

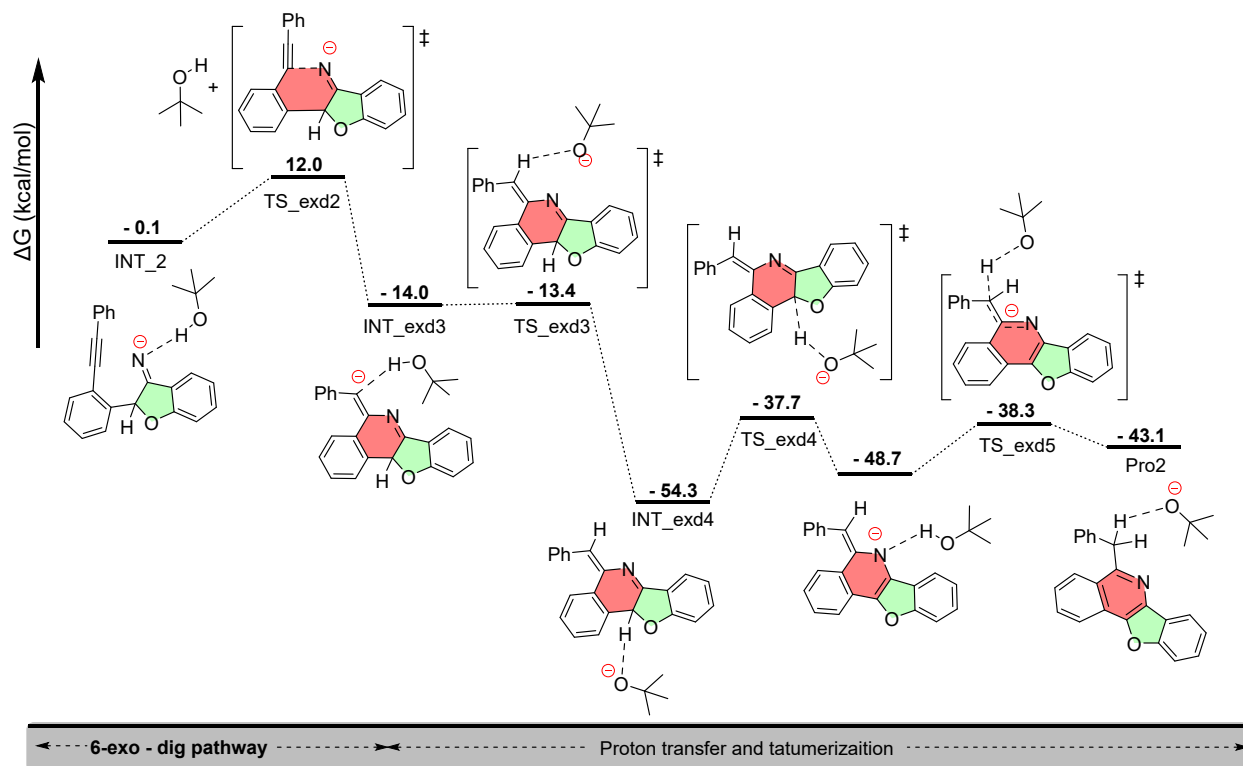
## Supporting Information

### **Anionic Aza $8\pi$ -electrocyclization as unprecedented pathway versus 7-end dig: DFT study on the mechanism of Base-Catalyzed of Benzofuroazepine synthesis via Cyclization of (2-Alkynylbenzyl)oxy Nitriles**

Omid Amiri, Ayoob Bazgir

### **Discussion of the M06-2X/6-311+G- (d,p)-CPCM(THF)//B3LYP/6-31G(d) study 6-exo-dig pathway**

**INT\_2** by deportation from tert-butanol through **TS\_exd2** result in **INT\_exd3**. It is worth noting that **TS\_exd2** is lower in terms of energy than **TS\_end2** (figure S1), and what is more important is that this mode of action 6-exo-dig result in a 6-membered ring that is not observed by experimental, but one of derivatives only as a trace amount as reported by Zeni.<sup>1</sup>

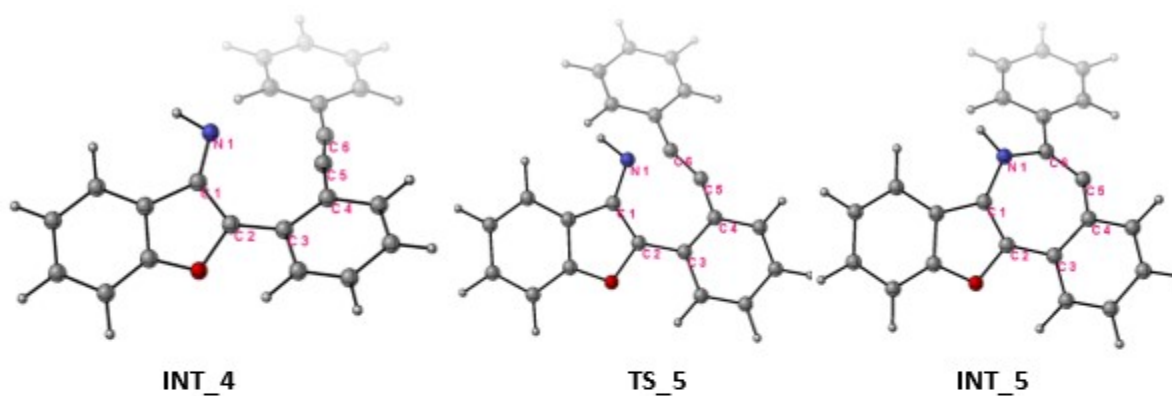


**Fig. S 1** calculated potential energy surface of the second cyclization through 6-exo-dig mode at M06-2X/6-311+G- (d,p)-CPCM(THF)//B3LYP/6-31G(d)

As it can be seen from **figure S 1**, INT\_exd4 can be easily formed through TS\_exd3. Pro\_2 can be formed from INT\_exd4 through intervention of tert-butoxide, tert-butanol (Figure S1).

## Comparison of bond length and bond order while going from Int\_4 to TS\_5 to Int\_5

As it can be seen from the tables in Fig. S2, the conjugation in forming 7-membered in TS\_5 can be deduced based on bond order and bond length in structure of TS\_5 relative to INT\_4 and INT\_5.



Bond length (Å)							
	N1-C1	C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	N1-C6
INT_4	1.32	1.44	1.42	1.45	1.41	1.22	3.26
TS_5	1.35	1.41	1.43	1.44	1.42	1.26	2.07
INT_5	1.40	1.38	1.44	1.44	1.43	1.34	1.48

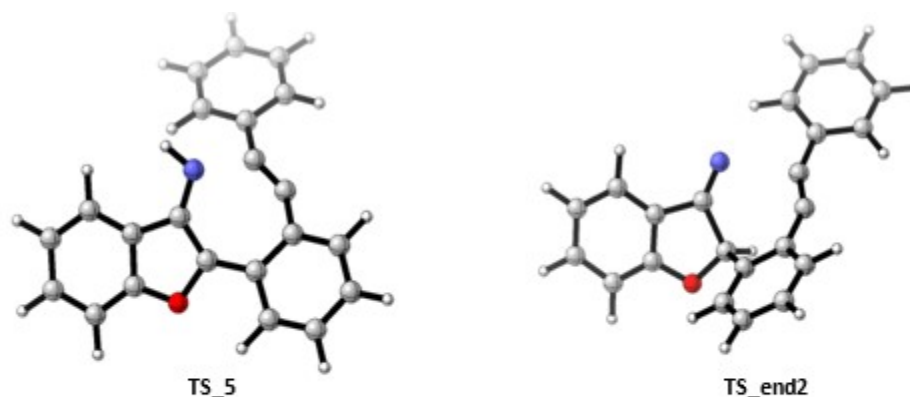
  

Bond order							
	N1-C1	C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	N1-C6
INT_4	1.71	0.74	1.14	1.35	1.01	2.37	-
TS_5	1.37	1.22	1.00	1.01	1.76	2.13	-
INT_5	1.08	1.29	0.85	1.15	1.34	2.06	0.76

**Fig. S 2** Bond length of forming 7-membered heterocycle in INT\_4, TS\_5, and INT\_5 at M06-2X/6-311+G- (d,p)-CPCM(THF)//B3LYP/6-31G(d)

**effect of functional on optimization and consequently the electronic energy calculated at M06-2X/6-311+G- (d,p)-CPCM(THF)**

As it can be seen from the Fig S3, the optimization of key transition states, namely **TS\_5** and **TS\_end2** at different functionals and subsequently calculating the electronic energy at M06-2X/6-311+G- (d,p)-CPCM(THF) level of theory has nearly no effect on the result that have been discussed in the main text with calculating at the M06-2X/6-311+G- (d,p)-CPCM(THF)//B3LYP/6-31G(d) level of theory.



Level of theory	TS_5 (hartree)	TS_end2 (hartree)	$\Delta G_{TS\_end2 - TS\_5}$ (kcal/mol)
wb97xd/6-31+g(d)	-976.3700	-976.3447	15.9
M062x/6-31+g(d)	-976.3706	-976.3454	15.8
b3lyp/6-31g(d)	-976.3709	-976.3477	14.6

**Fig. S 3** effect of different functional and basis set at the key transition state that is aza anionic 8 pi electrocyclization and 7-end-dig cyclization step (electronic energy calculated at M06-2X/6-311+G- (d,p)-CPCM(THF) at optimized structure at related level of theory)

## Cartesian coordinates, electronic energies, and imaginary frequencies

### INT\_2

E(B3lyp/6-31g(d) = -1210.380064 Hartree

Imaginary Freq= 0

-1 1

C	-4.86275400	1.59012900	-1.56324700
C	-4.35739400	0.32284800	-1.87915300
C	-3.11935500	-0.02469500	-1.34542600
C	-2.38597100	0.83519800	-0.52949900
C	-2.89380100	2.09841100	-0.22933400
C	-4.14162100	2.46948000	-0.74646700
H	-5.82954300	1.89172400	-1.96251800
H	-4.90016500	-0.36959800	-2.51765400
H	-2.30607400	2.77292500	0.38987000
H	-4.55349700	3.44979300	-0.51540400
C	-1.07278200	0.19974900	-0.16775200
N	-0.05558700	0.64124800	0.38999000
O	-2.51539600	-1.23369700	-1.57906100
C	-1.28224400	-1.30089300	-0.81508400
H	-0.46367900	-1.48029900	-1.51676400
C	-1.37256400	-2.40233000	0.19331900

C	-2.61499600	-2.83449400	0.68310600
C	-0.20061400	-3.02204300	0.71038700
C	-2.71354000	-3.83853400	1.64202500
H	-3.51376400	-2.37680000	0.28463100
C	-0.31662800	-4.04108400	1.67790300
C	-1.55963700	-4.44997900	2.14485500
H	-3.69424000	-4.14842700	1.99706000
H	0.59310100	-4.50077600	2.05465200
H	-1.63062200	-5.23600500	2.89298600
C	1.09088000	-2.62673900	0.26383800
C	2.19333300	-2.29014100	-0.12752000
C	3.36019100	-1.57632800	-0.52942700
C	4.59605600	-2.20212300	-0.77477000
C	3.25155000	-0.17594700	-0.67775600
C	5.70050900	-1.44577000	-1.16406000
H	4.67836100	-3.27943600	-0.65799400
C	4.36273000	0.56755400	-1.06537200
H	2.28726700	0.28414000	-0.46010500
C	5.58823500	-0.06107900	-1.31296300
H	6.65178000	-1.93889900	-1.35278300
H	4.27258000	1.64612600	-1.17006500
H	6.45176100	0.52562400	-1.61848600
C	0.89805400	3.88025600	1.14820200

C	0.69778600	5.28920500	1.72532600
H	1.54404100	5.94821900	1.48983800
H	-0.21653100	5.73558700	1.31703900
H	0.58901200	5.23582500	2.81491200
C	2.16471700	3.23654300	1.74884100
H	2.07575400	3.19298000	2.84082500
H	2.27282600	2.21114800	1.38095600
H	3.07422400	3.80000400	1.49612100
C	1.01415000	3.94784100	-0.38864100
H	1.89312500	4.52484100	-0.70956200
H	1.08591100	2.93581200	-0.79995100
H	0.11837900	4.41796200	-0.81157000
O	-0.24308900	3.13355200	1.52473700
H	-0.16875700	2.19975200	1.11063900

### INT\_1

E(B3lyp/6-31g(d) = -1210.369206 Hartree

Imaginary Freq= 0

-1 1

C	0.56676700	-3.93176200	0.56581200
C	-0.12808000	-2.85494200	0.02704500
C	0.48089000	-2.03445300	-0.94342200
C	1.79915900	-2.35695100	-1.37227800

C	2.47674800	-3.45399500	-0.81078200
C	1.87012000	-4.24498400	0.15679100
H	0.07995400	-4.53847400	1.32657900
H	-1.12729400	-2.61505300	0.37097300
H	3.48212900	-3.67394400	-1.15874900
H	2.39838700	-5.09307500	0.58334700
C	2.43876500	-1.60596800	-2.40807400
N	3.01043100	-1.06058800	-3.26420500
O	-0.08773100	-0.96973200	-1.51182600
C	-1.49698100	-0.74935000	-1.38603300
H	-2.53330600	-1.08951200	0.37300000
C	-1.94296800	0.57723300	-1.54306200
C	-3.28995600	0.78563400	-2.00202500
C	-1.20471500	1.77982400	-1.20699900
C	-3.84631200	2.03511400	-2.14881300
H	-3.87792100	-0.09589100	-2.25160600
C	-1.81072300	3.04943900	-1.38800600
C	-3.10352800	3.20173100	-1.85385300
H	-4.86876000	2.12207800	-2.51474100
H	-1.21592300	3.92365000	-1.13201800
H	-3.53848200	4.18956200	-1.98065200
C	0.08455600	1.76238600	-0.62582300
C	1.17156800	1.85820400	-0.07219000



C	2.43224900	1.95043700	0.56577300
C	2.98918400	3.20866500	0.89828900
C	3.17530400	0.79254600	0.89873600
C	4.22469900	3.30029300	1.53135000
H	2.43227700	4.10732800	0.64843300
C	4.40929000	0.89612300	1.53253100
H	2.76663700	-0.18102700	0.64740200
C	4.94573300	2.14686100	1.85545200
H	4.62954100	4.28087500	1.77458200
H	4.96037100	-0.01009800	1.77518500
H	5.91131000	2.22148000	2.35001100
H	-2.05217500	-1.53154900	-1.90667900
O	-3.05665900	-1.49078200	1.11932400
C	-3.04379500	-0.60258300	2.23913400
C	-3.85152600	0.66503100	1.90837200
H	-3.91015700	1.34054400	2.77225400
H	-3.39248700	1.21089700	1.07776700
H	-4.87052700	0.39178800	1.61101200
C	-1.59998400	-0.23570900	2.62346800
H	-1.57606700	0.41395600	3.50817300
H	-1.02410100	-1.14151700	2.84514400
H	-1.09895600	0.29193700	1.80449700
C	-3.71793000	-1.38283300	3.37514400

H	-3.77547600	-0.78213100	4.29115000
H	-4.73397600	-1.67224700	3.08296900
H	-3.15411600	-2.29729000	3.59219600

#### INT\_end4

E(B3lyp/6-31g(d) = -1210.390572 Hartree

Imaginary Freq= 0

-1 1

C	-4.80683400	-2.71889600	0.89932000
C	-4.76091500	-1.36782500	0.54334300
C	-3.52872500	-0.86991400	0.13569600
C	-2.36524700	-1.65343000	0.07421600
C	-2.42800600	-3.00509500	0.43490700
C	-3.65396200	-3.52639500	0.84532000
H	-5.75042800	-3.15211600	1.22368300
H	-5.64066600	-0.73167000	0.58032600
H	-1.52970900	-3.61367000	0.39131000
H	-3.72635000	-4.57372800	1.13124500
C	-1.29659700	-0.78908300	-0.39232200
N	-0.02297400	-1.27886700	-0.56009300
O	-3.26012600	0.40335900	-0.25148600
C	-1.89017900	0.44838500	-0.57072700
C	-1.40881800	1.74004900	-1.06022400

C	-2.30964600	2.78656000	-1.25918500
C	-0.01732500	1.92600300	-1.33550800
C	-1.89446500	4.04718100	-1.72442300
H	-3.35870200	2.61196100	-1.04347900
C	0.36194700	3.19547400	-1.80748300
C	-0.54995800	4.24375700	-1.99698000
H	-2.62149800	4.84400400	-1.86330200
H	1.41521200	3.36556600	-2.02255100
H	-0.19113200	5.20658400	-2.35734900
C	1.03047500	0.91764300	-1.16756200
C	0.97828000	-0.46235100	-0.91424200
C	2.28321200	-1.20369400	-1.06132600
C	2.26905100	-2.51506900	-1.56595600
C	3.52421000	-0.65002800	-0.70322900
C	3.45091100	-3.23119600	-1.74720700
H	1.30524500	-2.95285700	-1.80272100
C	4.70742800	-1.37176900	-0.87320700
H	3.55791500	0.33145200	-0.24099800
C	4.68062700	-2.66180000	-1.40570500
H	3.41273400	-4.24060700	-2.15327600
H	5.65397200	-0.92462300	-0.57538300
H	5.60414400	-3.22160600	-1.54066700
H	1.99642000	1.27142800	-1.52005500

H	1.77106100	1.44808600	0.81491700
C	1.72317200	1.24111200	2.78306300
C	0.27600700	1.74487900	2.91905400
H	0.25345100	2.83984700	2.88185000
H	-0.34205600	1.36388200	2.09850800
H	-0.17693700	1.41681000	3.86383400
C	1.76214100	-0.29713400	2.78267900
H	1.16376400	-0.70876000	1.96191000
H	2.79308600	-0.64686600	2.65727000
H	1.36990000	-0.70311100	3.72470300
C	2.59511100	1.79900500	3.91464600
H	2.23551300	1.46316400	4.89482100
H	3.63198600	1.46624700	3.79055500
H	2.58535100	2.89479200	3.89478900
O	2.30477300	1.75909500	1.58260700

### INT\_end5

E(B3lyp/6-31g(d) = -976.709065 Hartree

Imaginary Freq=0

-1 1

C	6.25770200	0.52949100	0.67072700
C	5.65758300	-0.33598600	-0.25065800
C	4.27737500	-0.24685300	-0.40203600

C	3.50749400	0.66821700	0.32891600
C	4.11796800	1.52595900	1.24375800
C	5.50256000	1.45083500	1.41107600
H	7.33469100	0.48308100	0.81409500
H	6.23576500	-1.05049100	-0.82810400
H	3.51289900	2.23220700	1.80471000
H	5.99987000	2.10807400	2.11938900
C	2.12557400	0.50752400	-0.11044900
N	1.12529700	1.23098800	0.22974800
O	3.54335200	-1.00884500	-1.26197800
C	2.13968200	-0.66360600	-1.09095000
C	1.33477700	-1.81734900	-0.54441100
C	1.88308900	-3.09074500	-0.36751000
C	-0.03705800	-1.58530700	-0.28342200
C	1.07118300	-4.15584400	0.01954400
H	2.93798100	-3.24476600	-0.56971700
C	-0.85557800	-2.69270300	0.04710100
C	-0.30337600	-3.95699700	0.20472700
H	1.50439700	-5.14670700	0.14064900
H	-1.92688200	-2.49184100	0.14546600
H	-0.94351000	-4.79597900	0.46911200
C	-0.70527000	-0.29728000	-0.35635900
C	-0.18399700	0.96025900	-0.17442000

C	-1.06383200	2.16297800	-0.24063600
C	-2.44483900	2.05959700	-0.51361100
C	-0.51468500	3.44463000	-0.05430200
C	-3.22799300	3.21009400	-0.59319800
H	-2.92291700	1.08337300	-0.63667700
C	-1.30702200	4.58900900	-0.13968500
H	0.54447600	3.52977300	0.16428700
C	-2.67117600	4.47923600	-0.41180400
H	-4.29171500	3.10616300	-0.79660000
H	-0.85451300	5.56818500	0.00748500
H	-3.29319700	5.36977000	-0.47945900
H	1.75134000	-0.35229200	-2.07145400
C	-4.70045400	-1.13389100	0.37953400
C	-5.21759800	-2.60639900	0.41337000
H	-4.46278700	-3.25045800	0.88455000
H	-6.16670500	-2.73646400	0.95928300
H	-5.35686500	-2.95963700	-0.61642900
C	-4.47481000	-0.67027800	1.85199000
H	-3.68928300	-1.28531300	2.31039300
H	-4.12445100	0.36964100	1.85740200
H	-5.37550700	-0.73454700	2.48507700
C	-5.83572700	-0.25410500	-0.23261900
H	-5.53106100	0.80097000	-0.22266300

H	-5.98723300	-0.54543700	-1.27984100
H	-6.79964500	-0.33499400	0.29628700
O	-3.56377500	-1.04355800	-0.36268000
H	-1.79826200	-0.40290900	-0.39625600

### INT\_end3

E(B3lyp/6-31g(d) = -1210.379707 Hartree

Imaginary Freq= 0

-1 1

C	-4.09455500	-2.92924600	-0.14681100
C	-3.88684300	-1.88970200	0.77038400
C	-2.68405100	-1.19645600	0.69214100
C	-1.70243800	-1.51218300	-0.26095100
C	-1.92005200	-2.55229200	-1.16372300
C	-3.12563200	-3.25934700	-1.10320000
H	-5.02753800	-3.48775900	-0.11175700
H	-4.63078600	-1.62731000	1.51682800
H	-1.15338700	-2.79535800	-1.89413600
H	-3.31383700	-4.07057400	-1.80258300
C	-0.56448000	-0.63302300	-0.00780900
N	0.59985500	-0.68890600	-0.54845400
O	-2.32600900	-0.17347800	1.51952700
C	-1.03414700	0.34154300	1.07221900

H	-0.35455900	0.34779200	1.93716300
C	-1.15945700	1.71405500	0.44947900
C	-2.37453600	2.39870100	0.37712100
C	0.03583500	2.24153700	-0.12580600
C	-2.46033300	3.62096000	-0.29047000
H	-3.25732300	1.95825500	0.83258700
C	-0.09530400	3.49296900	-0.78983500
C	-1.30999500	4.15582200	-0.89042900
H	-3.40778400	4.15443600	-0.33576700
H	0.80749600	3.91278100	-1.22778000
H	-1.36677800	5.10585000	-1.42091600
C	1.34053300	1.63425600	-0.02798700
C	1.55977900	0.28865400	-0.16092100
C	2.93723300	-0.26758000	-0.04581700
C	4.02345000	0.58186000	0.24477200
C	3.20949900	-1.64034500	-0.19955200
C	5.31415300	0.08297600	0.38257700
H	3.79566300	1.63967800	0.34801100
C	4.50797200	-2.13897800	-0.07390700
H	2.38484400	-2.30904300	-0.42488700
C	5.57162400	-1.28474600	0.22109000
H	6.13286800	0.76483900	0.61062300
H	4.68752800	-3.20586100	-0.20285600



H 6.58314900 -1.67417600 0.32304500

**Pro\_2**

E(B3lyp/6-31g(d) = -1210.471525 Hartree

Imaginary Freq= 0

-1 1

C 6.66162000 0.09858100 -0.70863200

C 5.94944700 -0.82082700 0.06629300

C 4.56530700 -0.72196600 0.03968200

C 3.87552900 0.24533000 -0.71965500

C 4.60726500 1.15714500 -1.48800400

C 5.99911300 1.07364100 -1.47473900

H 7.74786600 0.05700000 -0.71719000

H 6.44644200 -1.57910700 0.66342400

H 4.09099200 1.90891500 -2.07751100

H 6.58462600 1.77353300 -2.06575400

C 2.47148000 -0.00188400 -0.46150400

N 1.37050600 0.64266700 -0.92577600

O 3.69559800 -1.53268500 0.73263900

C 2.43106200 -1.07514300 0.40995700

C 1.21308400 -1.61060400 0.87191800

C 1.10131500 -2.71480500 1.74756100

C 0.03962500 -0.94749100 0.36819000

C	-0.15093500	-3.16606000	2.11228200
H	2.00487800	-3.19293100	2.11495100
C	-1.23224300	-1.45496700	0.74815100
C	-1.30872500	-2.54065400	1.60451400
H	-0.24370600	-4.01590000	2.78595800
H	-2.17240000	-1.04407600	0.33724900
H	-2.29039500	-2.91971000	1.87899100
C	0.18967100	0.19807000	-0.51619900
C	-1.01357300	0.99234700	-0.98788100
C	-1.38302600	2.11488400	-0.01612500
C	-2.65239000	2.13333000	0.58198500
C	-0.47480000	3.14379400	0.27391000
C	-2.99351000	3.17247900	1.45319400
H	-3.34613200	1.31935600	0.34133100
C	-0.82246000	4.17809200	1.14411000
H	0.51102000	3.12421100	-0.18536800
C	-2.08692800	4.19561100	1.73865700
H	-3.98014600	3.18008800	1.91369800
H	-0.10641200	4.96993200	1.35823800
H	-2.36095100	5.00106000	2.41821700
H	-0.72655900	1.43788100	-1.94807200
H	-1.90297800	0.36152600	-1.13972800
C	-4.76354500	-1.12358600	-1.06795000

C	-4.28843800	-2.37424700	-1.86609000
H	-3.60007500	-2.05726400	-2.65996000
H	-3.73473600	-3.04708400	-1.19828400
H	-5.11010800	-2.94594700	-2.32738200
C	-5.73766600	-1.60340900	0.04973100
H	-5.19953700	-2.26533100	0.74135200
H	-6.08194200	-0.73476500	0.62558300
H	-6.62151200	-2.14321500	-0.32771600
C	-5.55965100	-0.20401200	-2.04132800
H	-5.91635700	0.67948600	-1.49639800
H	-4.88847000	0.14695900	-2.83547700
H	-6.42728100	-0.69577500	-2.51078900
O	-3.70677600	-0.45224100	-0.53027700

### Pro\_1

E(B3lyp/6-31g(d) = -1210.456977 Hartree

Imaginary Freq= 0

-1 1

C	-6.40026700	0.27886300	1.01669000
C	-5.68873700	-0.86239500	0.63813800
C	-4.33526800	-0.69510300	0.37528900
C	-3.67469300	0.54053300	0.48283700
C	-4.40511400	1.67473500	0.85705300

C	-5.76633200	1.53051100	1.12117500
H	-7.46278500	0.19644000	1.23161200
H	-6.16295300	-1.83487000	0.54743900
H	-3.91175400	2.63904600	0.93472800
H	-6.35142900	2.39911800	1.41376700
C	-2.29085700	0.28349400	0.13768700
N	-1.35106300	1.26808300	-0.07134300
O	-3.46693500	-1.67392200	-0.02088900
C	-2.21840000	-1.07205200	-0.14673900
C	-1.11837700	-1.85569400	-0.65400100
C	-1.33402300	-3.00620100	-1.44037000
C	0.20410600	-1.43260400	-0.37406400
C	-0.25239700	-3.70077400	-1.96542000
H	-2.35206600	-3.32584000	-1.64345200
C	1.28702800	-2.13005200	-0.92904300
C	1.05385700	-3.25697300	-1.71658600
H	-0.42423500	-4.58551200	-2.57553500
H	2.29653400	-1.78629800	-0.66384000
H	1.89808900	-3.80895300	-2.12508300
C	0.44858500	-0.28254400	0.58327800
C	-0.07696000	1.03301400	0.02127400
C	0.85053300	2.10928400	-0.41727000
C	2.24631600	1.92695100	-0.44526300

C	0.31458300	3.34849900	-0.82754400
C	3.06722700	2.97548800	-0.87405000
H	2.72889400	0.98366000	-0.14099000
C	1.14352000	4.38306600	-1.24294000
H	-0.76289100	3.47373800	-0.80900200
C	2.53146000	4.19981300	-1.26884700
H	4.14349700	2.81765400	-0.89282000
H	0.71082200	5.33340400	-1.55009600
H	3.18359300	5.00769400	-1.59638100
H	-0.12589300	-0.47070900	1.50450800
H	1.51845000	-0.25788000	0.83233000
O	3.49119600	-0.65493900	0.44141300
C	4.64380400	-0.90723500	1.12407600
C	5.86285800	-0.92866300	0.15371000
H	6.82586100	-1.13610900	0.64831400
H	5.69778400	-1.69287000	-0.61675400
H	5.93800500	0.04125800	-0.35531700
C	4.57139900	-2.28889400	1.84050200
H	5.47787000	-2.54128500	2.41448500
H	3.71438100	-2.29582700	2.52598600
H	4.40492800	-3.07817300	1.09591900
C	4.90587100	0.18168400	2.20652100
H	5.82499800	0.01466100	2.79128100

H	4.97902400	1.16658200	1.72695400
H	4.05629900	0.21489000	2.90060200

**TS\_exd5**

E(B3lyp/6-31g(d) = -1210.453140 Hartree

Imaginary Freq= -1164.52

-1 1

C	-6.31014000	0.40572400	-1.16793500
C	-5.76919800	0.01013400	0.05850000
C	-4.38506900	-0.06791900	0.13855900
C	-3.53386000	0.22928100	-0.94639800
C	-4.09569700	0.62143700	-2.16590500
C	-5.48408300	0.70722400	-2.26523900
H	-7.38980300	0.48081800	-1.27275200
H	-6.39429100	-0.22638400	0.91430900
H	-3.45149700	0.85104800	-3.00952400
H	-5.93833800	1.01147200	-3.20520400
C	-2.18641100	0.02019800	-0.44933300
N	-1.00353500	0.11222000	-1.10050200
O	-3.67269000	-0.43775600	1.25267800
C	-2.33917500	-0.37303000	0.87000600
C	-1.22457300	-0.61278700	1.69845600
C	-1.28613100	-0.93946900	3.07394000

C	0.04114700	-0.44237700	1.04481900
C	-0.11972600	-1.05638600	3.80394100
H	-2.25756600	-1.07659200	3.54081900
C	1.20718900	-0.51144300	1.84390900
C	1.12822500	-0.81886500	3.19219300
H	-0.16629700	-1.30359900	4.86273800
H	2.16257900	-0.25860400	1.39662700
H	2.03724200	-0.86043200	3.78706700
C	0.10606700	-0.15534400	-0.39557600
C	1.40063200	-0.08010300	-1.07683200
C	2.26763100	-1.30913800	-1.12073300
C	3.64208600	-1.17362600	-1.40768300
C	1.77746600	-2.61519000	-0.92965000
C	4.47264300	-2.28730700	-1.51879200
H	4.04556600	-0.16827100	-1.48736000
C	2.61186100	-3.73044000	-1.02571300
H	0.72151600	-2.75738400	-0.71340000
C	3.96579300	-3.57679400	-1.32948100
H	5.53028700	-2.14723400	-1.73800200
H	2.19682000	-4.72595300	-0.87379500
H	4.61660300	-4.44549200	-1.41003100
H	1.23612100	0.29070400	-2.09582900
H	2.20454500	0.85468900	-0.51414800

C	2.97341700	2.91421900	-0.00586000
C	4.18297600	3.55978400	0.70872600
H	4.24364900	3.18583500	1.73787400
H	5.10895600	3.27346800	0.19531200
H	4.12376500	4.65834000	0.73821100
C	2.90721500	3.44515000	-1.46097900
H	3.81758300	3.15337000	-1.99907500
H	2.05202400	3.00239900	-1.98528200
H	2.80901100	4.54008700	-1.51175700
C	1.67580400	3.31604100	0.73988600
H	0.80046900	2.88232700	0.24233100
H	1.70455500	2.92534600	1.76388400
H	1.53503100	4.40636400	0.78685200
O	3.16264700	1.53704200	0.01140800

## INT\_8

E(B3lyp/6-31g(d) = -1210.470505 Hartree

Imaginary Freq= 0

-1 1

C	-2.31299300	4.50440600	-1.00295100
C	-3.16880600	3.44444600	-0.69685400
C	-2.57974400	2.19989400	-0.50260400
C	-1.19667000	1.97108400	-0.60142300



C	-0.35079800	3.04967900	-0.90610600
C	-0.92270300	4.30610800	-1.10257000
H	-2.72828400	5.49726400	-1.16222000
H	-4.24404500	3.57420100	-0.61233200
H	0.72366500	2.90363200	-0.95221900
H	-0.28171000	5.15367400	-1.33617400
C	-0.98926900	0.55142500	-0.34625800
N	0.26541100	-0.02003500	-0.38332200
O	-3.23271700	1.05028500	-0.20305400
C	-2.25479700	0.04406600	-0.10708600
C	-2.77641400	-1.27506600	0.24292600
C	-4.11512500	-1.42172100	0.61043900
C	-1.92427900	-2.41896200	0.18135600
C	-4.66543500	-2.67787600	0.92312800
H	-4.74294300	-0.53739000	0.64058200
C	-2.50396300	-3.65899500	0.49965100
C	-3.85192400	-3.79815000	0.86323200
H	-5.71418000	-2.75800300	1.20052700
H	-1.87294500	-4.54493400	0.45182100
H	-4.24764500	-4.78606000	1.09351700
C	-0.51698200	-2.39817800	-0.20634100
C	0.39847000	-1.37252400	-0.38371200
C	1.80645100	-1.81697500	-0.68031700

C	2.38258800	-2.94172900	-0.06482000
C	2.59267500	-1.09961800	-1.59769500
C	3.68173000	-3.34872400	-0.37016000
H	1.80586300	-3.48760500	0.67609000
C	3.88852600	-1.50785000	-1.90987800
H	2.16624900	-0.21451700	-2.05581300
C	4.44168700	-2.63652400	-1.30011800
H	4.10467700	-4.21867500	0.12891200
H	4.47170500	-0.93740700	-2.62996800
H	5.45600200	-2.95053000	-1.53840700
H	1.70475800	1.04345300	-0.03150100
H	-0.11444300	-3.39690500	-0.35161200
C	2.82488900	1.81665400	1.43529100
C	3.44652700	0.49855100	1.93519200
H	2.71504000	-0.31394300	1.87578000
H	4.30021400	0.22387400	1.30613000
H	3.78766500	0.58041200	2.97646200
C	3.86588400	2.94355200	1.48563500
H	4.72169400	2.69241500	0.84845600
H	3.42875400	3.87703500	1.11313000
H	4.22796200	3.11027900	2.50801300
C	1.59798400	2.18402300	2.29068200
H	1.14862200	3.11562500	1.92973000

H	0.83932200	1.39730100	2.22091100
H	1.86735400	2.31181500	3.34796400
O	2.46193300	1.69462100	0.06600900

### INT\_7

E(B3lyp/6-31g(d) = -1210.429413 Hartree

Imaginary Freq= 0

-1 1

C	-6.38249000	0.53905700	0.62150500
C	-5.67682700	-0.66514400	0.68576400
C	-4.32989100	-0.62263800	0.35286100
C	-3.66607800	0.55958500	-0.03297400
C	-4.39231400	1.75948100	-0.08891600
C	-5.74608600	1.73444500	0.23968900
H	-7.44002900	0.55131700	0.87201500
H	-6.15030200	-1.59619500	0.98179700
H	-3.91135600	2.69252900	-0.37280500
H	-6.32211700	2.65584900	0.20498400
C	-2.30619500	0.16485400	-0.30158000
N	-1.28599700	0.99396400	-0.75460800
O	-3.46857500	-1.67418900	0.35484100
C	-2.23011500	-1.18283000	-0.06309800
C	-1.13894100	-2.13636400	-0.21204400

C	-1.42204700	-3.50621000	-0.31397000
C	0.20818300	-1.68701200	-0.25437200
C	-0.39675100	-4.43930600	-0.47472100
H	-2.45613400	-3.83400000	-0.26455300
C	1.22718400	-2.64441300	-0.41747300
C	0.92734300	-4.00287500	-0.53270600
H	-0.63705100	-5.49762500	-0.55229600
H	2.25487000	-2.26592500	-0.43775800
H	1.73511300	-4.72140700	-0.65583100
C	0.67929600	-0.30261600	-0.08843500
C	0.06807200	0.87466700	-0.34813900
C	0.81032600	2.15970400	-0.25758400
C	2.21509300	2.18413700	-0.40999500
C	0.14007000	3.37902200	-0.04210100
C	2.89653100	3.39773400	-0.35225100
H	2.77989400	1.24984800	-0.54138100
C	0.83409400	4.58942700	0.00619200
H	-0.93336100	3.38612800	0.13473600
C	2.21856500	4.60569000	-0.15559500
H	3.97830200	3.39494100	-0.46789400
H	0.28934300	5.51536500	0.18073500
H	2.76438100	5.54658000	-0.12334200
H	-1.56951700	1.89879700	-1.09483800

H	1.73352200	-0.26267600	0.20854100
C	4.84310100	-0.73625800	0.41087800
C	5.05787900	-2.19430000	0.92187300
H	4.26456900	-2.44612100	1.63739400
H	4.97726200	-2.89141600	0.07708100
H	6.03193200	-2.35802100	1.41171600
C	5.97886500	-0.41760100	-0.61029300
H	5.87040400	-1.07590400	-1.48185900
H	5.87036900	0.61639300	-0.96407100
H	6.99719000	-0.53912400	-0.20490900
C	5.00937700	0.22011800	1.63149800
H	4.88456600	1.26064400	1.30444700
H	4.22094400	0.00966500	2.36547000
H	5.98570300	0.13412300	2.13678500
O	3.62182600	-0.59626500	-0.17433700

## INT\_5

E(B3lyp/6-31g(d) = -976.709065 Hartree

Imaginary Freq=0

-1 1

C	3.18856300	-3.84292900	-0.33705700
C	3.48391800	-2.52640200	-0.71295400
C	2.56594800	-1.54714400	-0.36590100

C	1.36767700	-1.81862400	0.33293500
C	1.09358500	-3.14612300	0.70443900
C	2.00690600	-4.14342500	0.36214800
H	3.88379500	-4.64014700	-0.58874800
H	4.38981500	-2.27263800	-1.25603000
H	0.18483600	-3.39647600	1.24770800
H	1.80139400	-5.17459300	0.64177800
C	0.72017600	-0.54619800	0.50585300
N	-0.47344100	-0.27178200	1.18589400
O	2.66719200	-0.22069300	-0.64205700
C	1.52948000	0.39677700	-0.09970300
C	1.44686300	1.83665400	-0.14870000
C	2.60454000	2.61172300	-0.36882500
C	0.18066100	2.47302400	0.12891800
C	2.59304300	3.98739500	-0.17844400
H	3.52806900	2.10720700	-0.64254300
C	0.23408100	3.87633300	0.36759400
C	1.40009000	4.61128400	0.23662800
H	3.49840500	4.57097500	-0.33282500
H	-0.70573300	4.37198000	0.60377900
H	1.38455000	5.68607100	0.41570900
C	-1.08386400	1.81740900	0.01339800
C	-1.41760600	0.58935500	0.42847300

C	-2.72102900	-0.02903000	0.09899600
C	-3.80044800	0.80246800	-0.28108300
C	-2.97499000	-1.41628600	0.13858500
C	-5.04645600	0.28082100	-0.60080600
H	-3.59751000	1.86878100	-0.31953300
C	-4.23027200	-1.94116000	-0.18105200
H	-2.17242200	-2.10851000	0.37996400
C	-5.27945300	-1.10116000	-0.54922600
H	-5.85182600	0.95541200	-0.88842400
H	-4.38064300	-3.01932400	-0.14810900
H	-6.25856600	-1.50916500	-0.79172300
H	-0.89608000	-1.12014200	1.54890800

#### INT\_4

E(B3lyp/6-31g(d) = -1210.430706 Hartree

Imaginary Freq= 0

-1 1

C	-4.74685300	-2.44686100	-0.84356100
C	-4.41508200	-1.29736200	-0.12268200
C	-3.22418500	-0.65452200	-0.45782300
C	-2.36742600	-1.12994300	-1.46064900
C	-2.71635500	-2.27871000	-2.17027700
C	-3.90867300	-2.93698600	-1.85891400

H	-5.67204200	-2.97091000	-0.61229200
H	-5.05482800	-0.90955500	0.66512200
H	-2.06120600	-2.65869400	-2.95252200
H	-4.19058800	-3.83646200	-2.40159700
C	-1.22173700	-0.19360100	-1.55376700
N	-0.25059600	-0.17719700	-2.43002700
O	-2.74642500	0.46414900	0.12288900
C	-1.46245200	0.74750900	-0.48056700
H	-0.19800000	-0.68777600	0.83630300
C	-0.99851800	2.07519200	-0.25516000
C	-1.89179600	3.07968000	0.22657800
C	0.36457600	2.49154200	-0.48268000
C	-1.51490300	4.40425700	0.35259500
H	-2.90974700	2.78435200	0.45558600
C	0.70447900	3.85893700	-0.38039900
C	-0.21294400	4.81958200	0.01834600
H	-2.24643700	5.13470900	0.69587500
H	1.73617500	4.13706900	-0.58277800
H	0.07991500	5.86320700	0.10381100
C	1.42163100	1.56277600	-0.64564000
C	2.38007500	0.80872400	-0.67180400
C	3.44754400	-0.12495300	-0.69705900
C	3.26484200	-1.43307800	-0.18966100



C	4.71615200	0.22271500	-1.21212400
C	4.31455100	-2.34653900	-0.20850300
H	2.29568700	-1.69822600	0.22365200
C	5.75812400	-0.70117500	-1.22426500
H	4.86542100	1.22459400	-1.60508100
C	5.56614200	-1.99193500	-0.72426800
H	4.15483500	-3.34818500	0.18564700
H	6.72648200	-0.41213700	-1.62856500
H	6.38119000	-2.71224000	-0.73542900
H	-0.38410700	-0.96205100	-3.07761900
C	0.01518400	-0.99155200	2.77959400
C	-1.47899800	-0.94623200	3.14652500
H	-2.00531000	-0.21886300	2.51951900
H	-1.93565600	-1.92818300	2.97808800
H	-1.62572200	-0.66844100	4.19898900
C	0.73514300	-2.07417600	3.59211100
H	0.29501000	-3.05610800	3.38444800
H	1.79533700	-2.11105800	3.31812900
H	0.65860400	-1.87724100	4.66839900
C	0.67259100	0.37975500	3.00625000
H	1.72392000	0.34936800	2.70175900
H	0.17382000	1.15140800	2.40998200
H	0.61996100	0.67704400	4.06209800

O 0.16202300 -1.39458800 1.41529700

### INT\_3

E(B3lyp/6-31g(d) = -1210.379707 Hartree

Imaginary Freq= 0

-1 1

C -4.93399700 0.13798000 -1.76280800

C -4.11745000 -0.97644700 -1.99186000

C -2.86428000 -0.97122300 -1.38799800

C -2.42589700 0.08367700 -0.58618100

C -3.23952600 1.19883300 -0.36440400

C -4.50370900 1.20766700 -0.96588700

H -5.92218800 0.16933500 -2.21875100

H -4.43603500 -1.80807600 -2.61385900

H -2.83867800 2.02187200 0.24667300

H -5.16285600 2.05993100 -0.81577100

C -1.05077400 -0.23166000 -0.13434000

N -0.20153700 0.41907600 0.54229500

O -1.94874700 -1.98551400 -1.52267600

C -0.76942900 -1.64301400 -0.74600500

H 0.07175200 -1.56769400 -1.44307300

C -0.49453600 -2.74185500 0.25921300

C -1.53853100 -3.52724800 0.75611400

C	0.82470100	-3.00146600	0.70844700
C	-1.30321200	-4.54946000	1.67489000
H	-2.54523400	-3.33725200	0.40026700
C	1.05082900	-4.04352100	1.62947300
C	-0.00283200	-4.81208300	2.11140400
H	-2.13562200	-5.14227400	2.04653900
H	2.06795500	-4.23023700	1.96169300
H	0.18882600	-5.60999400	2.82474000
C	1.91905300	-2.21083800	0.25381200
C	2.82954700	-1.49929300	-0.12392200
C	3.73848500	-0.46904400	-0.50795500
C	5.07308300	-0.73261300	-0.86636300
C	3.26805900	0.86148400	-0.51888700
C	5.91979400	0.31261900	-1.23079300
H	5.43376000	-1.75749900	-0.85638500
C	4.12387000	1.89710100	-0.88384000
H	2.23640800	1.04600200	-0.22720700
C	5.44886700	1.62810000	-1.24176600
H	6.95008000	0.10000800	-1.50716700
H	3.75227100	2.91847900	-0.88511100
H	6.11261400	2.44106200	-1.52671600
C	-0.73432100	4.00411900	1.16477200
C	-1.72812300	5.15432900	1.50222700

H	-1.27111100	6.15726800	1.48794800
H	-2.55709600	5.14303900	0.78238600
H	-2.15359100	4.97948000	2.49860400
C	0.44282000	4.06883600	2.18326600
H	0.05497400	3.87920700	3.19210900
H	1.16903300	3.27768200	1.95645400
H	0.97444700	5.03453700	2.18882200
C	-0.15887300	4.26558200	-0.26088900
H	0.35494900	5.23556200	-0.36468900
H	0.55379300	3.47097400	-0.51926200
H	-0.97386600	4.22721800	-0.99520200
O	-1.37212000	2.80063600	1.23848400
H	-0.58860900	1.37349600	0.84610500

### TS\_1

E(B3lyp/6-31g(d) = -1210.350781 Hartree

Imaginary Freq= -1006.20

-1 1

C	-1.53460500	-3.69159700	-1.28774600
C	-1.47418000	-2.31115900	-1.13552400
C	-0.50726200	-1.72931400	-0.28357800
C	0.35160000	-2.60101900	0.44722000
C	0.27180000	-3.99275100	0.26374100

C	-0.65447300	-4.54618000	-0.61158400
H	-2.29463200	-4.11051300	-1.94402100
H	-2.21059400	-1.67352500	-1.60839000
H	0.94603900	-4.62699500	0.83266600
H	-0.70820900	-5.62263300	-0.74759100
C	1.27581500	-2.09496100	1.41314000
N	2.03603400	-1.76384900	2.23184300
O	-0.34408500	-0.42256700	-0.11796100
C	-1.26992900	0.48539700	-0.79403400
H	-2.70251900	0.23464300	-0.59846700
C	-0.93328500	1.89767800	-0.50972100
C	-1.98907200	2.81836900	-0.71517100
C	0.31372300	2.43460000	-0.06716200
C	-1.85194700	4.17709600	-0.46935900
H	-2.94434100	2.40765100	-1.03206100
C	0.41867700	3.81792200	0.22112000
C	-0.64306200	4.68705500	0.02619100
H	-2.69894300	4.84112800	-0.63257700
H	1.37621000	4.19192300	0.57504700
H	-0.53411400	5.74557100	0.25137900
C	1.52957100	1.69360200	-0.00878800
C	2.65305900	1.22113400	-0.01343700
C	3.96170700	0.66836500	-0.06273100

C	5.08790200	1.45938300	0.25284000
C	4.17671800	-0.67193900	-0.44987800
C	6.37385500	0.93075700	0.18148700
H	4.93370600	2.49155900	0.55386300
C	5.46562000	-1.19182400	-0.51983900
H	3.31845600	-1.29177600	-0.68496400
C	6.57195800	-0.39691600	-0.20636500
H	7.22674800	1.55862800	0.43051800
H	5.60784000	-2.22829800	-0.81710700
H	7.57690900	-0.80880000	-0.26052200
H	-1.20161900	0.29024300	-1.87686400
O	-3.86769200	0.13586000	-0.76353100
C	-4.63380100	-0.08418300	0.38851100
C	-3.94087300	0.46748000	1.65533700
H	-4.55750300	0.32339600	2.55380800
H	-2.97992300	-0.03375700	1.81814900
H	-3.74044300	1.53897200	1.54176500
C	-4.89220200	-1.59978700	0.56833900
H	-5.54064700	-1.81924500	1.42961800
H	-5.36863100	-2.00042200	-0.33492300
H	-3.94337100	-2.12981900	0.70823800
C	-5.98637800	0.63597600	0.19541900
H	-6.67306400	0.47707500	1.03987400

H	-5.82086500	1.71385000	0.08043400
H	-6.47012900	0.27263300	-0.71941900

**ST**

E(B3lyp/6-31g(d) = -977.279048 Hartree

Imaginary Freq= 0

0 1

C	-0.52810800	-3.81727900	-1.65391400
C	-0.93403600	-2.48512200	-1.54853200
C	-1.29155000	-1.95816100	-0.30093100
C	-1.24073700	-2.79559800	0.84086800
C	-0.83117500	-4.13025900	0.71101300
C	-0.47281000	-4.64477500	-0.53232200
H	-0.25554900	-4.20759000	-2.63075100
H	-0.97599400	-1.86773700	-2.43772000
H	-0.79970100	-4.75326300	1.59923500
H	-0.15715200	-5.67908200	-0.62416500
C	-1.61101200	-2.28441300	2.12557600
N	-1.90779300	-1.90881500	3.18594200
O	-1.69777500	-0.68704000	-0.08205500
C	-1.75132100	0.22614200	-1.19356200
H	-2.52206500	-0.10936500	-1.89908600
C	-2.07455700	1.59488600	-0.66113300

C	-3.38677500	2.06799600	-0.68415500
C	-1.05176900	2.41392100	-0.12151000
C	-3.70735900	3.33296200	-0.18990100
H	-4.16923100	1.43372900	-1.09370300
C	-1.38525500	3.68953300	0.37262300
C	-2.70062700	4.14275800	0.33871300
H	-4.73543200	3.68237700	-0.21639500
H	-0.59825700	4.31406900	0.78329100
H	-2.93977700	5.12936800	0.72575300
C	0.30064200	1.96752700	-0.08108300
C	1.45534100	1.58569400	-0.04747500
C	2.80581900	1.13296800	-0.00500700
C	3.84624000	2.01319900	0.35404600
C	3.12203200	-0.20389200	-0.32093000
C	5.16358400	1.56530500	0.39429700
H	3.60644300	3.04319600	0.59937700
C	4.44246700	-0.64219700	-0.27820400
H	2.32304300	-0.88705600	-0.59267600
C	5.46688200	0.23853300	0.07842900
H	5.95671000	2.25353500	0.67363900
H	4.67327000	-1.67571300	-0.52179400
H	6.49623100	-0.10772000	0.11154500
H	-0.78127500	0.23090400	-1.70315300



## RC

E(B3lyp/6-31g(d) = -1210.383901 Hartree

Imaginary Freq= 0

-1 1

C	-2.85657300	-2.72778400	1.00856300
C	-2.19157800	-1.66373700	0.40316500
C	-0.80102600	-1.74834800	0.22405100
C	-0.11500500	-2.91802600	0.64451700
C	-0.81819500	-3.97443500	1.25270500
C	-2.18939100	-3.88014400	1.44405900
H	-3.93459700	-2.64867700	1.13419100
H	-2.77870700	-0.80485300	0.03013000
H	-0.26695000	-4.85705800	1.56474400
H	-2.73381900	-4.69380900	1.91608900
C	1.29309200	-3.04765700	0.43807700
N	2.43644700	-3.20978300	0.28082000
O	-0.02491200	-0.80635700	-0.35467400
C	-0.55638200	0.51418200	-0.66550900
H	-1.58946000	0.46173000	-1.03852000
C	-0.48666000	1.44890300	0.52456000
C	-1.67809200	1.94300000	1.07058400
C	0.75434000	1.86604100	1.06982700

C	-1.64481300	2.82326900	2.15568300
H	-2.62078300	1.63164700	0.59841800
C	0.76619100	2.75424800	2.16356700
C	-0.42628800	3.22468100	2.70611000
H	-2.57844700	3.19762600	2.57031500
H	1.72245900	3.06675400	2.57403400
H	-0.40041700	3.90856400	3.55219800
C	2.00425300	1.43590800	0.52777600
C	3.09492800	1.11414800	0.09521900
C	4.36773700	0.71456100	-0.41130300
C	5.37759100	1.67032000	-0.64505000
C	4.63893700	-0.64259700	-0.68210000
C	6.62032500	1.28109900	-1.13861500
H	5.17053200	2.71616500	-0.43704900
C	5.88614400	-1.01995700	-1.17517000
H	3.87409600	-1.38936800	-0.49061400
C	6.87995100	-0.06535100	-1.40700300
H	7.38808400	2.03098600	-1.31547500
H	6.08079800	-2.07049300	-1.37600500
H	7.85077600	-0.36796100	-1.79252700
H	0.11345800	0.85717400	-1.45949000
O	-3.60994200	0.65924600	-0.75576300
C	-4.76628700	0.79703100	-1.46749200

C	-6.00690300	0.64941200	-0.53827600
H	-6.97089500	0.76351500	-1.05981200
H	-5.98879900	-0.33936400	-0.06116900
H	-5.95415800	1.40189900	0.25911800
C	-4.86447500	-0.28209300	-2.58487600
H	-5.77920500	-0.20673900	-3.19450200
H	-3.99706100	-0.19433400	-3.25143100
H	-4.83385900	-1.28193300	-2.13295100
C	-4.82824900	2.19936700	-2.14111300
H	-5.73970400	2.36655800	-2.73731900
H	-4.77352700	2.97754600	-1.36887500
H	-3.95754600	2.32354800	-2.79748100

### TS\_9

E(B3lyp/6-31g(d) = -1210.436616 Hartree

Imaginary Freq= -316.30

-1 1

C	-5.68614200	-1.08951700	1.38009600
C	-5.22773600	0.13641800	0.89009400
C	-3.91576200	0.17240400	0.43552400
C	-3.06081900	-0.94033300	0.45061600
C	-3.53642000	-2.16204300	0.94390100
C	-4.85011500	-2.22228500	1.40532400

H	-6.70624100	-1.16763500	1.74838300
H	-5.85835600	1.02008200	0.86339300
H	-2.88281800	-3.02879700	0.96096600
H	-5.24047600	-3.15997600	1.79447200
C	-1.79954500	-0.49374800	-0.10144200
N	-0.74181400	-1.37295400	-0.26032000
O	-3.26826300	1.25451000	-0.08305000
C	-1.97563900	0.83889200	-0.40556200
C	-1.10434100	1.84971400	-0.98513500
C	-1.64353800	3.10801800	-1.30959900
C	0.26960700	1.58526800	-1.21380300
C	-0.85264400	4.12404000	-1.84039100
H	-2.70119600	3.27739900	-1.13735200
C	1.04546300	2.63838500	-1.72803500
C	0.50612200	3.88591900	-2.04057100
H	-1.29339700	5.08835100	-2.08249400
H	2.11273400	2.46681500	-1.83849700
H	1.15220600	4.66955600	-2.43096100
C	1.03262900	0.32396600	-0.91253300
C	0.44769400	-1.00950500	-0.64298600
C	1.41625700	-2.14987900	-0.78008300
C	2.79469300	-1.98335800	-0.54797400
C	0.93816000	-3.42241500	-1.13698200

C	3.65947500	-3.07250500	-0.68291700
H	3.17750200	-1.01606400	-0.21360100
C	1.80923100	-4.49928400	-1.28269500
H	-0.12881600	-3.54293200	-1.29395100
C	3.17836700	-4.32801800	-1.05743700
H	4.72073400	-2.93422700	-0.48612900
H	1.42096300	-5.47413200	-1.57218100
H	3.86121800	-5.16854800	-1.16768200
H	1.77353600	0.19435000	-1.71069500
H	1.87473900	0.61858500	-0.04312400
O	3.16902000	0.98710400	0.49699100
C	3.28008800	1.42542700	1.80215400
C	2.56452800	0.46787600	2.79181800
H	2.66771400	0.77946700	3.84264300
H	1.49387200	0.41571600	2.55830900
H	2.97625800	-0.54379800	2.69053900
C	2.67615500	2.84675400	1.95638400
H	2.78297500	3.25462100	2.97353000
H	3.16982400	3.53006600	1.25441900
H	1.60913400	2.82937700	1.70388300
C	4.78514100	1.48476600	2.17165900
H	4.96606100	1.84671500	3.19564700
H	5.22642500	0.48500700	2.07423200

H 5.30658400 2.14803400 1.47041300

**TS\_7**

E(B3lyp/6-31g(d) = -1210.409020 Hartree

Imaginary Freq= -810.52

-1 1

C 5.87950500 -0.53064600 1.15609300

C 5.13086900 0.64692300 1.24464800

C 3.87740900 0.64448800 0.64925400

C 3.34026600 -0.47741600 -0.01950900

C 4.11026200 -1.64901500 -0.09854000

C 5.37276900 -1.66231000 0.49220900

H 6.86784600 -0.57014800 1.60711300

H 5.50438400 1.53000000 1.75451800

H 3.73107900 -2.53256600 -0.60692900

H 5.97753900 -2.56475100 0.44166600

C 2.04677200 -0.05648500 -0.49617600

N 1.12763600 -0.76653300 -1.26922200

O 3.00027600 1.68327100 0.62549400

C 1.88118200 1.24378300 -0.08920000

C 0.82476300 2.18907500 -0.38945000

C 1.10546800 3.56794600 -0.37728000

C -0.47445300 1.71034200 -0.75445200

C	0.15711200	4.49647000	-0.79331400
H	2.09132600	3.89782000	-0.06075600
C	-1.40650200	2.68937000	-1.17613200
C	-1.09881600	4.04546300	-1.21622000
H	0.39442400	5.55834700	-0.79024700
H	-2.40789100	2.34487100	-1.41767400
H	-1.85224200	4.75909600	-1.54539700
C	-0.97810100	0.34168300	-0.58813900
C	-0.26472400	-0.78125800	-0.81025100
C	-0.80975800	-2.15099000	-0.61163200
C	-2.19283600	-2.40720100	-0.74747000
C	0.01938200	-3.25197400	-0.30982100
C	-2.70254600	-3.69316400	-0.59440800
H	-2.86304200	-1.57475500	-0.94121200
C	-0.49621000	-4.54072900	-0.15806500
H	1.08308100	-3.09792800	-0.14577000
C	-1.86194600	-4.77498900	-0.30747100
H	-3.77332800	-3.85407300	-0.70623900
H	0.17708900	-5.36094200	0.08563800
H	-2.26698800	-5.77891700	-0.19796900
H	1.47086400	-1.67611300	-1.55037700
H	-2.44130800	0.36311800	-0.29003400
C	-4.15061500	0.64108400	0.99788800

C	-3.94261300	2.10542400	1.45277500
H	-2.87353100	2.33559700	1.51447500
H	-4.38765900	2.78809600	0.71875500
H	-4.39767800	2.30697900	2.43397500
C	-5.66265900	0.35595000	0.89188300
H	-6.11112200	1.01319300	0.13703900
H	-5.82354200	-0.68024200	0.57115200
H	-6.18617600	0.51139400	1.84654600
C	-3.52227200	-0.31051700	2.04284600
H	-3.67200800	-1.35351700	1.74189900
H	-2.44273200	-0.13741400	2.11027400
H	-3.95927400	-0.17095400	3.04241400
O	-3.60312600	0.43694300	-0.27658200

### TS\_3

E(B3lyp/6-31g(d) = -1210.375826 Hartree

Imaginary Freq= -1016.29

-1 1

C	-4.93165100	1.22879200	-1.59933900
C	-4.33174700	0.00077500	-1.90423100
C	-3.07862500	-0.24813700	-1.35218700
C	-2.42626400	0.66796700	-0.52753500
C	-3.02616100	1.89444600	-0.23656900



C	-4.28932500	2.16398800	-0.77789600
H	-5.91265500	1.45630800	-2.01286800
H	-4.81301200	-0.73187400	-2.54654500
H	-2.48059300	2.60568200	0.38501600
H	-4.77701100	3.11229400	-0.56200900
C	-1.09141400	0.10674600	-0.14965700
N	-0.11162700	0.60003200	0.45772700
O	-2.37363800	-1.40525100	-1.57073600
C	-1.14512700	-1.35154200	-0.79575800
H	-0.30961400	-1.45927200	-1.49350200
C	-1.13635300	-2.48442900	0.20050000
C	-2.33614200	-3.01805500	0.68641000
C	0.08421900	-3.03136500	0.67573100
C	-2.34815500	-4.05967700	1.61205900
H	-3.27088500	-2.61255000	0.31519600
C	0.05835300	-4.08998800	1.60591500
C	-1.14597200	-4.60232200	2.07391100
H	-3.29784200	-4.45026300	1.97071700
H	1.00392900	-4.49571100	1.95452200
H	-1.14799400	-5.41726700	2.79385400
C	1.33577200	-2.51774200	0.23190500
C	2.39720900	-2.05908200	-0.14514200
C	3.50809500	-1.24923900	-0.52524700

C	4.77131500	-1.78340200	-0.83712700
C	3.31309000	0.14782500	-0.57938400
C	5.81918900	-0.93819800	-1.19866000
H	4.91947300	-2.85902400	-0.79340600
C	4.36818000	0.98115600	-0.94034100
H	2.32932100	0.53638300	-0.31908700
C	5.62157700	0.44393000	-1.25279700
H	6.79286700	-1.35951400	-1.43915200
H	4.20999700	2.05614100	-0.97332100
H	6.44166400	1.10005400	-1.53556000
C	0.42918300	3.83989200	1.15625800
C	-0.06185900	5.21398300	1.66510200
H	0.70069500	6.00190000	1.57018900
H	-0.95077400	5.52108700	1.10018900
H	-0.34989800	5.13194600	2.72022900
C	1.68455500	3.42344000	1.96591000
H	1.41960000	3.33360700	3.02648100
H	2.03813600	2.44191900	1.62999900
H	2.51314200	4.14235000	1.87307900
C	0.80919500	3.96596900	-0.34285400
H	1.60876100	4.70121200	-0.52220300
H	1.14089800	2.99424400	-0.72728900
H	-0.07249200	4.26655700	-0.92233300

O	-0.59394300	2.92074200	1.33939900
H	-0.32050000	1.78524000	0.90054400

## TS\_2

E(B3lyp/6-31g(d) = -976.675820 Hartree

Imaginary Freq= -110.01

-1 1

C	-4.96234900	-2.24254600	0.43066600
C	-4.29866100	-1.22282400	1.11523000
C	-3.00834400	-0.86754100	0.71119800
C	-2.37931700	-1.51897000	-0.35469200
C	-3.05666200	-2.53891900	-1.02810500
C	-4.34844800	-2.90216000	-0.64160800
H	-5.96846800	-2.52364000	0.73661200
H	-4.75875300	-0.70044700	1.94993900
H	-2.54708000	-3.03653500	-1.84971100
H	-4.87438600	-3.69610200	-1.16742600
C	-1.00808400	-1.08370200	-0.66260500
N	-0.08054000	-1.40265600	-1.35552900
O	-2.32742000	0.12047600	1.34789600
C	-1.04502300	0.37604300	0.74448500
H	-0.24659700	0.01653200	1.39159700
C	-0.90671200	1.72579100	0.26434900
C	-2.03027700	2.56350100	0.03208300

C	0.38426200	2.28010800	-0.04693500
C	-1.89710500	3.85700500	-0.44560600
H	-3.01497500	2.17038000	0.26256900
C	0.49043000	3.60152900	-0.52444800
C	-0.63024400	4.39712700	-0.72656700
H	-2.78945000	4.46311500	-0.59748900
H	1.48407100	3.98616000	-0.74301200
H	-0.52715000	5.41257600	-1.10139100
C	1.55832800	1.49617500	0.09556300
C	2.56112700	0.81140800	0.21175700
C	3.59286200	-0.16849600	0.17463400
C	4.91722500	0.11390600	0.56606200
C	3.27771300	-1.47076500	-0.27894900
C	5.89801000	-0.87466000	0.51203500
H	5.16251800	1.11434500	0.91265600
C	4.26750700	-2.44839000	-0.32658800
H	2.25792000	-1.66936900	-0.60676300
C	5.57880800	-2.16102000	0.06959900
H	6.91557500	-0.64057900	0.81910300
H	4.01438500	-3.44503500	-0.68206900
H	6.34526900	-2.93221600	0.03157600

**TS\_exd3**

E(B3lyp/6-31g(d) = -1210.410014 Hartree

Imaginary Freq= -739.04

-1 1

C	6.27710400	0.99189200	-0.23957800
C	5.76336600	-0.23983900	0.18563200
C	4.38245000	-0.35106700	0.30813400
C	3.52137200	0.72282700	0.01757300
C	4.04648600	1.93810300	-0.42072000
C	5.43336900	2.06995900	-0.53871600
H	7.35383800	1.10964000	-0.33905600
H	6.40944000	-1.08278100	0.41149100
H	3.37491700	2.75741100	-0.66084800
H	5.86153500	3.01316800	-0.86857600
C	2.16345300	0.22234200	0.19689400
N	1.04947000	0.73775600	-0.17407800
O	3.73194700	-1.48871500	0.69649500
C	2.31798900	-1.14750100	0.83392300
C	1.35603600	-2.10308800	0.19224400
C	1.62909400	-3.46487500	0.04233400
C	0.11229400	-1.54866600	-0.19048700
C	0.65964000	-4.31467100	-0.48396000
H	2.60322200	-3.84506000	0.33918300
C	-0.85805700	-2.42983900	-0.70999500

C	-0.58641400	-3.78866600	-0.84562700
H	0.86903400	-5.37544000	-0.60576900
H	-1.82936200	-2.03585100	-0.99789400
H	-1.35456100	-4.44493400	-1.25037900
C	-0.11617900	-0.07112500	-0.12125300
C	-1.37217100	0.47361000	-0.13814600
C	-1.57765100	1.92063000	-0.08809400
C	-0.87424200	2.81694400	0.75077800
C	-2.61659000	2.46786000	-0.88096500
C	-1.17184000	4.17869200	0.77156300
H	-0.09183100	2.42659400	1.39285200
C	-2.89062700	3.83296200	-0.88170800
H	-3.20374600	1.78292500	-1.48640500
C	-2.17165400	4.70120300	-0.05343700
H	-0.61265900	4.84051800	1.43183100
H	-3.68468100	4.22192200	-1.51739300
H	-2.39765400	5.76579700	-0.03989900
H	2.13499800	-1.08364500	1.92064900
H	-2.65514700	-0.25594400	-0.38269500
O	-3.63170700	-0.75155700	-0.76988800
C	-4.57269200	-1.00820000	0.23637100
C	-5.63162100	-1.95595900	-0.36246300
H	-6.43037900	-2.19823300	0.35372100

H	-6.08468500	-1.49204300	-1.24686700
H	-5.15528900	-2.89041000	-0.68235800
C	-5.26150800	0.30320800	0.68395800
H	-6.03494200	0.13115100	1.44730500
H	-4.52182600	1.00018500	1.09276600
H	-5.73100600	0.78728700	-0.18090300
C	-3.91763300	-1.68490000	1.46413700
H	-3.14942400	-1.03135600	1.89186700
H	-4.65209600	-1.91550500	2.24959200
H	-3.42854900	-2.61854200	1.16312900

### TS\_exd2

E(B3lyp/6-31g(d) = -976.669475 Hartree

Imaginary Freq= -139.98

-1 1

C	5.06170600	-2.38540900	-0.02543600
C	4.62691300	-1.30900700	0.75937100
C	3.32987200	-0.84727300	0.55643300
C	2.47503600	-1.42118700	-0.39026300
C	2.92223000	-2.48334000	-1.16851800
C	4.22138500	-2.97097000	-0.98005700
H	6.07065000	-2.76924500	0.11283400
H	5.27133400	-0.84487800	1.50128800

H	2.25119000	-2.91351600	-1.90857700
H	4.58196300	-3.80660400	-1.57621100
C	1.18410600	-0.67006700	-0.38987800
N	0.18612900	-0.71053500	-1.13621600
O	2.77722400	0.19776600	1.25109600
C	1.39556600	0.33327600	0.82819900
C	1.03099900	1.71331500	0.41239500
C	1.92048500	2.78995200	0.45287300
C	-0.27254400	1.88708100	-0.12208800
C	1.53839500	4.04937400	-0.00785700
H	2.91603200	2.62466500	0.85346700
C	-0.63339300	3.16626400	-0.59236200
C	0.25420100	4.23619200	-0.53075100
H	2.23897500	4.88074300	0.03870100
H	-1.63264100	3.29779000	-0.99793600
H	-0.05457200	5.21661700	-0.88856400
C	-1.22310500	0.80532400	-0.19098800
C	-2.39006300	0.41166200	0.00220400
C	-3.56726000	-0.34727500	0.07769500
C	-4.60971400	-0.20496400	-0.88168100
C	-3.79829300	-1.26433400	1.14215200
C	-5.78940500	-0.93120100	-0.77881700
H	-4.46214600	0.48458000	-1.70849100



C	-4.98498000	-1.98089300	1.23233700
H	-3.01908400	-1.39921700	1.88719900
C	-5.99837500	-1.82673300	0.27779200
H	-6.56101200	-0.79871100	-1.53635100
H	-5.12212900	-2.67638700	2.05946700
H	-6.92515700	-2.39038500	0.35430100
H	0.76333100	-0.01256300	1.65707500

### TS\_end2

E(B3lyp/6-31g(d) = -976.661498 Hartree

Imaginary Freq= -206.09

-1 1

C	-4.61264500	-2.56047500	0.06462000
C	-4.19948900	-1.48497600	0.86384900
C	-2.90413700	-1.00909200	0.68003100
C	-2.02986300	-1.56725000	-0.25149100
C	-2.44720600	-2.63958600	-1.03011500
C	-3.74913000	-3.13429100	-0.87644300
H	-5.62120000	-2.95302600	0.18241300
H	-4.85840200	-1.03573800	1.60295100
H	-1.74330500	-3.07398700	-1.73751800
H	-4.09261800	-3.96859600	-1.48534800
C	-0.69204900	-0.88964100	-0.15329800

N	0.40179200	-1.23338100	-0.63746900
O	-2.36266800	0.02749100	1.39331300
C	-1.03748300	0.32551000	0.86001800
H	-0.33416900	0.28535900	1.69753600
C	-1.04010900	1.71573500	0.26704400
C	-2.22535100	2.42258600	0.04331100
C	0.20002400	2.33752600	-0.05372200
C	-2.20994700	3.72811300	-0.46018000
H	-3.16888700	1.94248200	0.27886400
C	0.19703200	3.66641400	-0.51326000
C	-0.99629400	4.35829900	-0.72868900
H	-3.14954100	4.25065900	-0.63002300
H	1.15400100	4.13336000	-0.73190100
H	-0.97457400	5.37776000	-1.10890200
C	1.42413100	1.60185100	0.04388000
C	2.00815500	0.50483400	-0.02675000
C	3.22472300	-0.26463900	0.00993200
C	4.42254500	0.39142500	0.37461900
C	3.28133700	-1.63726000	-0.29747300
C	5.62876900	-0.30098700	0.43310400
H	4.37806300	1.45084000	0.61010600
C	4.49541700	-2.31990600	-0.23966200
H	2.34900900	-2.11363500	-0.58242400

C	5.67417200	-1.66419800	0.12615200
H	6.53774600	0.22553900	0.71908500
H	4.52051900	-3.38055900	-0.48338900
H	6.61654700	-2.20668800	0.17146200

#### TS\_end4

E(B3lyp/6-31g(d) = -1210.425178 Hartree

Imaginary Freq= -288.29

-1 1

C	-4.16675100	-3.12336000	-0.33736500
C	-3.97687000	-1.92409500	0.35205500
C	-2.80471100	-1.21059500	0.09126500
C	-1.84223400	-1.68604600	-0.81460200
C	-2.04268200	-2.88990400	-1.49059400
C	-3.21553600	-3.60734100	-1.25151400
H	-5.07459000	-3.69629800	-0.15971200
H	-4.70671500	-1.54872000	1.06283300
H	-1.28540700	-3.25014000	-2.18148400
H	-3.39411500	-4.54799300	-1.76655000
C	-0.74729700	-0.72260500	-0.79563400
N	0.38303800	-0.85139600	-1.40818200
O	-2.46881900	-0.03628700	0.66306200
C	-1.16164400	0.38191900	0.13088400

C	-1.29154500	1.68139000	-0.60813700
C	-2.48358100	2.41380900	-0.65162600
C	-0.13401400	2.19805900	-1.24768500
C	-2.54262100	3.65793900	-1.28311400
H	-3.35892500	2.01085500	-0.15401600
C	-0.21657200	3.45635700	-1.86791400
C	-1.40387900	4.18652300	-1.89232800
H	-3.47487200	4.21958000	-1.28129800
H	0.67576600	3.85764200	-2.34530000
H	-1.43718500	5.15933200	-2.37839800
C	1.14404100	1.48625000	-1.23381100
C	1.35118800	0.14153000	-1.24546300
C	2.73798000	-0.38441300	-1.12692400
C	3.26072800	-1.30863100	-2.04352900
C	3.52965600	0.02732400	-0.04220400
C	4.57043100	-1.76923700	-1.91340900
H	2.62934500	-1.65686600	-2.85606200
C	4.83930300	-0.43989400	0.08579500
H	3.06684500	0.65208000	0.71821800
C	5.36792600	-1.32915500	-0.85260000
H	4.97075800	-2.47488900	-2.63901600
H	5.44212100	-0.12333400	0.93449100
H	6.38856900	-1.69255100	-0.74953000

H	2.03136900	2.11617100	-1.25779900
H	-0.34046700	0.50154800	1.06620700
C	0.54941800	0.30493100	3.27566900
C	-0.71741600	0.95512000	3.89891300
H	-0.62995000	2.04724200	3.84046000
H	-1.60578300	0.66112400	3.32649400
H	-0.87812100	0.67360300	4.95168000
C	0.40638100	-1.24085200	3.35076700
H	-0.48198900	-1.56180900	2.79214700
H	1.28057500	-1.70757300	2.88099000
H	0.31590800	-1.62233100	4.38027300
C	1.78285300	0.72695700	4.11595000
H	1.70246500	0.44246900	5.17693300
H	2.68625400	0.26271200	3.70078100
H	1.90860600	1.81503900	4.05463000
O	0.73544000	0.72766200	1.97734200

**TS\_end3**

E(B3lyp/6-31g(d) = -1210.412158 Hartree

Imaginary Freq= -660.89

-1 1

C	6.02406900	0.92180700	0.73773700
C	5.49491900	0.15302800	-0.30670200

C	4.11057800	0.11595900	-0.43516200
C	3.26354300	0.81685300	0.43675300
C	3.80351800	1.58129900	1.46985900
C	5.19309600	1.62864400	1.61733800
H	7.10322200	0.96794500	0.86582700
H	6.13147000	-0.39612300	-0.99381200
H	3.14162500	2.12458100	2.13828900
H	5.63349200	2.21615000	2.41900900
C	1.89874500	0.59114000	-0.03094200
N	0.82448300	1.15174200	0.38104300
O	3.44238900	-0.57380000	-1.40415800
C	2.01240400	-0.42580900	-1.15945000
C	1.37389200	-1.71523700	-0.70490400
C	2.10683400	-2.90313800	-0.62187000
C	-0.00742700	-1.66779400	-0.36056700
C	1.49310800	-4.08663900	-0.21805700
H	3.15874100	-2.89213800	-0.89009400
C	-0.60570300	-2.90541800	-0.00435800
C	0.12579500	-4.08203100	0.08424100
H	2.06905100	-5.00852300	-0.16605100
H	-1.67593800	-2.90053000	0.17506000
H	-0.37106900	-5.00598000	0.37519300
C	-0.86974000	-0.48938000	-0.41150100

C	-0.42809700	0.79100600	-0.16362100
C	-1.33755700	1.96774700	-0.29885100
C	-2.55712700	1.87023000	-0.99868100
C	-0.98026200	3.23073000	0.21256300
C	-3.37825400	2.98351500	-1.16702600
H	-2.86304500	0.90437700	-1.38664600
C	-1.80660400	4.34209200	0.04515900
H	-0.04050700	3.32392900	0.74573700
C	-3.01223500	4.22968500	-0.64886100
H	-4.31440700	2.87509100	-1.71171000
H	-1.50260200	5.30285900	0.45809600
H	-3.65530300	5.09685200	-0.78635000
H	1.54691600	-0.05253100	-2.08284100
C	-4.23738700	-1.23551600	0.59785100
C	-4.81120800	-2.64043000	0.89647000
H	-4.00372700	-3.32618200	1.18081100
H	-5.55441800	-2.62858600	1.70752000
H	-5.28724000	-3.04148900	-0.00633900
C	-3.51197600	-0.70818000	1.85590600
H	-2.67913500	-1.36766300	2.12613200
H	-3.10033700	0.28990800	1.67482500
H	-4.19464800	-0.64880200	2.71553300
C	-5.41071200	-0.28670500	0.25424600

H	-5.03426200	0.72411500	0.06457000
H	-5.91015600	-0.63886800	-0.65664800
H	-6.15686000	-0.23125000	1.06083200
O	-3.38676400	-1.34244100	-0.51246500
H	-2.33453600	-0.88415000	-0.42667400

### TS\_5

E(B3lyp/6-31g(d) = -976.687692 Hartree

Imaginary Freq= -319.65

-1 1

C	-3.21589400	3.82726600	-0.46309400
C	-3.50079200	2.49121200	-0.76212900
C	-2.58831500	1.53342900	-0.33252000
C	-1.41655100	1.85674300	0.37726800
C	-1.15526000	3.19930000	0.67453300
C	-2.05455600	4.17796300	0.24679700
H	-3.90565000	4.60488500	-0.78410700
H	-4.39331700	2.20322300	-1.31075200
H	-0.26281700	3.47635800	1.23316300
H	-1.85789700	5.22497100	0.46768700
C	-0.73888700	0.59582000	0.67860400
N	0.36340700	0.40631500	1.44119000
O	-2.68358100	0.20161700	-0.53198900



C	-1.53253700	-0.39316200	0.06091300
C	-1.46203000	-1.81915600	-0.03656400
C	-2.63995700	-2.57523900	-0.28824600
C	-0.21831300	-2.53674400	0.11484200
C	-2.64140600	-3.95776500	-0.23143100
H	-3.56443900	-2.03997400	-0.48291800
C	-0.27040600	-3.95069900	0.20256100
C	-1.45179600	-4.65732100	0.05551000
H	-3.56925100	-4.50348600	-0.39616300
H	0.67208500	-4.47627500	0.34260600
H	-1.45429400	-5.74397500	0.11866000
C	1.02805900	-1.86966900	0.04027200
C	1.62057500	-0.78226500	0.29693400
C	2.84904000	-0.07170700	0.03609700
C	4.03189600	-0.81387400	-0.19646800
C	2.94938100	1.33395700	-0.02005700
C	5.24179000	-0.18300700	-0.46681300
H	3.96405700	-1.89683200	-0.16151100
C	4.16207900	1.96122700	-0.29891800
H	2.05568200	1.92598000	0.14171100
C	5.32069700	1.21276000	-0.51998800
H	6.13253300	-0.78535600	-0.63796400
H	4.20054500	3.04821900	-0.34423600

H 6.26748400 1.70637700 -0.72807700

H 0.73916600 1.32432400 1.70087700

#### TS\_4

E(B3lyp/6-31g(d) = -1210.368223 Hartree

Imaginary Freq= -410.95

-1 1

C -4.73916600 -2.41070000 -0.89171100

C -4.24541800 -1.52788800 0.06987200

C -3.09152100 -0.80752200 -0.24881400

C -2.43941600 -0.96754000 -1.47897300

C -2.95004800 -1.84810300 -2.43101100

C -4.10401100 -2.57603300 -2.13326500

H -5.63613100 -2.98574000 -0.67088900

H -4.72947900 -1.39905700 1.03308700

H -2.44756600 -1.97190700 -3.38899900

H -4.50967400 -3.27681300 -2.85869700

C -1.30153500 -0.02795900 -1.49081600

N -0.51697000 0.30822700 -2.45326800

O -2.50495500 0.10206400 0.54762500

C -1.22716200 0.50301200 -0.08103500

H -0.39673200 -0.21436600 0.53256900

C -1.02529200 1.97332800 0.08800700

C	-2.08362700	2.81394600	0.46748300
C	0.24933700	2.56829700	-0.13399000
C	-1.92031600	4.19204000	0.59386500
H	-3.05052900	2.36314000	0.66112200
C	0.39288900	3.96604500	-0.01928000
C	-0.67770100	4.77740900	0.33839400
H	-2.76791500	4.80993700	0.88393200
H	1.37401000	4.39685200	-0.19971800
H	-0.54163300	5.85272800	0.42953400
C	1.39899900	1.77882300	-0.41232000
C	2.38615900	1.09250700	-0.58935000
C	3.43465900	0.14514400	-0.75830200
C	3.21417800	-1.18530000	-0.33508400
C	4.67265800	0.49402100	-1.33196100
C	4.22470000	-2.13031700	-0.49675900
H	2.25063600	-1.42454700	0.12716300
C	5.67254100	-0.46481000	-1.48481700
H	4.83676600	1.51779600	-1.65796300
C	5.45298600	-1.78044200	-1.06873600
H	4.05189100	-3.15311800	-0.16840500
H	6.62490500	-0.18456000	-1.93072700
H	6.23527300	-2.52749900	-1.18787000
H	-0.75262600	-0.23890200	-3.29016400

C	0.36911600	-1.34545200	2.50980600
C	-1.02116900	-1.83375000	3.00037800
H	-1.79271400	-1.11123200	2.71313000
H	-1.26162900	-2.78809000	2.51521900
H	-1.06571100	-1.97682400	4.09148200
C	1.43093400	-2.38859500	2.94384500
H	1.22929100	-3.34337200	2.44226500
H	2.43040400	-2.05431600	2.63985600
H	1.44062300	-2.56138200	4.03111400
C	0.69812200	0.00691500	3.19665400
H	1.66935000	0.37052800	2.84126000
H	-0.05468600	0.75925500	2.93127200
H	0.73190100	-0.06671900	4.29486300
O	0.39562800	-1.23354400	1.13061900

(1) Gai, R.; Back, D. F.; Zeni, G. Potassium tert-Butoxide-Catalyzed Synthesis of Benzofuroazepines via Cyclization of (2-Alkynylbenzyl) oxy Nitriles. *The Journal of Organic Chemistry* **2015**, *80* (20), 10278-10287.