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**Fig. 1.** Step 3 of theoretical mechanism for the reaction between intermediate 5(I2) and intermediate 6(I2) for the generation of intermediate 7(I3)

The concerted reaction occurs with the C22-C31 bonds formation between intermediateI1 and intermediate I2 for the generation of another intermediate (intermediate 7(I3)). Herein, TS3 showed one imaginary frequency at 400.54i cm-1. The structure of TS3 is shown in Fig.9. To obtain the energy profile, we scanned the distance between C22- C31. The C22 and C31 atoms draw close and lead to the C22- C31 bond at intermediate **7(I3).** The TS3 energy at the HF/6-311G (d, p) level in the gas phase is 9.92kcal/mol, and 13.23 kcal/mol higher than the energy of the reactant and intermediate I3, respectively (**Fig. 1**). Hence, this process is exothermic (∆*r*=-3.31 kcal/mol), compared to the reactants.

**Fig. 2.** Step 3 of theoretical mechanism for the reaction between intermediate 5(I1) and intermediate 6(I2) for generation of intermediate 7(I3)

We have listed in Table 5 the major important geometrical features which undergo changes in this step.

**Table 1.** The major geometrical parameters containing bond lengths, bond angles and dihedral angles for stationary point of intermediate 5(I1), intermediate6(I2), Ts and intermediate 7(I3)

|  |  |  |  |
| --- | --- | --- | --- |
| Species | Bond length(Å) | bond angle (degree) | Dihedral angle (degree) |
| C22-C31  **C31-N34**  **C1-C22** | **C1-C22-C24** -  **C31-C34-C36** | **O17-C14-N12-C3** |
| I1+I2 |  4.50 1.20 1.34 |  123.88 \  127.21 |  179.28 |
| Ts3 |  2.15 1.31 1.40 |  118.09◦ 127.11  |  169.16 |
| Intermediate I3 |  1.57 1.46 1.50 |  111.57 118.92  |  143.99 |

As is evident, the major change can be expressed as follow: 1) **C31-N34**bond length increase in order of intermediate I1+intermediate I2 <TS3< intermediate I3; 2) **C1-C22** bond cleavage increase from reactant to Intermediate I3, 3) The **C1-C22-C24** angle changed in this order; reactant > TS3> intermediate I3. 4) The **O17-C14-N12-C3** dihedral angles in this step decrease. The Energies of the participating species in step3 at the HF/6-311G (d, p) and B3LYP/6-311g (d, p) levels are shown in **Table** **2**.

**Table 2.** Energies of participating species in step3 at the HF/6-311G (d, p) and B3LYP/6-311g (d, p) levels

|  |  |  |
| --- | --- | --- |
| Step3 | B3LYP/6-311G(d,p) (kcal/mol) | HF/6-311G(d,p)a(kcal/mol) |
| intermediate I1+ intermediate I2 | -719837.68 | -715450.00 |
| Ts3 | -719837.87 | -715433.50 |
| Intermediate I3  | -719839.63 | -715451.32 |

In the next step of the reaction an intramolecular reaction occurs at intermediate 7(I3).forming N13 and C27 bond at Intermediate I4 (Heterocycles) and causing H transfer from N to OMe and creating HOCH3.



**Fig. 3.** Step 4 of the theoretical mechanism for the intermediate 7(I3) intramolecular reaction for generation of intermediate 8(I4)

To obtain the energy profile, we utilized two dimensional scanning, thus, N13 approached C27, then the acidic hydrogen N34-H of the intermediate 7(I3) went near the oxygen atom with a 0.05Å magnitude. After obtaining the energy of each step, we again decreased the distance between N13-C27 and H went near O step by step until we obtained an energy diagram on the basis of the O-H distance which consists of an energy summit **Fig 3**. The TS4 energy at the HF/6-31G (d, p) level in the gas phase is 19.64 which is 26.93 kcalmol-1 higher than the energy of the reactants (**intermediate 7 I3)** and product, respectively (**Fig. 4**). So, this process is exothermic (*∆r* (HF) =-7.28 kcal/mol), in comparison with the reactants

 **Fig. 4. Step** 4 of theoretical mechanism for the intermediate7 (I3) intramolecular reaction for the generation of intermediate8 (I4)

These results are represented in separate diagrams and the energy values of the high energy points (TS) in each step was drawn versus the N13-C27 bond length changes forming, **Fig**. **5**. This diagram has a point with the lowest energy value that establishes the TS structure

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**Fig. 5.** The two dimensional scan of the obtained TS4 structure.

The Energies of participating species in step4 at the HF/6-311G (d, p) and B3LYP/6-311g (d, p) levels are shown in **Table** **3**.

**Table 3.** Energies of participating species in step4 at the HF/6-311G (d, p) and B3LYP/6-311g (d, p) levels

|  |  |  |
| --- | --- | --- |
| Step2 | B3LYP/6-311G(d,p) (kcal/mol) | HF/6-311G(d,p)a (kcal/mol) |
| intermediate7(I3) | -719838.05 | -715306.11 |
| Ts4 | -719807.93 | -715398.42 |
| intermediate8(I4) | -719831.46 | -715438.70 |

The major important geometrical features which undergo changes in this step4 have been listed in **Table 4**.

**Table 4.** The major geometrical parameters containing bond lengths, bond angles and dihedral angles for stationary point of intermediate 7(I3), TS4 and intermediate 8(I4)in step 4

|  |
| --- |
| Step4 Geometrical Reactant TS4 Product parameters |
| bond length (A) | N13-C10 | 1.45 | 1.49 | 1.50 |
| C26-C27 | 1.52 | 1.52 | 1.41 |
| C27-O28 | 1.18 | 1.21 | 1.18 |
| C27-o29 | 1.29 | 1.46 | 3.40 |
| C15-N13 | 1.42 | 1.45 | 1.47 |
| C26-N34 | 1.27 | 1.25 | 1.24 |
| C13-C10-C8 | 107.65 | 105.41 | 106.33 |
| bond angle (degree) | C27-C26-C8 | 119.13 | 110.29 | 108.15 |
| C26-N34-C36 | 129.96 | 128.26 | 130.18 |
| C26-C27-O29 | 116.69 | 100.25 | 119.25 |
|  | C10-N13-C15 | 118.69 | 116.69 | 113.91 |

As can be seen the most significant changes at HF/6-31G (d, p) can be expressed as the following: 1) C26-N34 bond decrease in order of reactant >TS>product 2 N13-C10, C27-o29, C15-N13 bond increase in order of reactant <TS<product

In the fifth step of the reaction an H-Shift occurred. The H16 transferred to N28. N28=C27 bond cleavage and C27=C15 bond formation **Fig. 6**.



**Fig. 6.** Step 5 of the theoretical mechanism for the H-Shift in intermediate 8(I4) for the generation of final product

To obtain a TS in this step of the mechanism, in the intermediateI4 of the proposed mechanism, proton H16 was transformed to carbon N28 (**Fig. 7**). **Fig. 7** shows the energy profile of step5 at HF /6-311G (d, p) level.

**Fig. 7 Step** 5 of theoretical mechanism for H-Shift in intermediate8 (I4) for generation of final product

The Energies of participating species in step5 in HF/6-311G (d, p) and B3LYP/6-311g (d, p) level is shown in Table **5**.

**Table 5.** Energy of participating species in step5 of the proposed mechanism

|  |  |  |
| --- | --- | --- |
| HF/6-311G(d,p) (kcal/mol) | B3LYP/6-31G(d,p) (kcal/mol) | Step2 |
| -642994.56 | -646956.47 | in intermediate8(I4) |
| -642916.75 | -646898.05 | TS5 |
| -643002.78 | -646341.57 | product |

The TS5 energy at the HF/6-311G (d, p) level in the gas phase is 52.21 and 53.14 kcalmol-1higher than the energy of the reactants (**intermediate I4)** and product, respectively (**Fig. 6**). So, this process is exothermic (*∆r* (HF) =-0.93 kcal/mol), in comparison with the reactants. We have listed the main optimized geometries which undergo changes in **Table 6** for step5 at this level

**Table 10.** The major geometrical parameters containing bond lengths, bond angles and dihedral angles for stationary point of intermediate8 (I4), TS5 and final product in step 5

|  |
| --- |
| Step5 Geometrical Reactant TS2 Product parameters |
| bond length (Å) | N28-C27 | 1.24 | 1.27 | 1.35 |
| C27-C15 | 1.50 | 1.45 | 1.30 |
| C15-C20 | 1.50 | 1.47 | 1.46 |
| C17-N3 | 1.46 | 1.48 | 1.45 |
| C20-C22 | 1.42 | 1.45 | 1.47 |
| C15-C17 | 1.52 | 1.52 | 1.49 |
| C27-C15-C20 | 112.15 | 118.83 | 130.46 |
| bond angle (degree)  | C28-C27-C15 | 123.69 | 109.23 | 130.17 |
| C29-N28-C22 | 124.69 | 133.40 | 125.77 |
| C20-C15-C17 | 114.21 | 115.21 | 119.30 |
|  | C1-C27-C15 | 106.38 | 110.73 | 107.95 |

The result at HF/6-31G (d, p) shows that the bond length of N28-C27 elongated from 1.24 Å in intermediate **I2** to 1.27 Å in the transition state TS5and 1.35 Å in the product which shows that the double bond N-C has changed to a simple bond. The C27-C15, C15-C20, and C15-C17 bond lengths, decreases along with the changing of reactants **(I4-)** to product and the C6-C7-C8, C8-C7 -C10, C6-C7-C10 **angles decrease**

STEP1 TS

 Z Y X

C 0.35902400 0.21836700 -0.69273800

C 1.13637700 -0.81984800 -0.95551100

H -0.16390300 -1.10041000 -1.58777200

C 2.55638400 -0.98224500 -0.61131000

O 3.45672200 -0.66325600 -1.31197900

O 2.70664200 -1.60070500 0.54949000

C 0.51867100 1.54603000 -0.07401900

O -0.29278200 2.40740700 -0.16306900

O 1.66480800 1.66428800 0.55996600

N -0.92585500 -0.12074900 -1.32760000

H -1.13297300 0.47226000 -2.10942100

C 4.03278300 -1.87284300 0.96174300

H 3.94756700 -2.38175100 1.91000100

H 4.53466300 -2.50422500 0.24078200

H 4.59144300 -0.95380400 1.07850600

C 1.96195500 2.92563600 1.13460400

H 1.22371200 3.18378100 1.88161400

H 2.93515400 2.81834500 1.58728800

H 1.98462200 3.69211000 0.37199300

C -2.10276900 -0.31742200 -0.52082600

C -3.32137600 0.15847900 -0.96840100

C -2.02074400 -1.02751800 0.66557300

C -4.46659000 -0.07538600 -0.22697500

H -3.37842900 0.71887800 -1.88511600

C -3.17027200 -1.25469100 1.40087900

H -1.07295100 -1.39548600 1.00971500

C -4.39529800 -0.78224100 0.95990000

H -5.41052400 0.30165500 -0.57687500

H -3.10550500 -1.80500000 2.32214300

H -5.28387300 -0.96089500 1.53758000

STEP1 INTERMEDIATE

 Z Y X

C 0.26007800 -0.38417200 -0.02956500

 C 0.35552800 0.94007800 0.07221800

 H -0.52775700 1.53289300 0.20061100

 C 1.59097500 1.73551400 0.00837800

 O 1.64425800 2.87490200 0.33338500

 O 2.63319000 1.08227600 -0.49166600

 C 1.43270700 -1.32930700 -0.17137100

 O 1.55052700 -2.04151100 -1.10812900

 O 2.19928700 -1.34613700 0.88787000

 N -0.90707600 -1.11470900 0.00339800

 H -0.84526000 -1.97772900 -0.48925900

 C 3.85587600 1.78891700 -0.57754700

 H 4.56455600 1.10182200 -1.01513300

 H 3.74605400 2.66229000 -1.20546300

 H 4.18769200 2.09686600 0.40508800

 C 3.32580600 -2.20794000 0.85447700

 H 3.97479200 -1.94275100 0.03122300

 H 3.83116600 -2.06303900 1.79618000

 H 3.01159700 -3.23721800 0.74828100

 C -2.20007500 -0.52401400 0.01279300

 C -2.70027100 0.02055200 1.18598700

 C -2.97825400 -0.52392000 -1.13341500

 C -3.96773800 0.57369400 1.20490000

 H -2.09547200 0.00475000 2.07412200

 C -4.25530600 0.01248000 -1.10474400

 H -2.58422700 -0.93999000 -2.04383300

 C -4.75077100 0.56748400 0.06148800

 H -4.34840200 0.99845600 2.11633500

 H -4.85576600 0.00362500 -1.99662100

 H -5.73887600 0.99053900 0.08140400

STEP1 REACTANTS

 Z Y X

 C -0.37795000 0.19586600 0.80745100

 C -1.08560100 -0.89606600 1.02430300

 H 0.92653000 -0.40315700 2.21901500

 C -2.44388600 -1.03472800 0.52446000

 O -3.42638500 -0.72656300 1.12106300

 O -2.47590500 -1.65641200 -0.65306700

 C -0.62431700 1.49082900 0.16225600

 O 0.12238000 2.42091100 0.28129700

 O -1.73439200 1.53262700 -0.52764600

 N 0.99725100 0.23469100 1.44595200

 H 1.15372800 1.16197500 1.80456600

 C -3.75148900 -1.93746700 -1.18624000

 H -3.57552300 -2.44891600 -2.12160900

 H -4.31910700 -2.57048900 -0.51663800

 H -4.30651700 -1.02468900 -1.36059400

 C -2.09884400 2.77031000 -1.11276300

 H -1.35256200 3.08414200 -1.82997700

 H -3.04249000 2.59256200 -1.60378600

 H -2.20920400 3.53049600 -0.35165100

 C 2.12526200 -0.14543000 0.59488500

 C 2.28632600 -1.47832600 0.26463000

 C 2.99428800 0.82461100 0.14298600

 C 3.35697800 -1.84228600 -0.52972700

 H 1.57561600 -2.20681500 0.60810600

 C 4.06281200 0.44683100 -0.65553100

 H 2.83014800 1.85762700 0.38732200

 C 4.24623300 -0.88224100 -0.98883700

 H 3.49355100 -2.87507400 -0.79304700

 H 4.74469200 1.19510700 -1.01585900

 H 5.07591100 -1.17152600 -1.60791600

STEP2 INTERMEDIATE

 Z Y X

C -1.65263000 1.38462000 -0.12588700

 C -0.33402700 0.97564600 -0.27791600

 C 0.00058600 -0.37490000 -0.17431800

 C -1.01928400 -1.29448800 0.09125900

 C -2.32699900 -0.87494300 0.24335000

 C -2.65895500 0.47071700 0.13598400

 H -1.88552400 2.42693500 -0.21251600

 H 0.41434600 1.71234800 -0.48190000

 H -0.77972800 -2.33658400 0.16918500

 H -3.08944700 -1.60022700 0.44486900

 H -3.67238000 0.79335100 0.25431500

 N 1.30532000 -0.84142000 -0.33934100

 H 1.46576000 -1.78550600 -0.08697800

 C 2.46134000 -0.01539200 -0.45457900

 H 3.26936900 -0.59579600 -0.85687600

 H 2.26081200 0.80934300 -1.11882300

 O 2.96560000 0.48186400 0.79305900

 H 2.33456600 0.98360200 1.29227600

STEP2 TS

Z Y X

C 1.70444500 1.38699900 0.02184900

 C 0.37392900 1.04186800 -0.14849600

 C 0.01386100 -0.29815400 -0.19302600

 C 0.97832200 -1.28507000 -0.07651900

 C 2.31163400 -0.93355200 0.08618700

 C 2.67729200 0.40204500 0.13774000

 H 1.98056700 2.42064800 0.05666300

 H -0.37834500 1.79743500 -0.24707300

 H 0.69745800 -2.31927600 -0.10856100

 H 3.05407200 -1.69979500 0.17428900

 H 3.70477500 0.67381800 0.26472100

 N -1.37132600 -0.64079100 -0.36801200

 H -1.49165200 -1.58910100 -0.65766300

 C -2.41719900 -0.19239700 0.68530900

 H -2.95812000 -1.05918500 1.03703600

 H -1.89780100 0.29485300 1.49530800

 O -3.10831100 0.63923100 -0.19469200

 H -2.09888600 0.12184700 -0.95936500

STEP2 REACTANTS

Z Y X

C -1.51516100 -1.50094400 -0.24388500

 C -0.36594100 -0.75610200 -0.45064400

 C -0.36633300 0.62310100 -0.22298900

 C -1.54855200 1.22738700 0.21244700

 C -2.69162700 0.47169700 0.41295500

 C -2.68866900 -0.89861000 0.18981000

 H -1.49318700 -2.55666400 -0.42814000

 H 0.52918800 -1.23175400 -0.79821500

 H -1.56596300 2.28404500 0.39402700

 H -3.58726800 0.95721500 0.74602500

 H -3.57460500 -1.47867300 0.34567600

 N 0.78376500 1.36812300 -0.41090900

 H 0.74434800 2.35502800 -0.39322600

 C 3.60776400 -0.45238400 0.79981600

 H 4.46267500 -0.97878600 1.20179600

 H 2.86036700 -0.10877100 1.50101900

 O 3.49267700 -0.25627100 -0.38915600

 H 1.60779000 0.94679600 -0.76441500

STEP3 REACTANTS

Z Y X

C 1.99563100 0.89567800 -0.54833300

 N 2.80837000 0.01182700 -1.16726400

 H 3.44343400 0.39247800 -1.83156500

 C 3.04275900 -1.34118200 -0.75727100

 C 3.95403800 -1.61638700 0.24939200

 C 2.38285300 -2.37319900 -1.40245500

 C 4.20147800 -2.92911500 0.61297900

 H 4.46523500 -0.80788700 0.73908700

 C 2.63336400 -3.68474200 -1.03766200

 H 1.68421600 -2.14402500 -2.18542000

 C 3.54184000 -3.96272800 -0.03042100

 H 4.91160500 -3.14290100 1.39028800

 H 2.12575400 -4.48623800 -1.54215300

 H 3.73941600 -4.98178600 0.24855300

 C 1.07296600 0.29184300 0.49029700

 O 0.04015200 -0.23281100 0.21729800

 O 1.58122900 0.38682300 1.67606300

 C 0.84522600 -0.14715600 2.77481800

 H -0.07142900 0.41030200 2.90179300

 H 0.63302100 -1.19207500 2.60501100

 H 1.48405400 -0.02155500 3.63186500

 C 1.98755100 2.21382300 -0.80847100

 H 2.70547600 2.63322700 -1.48519000

 C 1.06763300 3.13864900 -0.16543500

 O 0.08274600 2.82574800 0.45198300

 O 1.42148500 4.38880000 -0.34937600

 C 0.64419600 5.40635000 0.26211500

 H 0.61585400 5.26678600 1.33031700

 H 1.13365000 6.33249400 0.01605000

 H -0.36134000 5.40258600 -0.12927100

 C -2.34714500 1.51493500 -0.60580900

 H -2.05143100 2.43174400 -1.07342600

 H -1.69615200 1.06385700 0.11662700

 N -3.45197700 0.98962000 -0.93225000

 H -4.01158300 1.47311200 -1.60835500

 C -4.01877500 -0.23966400 -0.43839300

 C -5.39670600 -0.32005600 -0.37025700

 C -3.20287000 -1.29208600 -0.07245700

 C -5.97463500 -1.48543000 0.09546100

 H -6.01175800 0.51207100 -0.66410300

 C -3.79700500 -2.45079100 0.39562300

 H -2.13638800 -1.22424300 -0.15714300

 C -5.17472800 -2.54887900 0.48076600

 H -7.04304500 -1.56023300 0.15753200

 H -3.17852900 -3.28033100 0.68176000

 H -5.62572500 -3.45517500 0.83964900

STEP3 TS

Z Y X

C -0.85886900 0.58589600 -0.51257700

 N 0.17638600 0.83002900 -1.27151000

 H 0.14601300 0.46870200 -2.20172200

 C 1.33935600 1.61392800 -0.93211300

 C 1.48532800 2.86534600 -1.50622000

 C 2.29839900 1.09524400 -0.08392500

 C 2.61277100 3.61123800 -1.21902500

 H 0.72434500 3.25099700 -2.15988200

 C 3.42039800 1.85550200 0.20651300

 H 2.17698000 0.11637700 0.33931800

 C 3.57826300 3.10746100 -0.36024300

 H 2.73464100 4.58370300 -1.65878800

 H 4.17034300 1.46293500 0.86792800

 H 4.45227700 3.69114200 -0.13651000

 C -0.84597300 1.15400400 0.90186000

 O -0.58066400 0.44958300 1.81033800

 O -1.11300000 2.41404200 0.91278200

 C -1.23414400 3.05946700 2.18905900

 H -2.03134600 2.59300200 2.74784600

 H -0.29965700 2.98540100 2.72508000

 H -1.46974900 4.08592200 1.96537800

 C -1.90321600 -0.26453600 -0.91180200

 H -1.90712300 -0.56412900 -1.94626900

 C -3.24164100 -0.04793100 -0.32214500

 O -3.45322000 0.56588500 0.67199600

 O -4.16503300 -0.68553300 -1.00843500

 C -5.51937500 -0.55875600 -0.57143200

 H -5.81999900 0.47853400 -0.59512800

 H -6.10249800 -1.13802800 -1.26855800

 H -5.62715800 -0.94533400 0.43176600

 C -1.49752800 -2.15844600 0.04155600

 H -2.48205700 -2.47246700 -0.24344500

 H -1.36917700 -1.71652800 1.00878500

 N -0.49716900 -2.82856400 -0.48734300

 H -0.69060200 -3.36604500 -1.30373100

 C 0.86587800 -2.81346600 -0.06812900

 C 1.84473800 -3.02487200 -1.02609200

 C 1.20804500 -2.64483100 1.26321100

 C 3.17526100 -3.06304900 -0.65006000

 H 1.57204400 -3.16636200 -2.05757100

 C 2.54378200 -2.67281400 1.62662300

 H 0.45697700 -2.50739300 2.01764200

 C 3.52927300 -2.88289900 0.67666000

 H 3.93140400 -3.23472200 -1.39371200

 H 2.80837900 -2.54833900 2.66054300

 H 4.56227100 -2.91836700 0.96926100

STEP3 INTERMEDIATE

Z Y X

C -0.97350200 0.25875800 -0.40086900

 N -0.12767400 0.85495300 -1.13711000

 H 0.18245300 0.35939000 -1.95250600

 C 0.53287400 2.12552600 -0.87769800

 C -0.01727100 3.27958400 -1.40238300

 C 1.71796200 2.12606200 -0.16984300

 C 0.64007800 4.47777700 -1.19480300

 H -0.93945300 3.24475300 -1.95232400

 C 2.36409800 3.33502500 0.03228200

 H 2.13172300 1.20958900 0.20796800

 C 1.82700800 4.50413400 -0.47792900

 H 0.22734300 5.38645700 -1.59155000

 H 3.28627100 3.35703000 0.58219300

 H 2.33441400 5.43808000 -0.32098200

 C -1.33542000 0.83918900 0.96271400

 O -0.93558100 0.27494800 1.91448700

 O -2.02205000 1.92168600 0.87936800

 C -2.49840200 2.50718500 2.10519100

 H -3.14273600 1.80100800 2.60638400

 H -1.65916000 2.76988700 2.73128300

 H -3.04610700 3.38312900 1.80324700

 C -1.47737900 -1.10386000 -0.80414600

 H -1.51293500 -1.14204700 -1.88783300

 C -2.89635700 -1.34541500 -0.30791900

 O -3.49215600 -0.57270700 0.35989500

 O -3.34698000 -2.48747100 -0.73730900

 C -4.68183000 -2.86481300 -0.37091800

 H -5.38442200 -2.13870400 -0.75213100

 H -4.84046500 -3.82780700 -0.82617400

 H -4.76149800 -2.92934400 0.70403900

 C -0.48013900 -2.21228400 -0.33899200

 H -0.93740900 -3.16003800 -0.59107000

 H -0.37434000 -2.17663500 0.73379300

 N 0.79599600 -2.04117100 -0.99836500

 H 0.85130200 -2.60175900 -1.82091600

 C 2.00888500 -2.12342000 -0.26525800

 C 3.12543400 -2.67067900 -0.88821500

 C 2.13283500 -1.62495500 1.02561800

 C 4.34071800 -2.71877300 -0.23277600

 H 3.04335100 -3.06397100 -1.88712700

 C 3.35620500 -1.68806400 1.67720200

 H 1.29584000 -1.19107300 1.54045200

 C 4.46599200 -2.22947300 1.05729100

 H 5.19023300 -3.14953400 -0.73114000

 H 3.43179000 -1.30905000 2.68066700

 H 5.40896500 -2.27650800 1.56924200

STEP4 REACTANT

Z Y X

C 1.23767700 -1.48949200 -0.29592300

 O 1.14135100 -1.59685600 0.88504000

 O 1.91848100 -2.27563000 -1.08097000

 C 2.61473600 -3.37451100 -0.48003000

 H 3.08098100 -3.89902100 -1.29712200

 H 3.35585300 -3.00246500 0.21106000

 H 1.91627300 -4.01453900 0.03738700

 C 0.44956500 -0.45122700 -1.08715800

 H 0.85248100 -0.36904200 -2.09028700

 C -1.01856600 -0.95192200 -1.14117400

 H -1.01598300 -2.01844000 -1.35479000

 H -1.52704200 -0.45973500 -1.95100100

 N -1.64649600 -0.61041200 0.12084100

 H -1.21122600 -1.10541300 0.87270500

 C -3.06193600 -0.70437000 0.22690100

 C -3.61741200 -1.34338800 1.32838100

 C -3.90164300 -0.12421000 -0.71781900

 C -4.99138800 -1.40041200 1.48504900

 H -2.97654700 -1.79795500 2.06487200

 C -5.27587400 -0.19812900 -0.55840500

 H -3.49838300 0.39093800 -1.56974000

 C -5.82954900 -0.83235800 0.54069400

 H -5.40444700 -1.89867600 2.34369800

 H -5.91450400 0.24867400 -1.29943300

 H -6.89634100 -0.88461700 0.65826600

 C 0.49011000 0.91909600 -0.44301300

 C -0.69678400 1.85940400 -0.62295600

 O -1.23425600 1.92783600 -1.67208900

 O -0.89163800 2.59355500 0.43032100

 C -1.99119500 3.52861700 0.39734600

 H -1.96689500 4.02446400 1.35238900

 H -1.84642100 4.22880400 -0.41054600

 H -2.91202200 2.98225400 0.26827200

 N 1.48891500 1.43737600 0.15556000

 H 1.31703400 2.33589800 0.57154100

 C 2.83991600 0.94289800 0.30801500

 C 3.62333800 0.75900000 -0.81527300

 C 3.32932000 0.74873800 1.58824500

 C 4.93552200 0.34303500 -0.64922400

 H 3.23402300 0.95453700 -1.79806900

 C 4.63983400 0.33805700 1.73926100

 H 2.69447300 0.89337500 2.44316700

 C 5.44022400 0.13410000 0.62268400

 H 5.55952300 0.19850400 -1.51148100

 H 5.03535800 0.17563000 2.72456700

 H 6.46001400 -0.18071700 0.74771600

STEP4 TS

Z Y X

C -1.24235600 1.82894400 -0.01056900

 O -0.93551900 1.76913500 1.13456300

 O -2.17853000 2.56750600 -0.51567000

 C -2.96090200 3.36754100 0.38114300

 H -3.66120600 3.89415100 -0.24492300

 H -3.47617100 2.72818600 1.08244800

 H -2.32104200 4.05910500 0.90889500

 C -0.47290800 1.02737200 -1.05518500

 H -0.84311500 1.21330600 -2.05209700

 C 1.04064300 1.37797700 -0.93745600

 H 1.21363300 2.36475400 -0.53729700

 H 1.53185300 1.27307600 -1.88942600

 N 1.61576800 0.35124700 -0.01679300

 H 1.20280100 0.50246100 0.88997400

 C 3.06383600 0.36160700 0.15323100

 C 3.55696500 0.55020300 1.43240800

 C 3.91156500 0.18051300 -0.92601000

 C 4.92482700 0.56005900 1.63919800

 H 2.88763700 0.69414300 2.26328100

 C 5.27813700 0.19392500 -0.70441700

 H 3.52270700 0.00731200 -1.90844200

 C 5.78592800 0.38290900 0.57009500

 H 5.31158300 0.70987300 2.62998900

 H 5.94535600 0.05229100 -1.53428900

 H 6.84842200 0.39331300 0.72881000

 C -0.48121600 -0.43469600 -0.67702100

 C 0.93893500 -0.99421700 -0.68435500

 O 1.47196000 -1.33128600 -1.72195200

 O 0.83498900 -1.98230900 0.38964400

 C 1.60083500 -3.20245700 0.25489200

 H 1.29530800 -3.82951800 1.07739300

 H 1.38986700 -3.65621300 -0.69903100

 H 2.64519200 -2.94986000 0.33257900

 N -1.29390700 -1.22695300 -0.15168800

 H -0.33037400 -2.01144400 0.34078400

 C -2.69617700 -1.06486400 0.02018900

 C -3.49438900 -0.62908000 -1.02365300

 C -3.24747800 -1.40151000 1.24637000

 C -4.85953000 -0.50571900 -0.82642900

 H -3.06669100 -0.41966600 -1.98713800

 C -4.60912700 -1.26522100 1.43658400

 H -2.61657900 -1.75477700 2.04141000

 C -5.41644300 -0.81730300 0.40156100

 H -5.48478600 -0.17884100 -1.63657500

 H -5.04085900 -1.51661000 2.38759900

 H -6.47663300 -0.72535400 0.54930000

STEP4 INTERMEDIATE

Z Y X

C -0.82324000 2.05102500 -0.66334000

 O 0.03652400 2.65974600 -0.11282600

 O -1.96033000 2.54416400 -1.04684500

 C -2.22885000 3.92666900 -0.77165000

 H -3.20568100 4.11466700 -1.18416800

 H -2.22326300 4.09467600 0.29507700

 H -1.48502300 4.54549700 -1.25083700

 C -0.66506700 0.56961300 -0.98451800

 H -1.37552900 0.26482100 -1.73731100

 C 0.77575800 0.28016800 -1.43717900

 H 1.23313600 1.07901800 -1.99905600

 H 0.80857400 -0.63037200 -2.01557500

 N 1.57500000 0.04601600 -0.18701500

 H 1.92453900 0.94192000 0.18333000

 C 2.74958900 -0.82409600 -0.38267900

 C 3.98244400 -0.22733600 -0.54117000

 C 2.58633400 -2.19556700 -0.45404700

 C 5.08698100 -1.03170000 -0.77680000

 H 4.08566100 0.83958600 -0.47504700

 C 3.69564800 -2.98532600 -0.68657200

 H 1.62304600 -2.65326500 -0.31783400

 C 4.94475900 -2.40477900 -0.84889200

 H 6.05342600 -0.57976400 -0.90025500

 H 3.58481100 -4.05240100 -0.73596700

 H 5.80343500 -3.02490900 -1.02785400

 C -0.77637800 -0.26950300 0.28266500

 C 0.59580200 -0.41473200 0.86867400

 O 0.96386400 -0.78629500 1.89992000

 O 2.62080900 2.31440800 1.05867000

 C 3.30250300 2.41274200 2.29714400

 H 3.89798500 3.31724400 2.33324700

 H 2.60430000 2.40001100 3.12608600

 H 3.95590200 1.55593400 2.37495900

 N -1.68255300 -0.92267900 0.83501600

 H 2.01788200 3.03099500 0.94946300

 C -3.02808800 -1.08293100 0.47802900

 C -3.77365000 -0.21411400 -0.31801800

 C -3.63235000 -2.21507600 1.01711500

 C -5.09739100 -0.50265700 -0.58712500

 H -3.35453200 0.69604000 -0.69445900

 C -4.95039900 -2.50791800 0.72634600

 H -3.05031900 -2.85243400 1.65562800

 C -5.68395100 -1.65135200 -0.07741200

 H -5.67525900 0.17289400 -1.19063200

 H -5.40616500 -3.39022300 1.13572700

 H -6.71370100 -1.86825900 -0.29530600

STEP5 REACTANT

Z Y X

C -0.45184300 -0.53134600 -0.34116900

 O -0.39616100 -1.71071300 -0.44551900

 N -1.56200600 0.24679900 -0.21138000

 C -2.88637400 -0.24472200 -0.09368200

 C -3.28198000 -1.41330400 -0.73758600

 C -3.81538900 0.46775400 0.65390000

 C -4.58741400 -1.85205700 -0.62189100

 H -2.57443000 -1.97705800 -1.30833700

 C -5.12190200 0.02030600 0.75565900

 H -3.52940600 1.36593600 1.16709400

 C -5.51601100 -1.14169200 0.12085800

 H -4.87876600 -2.75797900 -1.12264200

 H -5.82647900 0.58474500 1.33985100

 H -6.52949300 -1.49028900 0.20261800

 C 0.16146700 1.81239700 -0.56542000

 H 0.14278700 2.01772500 -1.62976200

 C -1.26186600 1.66493200 -0.02539300

 H -1.29528800 1.94473100 1.01972400

 H -1.97423700 2.26707600 -0.57344200

 C 0.98221000 2.87430600 0.13125000

 O 0.83985800 3.18181000 1.26486400

 O 1.87011300 3.40494200 -0.67664700

 C 2.78179900 4.33813700 -0.11798900

 H 3.42336400 4.64198800 -0.93010700

 H 2.25134500 5.19008200 0.28481900

 H 3.36148900 3.86993400 0.66525700

 C 0.73461800 0.42433100 -0.36483900

 N 1.94673600 0.19155300 -0.24236700

 C 2.50141300 -1.08930200 -0.00318900

 C 2.37692300 -1.70377900 1.23221900

 C 3.28224700 -1.67028100 -0.99016500

 C 3.00755900 -2.91284000 1.46453200

 H 1.79282600 -1.23728000 2.00435200

 C 3.89669900 -2.88640300 -0.75400600

 H 3.39717900 -1.17086700 -1.93480700

 C 3.76397000 -3.51365900 0.47340400

 H 2.90235700 -3.38681700 2.42420100

 H 4.48738900 -3.34007300 -1.53000000

 H 4.24902000 -4.45530900 0.65687000

STEP5 TS

Z Y X

C -0.46391000 -0.51814700 0.35014900

 O -0.35834700 -1.41733800 1.12223000

 N -1.57991600 -0.02130900 -0.24185900

 C -2.87250300 -0.59268600 -0.10886700

 C -3.26467000 -1.22941500 1.06429200

 C -3.77689900 -0.48538600 -1.15826400

 C -4.53971300 -1.75396300 1.16902900

 H -2.57927200 -1.32164600 1.88016300

 C -5.05248500 -1.00835400 -1.03744700

 H -3.49661300 0.00173900 -2.07179200

 C -5.44160600 -1.64821700 0.12425500

 H -4.82803100 -2.24453000 2.08149400

 H -5.73851100 -0.91458400 -1.86015100

 H -6.43184700 -2.05613400 0.21599400

 C 0.08655300 1.55271200 -0.80709000

 H 1.47924000 1.23589900 -1.32309800

 C -1.33963300 1.14085600 -1.14181700

 H -2.06000500 1.91614900 -0.92912200

 H -1.44514500 0.82891100 -2.17396300

 C 0.21628500 2.81787800 -0.05976800

 O -0.53898700 3.73135700 -0.15211800

 O 1.30632400 2.86391700 0.70112900

 C 1.56722400 4.07616300 1.38282300

 H 2.48068900 3.91220700 1.93449600

 H 1.69444900 4.88885400 0.68018700

 H 0.75839700 4.31617400 2.05955800

 C 0.63344100 0.33906700 -0.22899000

 N 1.82502100 0.17586500 -0.64608400

 C 2.83555100 -0.76348000 -0.35078400

 C 3.92591500 -0.78395400 -1.20935600

 C 2.78598500 -1.62322700 0.73876200

 C 4.96022400 -1.67400800 -0.99141400

 H 3.95339800 -0.10203200 -2.03937900

 C 3.82525700 -2.51262100 0.94542500

 H 1.94539900 -1.60690700 1.40352000

 C 4.91134500 -2.54243600 0.08639200

 H 5.80169700 -1.68754100 -1.66017900

 H 3.78466400 -3.18192000 1.78562100

 H 5.71567300 -3.23470700 0.25833800

STEP5 PRODUCT

Z Y X

C -0.45402300 -0.49317300 -0.33977500

 O -0.31550200 -1.64204300 -0.60533900

 N -1.60895500 0.18395600 -0.07752500

 C -2.91474900 -0.35958600 -0.04664200

 C -3.16081800 -1.71922900 -0.23493800

 C -3.99353800 0.48944700 0.18921900

 C -4.45774000 -2.19730900 -0.18568800

 H -2.35177500 -2.39058400 -0.42025100

 C -5.28412700 -0.00714400 0.23474800

 H -3.84351400 1.54003800 0.34019800

 C -5.52925300 -1.35378300 0.04784800

 H -4.62454500 -3.24943800 -0.33444200

 H -6.09770000 0.67189000 0.41848700

 H -6.53234700 -1.73819800 0.08302500

 C 0.12008400 1.71832500 -0.02485600

 H 2.56659300 0.96160500 -0.57813800

 C -1.36840800 1.60478600 0.10650400

 H -1.70791300 1.93852900 1.08055200

 H -1.88580400 2.18642000 -0.64886800

 C 0.75376600 3.03174100 0.11164000

 O 0.15260000 4.02120600 0.37136400

 O 2.06752700 3.01140400 -0.08287400

 C 2.75871100 4.24467200 0.04891400

 H 3.79783600 4.02072400 -0.13752400

 H 2.39199500 4.96099000 -0.67291900

 H 2.63249300 4.64294400 1.04594400

 C 0.66511600 0.52080900 -0.26052400

 N 1.95293400 0.18096200 -0.52166800

 C 2.58287800 -1.04109400 -0.15109100

 C 3.50906500 -1.59010800 -1.02244900

 C 2.34831500 -1.64718100 1.07264600

 C 4.19658000 -2.73880000 -0.67206900

 H 3.67564600 -1.12143000 -1.97544500

 C 3.02217400 -2.80676700 1.41000400

 H 1.64175600 -1.21739900 1.75909300

 C 3.95178700 -3.35517500 0.54268600

 H 4.91313600 -3.15797200 -1.35564200

 H 2.82628600 -3.27618200 2.35741500

 H 4.47809000 -4.25349700 0.81057800