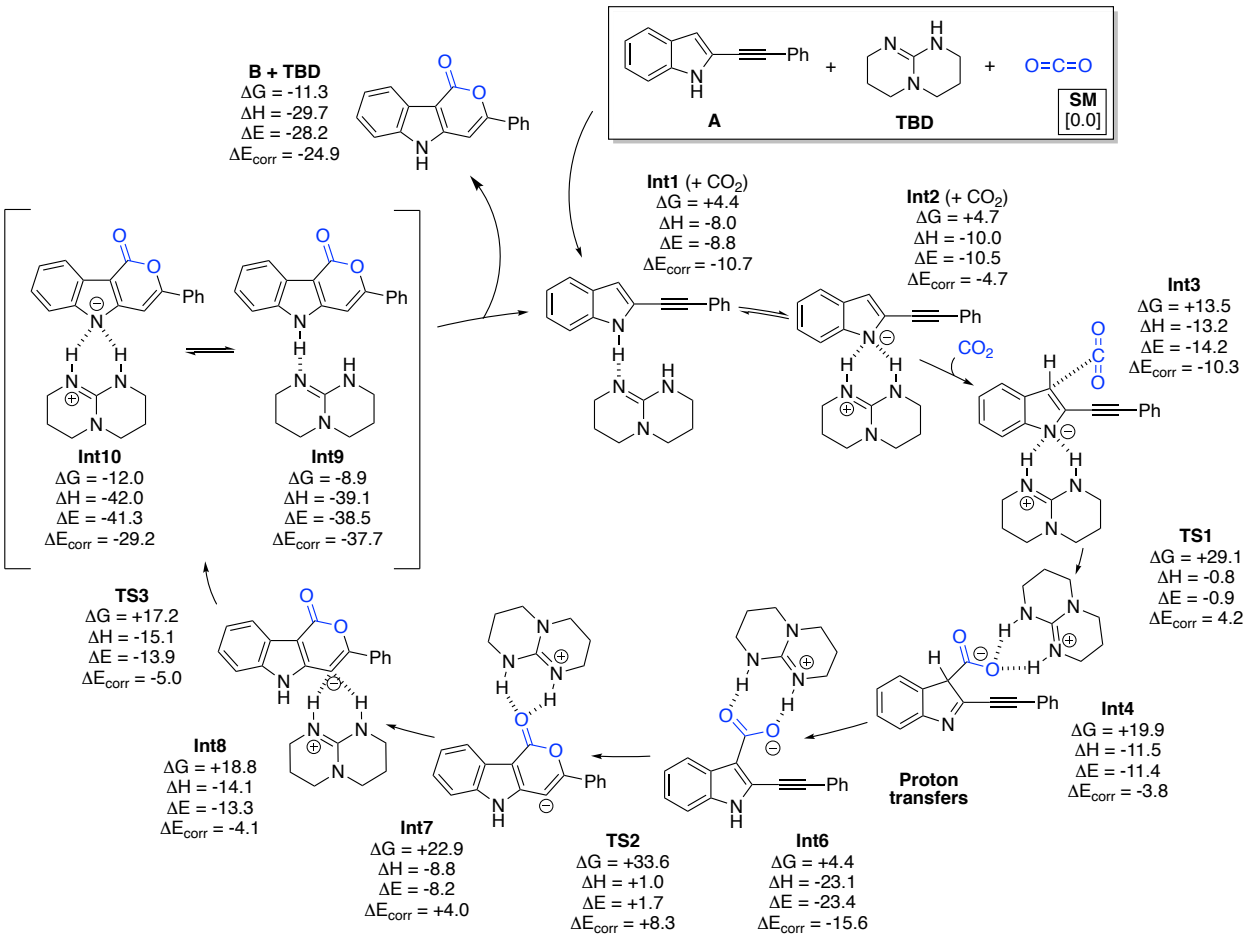


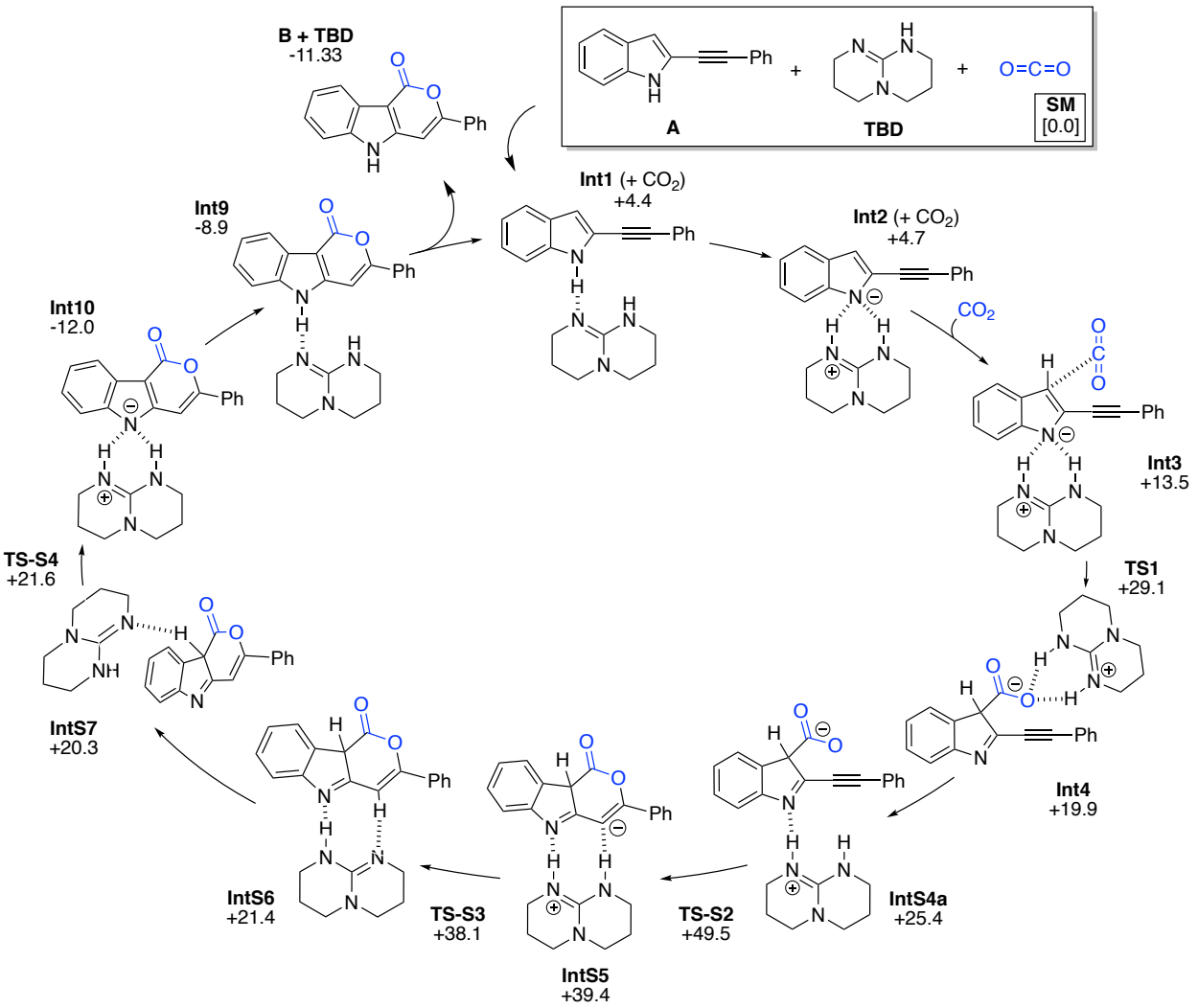
Figure S3: (a) Geometry of **Int3** (b) Non-covalent interactions of **Int3** (attractive, blue > green; repulsive, yellow < red).

In **Int3**, $TBDH^+$ preferentially orients CO_2 above the indole-3 position, stabilizing the complex though non-covalent interactions with both the substrate and the protonated catalyst (Figure S3). A non-covalent interaction (NCI) plot was generated for **Int3** which shows favourable interactions (green) between $TBDH^+$ and CO_2 as well as what is likely a $\pi \rightarrow \pi^*$ interaction between the π systems of the indole ring and CO_2.[7,8] The plot also shows strongly favourable interactions between the $TBDH^+$ and indole anion (blue-green), as well as a π-stacking interaction between the $TBDH^+$ and the phenyl ring of the substrate (green).

G. Computed Catalytic Cycles

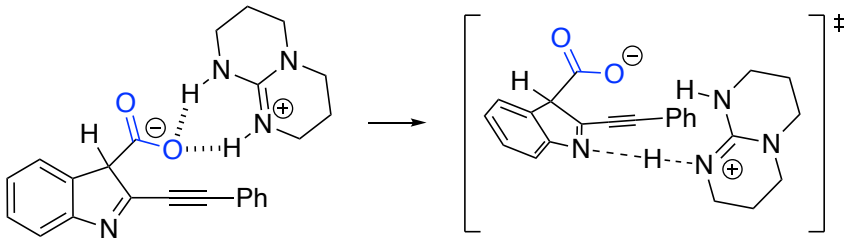


Scheme S1. Proposed catalytic cycle for carboxylative cyclization of indole derivatives. All values are relative to **SM** and are reported in kcal/mol.



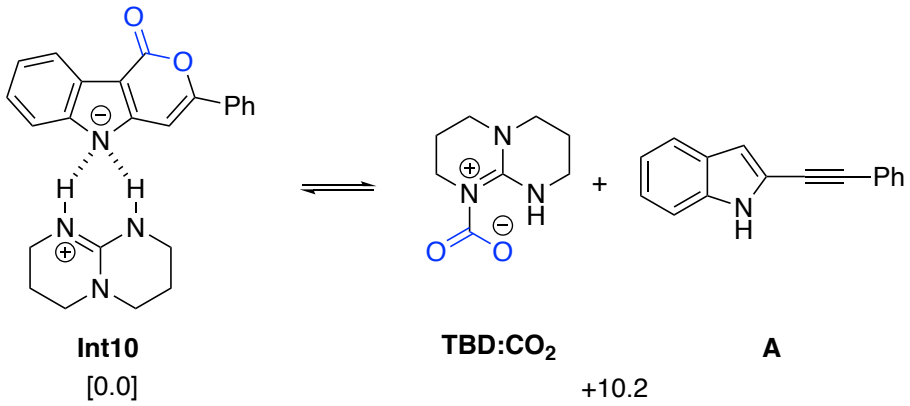
Scheme S2. Alternative catalytic cycle. All values are Gibbs free energies relative to **SM** and are reported in kcal/mol.

In this cycle (Scheme S2) only one molecule of TBD is invoked throughout and deprotonation of the indole-3 position occurs after cyclization. In this pathway, the cyclization was found to be the rate determining step, however the barrier was found to be unreasonably high for the given experimental conditions.



Scheme S3. Transition state of alternative catalytic cyclic.

An alternative catalytic cycle which proceeds from **Int4** through a transition state in which TBDH+ protonates the indole nitrogen was also considered (Scheme S3). However, all attempts to locate this transition state resulted in the loss of CO_2 from the indole-3 position, indicating that this pathway is likely not productive to forming the product (**B**).



Scheme S4. Relative Gibbs free energy (kcal/mol) between proposed catalyst resting state (**Int10**) and **TBD:CO_2** complex.

H. Computational Structures, Energies and Coordinates

CO2 (Optimized in diethyl ether)

Calculated using M06-2X/def2TZVP in diethyl ether at 373.15 K:

```
HF = -188.5986217 hartrees
Zero-point correction=                           0.011917 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=        -0.014974
Sum of electronic and zero-point Energies=           -188.586705
Sum of electronic and thermal Enthalpies=            -188.582072
Sum of electronic and thermal Free Energies=         -188.613596
```

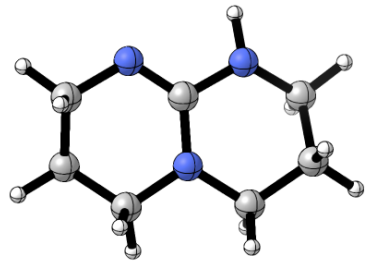
Calculated using M06-2X/def2TZVP in diethyl ether at 298.15 K:

```
Thermal correction to Gibbs Free Energy=        -0.008757
Sum of electronic and thermal Free Energies=         -188.607379
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	8	0	0.000000	0.000000	1.154562
3	8	0	0.000000	0.000000	-1.154562

TBD (Optimized in diethyl ether)



Calculated using M06-2X/def2TZVP in diethyl ether at 373.15 K:

```
HF = -438.8012035 hartrees
Zero-point correction=                           0.207149 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.162079
Sum of electronic and zero-point Energies=           -438.594055
Sum of electronic and thermal Enthalpies=            -438.579562
Sum of electronic and thermal Free Energies=         -438.639124
```

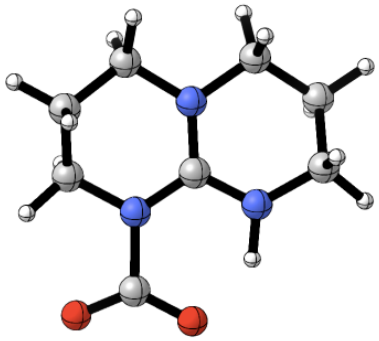
Calculated using M06-2X/def2TZVP in diethyl ether at 298.15 K:

```
Thermal correction to Gibbs Free Energy=         0.173505
Sum of electronic and thermal Free Energies=         -438.627698
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.068552	-0.739393	-0.083615
2	7	0	1.152866	-1.389945	-0.050388
3	1	0	1.039549	-2.362659	0.188140
4	7	0	-1.131858	-1.462098	-0.121165
5	7	0	-0.022357	0.630991	-0.128101
6	6	0	2.344320	-0.717959	0.425471
7	6	0	1.197738	1.418086	-0.015866
8	6	0	2.442329	0.603455	-0.311135
9	6	0	-1.253820	1.407154	-0.052036
10	6	0	-2.396877	-0.768576	-0.262291
11	6	0	-2.398725	0.563004	0.473531
12	1	0	-3.189778	-1.415050	0.117548
13	1	0	-2.620009	-0.591843	-1.323562
14	1	0	-2.260621	0.379813	1.541887
15	1	0	-3.341552	1.094551	0.339975
16	1	0	-1.070691	2.260414	0.607032
17	1	0	-1.496900	1.808796	-1.042327
18	1	0	1.119873	2.261083	-0.708214
19	1	0	1.262969	1.839363	0.996021
20	1	0	3.323465	1.164183	0.000262
21	1	0	2.520076	0.405920	-1.381679
22	1	0	2.320806	-0.540626	1.509338
23	1	0	3.203780	-1.351215	0.208806

TBD:CO2 (Optimized in diethyl ether)



Calculated using M06-2X/def2TZVP in diethyl ether at 373.15 K:

```
HF = -627.4235667 hartrees
Zero-point correction=                           0.222594 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.171781
Sum of electronic and zero-point Energies=           -627.200973
Sum of electronic and thermal Enthalpies=            -627.182901
Sum of electronic and thermal Free Energies=         -627.251786
```

Calculated using M06-2X/def2TZVP in diethyl ether at 298.15 K:

```
Thermal correction to Gibbs Free Energy=         0.184956
Sum of electronic and thermal Free Energies=         -627.238610
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.203119	-0.173779	-0.048814
2	7	0	-0.613188	-1.425322	-0.203502
3	1	0	0.177348	-2.089411	-0.231925
4	7	0	1.122863	0.087331	0.046050
5	7	0	-1.105074	0.820541	0.025437
6	6	0	-2.005297	-1.807931	-0.327169
7	6	0	-2.544352	0.557642	0.060146
8	6	0	-2.847479	-0.858591	0.500828
9	6	0	-0.754891	2.237772	-0.003423
10	6	0	1.555841	1.463964	0.283502
11	6	0	0.666891	2.423342	-0.475696
12	1	0	2.587622	1.525725	-0.041574
13	1	0	1.528790	1.682826	1.355568
14	1	0	0.740395	2.220236	-1.545870
15	1	0	0.982904	3.450938	-0.301791
16	1	0	-1.463108	2.733405	-0.670731
17	1	0	-0.890404	2.657666	0.997803
18	1	0	-2.982277	1.279894	0.751356
19	1	0	-2.964668	0.751368	-0.931748
20	1	0	-3.908471	-1.062720	0.366307
21	1	0	-2.604401	-0.982870	1.557422
22	1	0	-2.318026	-1.778083	-1.375173
23	1	0	-2.100198	-2.834201	0.021633
24	6	0	2.191969	-0.961845	0.046286
25	8	0	3.315249	-0.520487	0.245090
26	8	0	1.812864	-2.131522	-0.150232

CO2 (Optimized in acetonitrile)

Calculated using M06-2X/def2TZVP in acetonitrile at 373.15 K:

```
 HF = -188.5993547 hartrees
 Zero-point correction=                           0.011877 (Hartree/Particle)
 Thermal correction to Gibbs Free Energy=        -0.015835
 Sum of electronic and zero-point Energies=           -188.587478
 Sum of electronic and thermal Enthalpies=            -188.582842
 Sum of electronic and thermal Free Energies=         -188.615190
```

Calculated using M06-2X/def2TZVP in acetonitrile at 298.15 K:

```
Thermal correction to Gibbs Free Energy=        -0.008798
 Sum of electronic and thermal Free Energies=         -188.608153
```

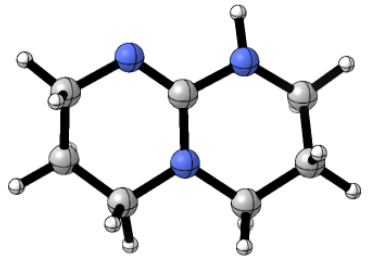
Single Points using M06-2X/def2TZVP in the gas phase:

```
 HF = -188.5969402 hartrees
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	-0.000000
2	8	0	0.000000	0.000000	-1.154562
3	8	0	0.000000	0.000000	1.154562

TBD (Optimized in acetonitrile)



Calculated using M06-2X/def2TZVP in acetonitrile at 373.15 K:

```
HF = -438.8044082 hartrees
Zero-point correction=                           0.207092 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.162080
Sum of electronic and zero-point Energies=           -438.597316
Sum of electronic and thermal Enthalpies=            -438.582827
Sum of electronic and thermal Free Energies=         -438.642328
```

Calculated using M06-2X/def2TZVP in acetonitrile at 298.15 K:

```
Thermal correction to Gibbs Free Energy=         0.173493
Sum of electronic and thermal Free Energies=         -438.630915
```

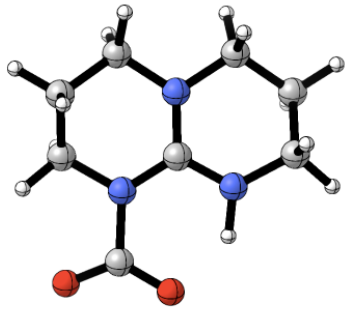
Single Points using M06-2X/def2TZVP in the gas phase:

```
HF = -438.794646 hartrees
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.066973	-0.738814	-0.082508
2	7	0	1.153189	-1.390464	-0.046725
3	1	0	1.043290	-2.360399	0.204886
4	7	0	-1.132906	-1.463803	-0.122652
5	7	0	-0.023150	0.628319	-0.127437
6	6	0	2.347948	-0.715911	0.423026
7	6	0	1.197625	1.417667	-0.014862
8	6	0	2.441845	0.604849	-0.314276
9	6	0	-1.254853	1.406342	-0.049844
10	6	0	-2.397889	-0.766738	-0.265353
11	6	0	-2.399706	0.562252	0.474226
12	1	0	-3.193618	-1.412802	0.109634
13	1	0	-2.618333	-0.584546	-1.326336
14	1	0	-2.262371	0.377311	1.542416
15	1	0	-3.342162	1.094042	0.340783
16	1	0	-1.069565	2.257467	0.610547
17	1	0	-1.496651	1.809515	-1.039375
18	1	0	1.115607	2.261323	-0.705166
19	1	0	1.262200	1.835248	0.997822
20	1	0	3.322876	1.166088	-0.004432
21	1	0	2.518138	0.409205	-1.385435
22	1	0	2.326874	-0.538758	1.506304
23	1	0	3.205792	-1.349941	0.203608

TBD:CO2 (Optimized in acetonitrile)



Calculated using M06-2X/def2TZVP in acetonitrile at 373.15 K:

```
HF = -627.4323609 hartrees
Zero-point correction=                           0.222749 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.171989
Sum of electronic and zero-point Energies=           -627.209612
Sum of electronic and thermal Enthalpies=            -627.191558
Sum of electronic and thermal Free Energies=         -627.260372
```

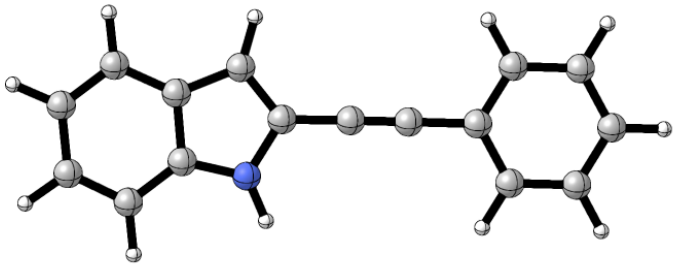
Calculated using M06-2X/def2TZVP in acetonitrile at 298.15 K:

```
Thermal correction to Gibbs Free Energy=         0.185150
Sum of electronic and thermal Free Energies=         -627.247211
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.205769	-0.175893	-0.055079
2	7	0	-0.622070	-1.425420	-0.208965
3	1	0	0.151443	-2.099434	-0.243922
4	7	0	1.128353	0.081665	0.034706
5	7	0	-1.098996	0.819488	0.024485
6	6	0	-2.018674	-1.802895	-0.324194
7	6	0	-2.541643	0.564180	0.065050
8	6	0	-2.850578	-0.849298	0.507837
9	6	0	-0.745823	2.237047	0.005599
10	6	0	1.565453	1.460824	0.267385
11	6	0	0.669845	2.421181	-0.481114
12	1	0	2.591881	1.525129	-0.072627
13	1	0	1.550992	1.678503	1.339498
14	1	0	0.731249	2.220707	-1.552469
15	1	0	0.990413	3.447061	-0.307029
16	1	0	-1.460087	2.738151	-0.649966
17	1	0	-0.870157	2.646342	1.011999
18	1	0	-2.970010	1.289709	0.757834
19	1	0	-2.961391	0.760601	-0.925690
20	1	0	-3.912800	-1.047421	0.376384
21	1	0	-2.604646	-0.974645	1.563538
22	1	0	-2.334747	-1.770736	-1.370461
23	1	0	-2.114082	-2.828409	0.025859
24	6	0	2.180933	-0.957978	0.049325
25	8	0	3.310417	-0.530023	0.277011
26	8	0	1.819392	-2.132314	-0.166184

A



Calculated using M06-2X/def2TZVP in acetonitrile at 373.15 K:

```
HF = -671.0070206 hartrees
Zero-point correction=                           0.222360 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.165889
Sum of electronic and zero-point Energies=           -670.784660
Sum of electronic and thermal Enthalpies=            -670.763591
Sum of electronic and thermal Free Energies=         -670.841131
```

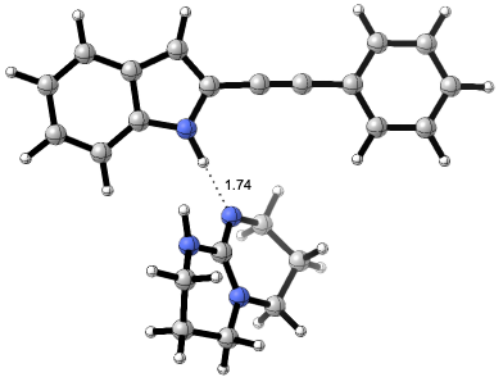
Single Points using M06-2X/def2TZVP in the gas phase:

```
HF = -670.9976774 hartrees
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.065096	-0.766068	-0.000016
2	6	0	2.970215	0.645336	0.000019
3	6	0	4.098966	1.467632	0.000112
4	6	0	5.332203	0.850356	0.000178
5	6	0	5.450818	-0.553040	0.000106
6	6	0	4.335469	-1.362400	0.000008
7	6	0	1.731477	-1.272763	-0.000141
8	6	0	0.890852	-0.186753	-0.000135
9	1	0	4.005674	2.545732	0.000139
10	1	0	6.228810	1.456719	0.000263
11	1	0	6.437460	-0.997807	0.000136
12	1	0	4.433659	-2.440774	-0.000040
13	1	0	1.417731	-2.303313	-0.000208
14	7	0	1.642478	0.970337	-0.000171
15	6	0	-0.523965	-0.141199	-0.000172
16	6	0	-1.728409	-0.091844	-0.000148
17	1	0	1.259540	1.901085	0.000157
18	6	0	-3.155405	-0.029819	-0.000081
19	6	0	-3.804404	1.209094	-0.000097
20	6	0	-3.915022	-1.204395	0.000060
21	6	0	-5.188469	1.267764	0.000012
22	1	0	-3.215829	2.117045	-0.000194
23	6	0	-5.298820	-1.135808	0.000192
24	1	0	-3.412075	-2.162440	0.000080
25	6	0	-5.938737	0.097697	0.000153
26	1	0	-5.683716	2.230015	0.000023
27	1	0	-5.880055	-2.048646	0.000321
28	1	0	-7.019727	0.147286	0.000238

Int1



Calculated using M06-2X/def2TZVP in acetonitrile at 373.15 K:

```
HF = -1109.8263091 hartrees
Zero-point correction=                           0.430276 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.349859
Sum of electronic and zero-point Energies=          -1109.396033
Sum of electronic and thermal Enthalpies=           -1109.359183
Sum of electronic and thermal Free Energies=        -1109.476450
```

Single Points using M06-2X/def2TZVP in the gas phase:

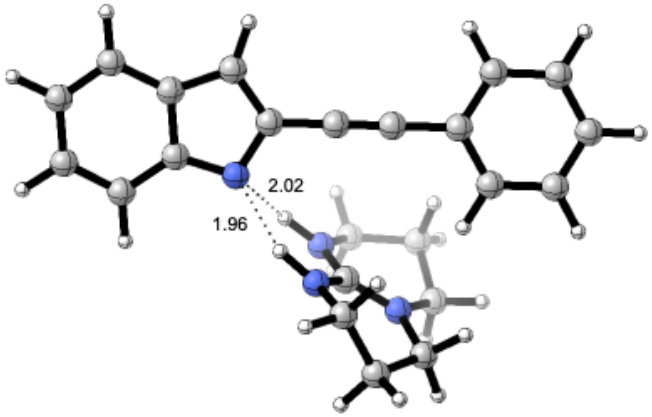
```
Counterpoise corrected energy =   -1109.810226776098
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.705369	-3.652340	-0.012248
2	6	0	-2.042333	-2.297058	0.232727
3	6	0	-3.362723	-1.889650	0.451135
4	6	0	-4.342176	-2.859355	0.419480
5	6	0	-4.027829	-4.212177	0.176534
6	6	0	-2.727509	-4.614869	-0.038172
7	6	0	-0.291394	-3.695353	-0.184571
8	6	0	0.159173	-2.401470	-0.043573
9	1	0	-3.599625	-0.849212	0.636998
10	1	0	-5.374618	-2.579047	0.585300
11	1	0	-4.826276	-4.942906	0.159360
12	1	0	-2.495611	-5.656451	-0.224414
13	1	0	0.323787	-4.556112	-0.388333
14	7	0	-0.896765	-1.558328	0.208790
15	6	0	1.480173	-1.892190	-0.120607
16	6	0	2.592608	-1.430348	-0.177785
17	6	0	-1.411162	2.087935	-0.002400
18	7	0	-2.299779	1.655991	-0.962313
19	1	0	-2.083641	0.731335	-1.301335
20	7	0	-0.666736	1.196505	0.574913
21	7	0	-1.417519	3.414922	0.292719
22	6	0	-2.900696	2.582512	-1.903980
23	6	0	-2.260949	4.402844	-0.371743
24	6	0	-3.420295	3.764399	-1.110435
25	6	0	-0.451685	3.968853	1.235534
26	6	0	0.207600	1.630991	1.649934

27	6	0	0.731535	3.037101	1.409280
28	1	0	1.032678	0.919007	1.726945
29	1	0	-0.322498	1.603792	2.610846
30	1	0	1.340202	3.046699	0.501990
31	1	0	1.351592	3.377804	2.238442
32	1	0	-0.127039	4.936001	0.844955
33	1	0	-0.942400	4.151607	2.197355
34	1	0	-2.627047	5.094646	0.390694
35	1	0	-1.645905	4.984156	-1.068612
36	1	0	-3.880407	4.501982	-1.766845
37	1	0	-4.174393	3.414975	-0.403003
38	1	0	-2.181274	2.925108	-2.657903
39	1	0	-3.708968	2.066372	-2.419181
40	1	0	-0.818034	-0.519131	0.345312
41	6	0	3.899977	-0.858578	-0.241801
42	6	0	5.034918	-1.672714	-0.311845
43	6	0	4.052193	0.531928	-0.232369
44	6	0	6.296234	-1.101695	-0.370547
45	1	0	4.917586	-2.748336	-0.318521
46	6	0	5.316863	1.094242	-0.290856
47	1	0	3.171831	1.159701	-0.182656
48	6	0	6.441479	0.280328	-0.360345
49	1	0	7.169838	-1.738372	-0.423212
50	1	0	5.425610	2.170968	-0.283519
51	1	0	7.428417	0.721772	-0.407497

Int2



Calculated using M06-2X/def2TZVP in acetonitrile at 373.15 K:

```
HF = -1109.8301982 hartrees
Zero-point correction=                           0.431497 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.354301
Sum of electronic and zero-point Energies=          -1109.398701
Sum of electronic and thermal Enthalpies=           -1109.362281
Sum of electronic and thermal Free Energies=        -1109.475897
```

Single Points using M06-2X/def2TZVP in the gas phase:

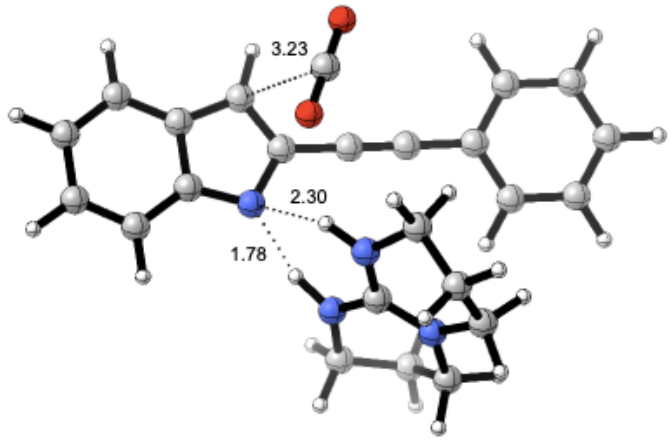
```
Counterpoise corrected energy =   -1109.801934275659
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.004919	-1.432000	-0.094955
2	6	0	-3.593565	-0.062489	-0.058960
3	6	0	-4.552826	0.963055	0.015548
4	6	0	-5.887400	0.621679	0.051604
5	6	0	-6.298492	-0.729920	0.015372
6	6	0	-5.375423	-1.749989	-0.057215
7	6	0	-2.807683	-2.184959	-0.164356
8	6	0	-1.783698	-1.243922	-0.167137
9	1	0	-4.240090	2.000966	0.043458
10	1	0	-6.638488	1.400099	0.110452
11	1	0	-7.356246	-0.960906	0.045281
12	1	0	-5.701593	-2.783782	-0.083920
13	1	0	-2.691814	-3.256672	-0.205814
14	7	0	-2.237885	0.048610	-0.103523
15	6	0	-0.387097	-1.522579	-0.218342
16	6	0	0.796891	-1.761278	-0.252490
17	6	0	0.602677	1.811931	0.228549
18	7	0	-0.075086	1.818121	-0.920949
19	1	0	-0.973047	1.321169	-0.888713
20	7	0	-0.026605	1.385986	1.323241
21	7	0	1.868794	2.235590	0.283438
22	6	0	0.573952	2.137280	-2.179408
23	6	0	2.537515	2.862322	-0.858549
24	6	0	1.547612	3.274253	-1.932262

25	6	0	2.677500	2.081892	1.493439
26	6	0	0.625604	1.282332	2.618100
27	6	0	2.102848	1.013513	2.403050
28	1	0	0.150899	0.471078	3.165877
29	1	0	0.483748	2.205104	3.186775
30	1	0	2.227188	0.030734	1.942749
31	1	0	2.636743	1.019881	3.351706
32	1	0	3.684506	1.808968	1.170605
33	1	0	2.740722	3.044539	2.008652
34	1	0	3.082755	3.728953	-0.480716
35	1	0	3.274913	2.160848	-1.261905
36	1	0	2.089514	3.523305	-2.842769
37	1	0	0.992550	4.157234	-1.611748
38	1	0	1.098379	1.262674	-2.579095
39	1	0	-0.196068	2.424509	-2.892020
40	1	0	-0.929867	0.942623	1.149153
41	6	0	2.197269	-2.042181	-0.282906
42	6	0	2.671367	-3.342476	-0.077639
43	6	0	3.118399	-1.013695	-0.511720
44	6	0	4.033168	-3.600032	-0.097453
45	1	0	1.964011	-4.142411	0.097619
46	6	0	4.478462	-1.276864	-0.527780
47	1	0	2.749104	-0.009167	-0.675330
48	6	0	4.940757	-2.571025	-0.319721
49	1	0	4.388659	-4.609765	0.062609
50	1	0	5.178514	-0.470161	-0.704719
51	1	0	6.002976	-2.777058	-0.332244

Int3



Calculated using M06-2X/def2TZVP in acetonitrile at 373.15 K:

```
HF = -1298.4362299 hartrees
Zero-point correction=                           0.444082 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.359093
Sum of electronic and zero-point Energies=          -1297.992148
Sum of electronic and thermal Enthalpies=           -1297.950282
Sum of electronic and thermal Free Energies=        -1298.077137
```

Single Points using M06-2X/def2TZVP in the gas phase:

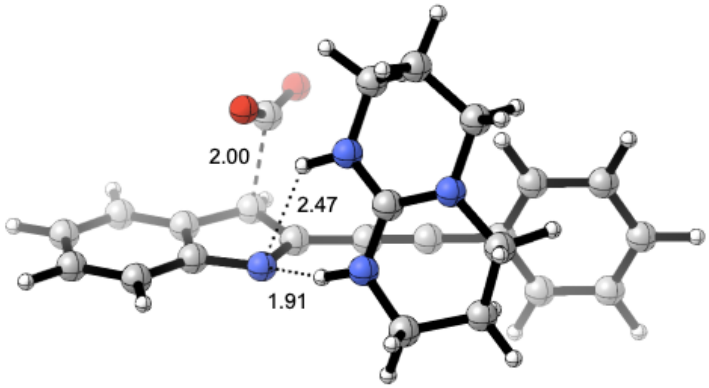
```
Counterpoise corrected energy =   -1298.408395134529
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.945025	-0.882866	-0.647165
2	6	0	3.455561	0.432894	-0.373471
3	6	0	4.349409	1.470768	-0.054911
4	6	0	5.697875	1.193232	-0.013299
5	6	0	6.187153	-0.105109	-0.283980
6	6	0	5.328943	-1.135472	-0.598451
7	6	0	2.796185	-1.664363	-0.922082
8	6	0	1.721585	-0.787600	-0.800528
9	1	0	3.975938	2.467293	0.152458
10	1	0	6.400197	1.981004	0.230624
11	1	0	7.254028	-0.286401	-0.242163
12	1	0	5.714979	-2.127657	-0.803912
13	1	0	2.741835	-2.713094	-1.169188
14	7	0	2.100057	0.484987	-0.468020
15	6	0	0.341900	-1.124796	-0.907182
16	6	0	-0.830495	-1.417014	-0.922598
17	6	0	1.198825	-2.434784	1.771964
18	8	0	1.060467	-3.496482	1.341856
19	8	0	1.329856	-1.383920	2.236181
20	6	0	-0.852968	1.923038	0.442764
21	7	0	-0.395507	1.074442	1.375347
22	1	0	0.514124	0.667244	1.186156

23	7	0	-0.016050	2.316268	-0.509236
24	7	0	-2.112853	2.366858	0.493284
25	6	0	-1.296350	0.417339	2.306048
26	6	0	-3.036139	2.014850	1.573832
27	6	0	-2.309178	1.443744	2.775232
28	6	0	-2.667052	3.216877	-0.561722
29	6	0	-0.401804	3.251118	-1.551831
30	6	0	-1.879506	3.081766	-1.850840
31	1	0	0.206113	3.038140	-2.428988
32	1	0	-0.192947	4.277166	-1.236780
33	1	0	-2.047030	2.096062	-2.290187
34	1	0	-2.218552	3.833081	-2.562014
35	1	0	-3.703428	2.907194	-0.709814
36	1	0	-2.675888	4.254399	-0.216658
37	1	0	-3.581005	2.920648	1.844260
38	1	0	-3.762745	1.293711	1.186210
39	1	0	-3.033073	0.990514	3.450179
40	1	0	-1.789963	2.238354	3.313069
41	1	0	-1.797235	-0.430373	1.823922
42	1	0	-0.703327	0.038281	3.134404
43	1	0	0.874509	1.775301	-0.568484
44	6	0	-2.214595	-1.769195	-0.903106
45	6	0	-2.605276	-3.112883	-0.900929
46	6	0	-3.198883	-0.775261	-0.865339
47	6	0	-3.949280	-3.448022	-0.859732
48	1	0	-1.847152	-3.884826	-0.930032
49	6	0	-4.540950	-1.117762	-0.821049
50	1	0	-2.896468	0.264839	-0.874402
51	6	0	-4.920592	-2.454694	-0.818085
52	1	0	-4.240395	-4.490603	-0.858474
53	1	0	-5.292084	-0.338550	-0.790479
54	1	0	-5.968907	-2.721224	-0.784874

TS1



Calculated using M06-2X/def2TZVP in acetonitrile at 373.15 K:

```
HF = -1298.4151163 hartrees
Zero-point correction=                           0.444244 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.362764
Sum of electronic and zero-point Energies=          -1297.970873
Sum of electronic and thermal Enthalpies=           -1297.930472
Sum of electronic and thermal Free Energies=        -1298.052352
```

Single Points using M06-2X/def2TZVP in the gas phase:

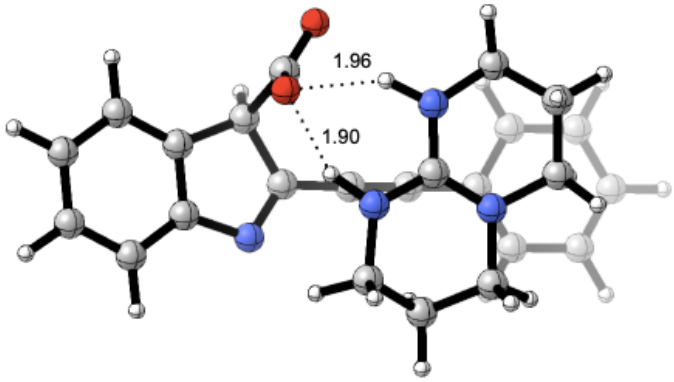
```
Counterpoise corrected energy =   -1298.385468815687
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.831043	-1.071843	-0.126851
2	6	0	3.338797	-0.074732	-0.995866
3	6	0	4.200430	0.829247	-1.619709
4	6	0	5.556315	0.707925	-1.377668
5	6	0	6.053829	-0.290574	-0.524569
6	6	0	5.202228	-1.178088	0.109642
7	6	0	2.663476	-1.736256	0.403095
8	6	0	1.584099	-1.165312	-0.351732
9	1	0	3.811350	1.597639	-2.276405
10	1	0	6.248965	1.391411	-1.852489
11	1	0	7.121610	-0.362090	-0.360396
12	1	0	5.593959	-1.936346	0.776946
13	1	0	2.641209	-2.731166	0.817990
14	7	0	1.958939	-0.147461	-1.114320
15	6	0	0.204541	-1.515040	-0.231458
16	6	0	-0.974595	-1.745249	-0.138886
17	6	0	2.219020	-0.715425	2.062192
18	8	0	1.873923	-1.531228	2.865204
19	8	0	2.400865	0.455667	1.884076
20	6	0	-0.886984	1.704477	-0.264826
21	7	0	-0.020051	1.666222	0.752416
22	1	0	0.916561	1.324661	0.571147
23	7	0	-0.443888	1.433166	-1.490610
24	7	0	-2.164276	2.028651	-0.048858
25	6	0	-0.440514	1.837257	2.132567

26	6	0	-2.654850	2.498101	1.247723
27	6	0	-1.519523	2.902476	2.167218
28	6	0	-3.172550	1.950822	-1.106117
29	6	0	-1.315600	1.442317	-2.655257
30	6	0	-2.719805	1.048314	-2.236235
31	1	0	-0.906349	0.740210	-3.378810
32	1	0	-1.319323	2.435369	-3.112276
33	1	0	-2.722938	0.009189	-1.901725
34	1	0	-3.410002	1.142168	-3.072945
35	1	0	-4.083662	1.561475	-0.647130
36	1	0	-3.383374	2.960553	-1.469859
37	1	0	-3.316626	3.344598	1.056177
38	1	0	-3.259377	1.704845	1.697967
39	1	0	-1.903036	3.029286	3.177910
40	1	0	-1.094253	3.852506	1.839986
41	1	0	-0.811731	0.892214	2.543126
42	1	0	0.433123	2.130306	2.708717
43	1	0	0.474676	0.975801	-1.546551
44	6	0	-2.392332	-1.919104	-0.044418
45	6	0	-3.075334	-2.763764	-0.922305
46	6	0	-3.111996	-1.181333	0.900125
47	6	0	-4.457484	-2.855475	-0.860256
48	1	0	-2.518657	-3.332869	-1.655055
49	6	0	-4.493177	-1.275603	0.954634
50	1	0	-2.574295	-0.540584	1.587344
51	6	0	-5.168877	-2.109762	0.071771
52	1	0	-4.981694	-3.508668	-1.545549
53	1	0	-5.042590	-0.698779	1.687547
54	1	0	-6.247852	-2.181549	0.112821

Int4



Calculated using M06-2X/def2TZVP in acetonitrile at 373.15 K:

```
HF = -1298.4345107 hartrees
Zero-point correction=                           0.446912 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.367612
Sum of electronic and zero-point Energies=          -1297.987598
Sum of electronic and thermal Enthalpies=           -1297.947517
Sum of electronic and thermal Free Energies=        -1298.066899
```

Single Points using M06-2X/def2TZVP in the gas phase:

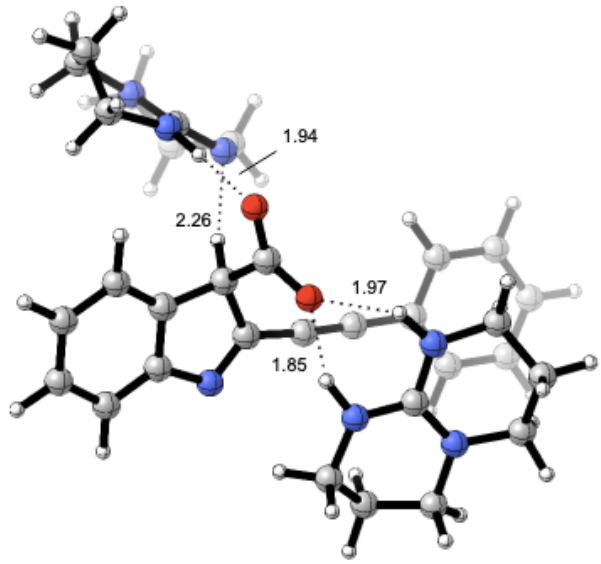
```
Counterpoise corrected energy =   -1298.400829386480
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.788757	-0.808072	-0.412352
2	6	0	3.638083	0.446200	-1.011369
3	6	0	4.701356	1.325198	-1.140409
4	6	0	5.938466	0.916261	-0.654037
5	6	0	6.096696	-0.333687	-0.058711
6	6	0	5.019611	-1.208949	0.069256
7	6	0	2.448254	-1.467448	-0.419831
8	6	0	1.645988	-0.398658	-1.135005
9	1	0	4.566919	2.293965	-1.604099
10	1	0	6.791050	1.577766	-0.738029
11	1	0	7.070650	-0.628070	0.310250
12	1	0	5.149714	-2.176758	0.537885
13	1	0	2.419647	-2.413282	-0.961242
14	7	0	2.309588	0.664218	-1.439635
15	6	0	0.250932	-0.532191	-1.373238
16	6	0	-0.940943	-0.656019	-1.504199
17	6	0	1.804018	-1.693698	0.986870
18	8	0	1.178539	-2.745216	1.154241
19	8	0	1.929299	-0.745376	1.804920
20	6	0	-0.933536	0.832340	1.470944
21	7	0	-0.901584	-0.348931	2.092255
22	1	0	0.022145	-0.744639	2.256280
23	7	0	0.224061	1.451966	1.233107
24	7	0	-2.094117	1.383295	1.111447
25	6	0	-2.095107	-1.136969	2.343087
26	6	0	-3.382555	0.777710	1.453576

27	6	0	-3.249434	-0.190845	2.612363
28	6	0	-2.147894	2.640234	0.365310
29	6	0	0.317944	2.730605	0.545626
30	6	0	-0.860224	2.877654	-0.398628
31	1	0	1.258811	2.739469	-0.001539
32	1	0	0.330603	3.547423	1.272033
33	1	0	-0.764314	2.146485	-1.203633
34	1	0	-0.874617	3.874742	-0.835552
35	1	0	-2.996341	2.568089	-0.317466
36	1	0	-2.347443	3.461161	1.060382
37	1	0	-4.062063	1.591782	1.709356
38	1	0	-3.780858	0.272253	0.567898
39	1	0	-4.178931	-0.746456	2.725453
40	1	0	-3.061726	0.356389	3.537768
41	1	0	-2.320016	-1.776907	1.485680
42	1	0	-1.897963	-1.776728	3.200773
43	1	0	1.061991	0.897266	1.403764
44	6	0	-2.360076	-0.751876	-1.621985
45	6	0	-3.093614	0.311728	-2.157377
46	6	0	-3.029073	-1.893338	-1.168734
47	6	0	-4.476128	0.238774	-2.218481
48	1	0	-2.573508	1.187466	-2.523972
49	6	0	-4.411871	-1.957187	-1.231675
50	1	0	-2.456470	-2.720743	-0.769662
51	6	0	-5.137227	-0.891380	-1.751509
52	1	0	-5.038603	1.066274	-2.630578
53	1	0	-4.924447	-2.840890	-0.875089
54	1	0	-6.217105	-0.943472	-1.797130

Int4a



Calculated using M06-2X/def2TZVP in acetonitrile at 373.15 K:

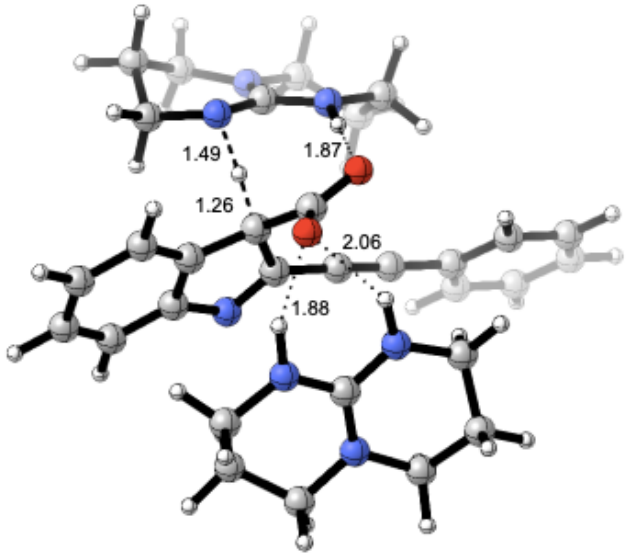
```
HF = -1737.2480143 hartrees
Zero-point correction=                           0.655752 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.553736
Sum of electronic and zero-point Energies=          -1736.592262
Sum of electronic and thermal Free Energies=        -1736.694278
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.949021	2.182612	-0.179786
2	6	0	1.283646	2.803055	-1.242623
3	6	0	1.700072	4.027585	-1.740808
4	6	0	2.803125	4.628246	-1.142185
5	6	0	3.458843	4.021194	-0.072899
6	6	0	3.034104	2.789103	0.421606
7	6	0	1.231305	0.898963	0.097562
8	6	0	0.153494	0.978001	-0.948856
9	1	0	1.179982	4.496771	-2.566018
10	1	0	3.154067	5.584553	-1.508081
11	1	0	4.308566	4.514997	0.380729
12	1	0	3.531188	2.321313	1.262274
13	1	0	1.850908	0.007053	-0.074522
14	7	0	0.187474	2.032365	-1.693332
15	6	0	-0.816629	-0.053091	-1.075151
16	6	0	-1.610814	-0.958621	-1.038623
17	6	0	0.741333	0.835020	1.568913
18	8	0	1.597862	0.507203	2.403921
19	8	0	-0.450970	1.154766	1.798294
20	6	0	-3.578338	1.032590	0.800758
21	7	0	-3.162684	0.165656	1.728089
22	1	0	-2.190767	0.249097	2.013236
23	7	0	-2.739513	1.989213	0.407226
24	7	0	-4.811158	0.945397	0.293515

25	6	0	-3.997578	-0.929423	2.192457
26	6	0	-5.822686	0.040079	0.840350
27	6	0	-5.437489	-0.452676	2.221406
28	6	0	-5.236913	1.780371	-0.828912
29	6	0	-3.061817	2.938707	-0.646009
30	6	0	-4.042028	2.294533	-1.607063
31	1	0	-2.132168	3.198344	-1.149093
32	1	0	-3.489559	3.848686	-0.216973
33	1	0	-3.547384	1.467963	-2.122602
34	1	0	-4.376201	3.013344	-2.353258
35	1	0	-5.875567	1.161463	-1.461768
36	1	0	-5.843397	2.609262	-0.452281
37	1	0	-6.763895	0.591119	0.874634
38	1	0	-5.949383	-0.800346	0.152253
39	1	0	-6.101466	-1.264860	2.512401
40	1	0	-5.539852	0.352837	2.950409
41	1	0	-3.900890	-1.796800	1.531221
42	1	0	-3.653196	-1.215985	3.183728
43	1	0	-1.782549	1.898986	0.754765
44	6	0	-2.561795	-2.015674	-0.919539
45	6	0	-3.838176	-1.892496	-1.476010
46	6	0	-2.231226	-3.166106	-0.195037
47	6	0	-4.771057	-2.902873	-1.300045
48	1	0	-4.090273	-1.004123	-2.041623
49	6	0	-3.169327	-4.171256	-0.025515
50	1	0	-1.242623	-3.255802	0.236151
51	6	0	-4.440830	-4.040540	-0.572777
52	1	0	-5.758625	-2.801279	-1.731441
53	1	0	-2.909468	-5.056797	0.539355
54	1	0	-5.173147	-4.825207	-0.435260
55	6	0	4.072125	-1.531169	0.337079
56	7	0	2.912046	-1.986285	-0.019040
57	7	0	4.124800	-0.617369	1.356519
58	7	0	5.271245	-1.913934	-0.205692
59	6	0	2.896915	-3.016650	-1.040651
60	6	0	5.318270	-2.747511	-1.399314
61	6	0	3.970849	-2.784473	-2.092526
62	6	0	6.569643	-1.426283	0.239426
63	6	0	5.315183	0.151485	1.643469
64	6	0	6.503487	-0.790402	1.613665
65	1	0	5.195233	0.611195	2.624391
66	1	0	5.472215	0.957683	0.913624
67	1	0	6.372287	-1.556111	2.380424
68	1	0	7.433833	-0.259024	1.812404
69	1	0	7.262895	-2.272108	0.240043
70	1	0	6.950944	-0.698750	-0.488078
71	1	0	6.084042	-2.338141	-2.064423
72	1	0	5.635134	-3.760444	-1.125947
73	1	0	3.968841	-3.567607	-2.851526
74	1	0	3.783563	-1.829246	-2.589429
75	1	0	3.046910	-4.009754	-0.593500
76	1	0	1.907494	-3.031476	-1.502519
77	1	0	3.223428	-0.275669	1.683435

TS-PT



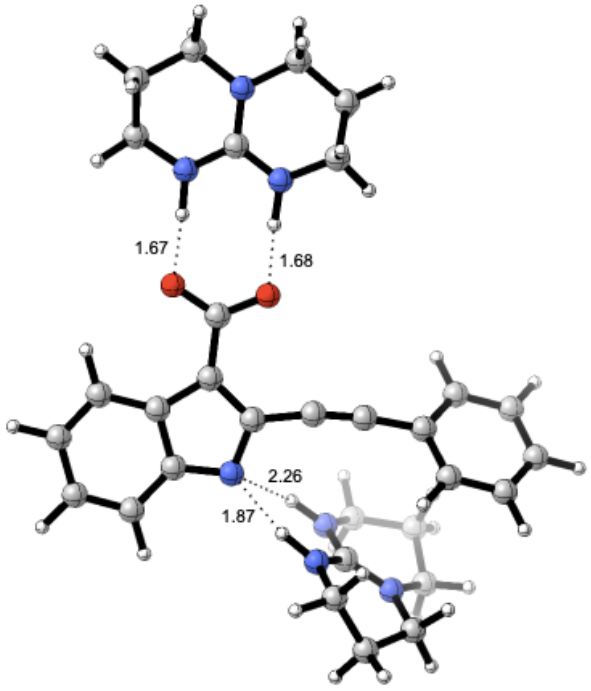
Calculated using M06-2X/def2TZVP in acetonitrile at 373.15 K:

```
HF = -1737.2418285 hartrees
Zero-point correction=                           0.651269 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.553061
Sum of electronic and zero-point Energies=          -1736.590560
Sum of electronic and thermal Free Energies=        -1736.688767

                      Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -1.416802   -2.362456   -0.294810
     2          6           0       -1.525698   -2.159850    1.092574
     3          6           0       -2.275363   -3.017162    1.894076
     4          6           0       -2.936429   -4.069849    1.280117
     5          6           0       -2.846832   -4.265761   -0.103398
     6          6           0       -2.082017   -3.422847   -0.899989
     7          6           0       -0.481888   -1.346595   -0.787322
     8          6           0       -0.287058   -0.522928    0.418595
     9          1           0       -2.344964   -2.852100    2.962332
    10          1           0       -3.536728   -4.746214    1.875222
    11          1           0       -3.383005   -5.089250   -0.558104
    12          1           0       -2.014673   -3.580472   -1.969085
    13          1           0        0.605479   -1.980389   -0.831898
    14          7           0       -0.833238   -1.020148    1.500377
    15          6           0        0.459809    0.690908    0.467504
    16          6           0        1.069124    1.730019    0.521717
    17          6           0       -0.593032   -0.668886   -2.141991
    18          8           0        0.413450   -0.054780   -2.553347
    19          8           0       -1.700480   -0.737051   -2.738772
    20          6           0       -3.141415    1.272156   -0.505395
    21          7           0       -2.297869    1.815567   -1.390794
    22          1           0       -1.990311    1.216096   -2.147782
    23          7           0       -3.508581    0.003183   -0.677995
    24          7           0       -3.607187    1.992719    0.515417
    25          6           0       -1.785657    3.169459   -1.266625
```

26	6	0	-3.288699	3.411975	0.677050
27	6	0	-2.858323	4.035729	-0.635570
28	6	0	-4.478553	1.406457	1.535058
29	6	0	-4.427563	-0.685453	0.215188
30	6	0	-4.299604	-0.096944	1.607257
31	1	0	-4.163765	-1.742458	0.207482
32	1	0	-5.452985	-0.583109	-0.150532
33	1	0	-3.311915	-0.329227	2.009235
34	1	0	-5.052098	-0.521894	2.269819
35	1	0	-4.214571	1.871102	2.485683
36	1	0	-5.516017	1.669214	1.309076
37	1	0	-4.186008	3.900169	1.058980
38	1	0	-2.503994	3.514388	1.432121
39	1	0	-2.478065	5.039246	-0.452703
40	1	0	-3.712665	4.108509	-1.310697
41	1	0	-0.880570	3.175290	-0.652738
42	1	0	-1.524506	3.520727	-2.262633
43	1	0	-3.028704	-0.506623	-1.424462
44	6	0	1.799655	2.957280	0.559068
45	6	0	2.022007	3.674605	-0.621887
46	6	0	2.299023	3.451719	1.768264
47	6	0	2.729483	4.865247	-0.589578
48	1	0	1.636121	3.287968	-1.557338
49	6	0	3.007936	4.642400	1.791222
50	1	0	2.126239	2.896112	2.680743
51	6	0	3.223885	5.351126	0.615481
52	1	0	2.897547	5.413945	-1.506975
53	1	0	3.392789	5.018767	2.730086
54	1	0	3.778349	6.280155	0.637699
55	6	0	2.887818	-1.899896	-0.540064
56	7	0	1.892542	-2.732030	-0.750484
57	7	0	2.890055	-0.739491	-1.235702
58	7	0	3.902366	-2.134011	0.328816
59	6	0	1.826821	-3.916988	0.087066
60	6	0	4.079194	-3.434071	0.966414
61	6	0	3.217753	-4.491493	0.303953
62	6	0	4.902119	-1.126771	0.659452
63	6	0	3.840366	0.332249	-1.013588
64	6	0	4.365462	0.268264	0.407721
65	1	0	3.330252	1.276810	-1.201077
66	1	0	4.675764	0.261287	-1.718383
67	1	0	3.552847	0.482545	1.106316
68	1	0	5.155171	1.003384	0.560090
69	1	0	5.157568	-1.257030	1.713365
70	1	0	5.814602	-1.299026	0.077019
71	1	0	5.138064	-3.698125	0.901909
72	1	0	3.827954	-3.346866	2.028884
73	1	0	3.190065	-5.383475	0.929751
74	1	0	3.642987	-4.767987	-0.663440
75	1	0	1.372935	-3.683835	1.061048
76	1	0	1.176478	-4.645747	-0.398657
77	1	0	2.020814	-0.517632	-1.726230

Int5



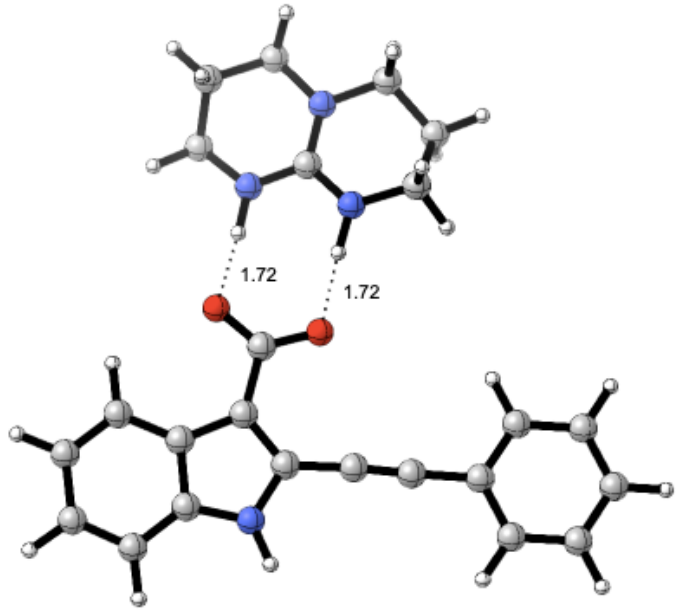
Calculated using M06-2X/def2TZVP in acetonitrile at 373.15 K:

```
HF = -1737.2778047 hartrees
Zero-point correction=                           0.655258 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.550874
Sum of electronic and zero-point Energies=          -1736.622547
Sum of electronic and thermal Free Energies=        -1736.726931

                      Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.620319   -3.201499   -0.007889
     2          6           0       -0.793321   -3.384966    0.000040
     3          6           0       -1.353251   -4.668524    0.094876
     4          6           0       -0.506487   -5.753458    0.179681
     5          6           0        0.893342   -5.581295    0.171004
     6          6           0        1.460373   -4.326105    0.079220
     7          6           0        0.826091   -1.792934   -0.113955
     8          6           0       -0.464439   -1.250950   -0.163631
     9          1           0       -2.430096   -4.794774    0.100059
    10          1           0       -0.917987   -6.752770    0.253790
    11          1           0        1.531970   -6.454026    0.236657
    12          1           0        2.534310   -4.198048    0.072073
    13          7           0       -1.447843   -2.190613   -0.094916
    14          6           0       -0.886529    0.109119   -0.252361
    15          6           0       -1.438845    1.181238   -0.285339
    16          6           0        2.113702   -1.069788   -0.156311
    17          8           0        3.171261   -1.759424   -0.086738
    18          8           0        2.099705    0.188350   -0.256725
    19          6           0        5.601872    0.850692   -0.080023
    20          7           0        4.495115    1.470982   -0.485029
    21          1           0        3.593070    0.950569   -0.413753
```

22	7	0	5.510506	-0.428779	0.276726
23	7	0	6.775613	1.496219	-0.032894
24	6	0	4.500814	2.850749	-0.934044
25	6	0	6.885167	2.929059	-0.300741
26	6	0	5.545869	3.623274	-0.150735
27	6	0	8.027303	0.811937	0.285923
28	6	0	6.650369	-1.178211	0.771027
29	6	0	7.907371	-0.684944	0.078933
30	1	0	6.470654	-2.231508	0.562942
31	1	0	6.747862	-1.062465	1.855033
32	1	0	7.845016	-0.909013	-0.987537
33	1	0	8.790285	-1.178308	0.482193
34	1	0	8.798730	1.229743	-0.363206
35	1	0	8.303831	1.038707	1.320042
36	1	0	7.610928	3.335804	0.405399
37	1	0	7.285211	3.073487	-1.308845
38	1	0	5.624704	4.646052	-0.515782
39	1	0	5.259246	3.654512	0.902101
40	1	0	4.716429	2.907261	-2.005615
41	1	0	3.504040	3.257557	-0.772694
42	1	0	4.593800	-0.910327	0.135891
43	6	0	-4.452392	-0.476766	0.258509
44	7	0	-3.709171	-0.538855	1.366340
45	1	0	-2.843160	-1.060247	1.282686
46	7	0	-4.050191	-1.174812	-0.801961
47	7	0	-5.570332	0.252368	0.229783
48	6	0	-4.022329	0.195221	2.581593
49	1	0	-4.623651	-0.425226	3.251441
50	1	0	-3.084409	0.425277	3.083454
51	6	0	-5.959898	1.121370	1.340155
52	1	0	-6.377417	2.029793	0.901737
53	1	0	-6.749637	0.631048	1.916214
54	6	0	-4.772447	1.463462	2.218053
55	1	0	-4.105763	2.143939	1.685355
56	1	0	-5.122454	1.963229	3.119896
57	6	0	-6.421815	0.290687	-0.956189
58	1	0	-7.452163	0.381386	-0.611181
59	1	0	-6.184664	1.187942	-1.537801
60	6	0	-4.768446	-1.178121	-2.064690
61	1	0	-4.594916	-2.138627	-2.546666
62	1	0	-4.384608	-0.398203	-2.729806
63	6	0	-6.245156	-0.959899	-1.795167
64	1	0	-6.789042	-0.850617	-2.731682
65	1	0	-6.650334	-1.821081	-1.260951
66	6	0	-2.228699	2.372065	-0.274193
67	6	0	-3.400677	2.421908	-1.038568
68	6	0	-1.906034	3.457867	0.545614
69	6	0	-4.243701	3.518572	-0.961342
70	1	0	-3.642423	1.586711	-1.684639
71	6	0	-2.753439	4.553523	0.617457
72	1	0	-1.000873	3.425400	1.137776
73	6	0	-3.926834	4.584617	-0.126905
74	1	0	-5.149334	3.544484	-1.554510
75	1	0	-2.499439	5.384817	1.262265
76	1	0	-4.588030	5.438859	-0.063168
77	1	0	-3.140400	-1.655687	-0.697817

Int6



Calculated using M06-2X/def2TZVP in acetonitrile at 373.15 K:

```
HF = -1298.4530985 hartrees
Zero-point correction=                           0.446374 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.361519
Sum of electronic and zero-point Energies=          -1298.006724
Sum of electronic and thermal Enthalpies=           -1297.965995
Sum of electronic and thermal Free Energies=        -1298.091580
```

Single Points using M06-2X/def2TZVP in the gas phase:

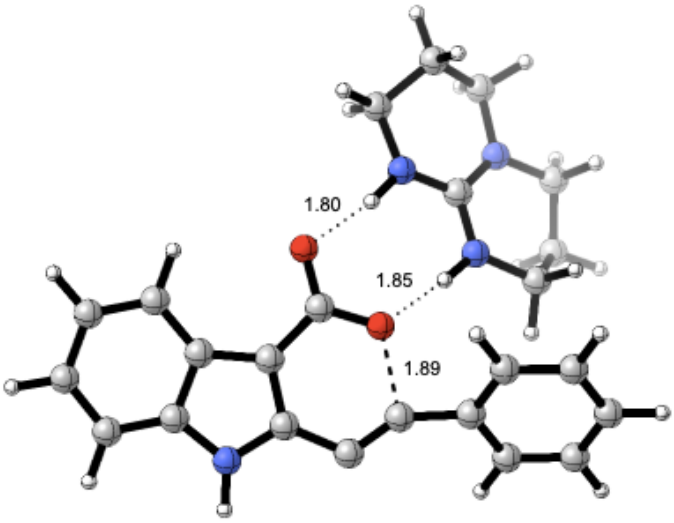
```
Counterpoise corrected energy =   -1298.419130951713
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.562885	3.244607	0.028756
2	6	0	-2.966303	3.398924	0.058356
3	6	0	-3.586874	4.648267	0.093547
4	6	0	-2.769122	5.759251	0.098563
5	6	0	-1.368059	5.632899	0.069466
6	6	0	-0.758916	4.395682	0.035123
7	6	0	-1.292343	1.834924	-0.000489
8	6	0	-2.521499	1.201952	0.011389
9	1	0	-4.665137	4.738147	0.116396
10	1	0	-3.212845	6.746179	0.126219
11	1	0	-0.759640	6.528331	0.074323
12	1	0	0.316606	4.295141	0.012376
13	7	0	-3.518980	2.146575	0.046548
14	6	0	-2.865413	-0.171454	-0.009874
15	6	0	-3.226504	-1.321307	-0.028865
16	6	0	0.046926	1.180520	-0.035853
17	8	0	1.045836	1.943398	-0.074647

18	8	0	0.092609	-0.073926	-0.024028
19	6	0	3.658494	-0.552010	0.001874
20	7	0	2.561243	-1.261205	0.261738
21	1	0	1.643937	-0.788019	0.158139
22	7	0	3.519592	0.740030	-0.291210
23	7	0	4.869578	-1.122970	0.033206
24	6	0	2.610590	-2.663160	0.635234
25	6	0	5.045172	-2.558483	0.245883
26	6	0	3.776820	-3.323517	-0.075735
27	6	0	6.099698	-0.347208	-0.120151
28	6	0	4.650306	1.584408	-0.630681
29	6	0	5.863278	1.124355	0.155749
30	1	0	4.384226	2.610788	-0.384625
31	1	0	4.856688	1.538490	-1.704283
32	1	0	5.683240	1.278665	1.221107
33	1	0	6.746777	1.693480	-0.128728
34	1	0	6.829201	-0.757068	0.580068
35	1	0	6.489965	-0.494391	-1.131503
36	1	0	5.864900	-2.882524	-0.397240
37	1	0	5.347711	-2.730677	1.283252
38	1	0	3.886576	-4.358519	0.243827
39	1	0	3.598639	-3.312607	-1.152436
40	1	0	2.720069	-2.769773	1.718787
41	1	0	1.663481	-3.116905	0.348185
42	1	0	2.571461	1.155523	-0.224975
43	6	0	-3.608723	-2.697097	-0.056149
44	6	0	-4.957160	-3.062700	0.003692
45	6	0	-2.629425	-3.692208	-0.145604
46	6	0	-5.315349	-4.400852	-0.026354
47	1	0	-5.714057	-2.292613	0.074659
48	6	0	-2.996539	-5.027564	-0.175024
49	1	0	-1.586643	-3.405947	-0.192664
50	6	0	-4.338381	-5.385319	-0.115520
51	1	0	-6.360897	-4.676585	0.019801
52	1	0	-2.233543	-5.791788	-0.246334
53	1	0	-4.622279	-6.429478	-0.138785
54	1	0	-4.502767	1.931905	0.057856

TS2



Calculated using M06-2X/def2TZVP in acetonitrile at 373.15 K:

```
HF = -1298.4136628 hartrees
Zero-point correction=                           0.446948 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.368512
Sum of electronic and zero-point Energies=          -1297.966715
Sum of electronic and thermal Enthalpies=           -1297.927607
Sum of electronic and thermal Free Energies=        -1298.045151
```

Single Points using M06-2X/def2TZVP in the gas phase:

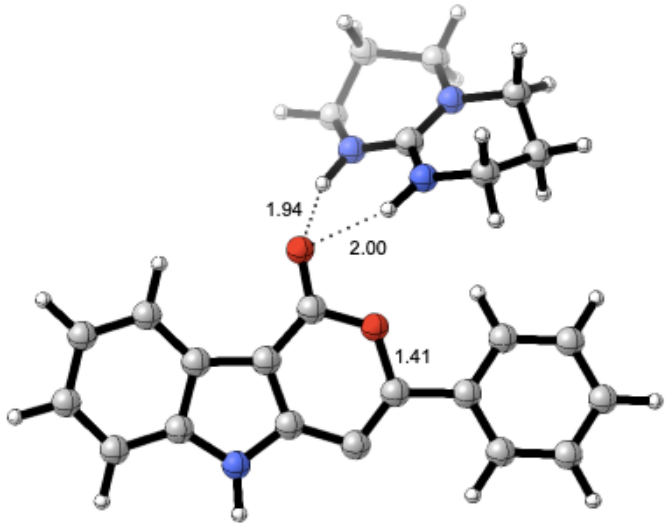
```
Counterpoise corrected energy =   -1298.381700714511
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.870551	-0.646708	0.038921
2	6	0	4.845382	0.268056	-0.424795
3	6	0	6.168920	-0.102792	-0.648784
4	6	0	6.512104	-1.418819	-0.400480
5	6	0	5.560823	-2.344086	0.059882
6	6	0	4.247866	-1.973380	0.281087
7	6	0	2.647736	0.092572	0.155125
8	6	0	2.913451	1.395126	-0.236366
9	1	0	6.898842	0.612958	-1.004758
10	1	0	7.532236	-1.741932	-0.563382
11	1	0	5.866262	-3.366211	0.244422
12	1	0	3.514984	-2.684973	0.636486
13	7	0	4.231920	1.489415	-0.583060
14	6	0	1.969032	2.466740	-0.271193
15	6	0	0.767808	2.295799	0.090689
16	6	0	1.320847	-0.361982	0.556794
17	8	0	0.377091	0.518921	0.613241
18	8	0	1.112453	-1.560956	0.821208
19	6	0	-2.516506	-1.567647	-0.071985
20	7	0	-1.557454	-2.358925	0.407898

21	1	0	-0.636129	-1.952719	0.620314
22	7	0	-2.277179	-0.257900	-0.162693
23	7	0	-3.694654	-2.071011	-0.451776
24	6	0	-1.695673	-3.804581	0.461111
25	6	0	-4.024752	-3.487372	-0.290656
26	6	0	-3.143973	-4.145149	0.752706
27	6	0	-4.732236	-1.245783	-1.071619
28	6	0	-3.283176	0.694444	-0.603608
29	6	0	-4.152526	0.028460	-1.651980
30	1	0	-2.766666	1.568263	-0.999708
31	1	0	-3.892261	1.024380	0.242724
32	1	0	-3.550503	-0.203892	-2.532227
33	1	0	-4.962602	0.689689	-1.954872
34	1	0	-5.196331	-1.848983	-1.853195
35	1	0	-5.498763	-1.020282	-0.324754
36	1	0	-5.074321	-3.541075	0.001757
37	1	0	-3.921154	-3.986734	-1.258264
38	1	0	-3.296821	-5.222660	0.729225
39	1	0	-3.409828	-3.782043	1.746952
40	1	0	-1.381602	-4.256071	-0.484784
41	1	0	-1.035629	-4.171210	1.244913
42	1	0	-1.360591	0.071792	0.145086
43	1	0	4.672096	2.337929	-0.900416
44	6	0	-0.537139	2.892783	0.292457
45	6	0	-1.003787	3.831387	-0.632758
46	6	0	-1.323803	2.587741	1.407001
47	6	0	-2.232325	4.448330	-0.445674
48	1	0	-0.396168	4.067335	-1.496676
49	6	0	-2.548488	3.210155	1.589335
50	1	0	-0.963871	1.863725	2.124261
51	6	0	-3.009128	4.139025	0.664182
52	1	0	-2.585868	5.168901	-1.171986
53	1	0	-3.147428	2.966175	2.457560
54	1	0	-3.968722	4.618938	0.806787

Int7



Calculated using M06-2X/def2TZVP in acetonitrile at 373.15 K:

```
HF = -1298.4316993 hartrees
Zero-point correction=                           0.449232 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.369508
Sum of electronic and zero-point Energies=          -1297.982467
Sum of electronic and thermal Enthalpies=           -1297.943269
Sum of electronic and thermal Free Energies=        -1298.062191
```

Single Points using M06-2X/def2TZVP in the gas phase:

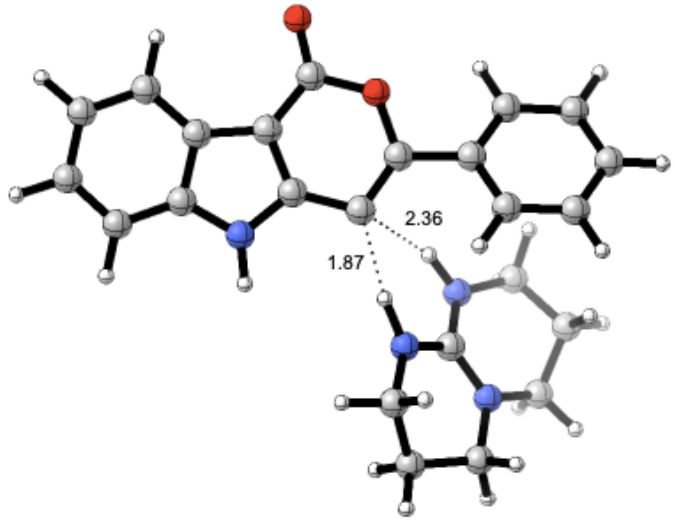
```
Counterpoise corrected energy =   -1298.390860274809
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.706252	1.003957	0.186440
2	6	0	-4.838527	0.221489	-0.137767
3	6	0	-6.119327	0.761104	-0.176554
4	6	0	-6.254958	2.108321	0.116923
5	6	0	-5.144209	2.898783	0.440430
6	6	0	-3.869254	2.358819	0.477061
7	6	0	-2.588222	0.105558	0.123591
8	6	0	-3.057195	-1.166349	-0.225046
9	1	0	-6.977107	0.150574	-0.427523
10	1	0	-7.239229	2.558151	0.094864
11	1	0	-5.289057	3.947774	0.664220
12	1	0	-3.011256	2.968460	0.728702
13	7	0	-4.411576	-1.069979	-0.378118
14	6	0	-2.279890	-2.350009	-0.392431
15	6	0	-0.975187	-2.082382	-0.162695
16	6	0	-1.208020	0.278436	0.353115
17	8	0	-0.451486	-0.824610	0.197105
18	8	0	-0.625337	1.318251	0.688314
19	6	0	2.680471	1.696897	0.188136
20	7	0	2.235544	0.757459	1.025137

21	1	0	1.226455	0.697841	1.129855
22	7	0	1.780800	2.472715	-0.420272
23	7	0	3.985040	1.856641	-0.031542
24	6	0	3.117756	-0.124906	1.769704
25	6	0	4.981565	0.962346	0.560574
26	6	0	4.364568	-0.368976	0.941985
27	6	0	4.498063	2.924874	-0.890888
28	6	0	2.143192	3.488961	-1.394401
29	6	0	3.497692	4.056975	-1.016767
30	1	0	1.373771	4.258002	-1.376828
31	1	0	2.174903	3.059949	-2.399657
32	1	0	3.417015	4.587472	-0.066486
33	1	0	3.840119	4.760079	-1.773836
34	1	0	5.425779	3.280723	-0.441789
35	1	0	4.738899	2.505845	-1.871887
36	1	0	5.766495	0.822190	-0.183048
37	1	0	5.427042	1.450926	1.431604
38	1	0	5.086715	-0.958248	1.504080
39	1	0	4.098991	-0.921229	0.038142
40	1	0	3.379166	0.320037	2.733526
41	1	0	2.579894	-1.052886	1.958342
42	1	0	0.806957	2.265714	-0.219401
43	1	0	-4.998058	-1.850083	-0.628791
44	6	0	0.140969	-3.049803	-0.249865
45	6	0	-0.137002	-4.419862	-0.290656
46	6	0	1.478410	-2.644695	-0.298839
47	6	0	0.883999	-5.351691	-0.372407
48	1	0	-1.171422	-4.734056	-0.255581
49	6	0	2.501098	-3.581465	-0.382591
50	1	0	1.715700	-1.588198	-0.285790
51	6	0	2.211561	-4.938464	-0.417062
52	1	0	0.645117	-6.407690	-0.397039
53	1	0	3.531241	-3.249288	-0.425002
54	1	0	3.010006	-5.666549	-0.480397

Int8



Calculated using M06-2X/def2TZVP in acetonitrile at 373.15 K:

```
HF = -1298.4389172 hartrees
Zero-point correction=                           0.448311 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.370151
Sum of electronic and zero-point Energies=          -1297.990606
Sum of electronic and thermal Enthalpies=           -1297.951705
Sum of electronic and thermal Free Energies=        -1298.068766
```

Single Points using M06-2X/def2TZVP in the gas phase:

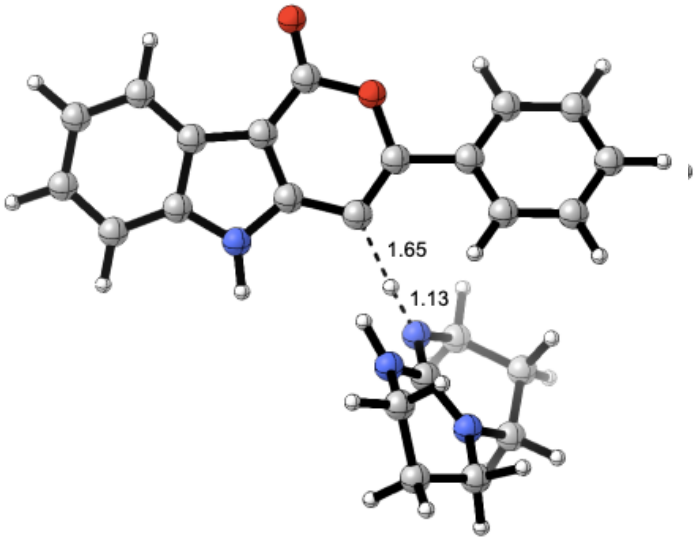
```
Counterpoise corrected energy =   -1298.402719660934
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.239334	-0.083125	0.153622
2	6	0	3.868221	-1.432827	-0.049505
3	6	0	4.790510	-2.471169	0.023570
4	6	0	6.104853	-2.139356	0.307113
5	6	0	6.491480	-0.807885	0.512622
6	6	0	5.571437	0.224016	0.438755
7	6	0	3.033163	0.677513	-0.003940
8	6	0	1.992702	-0.203913	-0.289732
9	1	0	4.490864	-3.499155	-0.135282
10	1	0	6.847391	-2.924232	0.372719
11	1	0	7.527963	-0.586441	0.732786
12	1	0	5.870535	1.251724	0.597339
13	7	0	2.512973	-1.467559	-0.311403
14	6	0	0.624518	0.144525	-0.513207
15	6	0	2.764680	2.071876	0.078813
16	8	0	1.463305	2.411434	-0.143515
17	8	0	3.553421	2.971127	0.317132
18	6	0	-2.451172	-1.402070	0.346446
19	7	0	-2.143982	-0.354268	1.126572
20	1	0	-1.229665	0.042791	0.940660

21	7	0	-1.512308	-1.852364	-0.477274
22	7	0	-3.656444	-1.968951	0.430548
23	6	0	-3.127948	0.473843	1.814735
24	6	0	-4.679068	-1.391940	1.298756
25	6	0	-4.524704	0.117089	1.341000
26	6	0	-3.993913	-3.164698	-0.340115
27	6	0	-1.751786	-2.965880	-1.377669
28	6	0	-2.739368	-3.922140	-0.734526
29	1	0	-0.798545	-3.457091	-1.570001
30	1	0	-2.143483	-2.606308	-2.334244
31	1	0	-2.287101	-4.369223	0.152719
32	1	0	-2.999619	-4.722811	-1.424749
33	1	0	-4.633501	-3.785194	0.287860
34	1	0	-4.569268	-2.875595	-1.224114
35	1	0	-5.646935	-1.669518	0.882953
36	1	0	-4.604353	-1.823682	2.301414
37	1	0	-5.265487	0.551115	2.010385
38	1	0	-4.687833	0.520006	0.339544
39	1	0	-3.040856	0.325178	2.893014
40	1	0	-2.900976	1.518389	1.590859
41	1	0	-0.673423	-1.203206	-0.596983
42	1	0	1.970740	-2.295379	-0.500810
43	6	0	0.458435	1.485330	-0.422181
44	6	0	-0.833888	2.192616	-0.564281
45	6	0	-1.061569	3.434656	0.034317
46	6	0	-1.877101	1.596806	-1.279635
47	6	0	-2.303250	4.049583	-0.060710
48	1	0	-0.263802	3.913898	0.585223
49	6	0	-3.113549	2.213424	-1.377171
50	1	0	-1.702151	0.640935	-1.757511
51	6	0	-3.335821	3.441694	-0.762303
52	1	0	-2.463395	5.007543	0.417830
53	1	0	-3.906985	1.737552	-1.940301
54	1	0	-4.302753	3.922407	-0.837983

TS3



Calculated using M06-2X/def2TZVP in acetonitrile at 373.15 K:

```
HF = -1298.4371368 hartrees
Zero-point correction=                           0.445578 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.365887
Sum of electronic and zero-point Energies=          -1297.991559
Sum of electronic and thermal Enthalpies=           -1297.953254
Sum of electronic and thermal Free Energies=        -1298.071250
```

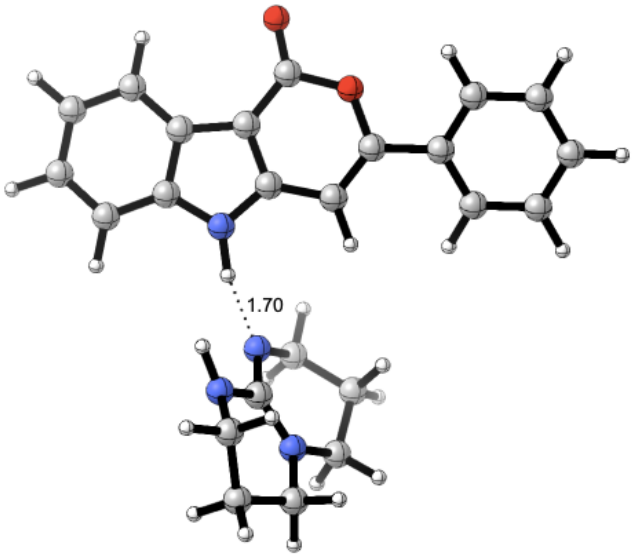
Single Points using M06-2X/def2TZVP in the gas phase:

```
Counterpoise corrected energy =   -1298.401475485965

                     Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -4.152652   -0.358778   -0.033539
     2          6           0       -3.594334   -1.638849   -0.255467
     3          6           0       -4.384658   -2.769455   -0.427813
     4          6           0       -5.758598   -2.602137   -0.376853
     5          6           0       -6.330538   -1.341057   -0.159698
     6          6           0       -5.540874   -0.217014    0.012629
     7          6           0       -3.036147    0.533390    0.093946
     8          6           0       -1.865114   -0.207312   -0.049851
     9          1           0       -3.941245   -3.742732   -0.594759
    10          1           0       -6.402759   -3.462141   -0.507200
    11          1           0       -7.408429   -1.247924   -0.126983
    12          1           0       -5.983441    0.756461    0.178817
    13          7           0       -2.218701   -1.510444   -0.259544
    14          6           0       -0.535479    0.310146    0.002871
    15          6           0       -2.955000    1.935378    0.314741
    16          8           0       -1.682333    2.427701    0.369266
    17          8           0       -3.872672    2.724706    0.458400
    18          6           0        2.466793   -1.552335   -0.123781
    19          7           0        1.763221   -0.874275   -1.010603
    20          1           0        0.806837   -0.425296   -0.614623
    21          7           0        1.841135   -1.914904    1.015489
```

22	7	0	3.746588	-1.891868	-0.318309
23	6	0	2.366552	-0.327024	-2.212248
24	6	0	4.471171	-1.402868	-1.490844
25	6	0	3.854601	-0.113892	-1.999706
26	6	0	4.505534	-2.700711	0.633819
27	6	0	2.541505	-2.530223	2.129106
28	6	0	3.587027	-3.472032	1.562488
29	1	0	1.812093	-3.068313	2.731000
30	1	0	3.014696	-1.772803	2.761979
31	1	0	3.089974	-4.274650	1.014923
32	1	0	4.174055	-3.917135	2.363980
33	1	0	5.130139	-3.383524	0.055934
34	1	0	5.169206	-2.045352	1.206074
35	1	0	5.505399	-1.241887	-1.184608
36	1	0	4.467535	-2.171954	-2.269161
37	1	0	4.339467	0.183853	-2.928214
38	1	0	4.005244	0.678238	-1.262603
39	1	0	2.199117	-0.997543	-3.060120
40	1	0	1.861383	0.615720	-2.430030
41	1	0	0.930010	-1.498305	1.156080
42	1	0	-1.560045	-2.258707	-0.405417
43	6	0	-0.543713	1.645444	0.218446
44	6	0	0.661111	2.498367	0.294820
45	6	0	0.616172	3.853290	-0.042071
46	6	0	1.882271	1.950123	0.696206
47	6	0	1.765584	4.630443	-0.002185
48	1	0	-0.323406	4.294532	-0.346065
49	6	0	3.028526	2.728899	0.739005
50	1	0	1.918128	0.911060	0.997026
51	6	0	2.976940	4.072226	0.384366
52	1	0	1.714154	5.676710	-0.276145
53	1	0	3.964134	2.288746	1.061833
54	1	0	3.872006	4.680009	0.417411

Int9



Calculated using M06-2X/def2TZVP in acetonitrile at 373.15 K:

```
HF = -1298.4779289 hartrees
Zero-point correction=                           0.447165 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.365103
Sum of electronic and zero-point Energies=          -1298.030764
Sum of electronic and thermal Enthalpies=           -1297.991531
Sum of electronic and thermal Free Energies=        -1298.112826
```

Single Points using M06-2X/def2TZVP in the gas phase:

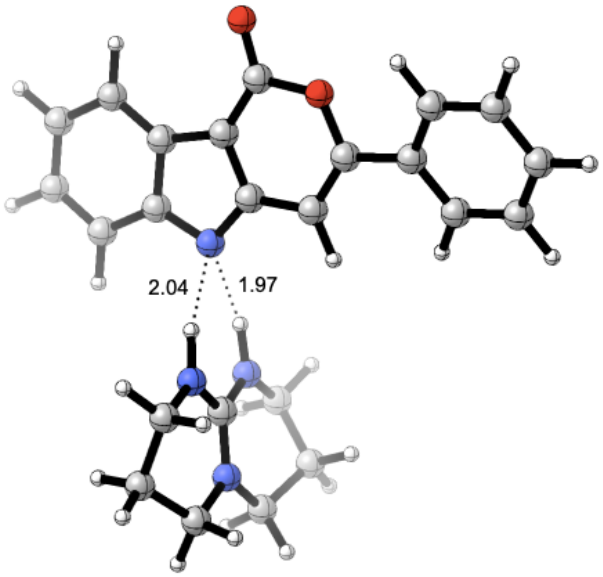
```
Counterpoise corrected energy =   -1298.455170564956
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.639355	3.148103	0.035870
2	6	0	-0.236556	3.017729	0.165898
3	6	0	0.598040	4.128054	0.257664
4	6	0	0.005549	5.377656	0.216505
5	6	0	-1.383816	5.523072	0.086432
6	6	0	-2.213848	4.420345	-0.004543
7	6	0	-2.143771	1.806726	-0.024130
8	6	0	-1.045973	0.955889	0.068564
9	1	0	1.669850	4.013211	0.356448
10	1	0	0.626573	6.261630	0.283721
11	1	0	-1.809898	6.517502	0.056467
12	1	0	-3.285340	4.534550	-0.104342
13	7	0	0.090122	1.674476	0.178468
14	6	0	-1.187642	-0.458595	0.035291
15	6	0	-2.445365	-0.935962	-0.076734
16	6	0	-3.454705	1.277242	-0.153430
17	8	0	-4.506420	1.868652	-0.249892
18	8	0	-3.518105	-0.109717	-0.163911
19	6	0	3.348226	-0.230388	-0.034445

20	7	0	3.635215	0.427539	-1.204353
21	1	0	2.885787	1.024383	-1.516470
22	7	0	2.329629	0.180173	0.660388
23	7	0	4.180865	-1.241089	0.327214
24	6	0	4.505420	-0.152754	-2.210005
25	1	0	4.014621	-0.970211	-2.751787
26	1	0	4.758157	0.624668	-2.928884
27	6	0	5.318855	-1.692830	-0.466437
28	1	0	6.140390	-1.904449	0.222054
29	1	0	5.055843	-2.636316	-0.958506
30	6	0	5.741404	-0.668118	-1.500102
31	1	0	6.250126	0.168401	-1.017973
32	1	0	6.431886	-1.128920	-2.205371
33	6	0	3.898575	-2.053588	1.505431
34	1	0	4.141684	-3.089229	1.257393
35	1	0	4.558184	-1.749631	2.324919
36	6	0	2.080580	-0.453637	1.943442
37	1	0	1.023150	-0.321973	2.189211
38	1	0	2.649823	0.045726	2.737742
39	6	0	2.445840	-1.928436	1.917115
40	1	0	2.297212	-2.393675	2.891449
41	1	0	1.813439	-2.446897	1.192091
42	1	0	-0.331223	-1.114863	0.065445
43	1	0	1.043057	1.229088	0.288650
44	6	0	-2.818978	-2.358362	-0.142898
45	6	0	-4.043409	-2.738580	-0.693712
46	6	0	-1.952564	-3.344206	0.333861
47	6	0	-4.384709	-4.080005	-0.781373
48	1	0	-4.722537	-1.981605	-1.060640
49	6	0	-2.297374	-4.682609	0.244110
50	1	0	-1.015381	-3.065684	0.797748
51	6	0	-3.513459	-5.055692	-0.316422
52	1	0	-5.334560	-4.363264	-1.216007
53	1	0	-1.619019	-5.436044	0.622592
54	1	0	-3.782252	-6.101900	-0.383253

Int10



Calculated using M06-2X/def2TZVP in acetonitrile at 373.15 K:

```
HF = -1298.4840367 hartrees
Zero-point correction=                           0.448721 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.366339
Sum of electronic and zero-point Energies=          -1298.035316
Sum of electronic and thermal Enthalpies=           -1297.996137
Sum of electronic and thermal Free Energies=        -1298.117698
```

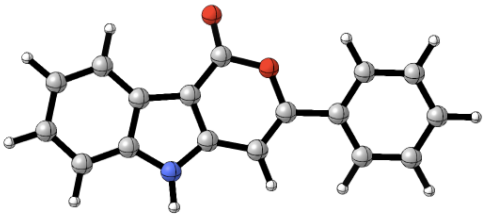
Single Points using M06-2X/def2TZVP in the gas phase:

```
Counterpoise corrected energy =   -1298.443117413520

                     Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.702984    3.187429    0.103392
     2          6           0        0.573253    2.563731    0.198005
     3          6           0        1.736601    3.337215    0.248929
     4          6           0        1.616280    4.714825    0.205969
     5          6           0        0.358076    5.332255    0.113107
     6          6           0       -0.803319    4.580816    0.060918
     7          6           0       -1.627186    2.097192    0.073044
     8          6           0       -0.841840    0.930343    0.151081
     9          1           0        2.707681    2.860462    0.321459
    10          1           0        2.506487    5.330540    0.243343
    11          1           0        0.299588    6.412994    0.081306
    12          1           0       -1.771058    5.061170   -0.013108
    13          1           0        1.807801    0.026113    1.092744
    14          7           0        0.472363    1.185266    0.225581
    15          6           0       -1.474329   -0.352268    0.132758
    16          6           0       -2.819006   -0.386893    0.048691
    17          6           0       -3.034807    2.035548   -0.023370
    18          8           0       -3.842531    2.942046   -0.102276
    19          8           0       -3.564499    0.749203   -0.025374
```

20	6	0	3.098216	-0.991330	-0.041013
21	7	0	2.590673	-0.633042	1.138852
22	7	0	2.542841	-0.475030	-1.140308
23	7	0	4.126239	-1.836298	-0.123460
24	6	0	3.144141	-1.083562	2.403781
25	6	0	4.704245	-2.462787	1.066124
26	6	0	3.715549	-2.476407	2.215755
27	6	0	4.740732	-2.183139	-1.405486
28	6	0	2.964570	-0.838909	-2.481864
29	6	0	4.453441	-1.128935	-2.457033
30	1	0	2.734809	-0.006148	-3.143064
31	1	0	2.411569	-1.715053	-2.831952
32	1	0	4.997789	-0.212900	-2.221512
33	1	0	4.788799	-1.486605	-3.428850
34	1	0	5.814068	-2.271401	-1.233611
35	1	0	4.370609	-3.161662	-1.724193
36	1	0	4.984930	-3.479483	0.789128
37	1	0	5.616151	-1.926208	1.342563
38	1	0	4.219202	-2.806926	3.122454
39	1	0	2.905518	-3.174910	1.998773
40	1	0	3.921820	-0.395834	2.747841
41	1	0	2.342570	-1.082311	3.139706
42	1	0	1.752617	0.147971	-0.976128
43	1	0	-0.895861	-1.263960	0.160523
44	6	0	-3.647592	-1.604586	-0.000888
45	6	0	-4.943683	-1.553372	-0.516040
46	6	0	-3.151384	-2.827766	0.456513
47	6	0	-5.718540	-2.702258	-0.586739
48	1	0	-5.339379	-0.610830	-0.868068
49	6	0	-3.927930	-3.972726	0.384396
50	1	0	-2.161118	-2.883745	0.889113
51	6	0	-5.214335	-3.915782	-0.139497
52	1	0	-6.720122	-2.646804	-0.993425
53	1	0	-3.531423	-4.911685	0.748795
54	1	0	-5.820613	-4.810845	-0.190508

B



Calculated using M06-2X/def2TZVP in acetonitrile at 373.15 K:

```
HF = -859.657192 hartrees
Zero-point correction=                           0.240111 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.182821
Sum of electronic and zero-point Energies=           -859.417081
Sum of electronic and thermal Enthalpies=            -859.393831
Sum of electronic and thermal Free Energies=         -859.474371
```

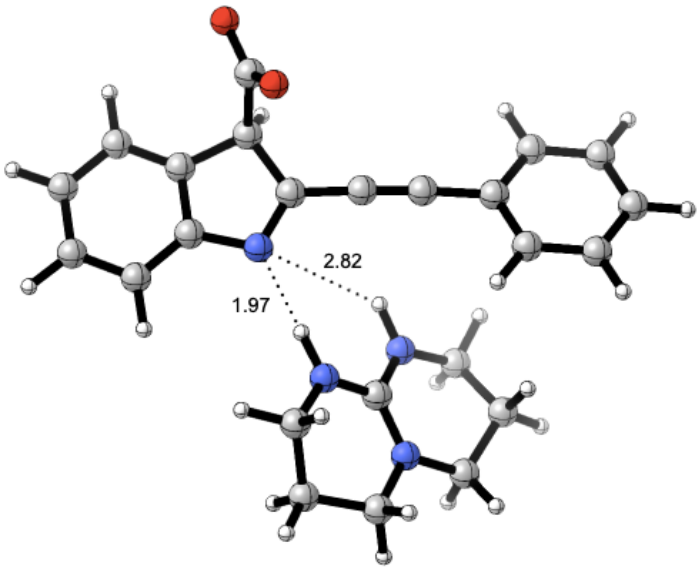
Single Points using M06-2X/def2TZVP in the gas phase:

```
HF = -859.640199 hartrees
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.711377	0.318071	0.019906
2	6	0	3.012169	-1.057073	-0.077607
3	6	0	4.319169	-1.528479	-0.115641
4	6	0	5.332572	-0.588297	-0.055305
5	6	0	5.053116	0.782760	0.040239
6	6	0	3.751329	1.247632	0.078505
7	6	0	1.279139	0.403811	0.034574
8	6	0	0.780755	-0.888895	-0.052757
9	1	0	4.532714	-2.586587	-0.189436
10	1	0	6.362659	-0.919014	-0.082184
11	1	0	5.873896	1.486513	0.085235
12	1	0	3.535308	2.305029	0.152803
13	7	0	1.817711	-1.758718	-0.120902
14	6	0	-0.612606	-1.160221	-0.071110
15	6	0	-1.434262	-0.091480	0.016566
16	6	0	0.390881	1.511597	0.112917
17	8	0	0.657400	2.688092	0.187695
18	8	0	-0.953350	1.172281	0.104991
19	1	0	-1.001274	-2.160554	-0.172696
20	1	0	1.732179	-2.760262	-0.189598
21	6	0	-2.905594	-0.139374	0.007979
22	6	0	-3.643299	1.003584	-0.304275
23	6	0	-3.580492	-1.325441	0.304211
24	6	0	-5.029036	0.954687	-0.333526
25	1	0	-3.128028	1.926715	-0.530035
26	6	0	-4.964277	-1.369164	0.274202
27	1	0	-3.027467	-2.213615	0.579503
28	6	0	-5.693454	-0.229970	-0.047064
29	1	0	-5.590423	1.845770	-0.582398
30	1	0	-5.476036	-2.292736	0.510695
31	1	0	-6.774826	-0.265698	-0.067952

IntS4a



Calculated using M06-2X/def2TZVP in acetonitrile at 373.15 K:

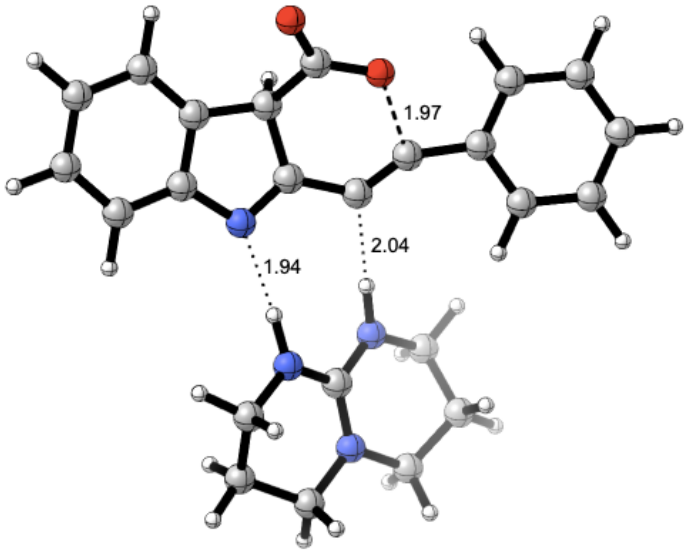
```
HF = -1298.4184906 hartrees
Zero-point correction=                           0.445870 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.360363
Sum of electronic and zero-point Energies=          -1297.972620
Sum of electronic and thermal Enthalpies=           -1297.931542
Sum of electronic and thermal Free Energies=        -1298.058127
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.895901	-0.264185	-0.521130
2	6	0	3.103289	0.850550	-0.231533
3	6	0	3.626687	2.132914	-0.204372
4	6	0	4.982425	2.279866	-0.476447
5	6	0	5.780087	1.173036	-0.761289
6	6	0	5.244293	-0.113162	-0.782913
7	6	0	3.015050	-1.470720	-0.427693
8	6	0	1.704911	-0.809484	-0.122133
9	1	0	2.998936	2.985590	0.020912
10	1	0	5.425164	3.267387	-0.464861
11	1	0	6.832828	1.316634	-0.967835
12	1	0	5.865753	-0.973078	-0.997497
13	1	0	2.968599	-2.053258	-1.349033
14	7	0	1.761946	0.476025	0.005193
15	6	0	0.475121	-1.509280	0.015374
16	6	0	-0.592419	-2.065031	0.087532
17	6	0	3.528950	-2.431283	0.715829
18	8	0	4.463194	-3.172755	0.373475
19	8	0	2.978941	-2.315142	1.823129
20	6	0	-1.700594	1.958267	-0.114247
21	7	0	-1.716862	0.871230	-0.894844
22	1	0	-0.915931	0.258951	-0.848438

23	7	0	-0.604159	2.208634	0.599055
24	7	0	-2.760869	2.761688	-0.055889
25	6	0	-2.846102	0.494498	-1.732658
26	6	0	-3.998955	2.465045	-0.778417
27	6	0	-4.122353	0.984514	-1.077070
28	6	0	-2.744002	4.010891	0.708665
29	6	0	-0.505497	3.340261	1.508681
30	6	0	-1.326518	4.487979	0.953281
31	1	0	0.545806	3.607205	1.592686
32	1	0	-0.864743	3.058321	2.501718
33	1	0	-0.883876	4.833440	0.017458
34	1	0	-1.341054	5.320902	1.653798
35	1	0	-3.303963	4.747092	0.131333
36	1	0	-3.270840	3.852774	1.653495
37	1	0	-4.824376	2.798448	-0.149099
38	1	0	-4.019353	3.053296	-1.699772
39	1	0	-4.972714	0.816332	-1.735492
40	1	0	-4.293986	0.433320	-0.150712
41	1	0	-2.736596	0.924105	-2.731313
42	1	0	-2.841291	-0.590972	-1.824321
43	1	0	0.214468	1.612880	0.445556
44	6	0	-1.888098	-2.659017	0.165108
45	6	0	-2.921169	-1.975872	0.815726
46	6	0	-2.139758	-3.900740	-0.425062
47	6	0	-4.189893	-2.529094	0.867183
48	1	0	-2.715492	-1.017250	1.276083
49	6	0	-3.411847	-4.445985	-0.367465
50	1	0	-1.336967	-4.424383	-0.926860
51	6	0	-4.437364	-3.762338	0.275385
52	1	0	-4.987246	-1.998718	1.371448
53	1	0	-3.603769	-5.406771	-0.826606
54	1	0	-5.429710	-4.191906	0.317883

TS-S2



Calculated using M06-2X/def2TZVP in acetonitrile at 373.15 K:

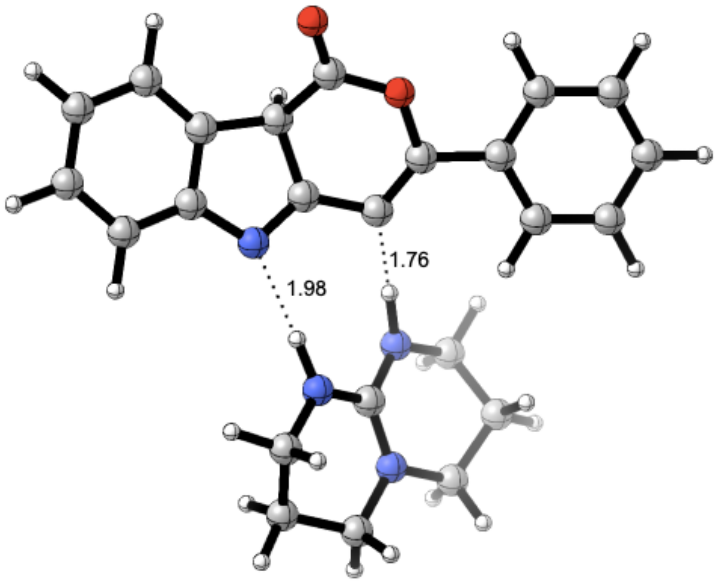
```
HF = -1298.3820817 hartrees
Zero-point correction=                           0.444869 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.362386
Sum of electronic and zero-point Energies=          -1297.937213
Sum of electronic and thermal Enthalpies=           -1297.897714
Sum of electronic and thermal Free Energies=        -1298.019696
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.500644	-1.228905	0.408389
2	6	0	2.461462	-2.135772	0.165166
3	6	0	2.709008	-3.483971	-0.038949
4	6	0	4.030966	-3.914706	0.007817
5	6	0	5.068924	-3.018581	0.251667
6	6	0	4.810531	-1.663966	0.457565
7	6	0	2.866283	0.109291	0.599872
8	6	0	1.412461	-0.241772	0.388990
9	1	0	1.896941	-4.174686	-0.227096
10	1	0	4.256306	-4.961823	-0.149416
11	1	0	6.089045	-3.379335	0.278512
12	1	0	5.616840	-0.965672	0.638494
13	1	0	2.998059	0.478883	1.624125
14	7	0	1.201181	-1.497086	0.158709
15	6	0	0.434929	0.795111	0.369704
16	6	0	0.662232	1.997492	0.081440
17	6	0	3.344762	1.286494	-0.293164
18	8	0	4.471618	1.222001	-0.773673
19	8	0	2.545251	2.268193	-0.418921
20	6	0	-2.656896	-1.427348	0.124816
21	7	0	-2.384669	-0.312408	0.806356
22	1	0	-1.436874	0.070488	0.729090
23	7	0	-1.645142	-2.120642	-0.396801

24	7	0	-3.917496	-1.839505	-0.027193
25	6	0	-3.420985	0.498042	1.424703
26	6	0	-5.060405	-1.027037	0.393979
27	6	0	-4.673355	0.427581	0.571583
28	6	0	-4.250775	-3.131404	-0.629047
29	6	0	-1.856400	-3.320026	-1.190314
30	6	0	-3.056846	-4.065130	-0.637832
31	1	0	-0.949865	-3.918811	-1.129090
32	1	0	-2.020041	-3.059765	-2.239746
33	1	0	-2.838052	-4.402653	0.376599
34	1	0	-3.285649	-4.937207	-1.247984
35	1	0	-5.070186	-3.556271	-0.047207
36	1	0	-4.616535	-2.960078	-1.645322
37	1	0	-5.828632	-1.132857	-0.373263
38	1	0	-5.459596	-1.437767	1.325603
39	1	0	-5.493493	0.963891	1.045865
40	1	0	-4.478313	0.884944	-0.400215
41	1	0	-3.628884	0.139753	2.436428
42	1	0	-3.041546	1.515658	1.499899
43	1	0	-0.682653	-1.855197	-0.164176
44	6	0	0.143124	3.328783	-0.117485
45	6	0	-1.199969	3.451800	-0.492122
46	6	0	0.902779	4.479505	0.097999
47	6	0	-1.772602	4.704860	-0.635943
48	1	0	-1.780756	2.555712	-0.672896
49	6	0	0.322405	5.729676	-0.050646
50	1	0	1.940600	4.380016	0.377800
51	6	0	-1.012965	5.847530	-0.415649
52	1	0	-2.811407	4.789010	-0.927700
53	1	0	0.916400	6.617885	0.121894
54	1	0	-1.459655	6.826527	-0.532189

IntS5



Calculated using M06-2X/def2TZVP in acetonitrile at 373.15 K:

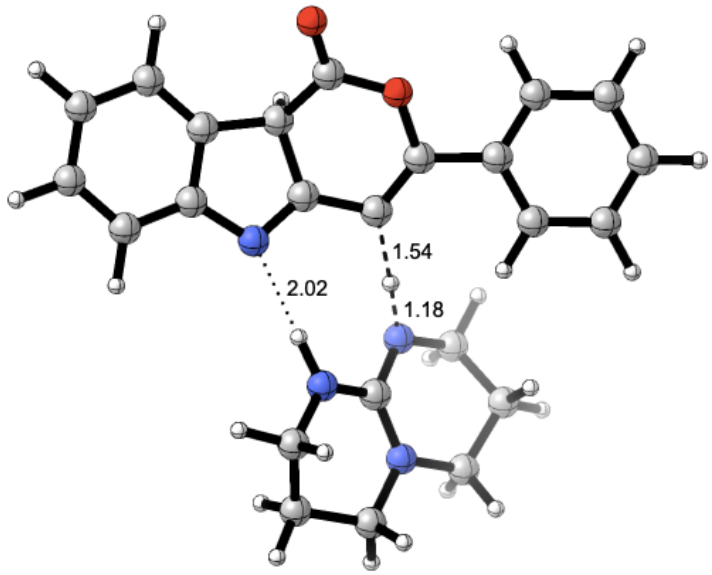
```
HF = -1298.4023978 hartrees
Zero-point correction=                           0.445868 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.366528
Sum of electronic and zero-point Energies=          -1297.956530
Sum of electronic and thermal Enthalpies=           -1297.917632
Sum of electronic and thermal Free Energies=        -1298.035869
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.725570	-0.539646	0.427969
2	6	0	2.915447	-1.643168	0.121492
3	6	0	3.471242	-2.892140	-0.105208
4	6	0	4.855557	-3.015997	-0.021746
5	6	0	5.659971	-1.922449	0.283683
6	6	0	5.095504	-0.668170	0.520133
7	6	0	2.787250	0.604009	0.642044
8	6	0	1.450947	-0.033137	0.328663
9	1	0	2.843401	-3.741598	-0.342457
10	1	0	5.314485	-3.980836	-0.197241
11	1	0	6.733649	-2.046331	0.337870
12	1	0	5.719338	0.182906	0.761127
13	1	0	2.789746	0.942820	1.686745
14	7	0	1.546711	-1.302606	0.069207
15	6	0	0.272942	0.775863	0.266563
16	6	0	0.529397	2.041857	-0.076716
17	6	0	2.949418	1.859393	-0.180236
18	8	0	4.002577	2.272248	-0.584509
19	8	0	1.828112	2.549017	-0.417158
20	6	0	-2.274264	-1.787846	0.143537
21	7	0	-2.083778	-0.691900	0.869039
22	1	0	-1.190180	-0.111492	0.668836
23	7	0	-1.218355	-2.334166	-0.470021

24	7	0	-3.486499	-2.346311	0.023707
25	6	0	-3.178267	-0.064568	1.585626
26	6	0	-4.694741	-1.688390	0.521589
27	6	0	-4.458953	-0.213362	0.783713
28	6	0	-3.697370	-3.637165	-0.629984
29	6	0	-1.330589	-3.509153	-1.315467
30	6	0	-2.403780	-4.418754	-0.747216
31	1	0	-0.358870	-3.999751	-1.329939
32	1	0	-1.579758	-3.224458	-2.341979
33	1	0	-2.091322	-4.775913	0.235533
34	1	0	-2.560689	-5.281735	-1.392358
35	1	0	-4.428884	-4.187469	-0.035369
36	1	0	-4.134801	-3.465341	-1.617970
37	1	0	-5.472764	-1.828595	-0.230839
38	1	0	-5.020704	-2.194477	1.435102
39	1	0	-5.310807	0.199000	1.322540
40	1	0	-4.359351	0.323389	-0.162533
41	1	0	-3.299438	-0.520036	2.572908
42	1	0	-2.914627	0.982788	1.735338
43	1	0	-0.288509	-1.961532	-0.263005
44	6	0	-0.458162	3.127448	-0.220802
45	6	0	-1.814375	2.806313	-0.338822
46	6	0	-0.089484	4.474155	-0.225787
47	6	0	-2.774104	3.799620	-0.429910
48	1	0	-2.099929	1.762682	-0.376686
49	6	0	-1.054136	5.469627	-0.319153
50	1	0	0.954760	4.743021	-0.147435
51	6	0	-2.398383	5.139402	-0.416920
52	1	0	-3.818655	3.529296	-0.522943
53	1	0	-0.750521	6.508977	-0.314455
54	1	0	-3.147461	5.916996	-0.493253

TS-S3



Calculated using M06-2X/def2TZVP in acetonitrile at 373.15 K:

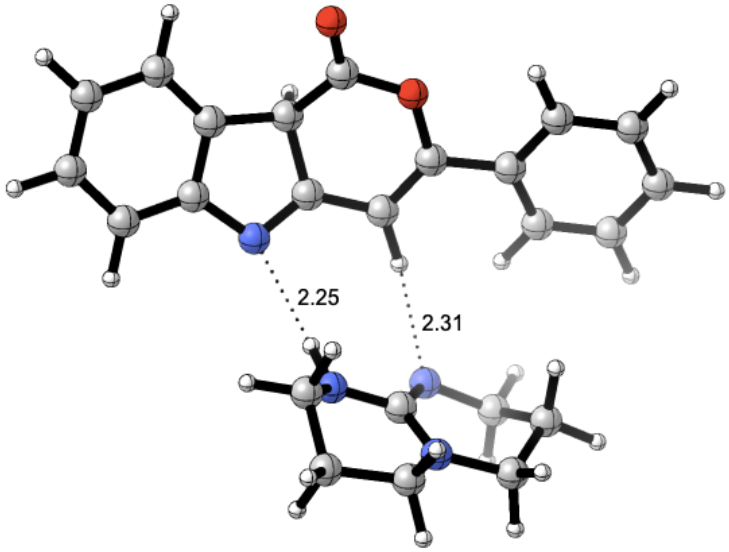
```
HF = -1298.4018223 hartrees
Zero-point correction=                           0.442501 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.363881
Sum of electronic and zero-point Energies=          -1297.959321
Sum of electronic and thermal Enthalpies=           -1297.920872
Sum of electronic and thermal Free Energies=        -1298.037942
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.781516	-0.335652	0.400787
2	6	0	3.047157	-1.500086	0.132670
3	6	0	3.684191	-2.712475	-0.074638
4	6	0	5.074720	-2.737864	-0.011195
5	6	0	5.804805	-1.583674	0.255684
6	6	0	5.158715	-0.366007	0.472657
7	6	0	2.766254	0.740797	0.611725
8	6	0	1.477351	0.005672	0.321039
9	1	0	3.113266	-3.608331	-0.282633
10	1	0	5.596979	-3.672091	-0.173738
11	1	0	6.885177	-1.630960	0.294829
12	1	0	5.725303	0.531693	0.684107
13	1	0	2.749133	1.076703	1.657910
14	7	0	1.656204	-1.257759	0.091015
15	6	0	0.243038	0.731514	0.255251
16	6	0	0.401675	2.017248	-0.079248
17	6	0	2.827279	2.006660	-0.202771
18	8	0	3.835395	2.497158	-0.629044
19	8	0	1.651597	2.622111	-0.403268
20	6	0	-2.146903	-1.858603	0.163283
21	7	0	-1.941810	-0.766894	0.878425
22	7	0	-1.096921	-2.407168	-0.471383

23	7	0	-3.358781	-2.432274	0.052274
24	6	0	-3.034346	-0.163815	1.615772
25	6	0	-4.564212	-1.785446	0.567109
26	6	0	-4.331540	-0.311546	0.838813
27	6	0	-3.571844	-3.720703	-0.602930
28	6	0	-1.220366	-3.569286	-1.330461
29	6	0	-2.275808	-4.492988	-0.751654
30	1	0	-0.247221	-4.055331	-1.375347
31	1	0	-1.495389	-3.274306	-2.348030
32	1	0	-1.941730	-4.856987	0.221498
33	1	0	-2.439289	-5.351118	-1.401909
34	1	0	-4.287397	-4.281489	0.001979
35	1	0	-4.030092	-3.549652	-1.582124
36	1	0	-5.351135	-1.923142	-0.177111
37	1	0	-4.879364	-2.299311	1.480548
38	1	0	-5.176174	0.092343	1.395854
39	1	0	-4.253562	0.233292	-0.105152
40	1	0	-3.138314	-0.629871	2.601212
41	1	0	-2.782385	0.886097	1.777013
42	1	0	-0.170648	-2.031762	-0.269514
43	1	0	-1.008587	-0.093735	0.608403
44	6	0	-0.671262	3.016752	-0.227432
45	6	0	-1.988091	2.587813	-0.418691
46	6	0	-0.415123	4.387545	-0.164769
47	6	0	-3.022738	3.502782	-0.517280
48	1	0	-2.184426	1.526653	-0.508701
49	6	0	-1.454539	5.303136	-0.263432
50	1	0	0.598977	4.737036	-0.029056
51	6	0	-2.760701	4.866700	-0.435865
52	1	0	-4.036074	3.152457	-0.669340
53	1	0	-1.240823	6.362770	-0.204714
54	1	0	-3.568385	5.582711	-0.516332

IntS6



Calculated using M06-2X/def2TZVP in acetonitrile at 373.15 K:

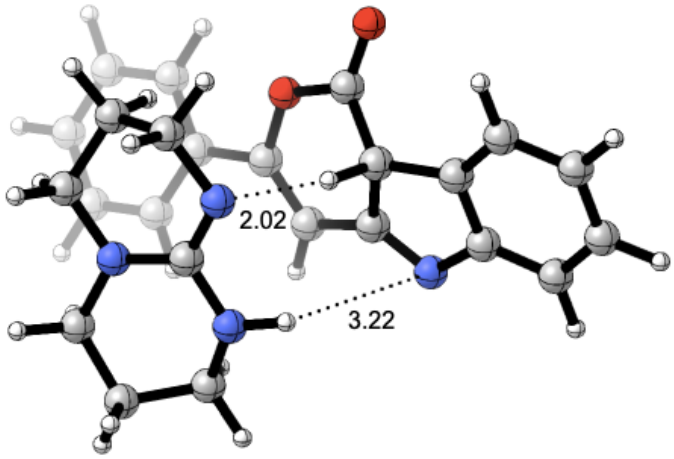
```
HF = -1298.4293094 hartrees
Zero-point correction=                           0.446815 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.364783
Sum of electronic and zero-point Energies=          -1297.982495
Sum of electronic and thermal Enthalpies=           -1297.943305
Sum of electronic and thermal Free Energies=        -1298.064527
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.895104	0.317865	-0.280275
2	6	0	-3.399368	-0.969616	-0.529699
3	6	0	-4.231583	-2.075274	-0.495837
4	6	0	-5.574526	-1.867005	-0.195293
5	6	0	-6.066628	-0.590014	0.057844
6	6	0	-5.227749	0.523493	0.008617
7	6	0	-2.733351	1.236654	-0.477373
8	6	0	-1.611110	0.250454	-0.677606
9	1	0	-3.841751	-3.065695	-0.691609
10	1	0	-6.247807	-2.713499	-0.155514
11	1	0	-7.114195	-0.458364	0.294419
12	1	0	-5.613204	1.516787	0.197951
13	1	0	-2.842156	1.784296	-1.426967
14	7	0	-2.003691	-0.972444	-0.766865
15	6	0	-0.271343	0.757031	-0.673759
16	6	0	-0.064902	1.968538	-0.127923
17	6	0	-2.374088	2.293848	0.519865
18	8	0	-3.116051	2.835517	1.277838
19	8	0	-1.072318	2.701906	0.466958
20	6	0	1.941231	-2.163240	-0.474087
21	7	0	2.215627	-1.392004	-1.477592
22	7	0	0.638355	-2.576671	-0.311745
23	7	0	2.849263	-2.650643	0.426233
24	6	0	3.616697	-1.080878	-1.697313

25	6	0	4.229252	-2.178464	0.419723
26	6	0	4.366208	-0.902212	-0.386690
27	6	0	2.504798	-3.475024	1.579089
28	6	0	0.157302	-3.071985	0.961913
29	6	0	1.139602	-4.120124	1.445203
30	1	0	-0.834227	-3.495297	0.805999
31	1	0	0.065342	-2.270838	1.707534
32	1	0	1.174964	-4.935118	0.719949
33	1	0	0.837348	-4.529746	2.408571
34	1	0	3.280795	-4.236946	1.690071
35	1	0	2.533438	-2.852950	2.482224
36	1	0	4.529659	-2.012335	1.457679
37	1	0	4.880934	-2.960235	0.014451
38	1	0	5.421151	-0.680779	-0.552087
39	1	0	3.925332	-0.067907	0.164843
40	1	0	4.101767	-1.875813	-2.280688
41	1	0	3.682080	-0.174507	-2.303909
42	1	0	-0.032381	-2.062367	-0.865634
43	1	0	0.559668	0.154098	-1.022730
44	6	0	1.238220	2.637604	-0.011054
45	6	0	2.331967	2.167527	-0.743424
46	6	0	1.403486	3.737107	0.832229
47	6	0	3.566643	2.781541	-0.624749
48	1	0	2.215744	1.322207	-1.410066
49	6	0	2.643743	4.348098	0.946992
50	1	0	0.563594	4.108444	1.401799
51	6	0	3.727501	3.872843	0.222194
52	1	0	4.406674	2.408634	-1.197251
53	1	0	2.761865	5.197014	1.607565
54	1	0	4.694058	4.351255	0.313294

IntS7



Calculated using M06-2X/def2TZVP in acetonitrile at 373.15 K:

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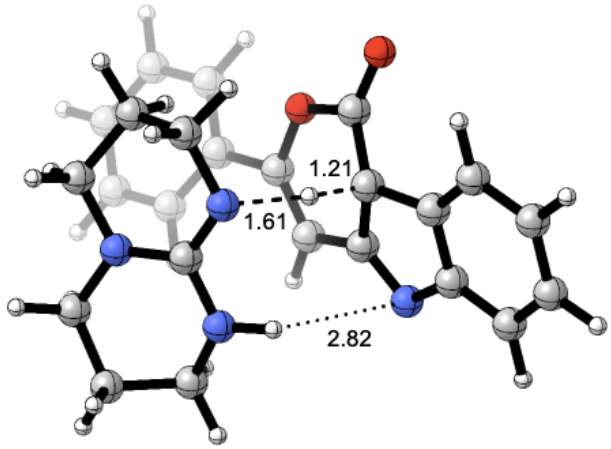
HF = -1298.4339656 hartrees
Zero-point correction=                           0.446622 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.367720
Sum of electronic and zero-point Energies=          -1297.987344
Sum of electronic and thermal Enthalpies=           -1297.948240
Sum of electronic and thermal Free Energies=        -1298.066246
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.446001	-0.408853	0.143883
2	6	0	-3.673437	0.172168	-1.114112
3	6	0	-4.947541	0.553497	-1.504099
4	6	0	-5.994340	0.326624	-0.616791
5	6	0	-5.770932	-0.259344	0.627007
6	6	0	-4.486311	-0.626167	1.024965
7	6	0	-1.973107	-0.593103	0.229468
8	6	0	-1.543295	-0.210588	-1.156293
9	1	0	-5.114963	1.007123	-2.472385
10	1	0	-7.001078	0.607984	-0.897997
11	1	0	-6.605432	-0.429671	1.294557
12	1	0	-4.313181	-1.072970	1.995375
13	1	0	-1.497208	0.178643	0.892827
14	7	0	-2.490719	0.277315	-1.882315
15	6	0	-0.171002	-0.439741	-1.499007
16	6	0	0.547274	-1.254056	-0.705234
17	6	0	-1.324041	-1.838591	0.711725
18	8	0	-1.786856	-2.665628	1.435732
19	8	0	-0.011431	-1.961548	0.335672
20	6	0	0.750230	1.795729	0.914679
21	7	0	0.012449	1.179349	1.783448
22	7	0	0.121546	2.531839	-0.057726
23	7	0	2.113564	1.800267	0.891118
24	6	0	0.698174	0.541102	2.893549
25	6	0	2.883920	0.961755	1.800492
26	6	0	2.014839	-0.088833	2.465884
27	6	0	2.926158	2.610000	-0.008805

28	6	0	0.816041	3.026527	-1.225380
29	6	0	2.113232	3.654506	-0.751154
30	1	0	0.179319	3.759546	-1.717527
31	1	0	1.026928	2.228925	-1.949722
32	1	0	1.877806	4.491488	-0.091767
33	1	0	2.694592	4.033297	-1.590993
34	1	0	3.710120	3.089296	0.584565
35	1	0	3.429018	1.945632	-0.721325
36	1	0	3.680031	0.485190	1.218201
37	1	0	3.364139	1.598566	2.551996
38	1	0	2.547062	-0.513852	3.317631
39	1	0	1.810727	-0.898019	1.764541
40	1	0	0.887335	1.271006	3.692180
41	1	0	0.036487	-0.218078	3.316201
42	1	0	-0.877956	2.412897	-0.086911
43	1	0	0.260865	-0.017920	-2.393335
44	6	0	1.977637	-1.553237	-0.862859
45	6	0	2.534105	-2.703554	-0.301478
46	6	0	2.801889	-0.668360	-1.560410
47	6	0	3.887761	-2.966485	-0.448867
48	1	0	1.905415	-3.389280	0.249401
49	6	0	4.153340	-0.933881	-1.704363
50	1	0	2.389327	0.241307	-1.976930
51	6	0	4.700518	-2.084723	-1.148996
52	1	0	4.308546	-3.863574	-0.014108
53	1	0	4.782330	-0.236368	-2.242154
54	1	0	5.757527	-2.289519	-1.258060

TS-S4



Calculated using M06-2X/def2TZVP in acetonitrile at 373.15 K:

```
HF = -1298.4333412 hartrees
Zero-point correction=                           0.444083 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=         0.369055
Sum of electronic and zero-point Energies=          -1297.989258
Sum of electronic and thermal Enthalpies=           -1297.951368
Sum of electronic and thermal Free Energies=        -1298.064287
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.287575	-0.583380	0.087968
2	6	0	-3.517555	0.069232	-1.138149
3	6	0	-4.791604	0.497231	-1.487959
4	6	0	-5.831308	0.243468	-0.602538
5	6	0	-5.605743	-0.414774	0.606969
6	6	0	-4.327008	-0.827602	0.968778
7	6	0	-1.831271	-0.799032	0.136784
8	6	0	-1.401063	-0.359248	-1.212293
9	1	0	-4.962543	1.005032	-2.428485
10	1	0	-6.835463	0.559019	-0.855541
11	1	0	-6.437005	-0.603970	1.273739
12	1	0	-4.151733	-1.329821	1.911400
13	1	0	-1.296526	0.051641	0.816436
14	7	0	-2.344559	0.194288	-1.908289
15	6	0	-0.018297	-0.538463	-1.542792
16	6	0	0.719485	-1.323143	-0.736124
17	6	0	-1.152441	-1.991983	0.646205
18	8	0	-1.577040	-2.830165	1.387639
19	8	0	0.174703	-2.066264	0.283269
20	6	0	0.441846	1.788984	0.827349
21	7	0	-0.292759	1.034221	1.598966
22	7	0	-0.176327	2.446855	-0.194727
23	7	0	1.776746	1.980557	0.967230
24	6	0	0.341750	0.413530	2.749751
25	6	0	2.538361	1.261358	1.982069
26	6	0	1.790056	0.038181	2.474024
27	6	0	2.565053	2.914080	0.168024

28	6	0	0.561187	3.078516	-1.268121
29	6	0	1.699526	3.861101	-0.641341
30	1	0	-0.118508	3.733360	-1.809732
31	1	0	0.954111	2.341303	-1.979706
32	1	0	1.281390	4.634917	0.004343
33	1	0	2.308280	4.343760	-1.404561
34	1	0	3.209351	3.475682	0.849338
35	1	0	3.222375	2.338311	-0.493331
36	1	0	3.491509	0.971738	1.530627
37	1	0	2.760447	1.941377	2.811535
38	1	0	2.271770	-0.345200	3.373669
39	1	0	1.827942	-0.746706	1.716656
40	1	0	0.296491	1.087362	3.613721
41	1	0	-0.236119	-0.474846	3.016811
42	1	0	-1.144627	2.206973	-0.335088
43	1	0	0.422315	-0.072569	-2.411088
44	6	0	2.172031	-1.523282	-0.841400
45	6	0	2.771250	-2.683631	-0.350474
46	6	0	2.970678	-0.526272	-1.403928
47	6	0	4.145104	-2.848565	-0.440569
48	1	0	2.159097	-3.453974	0.098001
49	6	0	4.343184	-0.693763	-1.489609
50	1	0	2.516609	0.392465	-1.753620
51	6	0	4.933838	-1.856771	-1.009378
52	1	0	4.600875	-3.754234	-0.062363
53	1	0	4.953482	0.089449	-1.920197
54	1	0	6.006565	-1.985723	-1.071557

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