

Electronic Supplementary Information.

Meisenheimer complex as hidden intermediates in the aza-S_NAr mechanism.

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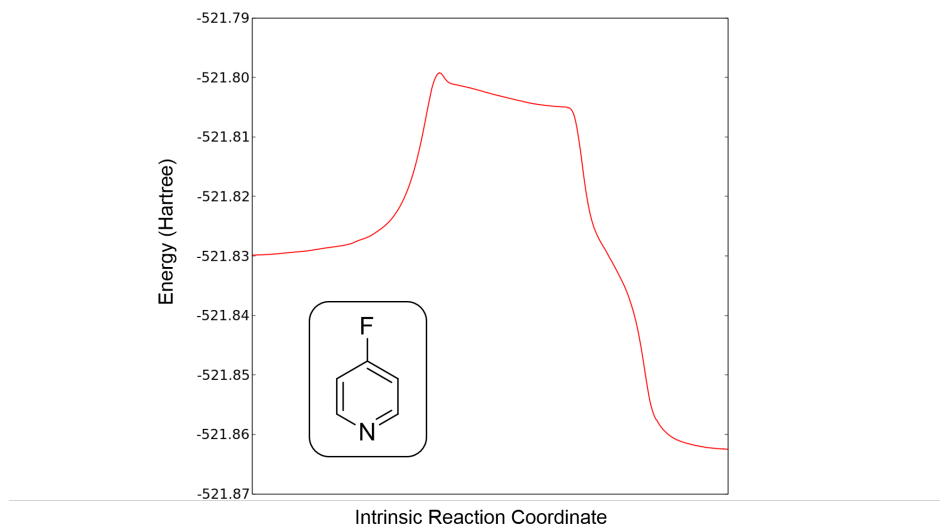
⁴Caltech.

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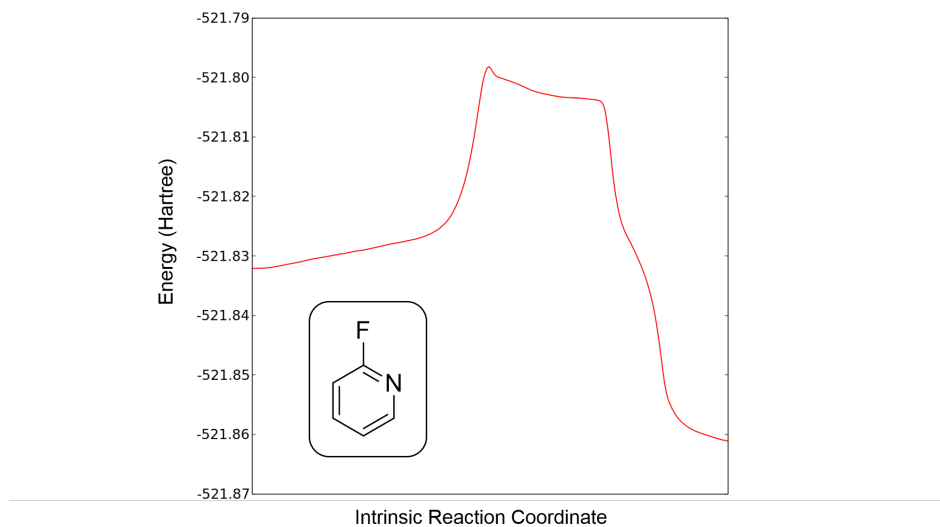
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1 Computed (M06-2X/6-31+G(d,p)/SMD=water) reaction profiles for the reaction between propylamine and different substrates considered in present study

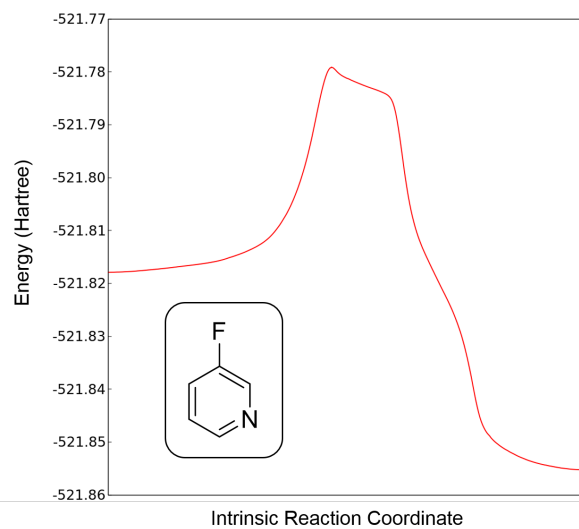
- TS1-1A-F



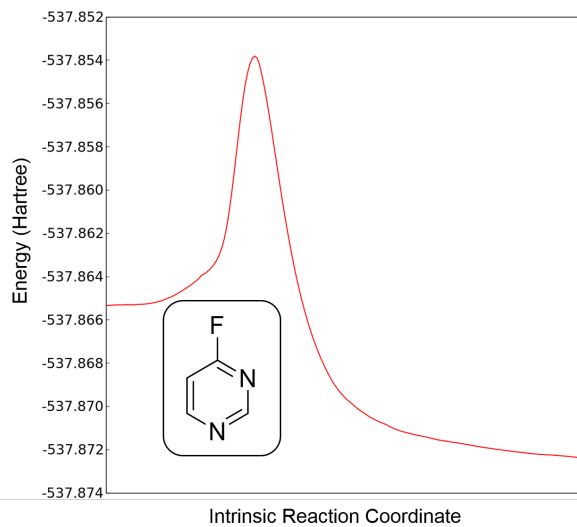
- TS1-1B-F



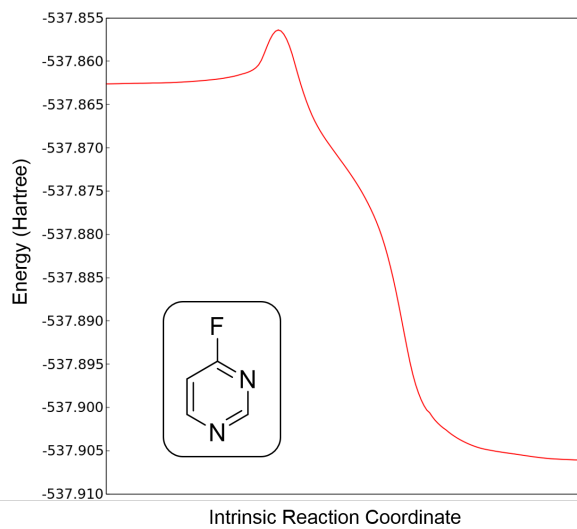
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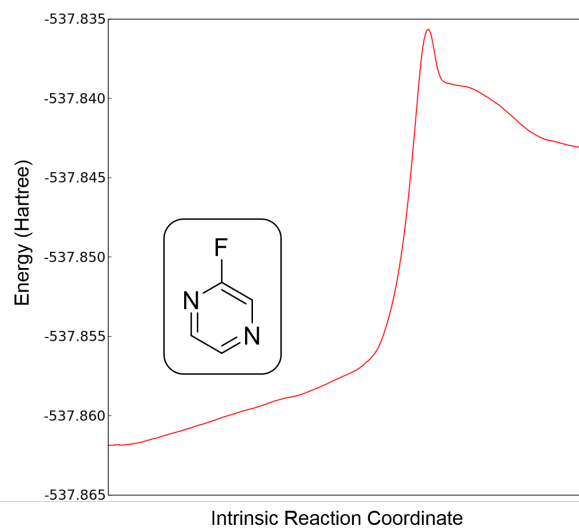
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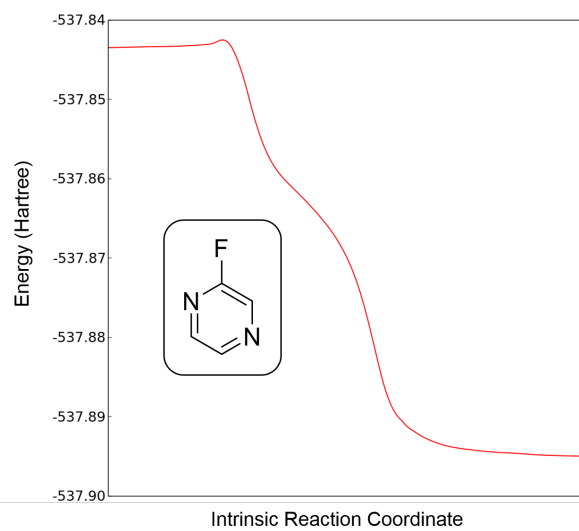
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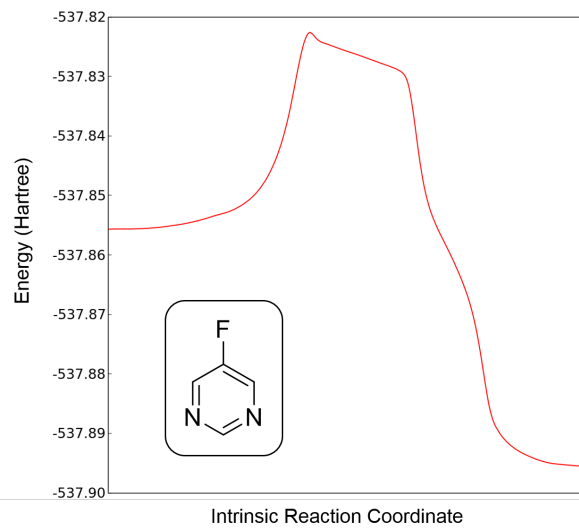
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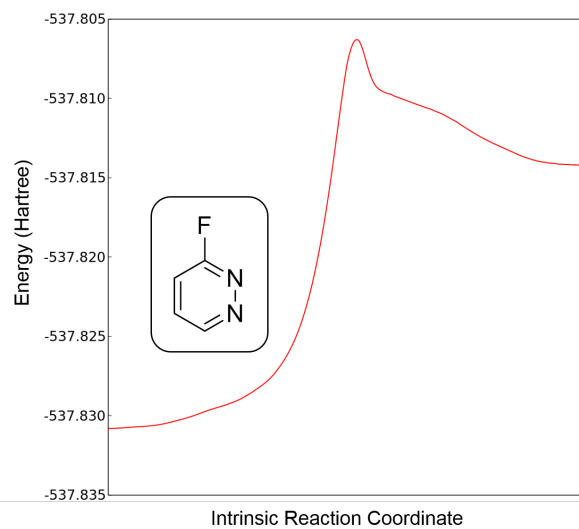
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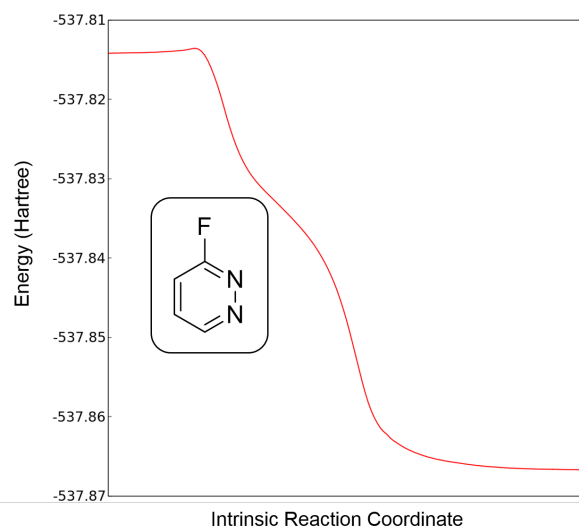
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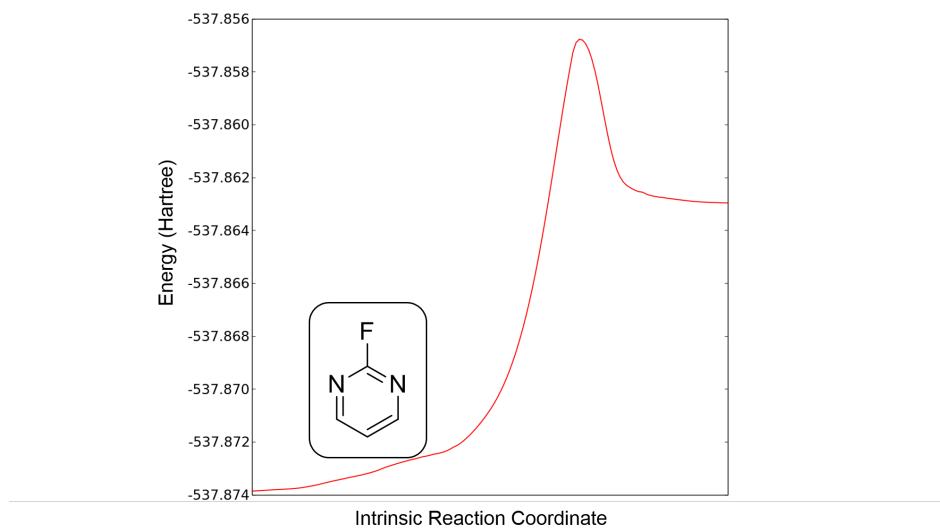
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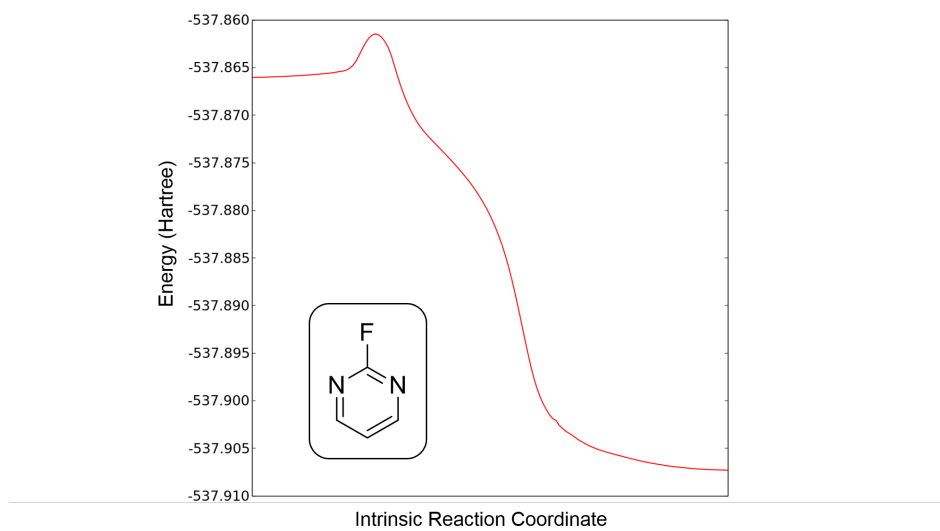
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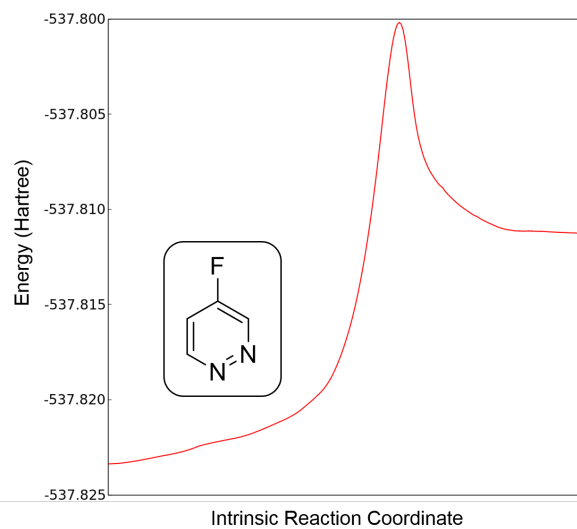
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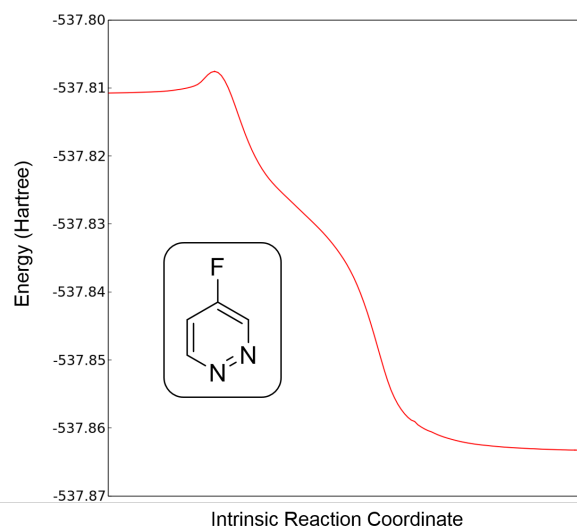
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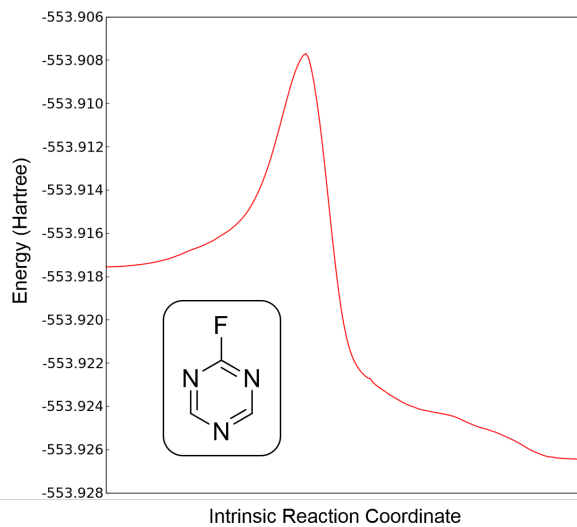
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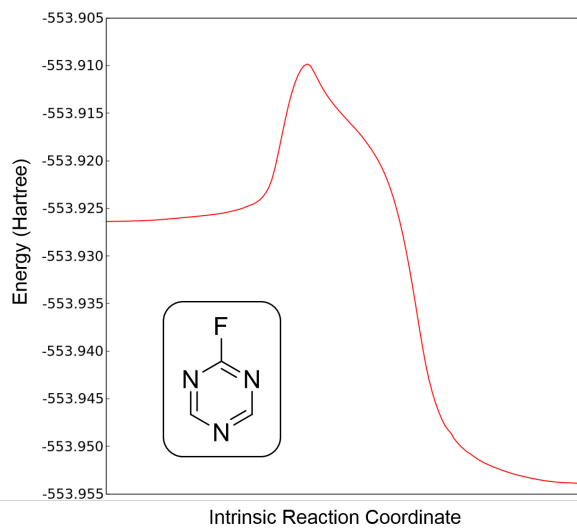
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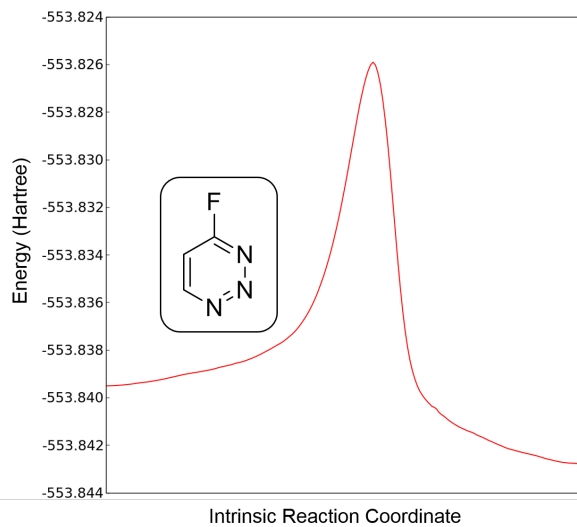
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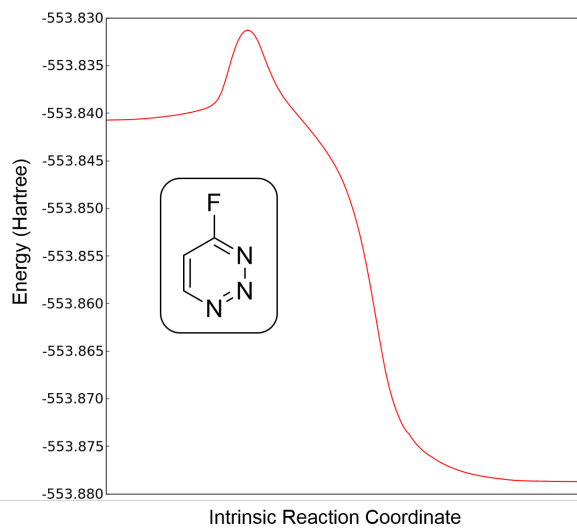
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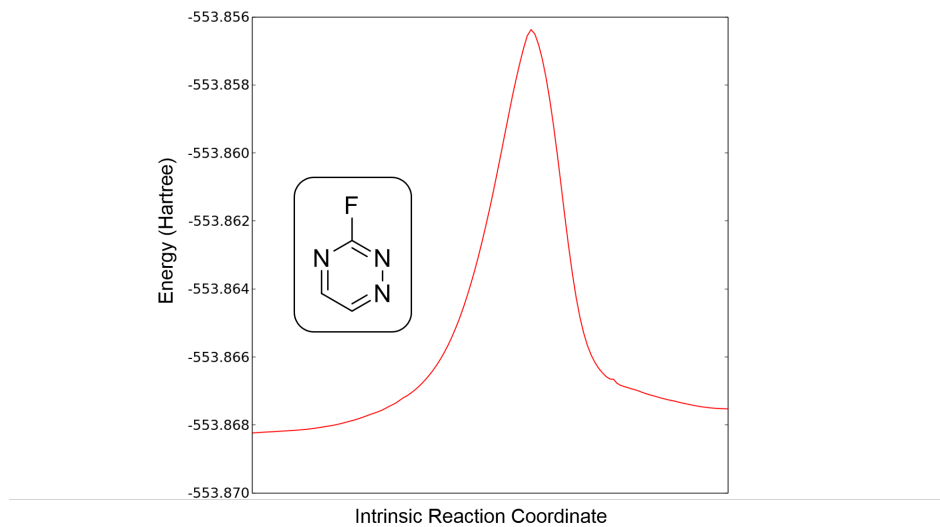
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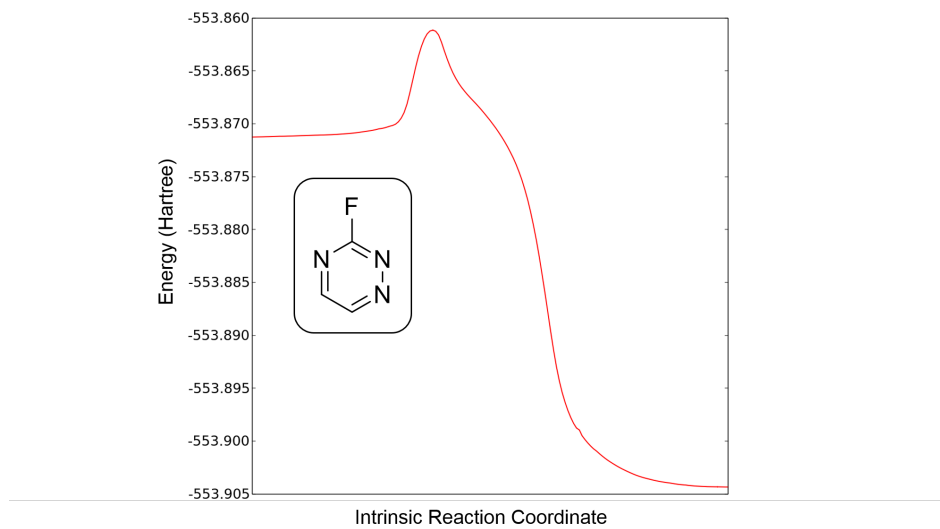
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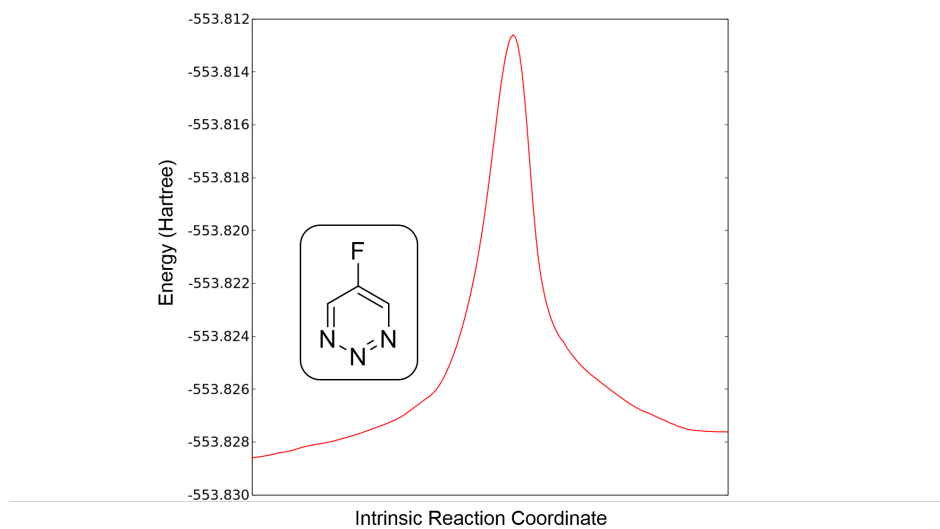
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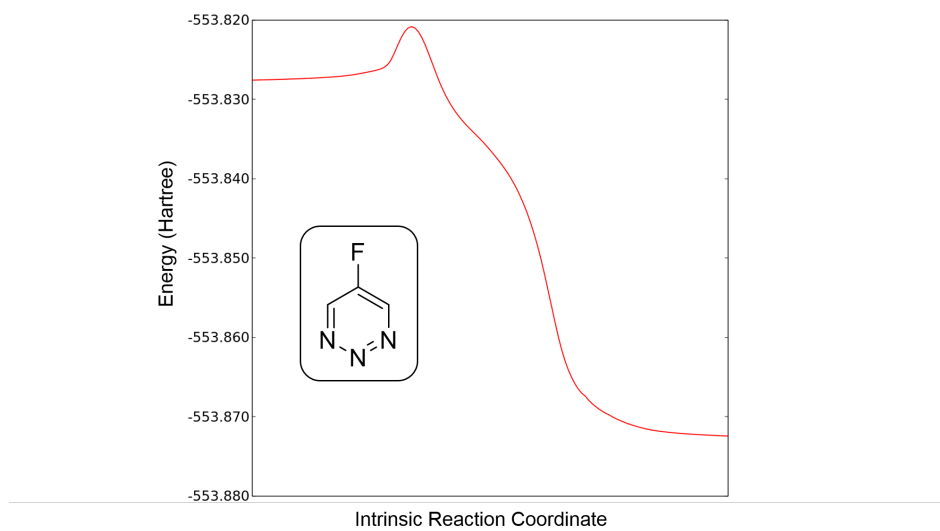
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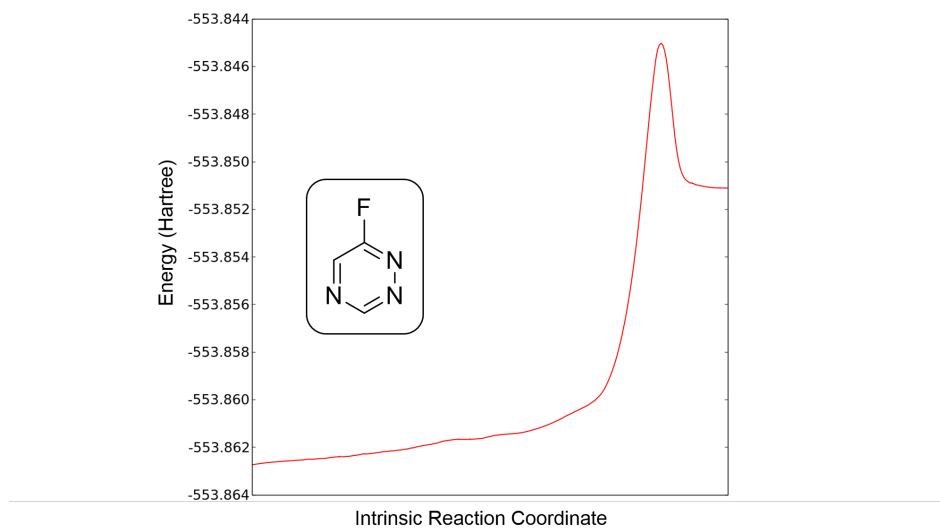
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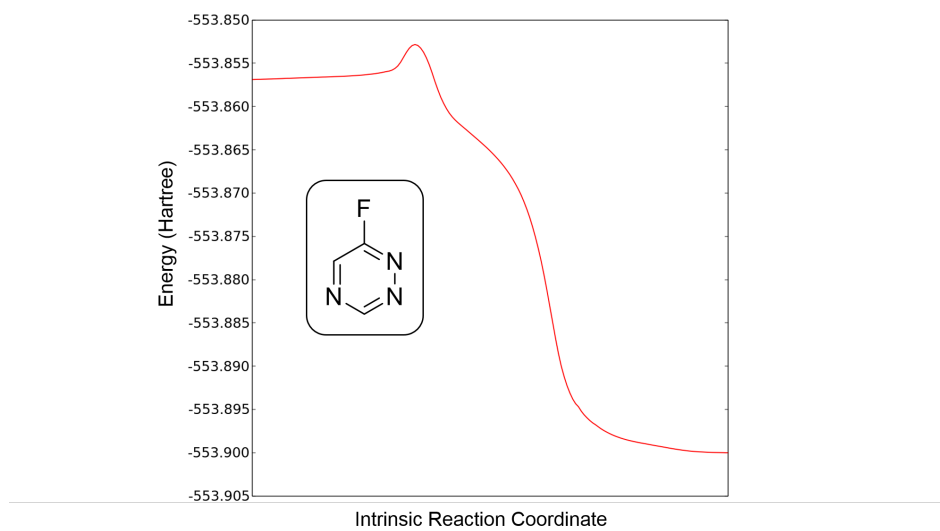
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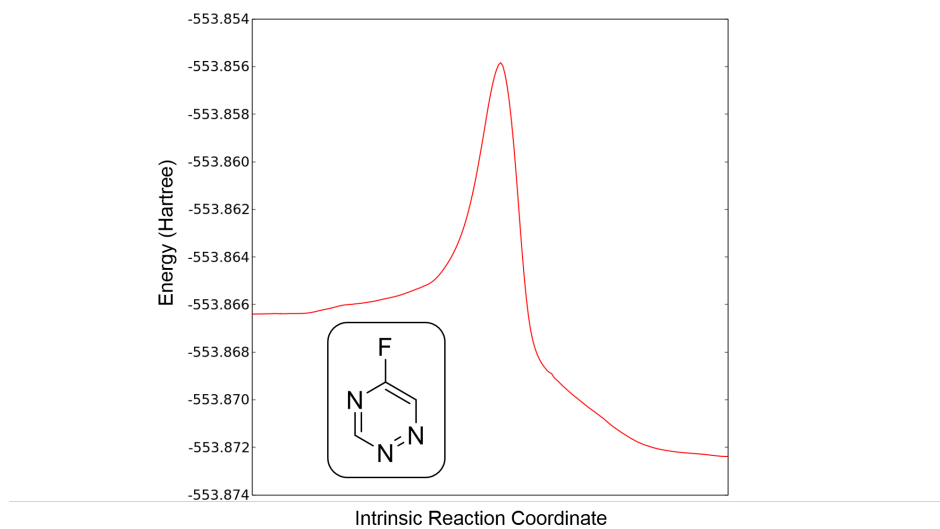
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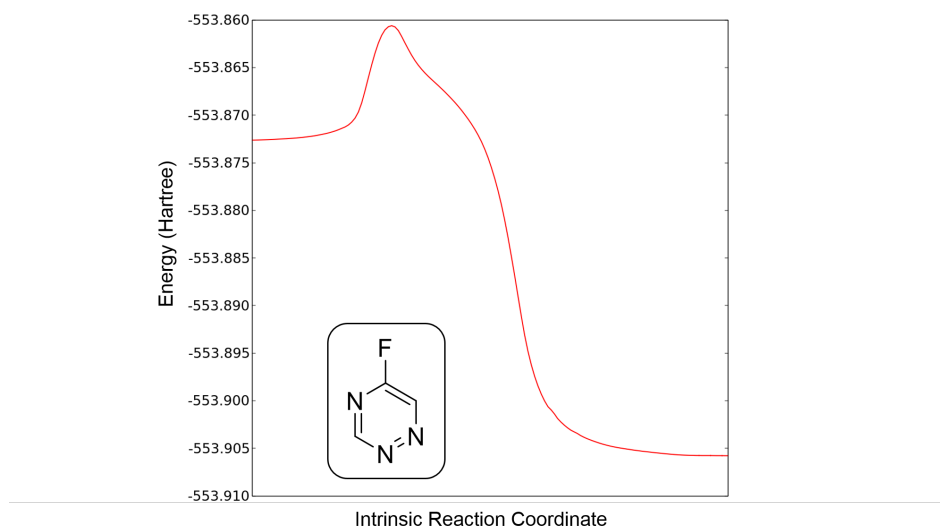
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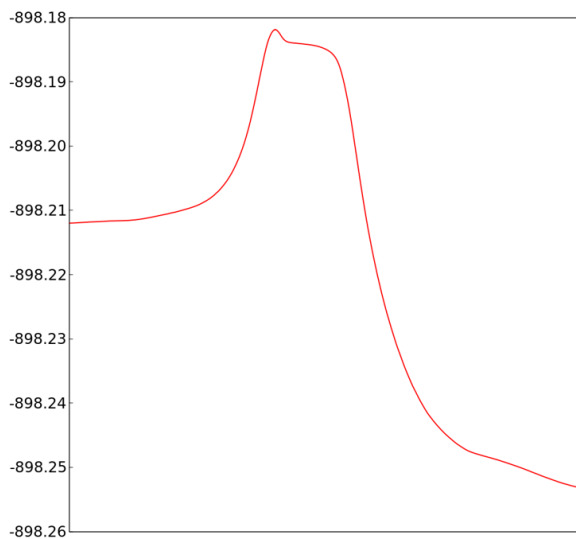
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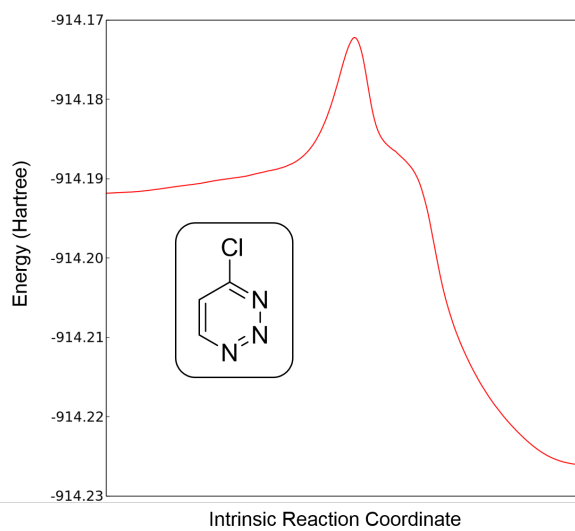
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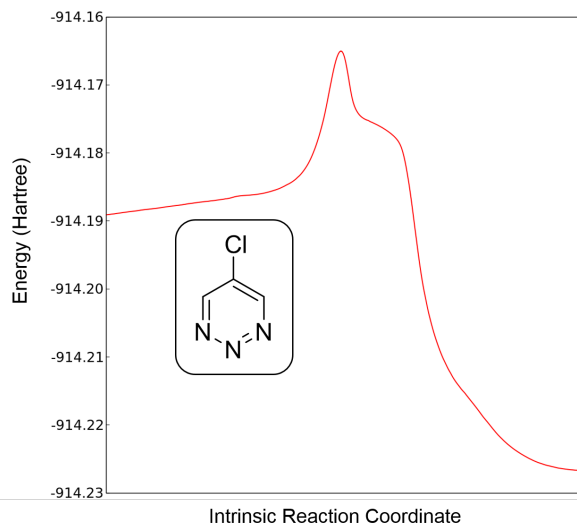
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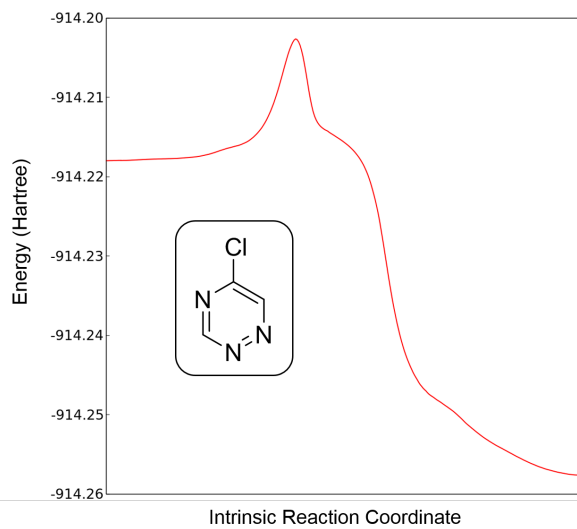
- TS1-3B-Cl



- TS1-3D-Cl



- TS1-3F-Cl



2 Number of Imaginary frequencies (NIMAG), characteristic frequencies and energies for transition states in the reaction of the substrates considered in present study with propylamine.

Entry	NIMAG	Frequency (cm^{-1})	E (hartree)
TS1-1A-F	1	-336	-521.794273027
TS1-1B-F	1	-289	-521.799264074
TS1-1C-F	1	-323	-521.779374038
TS1-2A-F	1	-328	-537.853881072
TS2-2A-F	1	-326	-537.856454903
TS1-2B-F	1	-295	-537.835690772
TS2-2B-F	1	-259	-537.842702066
TS1-2C-F	1	-328	-537.822654392
TS1-2D-F	1	-291	-537.806256486
TS2-2D-F	1	-227	-537.813697232
TS1-2E-F	1	-293	-537.856690009
TS2-2E-F	1	-285	-537.861557559
TS1-2F-F	1	-332	-537.800238593
TS2-2F-F	1	-336	-537.807536908
TS1-3A-F	1	-443	-553.907619645
TS2-3A-F	1	-365	-553.909999411
TS1-3B-F	1	-381	-553.826007006
TS2-3B-F	1	-308	-553.831408583
TS1-3C-F	1	-427	-553.856540644
TS2-3C-F	1	-286	-553.861353973
TS1-3D-F	1	-314	-553.812712875
TS2-3D-F	1	-362	-553.820847796
TS1-3E-F	1	-384	-553.855793396
TS2-3E-F	1	-300	-553.860713505
TS1-3F-F	1	-289	-553.845032697
TS2-3F-F	1	-297	-553.853003565

Entry	NIMAG	Frequency (cm ⁻¹)	E (hartree)
1A-C1	1	-365	-882.143830648
1B-C1	1	-320	-882.144554693
1C-C1	1	-392	-882.129523553
2A-C1	1	-325	-898.198898020
2B-C1	1	-316	-898.181998032
2C-C1	1	-334	-898.173921842
2D-C1	1	-308	-898.152514497
2E-C1	1	-273	-898.198820863
2F-C1	1	-348	-898.151075575
3A-C1	1	-453	-914.250010079
3B-C1	1	-363	-914.172232183
3C-C1	1	-347	-914.200531645
3D-C1	1	-329	-914.165117787
3E-C1	1	-361	-914.202748899

3 Cartesian coordinates for Transition States.

- **TS1-1A-F**

```
C 1.16143100 0.81898400 0.00009100
N -0.71167900 1.24452200 -0.00013800
H -0.89204600 1.81324100 0.82824600
C 1.74258900 -1.22404000 -1.13579800
C 1.42835700 0.11810000 1.20621800
C 1.74231300 -1.22426500 1.13571100
H 1.90683800 -1.76869100 -2.06318300
H 1.90634300 -1.76909200 2.06303100
H 1.33474000 0.62563000 2.16070200
F 1.47098200 2.17198800 0.00027200
H -0.89183800 1.81297100 -0.82875200
C -1.52189500 0.02608200 -0.00003900
H -1.23606500 -0.55427900 -0.88506600
H -1.23620900 -0.55402500 0.88520000
C -3.02406900 0.28462000 -0.00018600
H -3.28513600 0.88121900 -0.88227500
H -3.28522300 0.88160500 0.88161700
C -3.81084500 -1.02283000 0.00007000
H -3.57267900 -1.62177700 0.88531400
H -4.88803900 -0.83533200 0.00000900
H -3.57264000 -1.62215900 -0.88490500
N 1.89147400 -1.93498400 -0.00009400
C 1.42866100 0.11834200 -1.20611100
H 1.33529700 0.62607800 -2.16051100
```

• **TS1-1B-F**

C 0.92984600 0.68283500 0.28924000
N -0.62037500 0.43324600 -0.65081400
H -0.77576900 1.29610500 -1.17578400
C 2.68654400 -0.01833300 -1.00366200
C 2.74989800 -1.25527600 -0.38694300
C 1.08681400 -0.45006800 1.16377200
C 1.96003500 -1.43208500 0.77265100
H 3.37193200 0.21906500 -1.81472400
H 2.06812200 -2.32926100 1.37676300
H 0.48039200 -0.51876400 2.06004000
F 0.45082600 1.81443000 0.93849500
H -0.39119600 -0.30807700 -1.31602900
C -1.80703500 0.07010900 0.13881500
H -1.53449500 -0.78968500 0.76030200
H -2.03243000 0.91105600 0.80150200
C -3.01645600 -0.27214900 -0.72346300
H -2.75471100 -1.10273100 -1.39002000
H -3.26103400 0.58869200 -1.35682900
C -4.21854700 -0.64889000 0.13724500
H -4.50219500 0.17861000 0.79572000
H -5.08398500 -0.89794100 -0.48269300
H -3.99274200 -1.51708600 0.76510400
H 3.45201200 -2.00817700 -0.72354300
N 1.85924300 0.97982100 -0.64521400

• **TS1-1C-F**

C 0.84975000 0.54938200 0.35331100
N -0.70089000 0.53790500 -0.57436100
H -0.87659800 1.50254300 -0.86606800
C 2.98823400 -1.01802200 -0.49001800
C 1.08736000 -0.71274200 0.96783600
C 2.12627100 -1.49905900 0.49688900
H 2.29310100 -2.48334700 0.92573200
H 0.43127700 -1.04675900 1.76569100
F 0.36895400 1.54780400 1.22633700
H -0.50079400 -0.01681100 -1.40854300
C -1.86150100 -0.01441400 0.14530100
H -1.58053100 -1.01233500 0.49867800
H -2.03956700 0.62064800 1.01778600
C -3.10907900 -0.09808900 -0.72582600
H -2.88482900 -0.70635300 -1.61013100
H -3.36775300 0.90661400 -1.08012000
C -4.28044500 -0.70091100 0.04364100
H -4.52630300 -0.09477000 0.92180000
H -5.17404000 -0.75978200 -0.58350800
H -4.04227500 -1.71239800 0.38863200
H 3.81158300 -1.61600300 -0.86533500
N 2.87521200 0.23592400 -0.96403500
C 1.88172600 1.00231100 -0.53463000
H 1.82198800 2.02096600 -0.91190400

● **TS1-2A-F**

C 1.30992400 0.74641700 -0.03491300

N -0.64020900 1.28015300 0.02361500
H -0.78570800 1.81130900 0.88265700
C 1.53342100 -1.22097500 -1.13348900
C 1.50578100 0.07306000 1.20030900
C 1.61255300 -1.28907200 1.12477900
H 1.58684900 -1.73705000 -2.08874700
H 1.73079400 -1.87809300 2.02994200
H 1.52037200 0.61682100 2.13723700
F 1.66812400 2.06181700 -0.07170100
H -0.82052100 1.89704700 -0.76843500
C -1.49698600 0.09556600 -0.01678300
H -1.25977600 -0.45210900 -0.93697500
H -1.21575000 -0.54139900 0.83100900
C -2.99166500 0.39588800 0.03747800
H -3.25717900 1.04340200 -0.80692000
H -3.20976800 0.95587200 0.95493000
C -3.81844700 -0.88571600 -0.00428800
H -3.57723800 -1.53388800 0.84482600
H -4.88936500 -0.66741000 0.03198000
H -3.62079600 -1.44804700 -0.92303100
N 1.44613700 0.11138200 -1.20325500
N 1.60228400 -1.97922300 -0.04631900

● **TS2-2A-F**

C 0.68781600 0.23833400 0.04832100
C 2.99184200 0.60718300 0.42263800
C 2.19096100 -1.44991100 -0.06301000

H 3.84551600 1.23380200 0.66342400
H 2.36836400 -2.50989400 -0.22630600
N -0.68566900 0.62091500 0.47488100
H -0.86533900 1.54569300 0.06750500
H -0.68882600 0.72652700 1.49693900
C -1.79337700 -0.30427500 0.07751400
H -1.66734500 -1.22314900 0.65070800
H -1.65606300 -0.51405700 -0.98347200
C -3.13253900 0.35679800 0.35876300
H -3.20550400 1.28223000 -0.22428200
H -3.18976400 0.63033800 1.41866800
C -4.27883200 -0.58245000 -0.00278400
H -4.23487200 -1.50180300 0.58938800
H -5.24398100 -0.10546000 0.18525400
H -4.23928900 -0.85816500 -1.06129800
F 0.28120400 0.80131300 -1.64656200
N 3.26080500 -0.69323600 0.13597500
C 1.72641900 1.12711800 0.43415100
H 1.52379500 2.16540600 0.67165200
N 0.90611000 -1.07626000 -0.05123900

● **TS1-2B-F**

C -0.95196300 -0.66893700 0.30398100
N 0.60739900 -0.29716800 -0.69811200
H 0.70874800 -1.03903200 -1.39284500
C -2.66756200 1.28745900 -0.27986600
C -1.87994900 1.31588400 0.85150100

H -1.93089600 2.16213100 1.53123600
F -0.45495300 -1.84576500 0.80457400
H 0.39401400 0.57208700 -1.19139800
C 1.82435800 -0.14916800 0.11255600
H 1.57862100 0.51834600 0.94603200
H 2.06611700 -1.13184400 0.52787200
C 3.00727500 0.40510400 -0.67312800
H 2.73128100 1.38238500 -1.08743600
H 3.21781800 -0.25843600 -1.52032900
C 4.24583200 0.53832600 0.20765400
H 4.54464500 -0.43449700 0.61192100
H 5.09025500 0.94063400 -0.35863600
H 4.05530700 1.20931200 1.05182600
H -3.30774400 2.11833300 -0.54875400
N -2.76938500 0.14548500 -1.01787200
C -1.96845600 -0.83981600 -0.70586900
H -2.04076100 -1.78445900 -1.23801800
N -1.07659000 0.29794100 1.21975500

• **TS2-2B-F**

C 0.68861300 -0.27095500 0.00086700
C 2.87440800 -0.76629900 -0.36039300
C 3.23351800 0.54707700 -0.14478200
H 3.63202100 -1.51406200 -0.57787400
N -0.69036400 -0.66135900 -0.42615200
H -0.87685300 -1.56203900 0.03070400
H -0.67427500 -0.83406300 -1.43827900

C -1.80729600 0.28281900 -0.10313200
H -1.70132400 1.14928300 -0.75849100
H -1.67140400 0.58648600 0.93615400
C -3.14565000 -0.40359100 -0.31861900
H -3.20111900 -1.29064700 0.32289000
H -3.21676900 -0.74309900 -1.35826000
C -4.29126900 0.55051800 0.00352300
H -4.25622800 1.43728900 -0.63709100
H -5.25665800 0.06193500 -0.14937200
H -4.24143600 0.88281800 1.04517400
H 0.25697900 1.89261500 -0.01626000
F 0.34962000 -0.55769600 1.63093400
C 1.02802400 1.12972700 -0.04539800
H 4.27024300 0.86063400 -0.13490700
N 1.59554300 -1.18286400 -0.38969000
N 2.28170000 1.51227100 -0.06061300

● **TS1-2C-F**

C 0.89554300 0.64739100 0.28402700
N -0.66823000 0.55979800 -0.64079500
H -0.87090600 1.50306800 -0.97985300
C 2.72278900 -1.25419800 -0.34913000
C 1.08746700 -0.52920900 1.06861400
H 0.50002800 -0.66973300 1.97198000
F 0.48149500 1.76518600 1.00623700
H -0.46925900 -0.03669600 -1.44634000
C -1.79677700 0.01840300 0.13511100

H -1.48568600 -0.95824600 0.52191900
H -1.96110800 0.68570700 0.98665900
C -3.06859200 -0.12545800 -0.69113800
H -2.85606800 -0.75485600 -1.56351000
H -3.36748700 0.86008500 -1.06682100
C -4.19560900 -0.73710200 0.13565300
H -4.42828800 -0.11248800 1.00434300
H -5.10771600 -0.83801700 -0.45858400
H -3.91759000 -1.73143300 0.50000500
H 3.39915800 -2.04337200 -0.65537200
N 2.80635100 -0.08130300 -0.98948800
C 1.96199100 0.87880600 -0.63567600
H 2.05862800 1.85655300 -1.10117400
N 1.93787400 -1.48407300 0.70826100

● **TS1-2D-F**

C -0.97016300 -0.69027900 0.28637300
N 0.61000800 -0.40431000 -0.68734300
H 0.78227100 -1.27490500 -1.19332600
C -2.67034400 1.22378800 -0.42155800
C -1.09177600 0.42863900 1.17832900
C -1.91544700 1.42864300 0.76194900
H -2.04251000 2.33974400 1.33785100
H -0.51170500 0.45852400 2.09424600
F -0.49476900 -1.83746600 0.87166700
H 0.37907400 0.32212100 -1.36765400
C 1.77389600 -0.01213700 0.12018300

H 1.50684800 0.90561700 0.65560000
H 1.93851800 -0.79953300 0.86286500
C 3.03791400 0.21276400 -0.70162900
H 2.84678400 0.99081300 -1.45029800
H 3.27871400 -0.70813400 -1.24576000
C 4.20867900 0.61781300 0.18916000
H 4.41255600 -0.15201700 0.94068500
H 5.11868000 0.76367300 -0.39910600
H 3.99425600 1.55376600 0.71558700
H -3.33571000 1.98610700 -0.81031600
N -2.70841700 0.05446500 -1.03167600
N -1.92322100 -0.95072300 -0.63272700

• **TS2-2D-F**

C 0.68341700 -0.24512500 0.03457300
C 3.26709100 0.38231500 -0.20243900
N -0.68853500 -0.64969700 -0.40586200
H -0.87117100 -1.55532500 0.04229400
H -0.65988100 -0.81583200 -1.41858600
C -1.81259100 0.28591000 -0.08788000
H -1.69890500 1.16050300 -0.73131400
H -1.69349300 0.57873300 0.95661400
C -3.14643500 -0.40048100 -0.32959100
H -3.21244100 -1.29010300 0.30721400
H -3.20024600 -0.73550000 -1.37169700
C -4.29750600 0.55243200 -0.02344100
H -4.25346600 1.43959800 -0.66298100

H -5.26030800 0.06347400 -0.19078200
H -4.26323100 0.88415400 1.01903500
F 0.35268600 -0.54773700 1.64093900
H 4.33652100 0.55721000 -0.23526600
N 1.57568100 -1.17479100 -0.38571300
C 2.34488600 1.44677600 -0.06442800
H 2.69622500 2.47307100 -0.03950400
C 1.01642200 1.15193200 -0.01328700
H 0.25093500 1.91566400 0.06015700
N 2.87336500 -0.85959300 -0.40623600

• **TS1-2E-F**

C -1.09855900 0.75773900 -0.28418300
N 0.57181200 0.33948600 0.73708100
H 0.75017500 1.17279700 1.29720700
C -2.58254400 -0.32635600 0.99883100
C -2.37261500 -1.48232200 0.24620200
C -1.67923900 -1.30044800 -0.94873800
H -3.27880500 -0.32683600 1.83368100
H -1.64099900 -2.09046300 -1.69505500
F -0.63211100 1.97000400 -0.67562000
H 0.35946500 -0.42937100 1.37290600
C 1.72498200 0.01331300 -0.10522500
H 1.47099800 -0.88550800 -0.67699800
H 1.85510300 0.83237500 -0.82207100
C 3.01820000 -0.21054100 0.67259400
H 2.86547300 -1.02462400 1.39170100

H 3.24688500 0.69185100 1.25246400
C 4.18016500 -0.54344900 -0.25837100
H 4.35766700 0.27090800 -0.96887900
H 5.10421800 -0.70549000 0.30345700
H 3.97247700 -1.45148400 -0.83422400
H -2.84894500 -2.42171900 0.49433700
N -2.00427400 0.83755600 0.71118800
N -1.09140300 -0.14991000 -1.27606800

• **TS2-2E-F**

C 0.69784000 -0.22156400 -0.11114500
C 2.86751000 -0.78410500 -0.32126500
C 3.23251700 0.53428300 -0.05978300
H 3.62164100 -1.54395300 -0.50859900
N -0.68055100 -0.64164800 -0.46667000
H -0.83236000 -1.53211500 0.01943700
H -0.70838400 -0.83395400 -1.47588100
C -1.78834600 0.29837900 -0.11242900
H -1.69130300 1.17226200 -0.75683000
H -1.62314300 0.58907400 0.92532100
C -3.12650700 -0.39568200 -0.30573200
H -3.16095900 -1.29280400 0.32355000
H -3.22022800 -0.72238300 -1.34793000
C -4.27398800 0.54130100 0.05681200
H -4.26226300 1.43867600 -0.56968500
H -5.23764300 0.04508900 -0.08275700
H -4.20493500 0.85706900 1.10253700

F 0.34088800 -0.56707000 1.65766700
H 4.26874400 0.83950700 0.00661700
N 1.59858400 -1.17618700 -0.41238300
N 0.90791700 1.10213800 -0.13849800
C 2.19218700 1.45625300 -0.04964300
H 2.39392000 2.52384600 -0.01281700

● **TS1-2F-F**

C -0.94957700 -0.63035400 0.37744000
N 0.71004600 -0.57079500 -0.65757300
H 0.90343900 -1.51763300 -0.98592700
C -1.09958700 0.57836000 1.07539700
C -2.01855500 1.47779900 0.55987200
H -2.12773300 2.45778600 1.01557100
H -0.48839900 0.81403000 1.93916900
F -0.49786000 -1.71935600 1.07966900
H 0.50253300 0.01794400 -1.46481000
C 1.83499900 -0.03136400 0.11234000
H 1.52439800 0.94261800 0.50876100
H 2.00382900 -0.70048700 0.96284000
C 3.11567400 0.12483000 -0.70059100
H 2.91180900 0.77074700 -1.56310800
H 3.41345600 -0.85483800 -1.09291700
C 4.23983600 0.71554500 0.14506800
H 4.46542700 0.07056500 1.00086000
H 5.15647000 0.82835800 -0.44021900
H 3.96197700 1.70190100 0.53101700

N -2.82156300 0.01236800 -1.00595200
C -1.96246000 -0.89376300 -0.59559400
H -2.01513800 -1.87384000 -1.06107100
N -2.84467000 1.23996200 -0.46658800

● **TS2-2F-F**

C 0.67668700 -0.29367800 0.03834000
C 2.98337300 -0.59136100 -0.47686500
H 3.82595900 -1.21679000 -0.75627400
N -0.69820000 -0.65392500 -0.41014600
H -0.89768200 -1.58204400 -0.01756300
H -0.68192800 -0.75179000 -1.43249800
C -1.81342300 0.27265000 -0.03331600
H -1.64554700 1.21245000 -0.56274000
H -1.73606200 0.43527600 1.04271800
C -3.14613300 -0.34354300 -0.42402700
H -3.26458000 -1.30533200 0.08793300
H -3.15072000 -0.54129600 -1.50198900
C -4.29461100 0.59157200 -0.05747200
H -4.19405400 1.55436900 -0.56806300
H -5.25388200 0.15438600 -0.34512200
H -4.31668900 0.77914400 1.02050200
H 0.28504800 1.84364000 0.33258400
F 0.28544900 -0.76371600 1.68093200
C 1.03288800 1.08653900 0.12416100
N 2.27545900 1.51952300 0.03973500
N 3.28642200 0.68990100 -0.23150400

C 1.71000400 -1.12726100 -0.42702600
H 1.52261900 -2.16656300 -0.67724900

• **TS1-3A-F**

C -1.16833700 0.75173800 -0.29461000
N 0.60582200 0.43942800 0.76161100
H 0.79010100 1.31049500 1.25817600
C -2.54721300 -0.44643000 0.96340600
C -1.62771200 -1.33728000 -0.87511100
H -3.22719600 -0.53456000 1.80561700
H -1.53540300 -2.16958700 -1.56702800
F -0.78015400 1.97344100 -0.69226500
H 0.42062100 -0.28522600 1.45530300
C 1.73281800 0.06320300 -0.09358000
H 1.45111000 -0.85407600 -0.62280800
H 1.85798200 0.85010300 -0.84631500
C 3.04371100 -0.15463300 0.65650600
H 2.89528800 -0.93349500 1.41449400
H 3.30847800 0.76656000 1.18948700
C 4.16901900 -0.55488700 -0.29288000
H 4.33884000 0.22039100 -1.04759100
H 5.10777200 -0.70970200 0.24614100
H 3.92522300 -1.48496000 -0.81738500
N -2.05552700 0.75605200 0.71510000
N -1.08723100 -0.18713300 -1.24939200
N -2.30951400 -1.56080200 0.25552400

• **TS2-3A-F**

C 0.70936500 -0.20319800 -0.19588100
C 2.87775000 -0.62969300 -0.42353600
H 3.68523900 -1.31555400 -0.65975100
N -0.66330700 -0.64087600 -0.48900400
H -0.78405400 -1.50501700 0.05550800
H -0.72389100 -0.87615300 -1.48904000
C -1.76105700 0.31171500 -0.12902500
H -1.66020400 1.18234100 -0.77802000
H -1.58628900 0.60429500 0.90662800
C -3.10486200 -0.37340400 -0.30693700
H -3.14426300 -1.26023400 0.33619000
H -3.20735200 -0.71337400 -1.34383000
C -4.23887700 0.58323500 0.04781600
H -4.22233700 1.46786900 -0.59645800
H -5.20887900 0.09513700 -0.07421200
H -4.15688500 0.91898400 1.08632700
F 0.33358400 -0.84451200 1.69066200
N 1.63998900 -1.08750900 -0.55705800
N 0.89661000 1.09573000 0.00615200
C 2.17952500 1.42998500 0.10980300
H 2.39792200 2.47191200 0.32273200
N 3.21780400 0.60673300 -0.04515600

• **TS1-3B-F**

C 1.35051200 0.72261200 -0.00574600
N -0.63763900 1.29046200 0.03943800

H -0.79734300 1.84491500 0.88085400
C 1.53367300 0.03035000 1.20730300
C 1.57810400 -1.32714100 1.07382000
H 1.67363300 -1.98271400 1.93238000
H 1.59014000 0.54509200 2.15910900
F 1.71723500 2.02125200 -0.05893700
H -0.79353700 1.88809700 -0.77216100
C -1.50196900 0.11116400 0.00671600
H -1.24839800 -0.45880900 -0.89565400
H -1.24674800 -0.51005000 0.87422500
C -2.99624600 0.41977800 0.01757300
H -3.23915600 1.04315100 -0.85135000
H -3.23281600 1.00760700 0.91264800
C -3.82771400 -0.85936900 -0.00507600
H -3.60845600 -1.48239700 0.86846200
H -4.89817700 -0.63613300 0.00038800
H -3.61105200 -1.44992100 -0.90150900
N 1.46335000 0.09001800 -1.18599100
N 1.53897500 -1.95295100 -0.13243500
N 1.51226100 -1.22531000 -1.21308200

● **TS2-3B-F**

C 0.68851000 -0.20954000 -0.09664400
N -0.67315800 -0.64837000 -0.44447600
H -0.82278300 -1.52578700 0.06957000
H -0.69806800 -0.86265200 -1.45061800
C -1.78475100 0.30061000 -0.11318200

H -1.67281100 1.16911500 -0.76548200
H -1.64080600 0.59396900 0.92798400
C -3.12408800 -0.38276400 -0.32722100
H -3.18061200 -1.26944500 0.31443500
H -3.19816500 -0.72116800 -1.36691300
C -4.26539000 0.57588500 -0.00304100
H -4.22894400 1.46135300 -0.64530200
H -5.23231800 0.08969100 -0.15321800
H -4.21204300 0.90933500 1.03798500
F 0.31773300 -0.72910900 1.70555200
N 1.61130800 -1.10115600 -0.48765000
C 2.35555400 1.39901000 0.03926900
H 2.74963500 2.39703200 0.19437900
C 1.00975700 1.14769800 0.03578900
H 0.27188600 1.92558900 0.18469500
N 2.88265200 -0.77067200 -0.46112600
N 3.28317900 0.43584800 -0.16493500

● **TS1-3C-F**

C 1.19289500 0.77131300 0.26923200
N -0.54502700 0.37856100 -0.75384000
H -0.72535000 1.25282800 -1.24663000
C 2.11089300 -1.54270100 -0.27809700
C 1.52642900 -1.29479100 0.97270000
H 1.46776900 -2.07668500 1.72455200
F 0.83320100 2.02926500 0.56212400
H -0.38214300 -0.34560300 -1.45330600

C -1.67413300 0.01674800 0.10726100
H -1.42672500 -0.93306900 0.59439500
H -1.75485200 0.77740400 0.89251300
C -3.00042900 -0.10805600 -0.63624300
H -2.89349500 -0.85708800 -1.43026400
H -3.22482900 0.84865000 -1.12346600
C -4.13643700 -0.49859400 0.30416000
H -4.26082100 0.24444400 1.09896700
H -5.08536400 -0.57717400 -0.23356800
H -3.93741200 -1.46614600 0.77715500
H 2.42748500 -2.53086400 -0.58567800
N 2.09539400 0.69714200 -0.72990600
N 1.12075200 -0.08225200 1.30512400
N 2.49768400 -0.51682200 -1.03678800

● **TS2-3C-F**

C 0.70327400 -0.20632700 -0.18945200
C 3.18158800 0.45220900 -0.03505700
N -0.66647900 -0.65706100 -0.47129600
H -0.79253300 -1.51260600 0.08345000
H -0.73170400 -0.91205600 -1.46609500
C -1.76720300 0.30108500 -0.13005900
H -1.67538900 1.15302800 -0.80414300
H -1.58425500 0.62065900 0.89616100
C -3.10801800 -0.39596200 -0.28361600
H -3.13454500 -1.27530900 0.37045400
H -3.21886400 -0.74956600 -1.31508700

C -4.24622200 0.55516100 0.07191400
H -4.24176300 1.43467400 -0.57947900
H -5.21307800 0.05816500 -0.03884100
H -4.15878000 0.89951500 1.10711300
F 0.36027500 -0.58979300 1.69950700
H 4.22981100 0.68965100 0.09622800
N 1.61142500 -1.14223800 -0.47946600
N 0.91005800 1.11268400 -0.15397000
C 2.18589500 1.43515000 -0.02440100
H 2.43937500 2.48909800 0.03805200
N 2.87976200 -0.80410000 -0.34374700

● **TS1-3D-F**

C 1.05024400 0.72018200 0.31396400
N -0.70226700 0.65350200 -0.71212900
H -0.93199700 1.60479800 -0.99955200
C 1.08707000 -0.43730900 1.11415300
H 0.52346200 -0.50377500 2.03890700
F 0.68529500 1.88511400 0.90282500
H -0.52585600 0.09539900 -1.54760200
C -1.77508200 0.06599600 0.09420700
H -1.42433100 -0.91008900 0.45146800
H -1.92144400 0.70691100 0.97096700
C -3.08955800 -0.10542200 -0.66039500
H -2.91104600 -0.73320100 -1.54178100
H -3.42344300 0.87388900 -1.02335200
C -4.16316800 -0.73228300 0.22432300

H -4.36400500 -0.10487700 1.09909800
H -5.10212500 -0.85644000 -0.32200100
H -3.84861600 -1.71801800 0.58288300
N 2.72769400 -0.34026700 -0.99247800
C 2.06504200 0.75497000 -0.66253800
H 2.29360100 1.66633200 -1.20579700
N 1.77599400 -1.50317400 0.73424400
N 2.54441500 -1.47917100 -0.33977200

● **TS2-3D-F**

C 0.66967300 -0.25134700 -0.04648000
N -0.69290700 -0.65428200 -0.44018400
H -0.87275100 -1.55364700 0.02402000
H -0.70987700 -0.82005800 -1.45539800
C -1.79918700 0.29564000 -0.08374700
H -1.66427800 1.19006700 -0.69517400
H -1.66781800 0.54174600 0.97146600
C -3.14261800 -0.36035400 -0.35043600
H -3.22049600 -1.27510500 0.24799400
H -3.20273000 -0.64859200 -1.40600900
C -4.27847500 0.59612700 -0.00068100
H -4.21815300 1.51248500 -0.59598700
H -5.24768600 0.13026000 -0.19456700
H -4.24275000 0.87476700 1.05702700
H 0.29467900 1.89188600 0.20050400
F 0.32795200 -0.80458700 1.66333200
C 1.02462700 1.10386000 0.05754800

N 2.29904400 1.47480500 0.07351800
N 3.27084600 0.60916500 -0.13467600
C 1.72987700 -1.06156700 -0.49434400
H 1.56138800 -2.08237100 -0.82502200
N 2.98237800 -0.63744700 -0.46865700

● **TS1-3E-F**

C 1.07037000 0.69712200 0.37164900
N -0.64275800 0.44279800 -0.77167900
H -0.84151900 1.32953100 -1.23423800
C 1.76026200 -1.37929700 0.74854600
H 1.70899900 -2.28855200 1.33939500
F 0.62007000 1.86694500 0.86348500
H -0.44311200 -0.25473100 -1.48875900
C -1.75871300 0.01757400 0.07538100
H -1.46819700 -0.92651200 0.54978500
H -1.87574800 0.76324300 0.87011300
C -3.07727600 -0.15897000 -0.67173800
H -2.94347100 -0.90879200 -1.46078800
H -3.33672900 0.78571400 -1.16473500
C -4.19831900 -0.58300200 0.27237700
H -4.35191800 0.16509000 1.05731500
H -5.14334800 -0.70551200 -0.26393300
H -3.96150100 -1.53553600 0.75822100
N 2.72431800 -0.28086600 -1.01024300
C 2.04811300 0.77736700 -0.67357100
H 2.21653600 1.70389100 -1.21311800

N 1.08124800 -0.31606800 1.21603100
N 2.52187100 -1.43944800 -0.32789300

• **TS2-3E-F**

C 0.70376100 -0.26276800 -0.13791900
C 2.88315900 -0.66401200 -0.40199300
H 3.68411100 -1.36958800 -0.59446000
N -0.67124700 -0.69399100 -0.43223600
H -0.82000000 -1.53385200 0.14252600
H -0.71687700 -0.97221200 -1.42210100
C -1.77244600 0.28081300 -0.13862900
H -1.65788000 1.11792000 -0.83020600
H -1.62017400 0.61763200 0.88776100
C -3.11830000 -0.40042400 -0.31490000
H -3.17768600 -1.25855900 0.36436400
H -3.20303400 -0.78153300 -1.33880200
C -4.24870300 0.58166000 -0.02353100
H -4.21070800 1.43569000 -0.70698400
H -5.22091600 0.09740700 -0.14231700
H -4.18129700 0.96222500 1.00033200
H 0.27232900 1.88050500 0.14200200
F 0.29357400 -0.64203600 1.75927900
C 1.02519900 1.11346600 0.00685100
N 1.62604800 -1.13540400 -0.47676000
N 2.27686400 1.49405800 0.01717300
N 3.25032700 0.57680500 -0.14744900

• **TS1-3F-F**

C 1.01495200 0.71819300 0.26579400
N -0.58396100 0.26166200 -0.77830300
H -0.69096400 0.96094100 -1.51400400
C 2.44096900 -1.39638400 -0.13429200
F 0.53217000 1.92456800 0.64227700
H -0.39328400 -0.63926800 -1.22010200
C -1.77877500 0.18120700 0.06952200
H -1.51573900 -0.42265500 0.94614700
H -2.00713800 1.19283300 0.41865000
C -2.98795000 -0.42186100 -0.63667000
H -2.72770200 -1.42641800 -0.99194100
H -3.22608800 0.18217500 -1.52024400
C -4.19707200 -0.49182900 0.29120300
H -4.48046100 0.50634300 0.64118100
H -5.06028000 -0.92633900 -0.22048400
H -3.98097700 -1.10813600 1.17011400
H 2.92274900 -2.34402200 -0.33903100
N 2.71695700 -0.35176200 -0.97070100
C 2.04440300 0.73680800 -0.73786600
H 2.25006900 1.64544500 -1.29791900
N 1.10002500 -0.16340500 1.26107200
N 1.75285400 -1.30346900 0.97950200

• **TS2-3F-F**

C 0.69274700 -0.25297500 -0.08262200
C 3.19301800 0.43093000 -0.10593700

N -0.67756200 -0.68109200 -0.42582500
H -0.84202400 -1.54392600 0.10805500
H -0.70025500 -0.92946300 -1.42341600
C -1.79024200 0.28243000 -0.13130600
H -1.69923100 1.10922600 -0.83825000
H -1.62820000 0.64041400 0.88611400
C -3.12853200 -0.42035900 -0.27997500
H -3.16303200 -1.27496600 0.40565000
H -3.22397700 -0.81021700 -1.29961800
C -4.27068800 0.54347000 0.02496100
H -4.25977700 1.39497200 -0.66256100
H -5.23579400 0.04109900 -0.07542600
H -4.19337500 0.92974300 1.04599500
H 0.30047900 1.91513400 -0.20846300
F 0.34985500 -0.43159000 1.68261200
C 1.04917100 1.13134200 -0.14498200
H 4.24540500 0.66841800 -0.01164400
N 1.59365600 -1.17577600 -0.40472600
N 2.31059400 1.46409200 -0.10329300
N 2.88448900 -0.82796000 -0.31626700

● **TS1-1A-C1**

C 1.09443900 -0.34065400 -0.00248900
N -0.63454600 -1.16108300 0.00931600
H -0.69521100 -1.80019500 -0.78539600
C 1.19742700 1.78606500 1.14206300
C 1.18609200 0.41908500 -1.20383700

C 1.18398000 1.79725000 -1.12517700
H 1.23975700 2.34561200 2.07426000
H 1.21404400 2.36679400 -2.05173200
H 1.21804400 -0.07957900 -2.16667700
H -0.69633000 -1.70671500 0.87120000
C -1.67571600 -0.13278400 -0.04797400
H -1.47900400 0.57205400 0.76869000
H -1.55133000 0.40446600 -0.99430500
C -3.09094400 -0.68911200 0.06438700
H -3.19106600 -1.22275700 1.01694700
H -3.25354800 -1.42139300 -0.73522600
C -4.13056300 0.42424100 -0.02445200
H -4.05647600 0.95268300 -0.98053900
H -5.14381200 0.02242200 0.06166300
H -3.98962600 1.15717300 0.77681700
N 1.17602000 2.52008200 0.01234600
C 1.19809300 0.40694800 1.20578000
H 1.24318600 -0.10201700 2.16271000
Cl 1.97495300 -1.94281000 -0.01293200

• **TS1-1B-Cl**

C 0.92920000 0.47484800 -0.01311400
N -0.65329900 -0.00395400 -0.78664700
H -0.80294300 0.61744400 -1.58456000
C 2.60263200 -0.76535200 -0.98417300
C 2.61304800 -1.70184900 0.03306600
C 1.04445800 -0.28837700 1.20635900

C 1.84501800 -1.40103600 1.18086600
H 3.27415300 -0.87409400 -1.83337100
H 1.91333800 -2.02841700 2.06598100
H 0.47116000 -0.00580800 2.08153100
H -0.43346800 -0.93604800 -1.14652300
C -1.84107700 -0.06145300 0.07924300
H -1.57169900 -0.65313500 0.96049600
H -2.06191400 0.95870500 0.40611500
C -3.05075000 -0.67432400 -0.61666800
H -2.79240400 -1.68218300 -0.96273200
H -3.29599700 -0.07869300 -1.50364700
C -4.25202800 -0.73583100 0.32209700
H -4.53085300 0.26492800 0.66785800
H -5.11927600 -1.17225600 -0.18075000
H -4.02956800 -1.34742700 1.20256100
H 3.26247300 -2.56745100 -0.01204600
N 1.84338200 0.34674500 -1.00233000
Cl 0.47314200 2.23677400 0.30093300

• **TS1-1C-Cl**

C 0.85803800 0.41724400 0.00405400
N -0.72252700 -0.00407000 -0.78780200
H -0.87085900 0.64160900 -1.56809200
C 2.86367800 -1.51522500 -0.00101700
C 1.05905000 -0.39975900 1.15407400
C 2.03099400 -1.38682000 1.11056100
H 2.16345300 -2.04474400 1.96501700

H 0.43825000 -0.26027500 2.03302400
H -0.51420700 -0.92695400 -1.17652700
C -1.90776500 -0.07814100 0.08325100
H -1.62857900 -0.67419800 0.95899600
H -2.13816700 0.93658900 0.41763200
C -3.11072600 -0.69991100 -0.61624600
H -2.84210000 -1.70348800 -0.96663900
H -3.36112900 -0.10242100 -1.50047400
C -4.31179100 -0.77707300 0.32162900
H -4.60132600 0.21944400 0.67070500
H -5.17369600 -1.22077900 -0.18397600
H -4.08389300 -1.38972000 1.19993900
H 3.63250200 -2.27848600 -0.05088700
N 2.79407100 -0.64646200 -1.02481500
C 1.86982400 0.30385500 -1.00889800
H 1.86219600 1.01260500 -1.83338200
Cl 0.38287800 2.18585500 0.37873700

● **TS1-2A-Cl**

C -1.20758000 -0.24952400 -0.02310000
N 0.56743800 -1.18743200 0.05207700
H 0.60171900 -1.69460100 0.93785200
C -0.95079600 1.71494500 -1.13783300
C -1.25112200 0.47547400 1.20414900
C -1.04611400 1.82561900 1.11481300
H -0.86171500 2.21429200 -2.09955400
H -1.04429300 2.43412400 2.01486100

H -1.40337000 -0.02590200 2.15222300
H 0.60867600 -1.86412100 -0.71084600
C 1.65154800 -0.21008700 -0.04184700
H 1.54587600 0.30844500 -1.00198800
H 1.49918800 0.52615200 0.75695700
C 3.04693100 -0.81729000 0.07372600
H 3.17994800 -1.56126600 -0.72070800
H 3.12486100 -1.34896500 1.02970500
C 4.13039500 0.25280800 -0.02062300
H 4.01784300 0.99477000 0.77695200
H 5.12770400 -0.18674600 0.06823000
H 4.07740900 0.77965400 -0.97912800
N -1.17686900 0.39837700 -1.19806600
N -0.86486200 2.48392700 -0.06003300
Cl -2.14078700 -1.78774200 -0.04694800

• **TS1-2B-Cl**

C 0.97259500 0.48147500 0.07958000
N -0.58962100 -0.00256300 -0.76841900
H -0.70193100 0.59581800 -1.58964600
C 2.21995100 -1.87098300 0.02822100
C 1.54485200 -1.42531500 1.14667400
H 1.48909500 -2.04837800 2.03574800
H -0.39947700 -0.95433800 -1.09369400
C -1.79105400 0.01075400 0.08045000
H -1.54995700 -0.55639400 0.98475800
H -1.98224300 1.04911200 0.36744200

C -3.00993100 -0.58516900 -0.61430100
H -2.77978700 -1.61190400 -0.92278500
H -3.22362800 -0.01177300 -1.52378800
C -4.22534700 -0.57619700 0.30815200
H -4.47724600 0.44496700 0.61237900
H -5.09880900 -1.00364900 -0.19159700
H -4.03342400 -1.16126700 1.21337900
H 2.64203500 -2.86659000 -0.02702400
N 2.54382400 -0.98957200 -0.96203000
C 1.99418000 0.19365900 -0.91547200
H 2.27641000 0.94725400 -1.64478500
N 1.01139600 -0.19265400 1.24877800
Cl 0.63813500 2.24125400 0.26302900

● **TS1-2C-Cl**

C 0.87795300 0.46170000 -0.01250000
N -0.65440200 0.01746100 -0.80138400
H -0.79802000 0.63804800 -1.60325700
C 2.52315600 -1.70209400 0.07698000
C 1.06482200 -0.32664600 1.17579100
H 0.56439900 -0.04602900 2.09782500
H -0.45360800 -0.91969500 -1.16194000
C -1.84217100 -0.02206800 0.07255100
H -1.56396300 -0.58673000 0.96898600
H -2.06999500 1.00540400 0.36738400
C -3.04392600 -0.66656300 -0.60628600
H -2.77568200 -1.68105100 -0.92366300

H -3.29679200 -0.09730400 -1.50801900
C -4.24111800 -0.71359600 0.33866000
H -4.53250800 0.29398600 0.65244500
H -5.10311600 -1.17849900 -0.14706800
H -4.00694000 -1.29310800 1.23746300
H 3.10332200 -2.61682500 0.06716400
N 2.67780300 -0.85103500 -0.94552800
C 1.94432600 0.25204600 -0.95398900
H 2.12648600 0.98783300 -1.73252000
N 1.80312900 -1.42874100 1.17066400
Cl 0.48955600 2.21373500 0.30421800

• **TS1-2D-Cl**

C 0.98199600 0.48967700 0.01429200
N -0.61294300 0.01217100 -0.77517300
H -0.73822400 0.61954500 -1.58768700
C 2.32450700 -1.80727600 -0.05191200
C 1.05389200 -0.26169400 1.24657800
C 1.67733700 -1.46808900 1.16346300
H 1.73983500 -2.13260300 2.01959200
H 0.59513800 0.11322300 2.15424400
H -0.41905200 -0.93404400 -1.11304500
C -1.80701800 0.00893600 0.08374300
H -1.55699700 -0.55776300 0.98730000
H -2.00990000 1.04423400 0.37361700
C -3.02368100 -0.60321200 -0.60118500
H -2.77912300 -1.62409600 -0.91789700

H -3.25400500 -0.02804000 -1.50544800
C -4.23095500 -0.62062400 0.33136900
H -4.49637600 0.39350900 0.64726500
H -5.10164000 -1.05742200 -0.16517100
H -4.02279700 -1.21120700 1.22941300
H 2.82182000 -2.76099800 -0.18612900
N 2.49539500 -0.91895400 -1.01411600
N 1.92130800 0.28559200 -0.95374900
Cl 0.63167900 2.23868800 0.24394900

• **TS1-2E-Cl**

C 1.07039300 0.50930700 0.06475600
N -0.58382800 -0.06519900 -0.77606900
H -0.73938700 0.56966100 -1.55978200
C 2.44329100 -0.96232200 -0.94021300
C 2.15420100 -1.89761100 0.05465100
C 1.53371900 -1.37933500 1.19020200
H 3.12214700 -1.20961900 -1.75290700
H 1.47440400 -1.96448000 2.10517700
H -0.38312200 -0.99173700 -1.15600400
C -1.75497500 -0.11714100 0.10431300
H -1.53681400 -0.83651700 0.89988200
H -1.86715600 0.86959600 0.56754300
C -3.03799700 -0.50515000 -0.62436200
H -2.90222600 -1.49006800 -1.08700300
H -3.21707000 0.21172100 -1.43468100
C -4.23168900 -0.53063300 0.32544200

H -4.39502500 0.45509500 0.77333500
H -5.14663800 -0.81805100 -0.19986100
H -4.07070500 -1.24704700 1.13778400
H 2.54380300 -2.90667400 0.02415000
N 1.97325300 0.28226000 -0.92713700
N 1.05616100 -0.13771300 1.25663000
Cl 0.64335400 2.24117700 0.22115700

• **TS1-2F-Cl**

C 0.93736600 0.47931000 0.04924600
N -0.72028200 0.14572700 -0.85172900
H -0.91228300 0.90994700 -1.50207100
C 1.01527300 -0.37523100 1.17200500
C 1.77414000 -1.52343500 1.03262600
H 1.79268400 -2.25619900 1.83492700
H 0.45891600 -0.17405100 2.08015700
H -0.52532800 -0.70020000 -1.39112800
C -1.84232100 -0.07380500 0.06779400
H -1.53922800 -0.86053100 0.76751200
H -1.99103600 0.84911100 0.63884100
C -3.13107700 -0.47547500 -0.64147000
H -2.93997800 -1.37152000 -1.24377000
H -3.42709300 0.32380700 -1.33073400
C -4.24928400 -0.74758500 0.36030400
H -4.46520900 0.14338900 0.95909700
H -5.17042100 -1.04146600 -0.15016300
H -3.97080700 -1.55524600 1.04518900

N 2.65486400 -0.88763500 -0.97848900
C 1.94419500 0.21630400 -0.94383400
H 2.11356000 0.93070300 -1.74419200
N 2.54896100 -1.81912700 -0.01939200
Cl 0.61774500 2.21935300 0.37668100

• **TS1-3A-Cl**

C 1.14562100 0.49380500 0.07533900
N -0.65473000 0.01192600 -0.83667100
H -0.80747500 0.70379500 -1.57023500
C 2.39317300 -1.08284800 -0.88423400
C 1.48374300 -1.43825100 1.12912600
H -0.49997000 -0.89161200 -1.28580800
C -1.79599500 -0.05643400 0.07595300
H -1.55433100 -0.79272300 0.85077200
H -1.89305300 0.92025000 0.56485900
C -3.10715900 -0.43136300 -0.61018100
H -2.98982200 -1.41264500 -1.08587700
H -3.30959800 0.29260000 -1.40872500
C -4.26880500 -0.46072200 0.37799000
H -4.41739800 0.52332000 0.83475600
H -5.20141800 -0.74655700 -0.11636300
H -4.08114100 -1.17953400 1.18269100
N 2.00032300 0.17958800 -0.92410300
N 1.04342900 -0.19310000 1.23089000
N 2.10358800 -1.97745400 0.07203700
Cl 0.81228100 2.22245700 0.23209800

H 1.35873400 -2.07175600 2.00305900
H 3.03496300 -1.41874500 -1.69382000

• **TS1-3B-C1**

C -1.24319100 -0.23412700 0.00379900
N 0.57140500 -1.18265700 0.07082900
H 0.61056100 -1.69731500 0.95214800
C -1.27438100 0.50681400 1.20961800
C -1.00737500 1.83696700 1.06864000
H -0.96929000 2.50302400 1.92391300
H -1.45934100 0.04028200 2.16999100
H 0.60449200 -1.85388200 -0.69731300
C 1.65995300 -0.21043600 -0.02556600
H 1.54861600 0.31732200 -0.98020300
H 1.52550300 0.51956900 0.78223300
C 3.05271300 -0.82831800 0.06639900
H 3.16953600 -1.56554500 -0.73683100
H 3.13778800 -1.36943100 1.01643300
C 4.14259800 0.23470200 -0.03219100
H 4.04417700 0.97155400 0.77196100
H 5.13776400 -0.21229500 0.04222700
H 4.08253200 0.76881400 -0.98625000
N -1.20341600 0.41230600 -1.18413500
N -0.80788100 2.42739500 -0.13926500
N -0.93682100 1.70160600 -1.21345200
C1 -2.16336800 -1.75095600 -0.04355000

• **TS1-3C-C1**

C 1.14943000 0.49280600 0.09419500
N -0.58110800 -0.04963000 -0.79537300
H -0.71300700 0.63018900 -1.54449600
C 1.90077600 -1.94837800 -0.03219900
C 1.38843400 -1.43283400 1.16677400
H 1.31999800 -2.05345300 2.05589800
H -0.44975900 -0.96546500 -1.22635200
C -1.73813100 -0.07456700 0.10354800
H -1.54502900 -0.83018100 0.87236400
H -1.79701700 0.89951600 0.60345100
C -3.05080700 -0.37812600 -0.61256200
H -2.96523200 -1.35142900 -1.11080000
H -3.21020900 0.37350900 -1.39501100
C -4.22832500 -0.38477200 0.35710300
H -4.33993700 0.59022300 0.84288400
H -5.16450800 -0.61104900 -0.16070700
H -4.08709000 -1.13698700 1.14023300
H 2.13435400 -2.99714100 -0.16306900
N 2.04283600 0.17206100 -0.88172000
N 1.07623500 -0.15493300 1.28062600
N 2.34532800 -1.10406800 -0.96456300
Cl 0.82977300 2.22138100 0.18539200

• **TS1-3D-C1**

C 1.01573200 0.50927100 0.03583400
N -0.69800900 0.03416200 -0.87041800

H -0.83604000 0.65922400 -1.66565300
C 1.08010700 -0.32041300 1.18329900
H 0.60042200 -0.04444200 2.11642100
H -0.50291000 -0.90354200 -1.22517500
C -1.85609400 0.02566200 0.02661800
H -1.57095800 -0.52988500 0.92893500
H -2.06005600 1.06101900 0.31803700
C -3.10131200 -0.60222300 -0.59263500
H -2.86665100 -1.62865900 -0.89882200
H -3.36965000 -0.04533800 -1.49792900
C -4.26649500 -0.60092100 0.39209300
H -4.52622800 0.42076800 0.68823100
H -5.15599000 -1.05971200 -0.04810700
H -4.01250100 -1.16023900 1.29850600
N 2.59830900 -1.00973600 -0.89775800
C 2.02102700 0.17714900 -0.90705800
H 2.30027300 0.85946200 -1.70322200
N 1.67981700 -1.49853500 1.13664600
N 2.37203400 -1.88021500 0.07651200
Cl 0.64573200 2.21885000 0.27911800

• **TS1-3E-Cl**

C -1.06575700 0.48881200 -0.11029000
N 0.68075300 0.02897100 0.87438500
H 0.81670300 0.66975900 1.65623400
C -1.56067000 -1.45753000 -1.08640600
H -1.43855800 -2.13574200 -1.92565700

H 0.50974200 -0.90530900 1.24944700
C 1.83079900 0.02185200 -0.02956300
H 1.55459300 -0.57811300 -0.90491100
H 1.99606000 1.05025000 -0.36939100
C 3.10528000 -0.53175600 0.60167100
H 2.91189900 -1.55069700 0.95841900
H 3.36251000 0.07449500 1.47828300
C 4.26136300 -0.53396500 -0.39356500
H 4.46462200 0.47858700 -0.75795400
H 5.17768300 -0.91584200 0.06482800
H 4.03078700 -1.16263900 -1.25999700
N -2.55147500 -1.04872600 0.92960600
C -2.00563900 0.13067700 0.92088800
H -2.25295900 0.81921400 1.72235400
N -1.01976900 -0.23319700 -1.22252600
N -2.26354200 -1.92316700 -0.07165000
Cl -0.73218200 2.21649000 -0.28804600