**Exploration of the Mechanism, Chemospecificity, Regiospecificity and Stereoselectivity of the Cycloaddition Reaction between Hydroxyparthenolide and Nitrilimine: MEDT Study**

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**B3LYP/6-31G(d) Cartesian coordinates and electronic energies for TSs structures, together with the single imaginary frequencies.**

**TS-1 GAS**

E(RB3LYP) = -1630.63298304A.U.

1 imaginary frequency -327.0418 cm-1

Sum of electronic and zero-point Energies= -1630.122574

Sum of electronic and thermal Energies= -1630.089902

Sum of electronic and thermal Enthalpies= -1630.088958

Sum of electronic and thermal Free Energies= -1630.188629

E (Thermal) CV S

KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin

Total 340.788 124.329 209.776

C 1.84807253 -0.83900225 0.00000000

C 0.54961553 -0.65389925 0.78494900

C -0.02222947 -1.84754725 1.44250100

C -0.37225447 -2.99334625 -1.75041300

C 0.86333153 -2.69561625 -1.31815200

C 1.63650853 -1.41220525 -1.43271100

C -1.48521047 -2.18193025 1.69908500

C -2.39029947 -2.42871625 0.45455300

C -2.34306947 -3.77484925 -0.28861100

C -1.07649947 -4.16695725 -1.09253500

C -1.13606747 -2.23139625 -2.80531200

C -0.28773247 0.54400575 0.39227400

O -2.15062047 -1.11970425 2.42209500

C -3.50632947 -1.19346025 2.20757100

C -3.74939147 -2.13275225 1.09063200

O -4.28558347 -0.55116625 2.87766900

O -1.54570747 -5.14257425 -2.03327800

O 0.65960453 -0.85886125 2.21713400

C -4.85566247 -0.26733025 -0.23926000

N -5.78388347 -0.96910425 -0.54745300

N -6.14250847 -2.20471225 -0.43308800

C -4.87156747 -2.93616525 1.07081800

C -4.15066147 0.95679375 -0.47203400

C -3.88713747 1.82938575 0.60395300

C -3.22478847 3.03093175 0.37874200

C -2.82144947 3.34338175 -0.91667900

C -3.05855247 2.49698775 -1.99826500

C -3.72494247 1.29873575 -1.77311700

C -7.49458447 -2.49547925 -0.23842500

O -7.85745547 -3.59192625 0.13571400

O -8.31834047 -1.46364525 -0.53002300

C -10.48354947 -0.47930725 -0.73417900

C -9.72853947 -1.74203425 -0.36445500

H 2.38036553 0.11903975 -0.06406200

H 2.49234553 -1.52110425 0.56800300

H 0.55425153 -2.76845925 1.34107700

H 1.32160253 -3.40781825 -0.62903200

H 1.11566053 -0.68187125 -2.06113600

H 2.62540053 -1.57344925 -1.88380400

H -1.51394547 -3.07144925 2.34642000

H -2.14965747 -1.63081125 -0.25782500

H -3.16591647 -3.76429925 -1.01395800

H -2.56425747 -4.59657025 0.40343100

H -0.35948247 -4.63954525 -0.40300600

H -0.51496247 -1.48473525 -3.30691200

H -1.50503947 -2.93399925 -3.56181100

H -2.02143547 -1.72174625 -2.40302500

H 0.31130153 1.45740775 0.49499300

H -0.61628547 0.47839275 -0.65151000

H -1.16282547 0.63414275 1.03486800

H -0.76641547 -5.49247625 -2.49378300

H -4.87229047 -3.90320425 0.58535000

H -5.62154647 -2.79470225 1.84273300

H -4.20124947 1.54866775 1.60358100

H -3.01549747 3.72248875 1.18763800

H -2.72847747 2.78836875 -2.98965900

H -3.93358347 0.62689775 -2.59952600

H -11.56045447 -0.64556425 -0.62147600

H -10.19332047 0.35369775 -0.08599600

H -10.28513147 -0.19432125 -1.77237000

H -9.99887747 -2.58655225 -1.00626400

H -9.90993147 -2.04152225 0.67253100

F -2.18099447 4.50340575 -1.13572200

**TS-1 DCM**

E(RB3LYP) = -1630.65377774 A.U.

1 imaginary frequency -333.4895 cm-1

Sum of electronic and zero-point Energies= -1630.143729

Sum of electronic and thermal Energies= -1630.111038

Sum of electronic and thermal Enthalpies= -1630.110094

Sum of electronic and thermal Free Energies= -1630.209368

E (Thermal) CV S

KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin

Total 340.574 124.505 208.939

C 0.17006802 1.42857134 0.00000000

C -1.14380498 1.59782834 0.76085000

C -1.71899798 0.39271634 1.39091300

C -2.02812998 -0.69392966 -1.82508100

C -0.80065698 -0.40427866 -1.36310300

C -0.02073798 0.87792634 -1.44463600

C -3.18299398 0.04193634 1.61646100

C -4.07634898 -0.16844466 0.35840600

C -4.02130698 -1.50017766 -0.41068900

C -2.74089798 -1.87915566 -1.19897200

C -2.77210198 0.08398434 -2.88176900

C -1.97932898 2.79400634 0.36219400

O -3.86407798 1.08179334 2.37040600

C -5.21354398 1.00570034 2.13781300

C -5.44286498 0.11151334 0.98899500

O -6.00121098 1.61394434 2.83770900

O -3.19339498 -2.84342866 -2.16450600

O -1.06303298 1.37958034 2.20041000

C -6.53103698 1.99876134 -0.33133300

N -7.47224498 1.31152634 -0.62973300

N -7.83803598 0.07222734 -0.51478900

C -6.56496998 -0.69484966 0.94112600

C -5.79929398 3.20628834 -0.55322300

C -5.57335698 4.09681834 0.51690300

C -4.89250698 5.28825434 0.29798200

C -4.43229398 5.56830934 -0.98644700

C -4.62867798 4.70345434 -2.06145200

C -5.31515798 3.51571134 -1.84274700

C -9.19104198 -0.20388666 -0.33419600

O -9.56698998 -1.31496766 -0.00212700

O -10.00350498 0.84197934 -0.58416000

C -12.15515898 1.86794134 -0.76804900

C -11.42413798 0.58046234 -0.44132200

H 0.69977602 2.38881734 -0.04162700

H 0.80550602 0.73594034 0.56509800

H -1.13148398 -0.52011666 1.29451300

H -0.35501798 -1.13006166 -0.68038900

H -0.52400498 1.62165234 -2.07097200

H 0.97597102 0.71759234 -1.87748400

H -3.21667698 -0.86388866 2.23773800

H -3.83040798 0.64352534 -0.33526200

H -4.83199498 -1.46737466 -1.14923700

H -4.25610698 -2.33278666 0.26336300

H -2.03755898 -2.36455166 -0.50670800

H -2.17612598 0.90429534 -3.28918400

H -3.03578198 -0.58717966 -3.70831200

H -3.71755198 0.50151234 -2.51321900

H -1.38875998 3.70992134 0.48694900

H -2.27897398 2.73528234 -0.68977900

H -2.87454298 2.87377834 0.97826800

H -2.40297698 -3.18378866 -2.61438900

H -6.54721098 -1.65053666 0.43424600

H -7.31060198 -0.58953166 1.72286900

H -5.93541898 3.84440734 1.50722500

H -4.71451498 5.99508634 1.10078500

H -4.25247098 4.96881134 -3.04332300

H -5.49039698 2.82894434 -2.66379000

H -13.23432398 1.70985034 -0.67048800

H -11.86131198 2.67019634 -0.08367900

H -11.94513198 2.18888034 -1.79333600

H -11.70017298 -0.23139966 -1.12077300

H -11.61740298 0.24747034 0.58263700

F -3.77327598 6.71981534 -1.19952200

**TS-2 GAS**

E(RB3LYP) = -1630.63620471 A.U.

1 imaginary frequency -320.0754 cm-1

Sum of electronic and zero-point Energies= -1630.125916

Sum of electronic and thermal Energies= -1630.093190

Sum of electronic and thermal Enthalpies= -1630.092246

Sum of electronic and thermal Free Energies= -1630.192643

E (Thermal) CV S

KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin

Total 340.747 124.383 211.304

C 5.44018600 0.04394700 -0.68896200

C 4.06001600 0.24864500 -1.31344100

C 3.04067400 0.92813000 -0.48697900

C 3.37095700 -1.87215000 1.50064500

C 4.43432800 -1.07891600 1.29170400

C 5.52457300 -1.18800400 0.26158800

C 1.53501700 0.68354900 -0.47793100

C 1.09507500 -0.76431200 -0.10918800

C 0.91943800 -1.13612300 1.37534400

C 2.19120700 -1.27787900 2.25229500

C 3.22030300 -3.28548700 0.99456300

C 3.70084600 -0.68950200 -2.44810000

O 0.94963200 0.95552600 -1.76787100

C -0.12568400 0.12563800 -2.00205100

C -0.16550700 -0.90101600 -0.94798700

O -0.85237300 0.29854200 -2.95677500

O 1.76888700 -2.06954500 3.37019800

O 3.68424500 1.63076000 -1.55014600

C -1.98283200 0.60686700 0.13265500

N -2.67645700 -0.35608200 0.33320900

N -2.61720700 -1.64193300 0.24513000

C -0.99115500 -2.00055700 -1.03283900

C -1.74664800 1.99729500 0.38377600

C -1.75901000 2.49771800 1.70365700

C -1.53149800 3.84708200 1.94110300

C -1.28708600 4.68536700 0.85446600

C -1.26333900 4.22019700 -0.45720600

C -1.49116900 2.86956500 -0.69494000

C -3.77364400 -2.34345300 -0.10801600

O -3.72544400 -3.50287100 -0.46376500

O -4.90559900 -1.61622400 0.01854800

C -7.27428300 -1.35005200 -0.11174700

C -6.12602100 -2.32126200 -0.31037600

H 6.19526700 -0.05422500 -1.47978500

H 5.69033500 0.95042900 -0.12428000

H 3.37242800 1.26375100 0.49695100

H 4.43501400 -0.12032900 1.81405800

H 5.44410000 -2.11730500 -0.31229300

H 6.52085400 -1.18812300 0.72543400

H 1.08458300 1.39495400 0.22778400

H 1.84533500 -1.44018200 -0.53659000

H 0.41357900 -2.10776700 1.41518800

H 0.24107900 -0.42796100 1.86693900

H 2.48928500 -0.27702500 2.60422600

H 4.14024400 -3.66474600 0.54267500

H 2.95413000 -3.94322000 1.83046100

H 2.41268900 -3.38719500 0.25798900

H 4.44068100 -0.58807900 -3.25158900

H 3.70777600 -1.73666100 -2.12289700

H 2.71955400 -0.45078900 -2.86016600

H 2.52185800 -2.12624400 3.97980400

H -1.63502400 -2.09692600 -1.90139500

H -0.76694800 -2.91969200 -0.50466700

H -1.95578600 1.82317400 2.53075900

H -1.54298600 4.25898500 2.94451400

H -1.06585900 4.91165500 -1.26899700

H -1.47081600 2.47903800 -1.70663800

H -8.22211600 -1.84336600 -0.35316900

H -7.31968000 -1.00427500 0.92592600

H -7.16429500 -0.47669300 -0.76239700

H -6.06097700 -2.67617900 -1.34364900

H -6.21132100 -3.19887600 0.33816500

F -1.06673100 5.98986000 1.08506400

**TS-2 DCM**

E(RB3LYP) = -1630.65692161 A.U.

1 imaginary frequency -327.5502 cm-1

Sum of electronic and zero-point Energies= -1630.147028

Sum of electronic and thermal Energies= -1630.114263

Sum of electronic and thermal Enthalpies= -1630.113319

Sum of electronic and thermal Free Energies= -1630.213404

E (Thermal) CV S

KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin

Total 340.523 124.579 210.648

C 5.43300300 -0.02919400 -0.74001500

C 4.04833200 0.13775100 -1.36280400

C 3.04724500 0.88962600 -0.57947500

C 3.35287700 -1.80519000 1.55594700

C 4.41691500 -1.02413900 1.30549400

C 5.51182200 -1.19711200 0.28921400

C 1.53867700 0.66395700 -0.53155500

C 1.07984600 -0.76052200 -0.10203000

C 0.90416100 -1.06584100 1.39779700

C 2.17613300 -1.17166300 2.27923500

C 3.19965800 -3.24184500 1.12061400

C 3.66982800 -0.88610600 -2.41331800

O 0.93651000 0.89391000 -1.82979000

C -0.14216500 0.06513200 -2.01958500

C -0.18814100 -0.91416700 -0.92966600

O -0.86607900 0.20404000 -2.98891200

O 1.74992400 -1.91127300 3.43496900

O 3.67719400 1.50384400 -1.71144200

C -1.99225900 0.62381500 0.14797300

N -2.69395700 -0.33228600 0.34575300

N -2.63701700 -1.62403100 0.26238300

C -1.01677400 -2.01695300 -0.97790900

C -1.72128800 2.00831500 0.38153500

C -1.51479000 2.87489600 -0.71242000

C -1.25608200 4.22220100 -0.49259900

C -1.19771200 4.68584300 0.81916000

C -1.39090400 3.85408000 1.92077100

C -1.65193600 2.50817800 1.70063200

C -3.80185800 -2.31560400 -0.07001600

O -3.76588800 -3.49233800 -0.38391900

O -4.92220500 -1.57415600 0.02186400

C -7.28990500 -1.27059300 -0.11464900

C -6.16102000 -2.26889300 -0.28042600

H 6.18004300 -0.18783600 -1.52819900

H 5.69350700 0.90958200 -0.23650700

H 3.39792400 1.30553700 0.36481800

H 4.42046700 -0.03999800 1.77719900

H 5.43776400 -2.16081300 -0.22493100

H 6.50511400 -1.16246400 0.75702700

H 1.10851400 1.41251800 0.14502100

H 1.81527500 -1.46816200 -0.50090600

H 0.39891600 -2.03603400 1.47269400

H 0.22834800 -0.33564800 1.85870700

H 2.47560700 -0.15895700 2.58790500

H 4.10827800 -3.63478700 0.65816300

H 2.96760000 -3.86348700 1.99375900

H 2.37119400 -3.38326800 0.41433300

H 4.39252100 -0.84491200 -3.23735400

H 3.69297800 -1.90298300 -2.00639200

H 2.67664900 -0.69177300 -2.82095300

H 2.49933300 -1.92802400 4.05225000

H -1.65141500 -2.14927100 -1.84848900

H -0.77639800 -2.91805200 -0.42636500

H -1.56058600 2.48428400 -1.72276100

H -1.10001400 4.91056100 -1.31567300

H -1.33834400 4.26499100 2.92293000

H -1.80942400 1.83954500 2.54011300

H -8.24431400 -1.75903600 -0.33737100

H -7.32900000 -0.88911100 0.91063800

H -7.16819500 -0.42436200 -0.79824400

H -6.10353600 -2.65732900 -1.30141800

H -6.26027400 -3.11801200 0.40212700

F -0.94548100 5.98816500 1.03303800

**TS-3 GAS**

E(RB3LYP) = -1630.61877604 A.U.

1 imaginary frequency -325.3324 cm-1

Sum of electronic and zero-point Energies= -1630.108746

Sum of electronic and thermal Energies= -1630.075893

Sum of electronic and thermal Enthalpies= -1630.074949

Sum of electronic and thermal Free Energies= -1630.176458

E (Thermal) CV S

KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin

Total 340.664 124.638 213.644

C 4.37199400 -0.89665100 -1.30807500

C 2.98941700 -0.35295500 -1.23623800

C 2.35970100 0.57526400 -0.20011400

C 1.05019300 0.20475700 0.58576400

C 4.63532600 -2.03884600 -2.27779200

O 1.85486500 1.68917900 -1.01859600

C 0.56367800 1.43848700 -1.39388200

C 0.05302100 0.31635400 -0.55104500

O 0.00319400 2.05928800 -2.26486800

O 4.01925900 0.31688900 -1.98825700

N -1.53524400 1.82792300 0.68299700

N -2.55834100 1.14068700 0.35121700

C -2.86217600 0.08578200 -0.16004700

C -0.89321800 -0.56017500 -1.00651400

C -3.95650700 -0.85446700 -0.16346700

C -4.04032300 -1.84432100 -1.15870500

C -5.09513900 -2.75123400 -1.16851700

C -6.06710700 -2.65640900 -0.17753900

C -6.01747800 -1.68616500 0.82096300

C -4.95776300 -0.78798000 0.82816200

C -1.59844800 3.19101400 0.32753900

O -2.55560800 3.79457500 -0.10844300

O -0.37997400 3.71127600 0.57459400

C -0.63475000 6.06787000 1.20509200

C -0.17702900 5.07782100 0.14494300

H 3.12009000 1.00804200 0.44982900

H 0.89876400 1.12928500 1.15274200

H 4.62103000 -3.01793500 -1.78898600

H 3.88814900 -2.03971700 -3.07638300

H 5.62165800 -1.90569400 -2.73882800

H -0.98801100 -1.54589000 -0.56072800

H -3.27937400 -1.89497300 -1.92989700

H -5.17837100 -3.51905300 -1.93006200

H -6.79982700 -1.64838700 1.57149600

H -4.89740900 -0.02205000 1.59432300

H -0.39929900 7.08945900 0.88436900

H -1.71518800 5.99540500 1.35712100

H -0.12796700 5.88180700 2.15805900

H 0.89900200 5.14175700 -0.03170000

H -0.70550000 5.22936200 -0.79894700

C 0.83592700 -0.90684600 1.64881200

H -0.23172400 -1.16436400 1.61780200

C 1.63046500 -2.22628600 1.65779700

O 1.41821200 -2.97114100 0.45723800

C 3.11360600 -1.98273000 1.86144000

C 3.98551100 -2.45959600 0.96780500

C 5.40444000 -2.01253700 0.75616300

C 5.37589200 -0.76165800 -0.16989300

H 0.97528100 -0.44969300 2.63454100

H 3.57345700 -3.08161900 0.18047800

H 5.98922200 -2.81168900 0.28546700

H 5.91789500 -1.75312800 1.68859900

F -7.08805700 -3.52999000 -0.18265300

C 3.49198500 -1.14280100 3.05995100

H 2.93719000 -1.46067300 3.95311700

H 4.55719500 -1.23155800 3.28877000

H 3.27488500 -0.07515800 2.92135700

H 0.51505900 -3.31922800 0.49125900

H -1.25621500 -0.43974100 -2.02308400

H 6.37136000 -0.58321200 -0.59867400

H 5.12697400 0.12374200 0.42324900

H 1.24604600 -2.80328400 2.51895400

H 2.24634500 -0.85684100 -1.85882500

**TS-3 DCM**

E(RB3LYP) = -1630.66252482 A.U.

1 imaginary frequency -357.0648 cm-1

Sum of electronic and zero-point Energies= -1630.152745

Sum of electronic and thermal Energies= -1630.119993

Sum of electronic and thermal Enthalpies= -1630.119049

Sum of electronic and thermal Free Energies= -1630.219678

E (Thermal) CV S

KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin

Total 340.444 124.522 211.791

C 4.42490500 -0.97682200 -1.39749100

C 3.01897100 -0.50313000 -1.49576000

C 2.26048900 0.35010600 -0.49245100

C 0.96570500 -0.27266200 0.12770800

C 4.82474600 -2.18200100 -2.22853300

O 1.76943000 1.50852700 -1.24304300

C 0.47214100 1.32901500 -1.61370300

C -0.06409500 0.14146200 -0.90752600

O -0.07274200 2.06068500 -2.41508900

O 4.07722000 0.18191500 -2.18935200

N -1.35737100 1.75922800 0.61853500

N -2.46133700 1.16923000 0.32899300

C -2.87243400 0.17375500 -0.22944800

C -1.17479000 -0.51960900 -1.36686200

C -4.02397400 -0.69576100 -0.19235200

C -4.34416100 -1.50873600 -1.29471900

C -5.46168400 -2.33558100 -1.25859300

C -6.25064800 -2.33950400 -0.11228800

C -5.96256900 -1.54793200 0.99736800

C -4.84329500 -0.72656000 0.95609100

C -1.37530500 3.14438900 0.38813700

O -2.32238500 3.82208300 0.02959900

O -0.13617200 3.60671900 0.63942100

C -0.30547400 5.83474300 1.65145900

C 0.07923200 5.02377700 0.42405700

H 2.92624200 0.75829100 0.26505800

H 0.75627000 0.31730300 1.02832200

H 4.75485400 -3.10896200 -1.64949200

H 4.18123500 -2.27592100 -3.10799200

H 5.86145200 -2.07641500 -2.56931800

H -1.35980100 -1.54925600 -1.07730300

H -3.72327100 -1.48898400 -2.18327000

H -5.72718500 -2.96690700 -2.09922800

H -6.60675400 -1.58464900 1.86903300

H -4.59663900 -0.10115600 1.80735500

H -0.06359700 6.89040700 1.48479100

H -1.37824200 5.75438400 1.84931600

H 0.24441200 5.49109600 2.53368100

H 1.14757800 5.10100700 0.21170300

H -0.48631400 5.33620800 -0.45654700

C 0.96547000 -1.75760500 0.52881100

H 1.46695700 -2.37415200 -0.22526700

C 1.58685500 -2.06055000 1.91255300

O 1.51196800 -3.46685700 2.17829000

C 3.04563600 -1.62908000 1.99590400

C 3.92998200 -2.22470300 1.18534600

C 5.33772600 -1.78766000 0.87916900

C 5.31889100 -0.67349300 -0.20172300

H -0.07846900 -2.09654100 0.56808000

H 3.55628500 -3.03961300 0.56614600

H 5.92375000 -2.64178800 0.52114900

H 5.85693200 -1.40078400 1.76274200

F -7.33181400 -3.13841800 -0.07270700

C 3.35972400 -0.51037200 2.95639000

H 3.07663100 -0.79692800 3.97857400

H 4.41990700 -0.24459800 2.96229100

H 2.78842900 0.39943500 2.72571600

H 0.57705300 -3.72367100 2.11372200

H -1.60014000 -0.19344000 -2.31203000

H 6.33776700 -0.50572700 -0.57621700

H 4.99734700 0.26704700 0.25486300

H 1.01075900 -1.51095200 2.67391900

H 2.36302300 -1.06567100 -2.16600000

**TS-4 GAS**

E(RB3LYP) = -1630.64419070 A.U.

1 imaginary frequency -327.8407 cm-1

Sum of electronic and zero-point Energies= -1630.133882

Sum of electronic and thermal Energies= -1630.101198

Sum of electronic and thermal Enthalpies= -1630.100254

Sum of electronic and thermal Free Energies= -1630.199849

E (Thermal) CV S

KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin

Total 340.733 124.442 209.615

C 3.84840200 -0.22495900 -0.95703900

C 2.63152600 0.29415900 -0.27430500

C 2.12149700 -0.07758800 1.10821800

C 0.74958800 -0.83092000 1.22820100

C 3.92036100 -0.07513600 -2.46715000

O 1.91540600 1.17991700 1.81362000

C 0.59350600 1.47108600 1.97611200

C -0.20630100 0.28746700 1.58119100

O 3.86875700 1.03086900 -0.25692600

N -0.59931600 1.48375000 -0.74835700

N -1.84177500 1.21379100 -0.64529700

C -2.65658700 0.62634000 0.03045600

C -1.54372300 0.18269700 1.85711100

C -3.97565700 0.05506600 -0.12153200

C -4.77115200 -0.20844700 1.00701700

C -6.04407600 -0.75092400 0.86440300

C -6.51247700 -1.02794000 -0.41604100

C -5.75106100 -0.77904500 -1.55561200

C -4.48009700 -0.23876800 -1.40513200

C -0.34293000 2.87467000 -0.87807000

O -1.16771800 3.75124100 -1.02248800

O 0.98699800 3.03370800 -0.81331900

C 2.69426600 4.39270800 0.17593500

C 1.49325300 4.39057800 -0.75214100

H 1.87184500 0.74883000 -0.90665800

H 2.90382000 -0.59431500 1.66516900

H 0.82756800 -1.44734500 2.13829500

H 3.56848900 -0.97564400 -2.98311600

H 3.31025200 0.77103900 -2.79465600

H 4.95570400 0.10915000 -2.77928300

H -2.01011400 0.99484000 2.40833600

H -2.01097000 -0.79646500 1.92297200

H -4.39364600 0.02257300 1.99719100

H -6.67454500 -0.95658500 1.72260800

H -6.15802500 -1.01022800 -2.53419100

H -3.86767600 -0.03507200 -2.27726500

H 3.13815300 5.39486300 0.19976300

H 2.38780200 4.11504600 1.18856700

H 1.76029000 4.68507400 -1.77380900

H 0.69166700 5.04503900 -0.40379900

C 0.29564000 -1.75905000 0.08430500

H 0.61643600 -1.36396800 -0.88394100

C 0.77646900 -3.21932500 0.19484200

C 2.29669400 -3.31556100 0.29129800

C 3.01683200 -3.01911900 -0.79923700

C 4.49246700 -2.72962900 -0.86480000

C 4.76586300 -1.28672000 -0.36112200

H -0.80002400 -1.78507000 0.05868600

H 2.45428800 -2.81246500 -1.70938200

H 5.08101500 -3.42692600 -0.25703100

H 5.80209300 -1.00530900 -0.59484500

H 4.67895700 -1.26157500 0.72899200

F -7.74059900 -1.55381800 -0.55889500

H 3.44920100 3.67652800 -0.16141500

H 4.84958700 -2.83950300 -1.89517100

C 2.87286200 -3.65847100 1.64259600

H 2.47137800 -4.61625900 2.00160200

H 3.96299200 -3.73795200 1.62537600

H 2.60837200 -2.91335800 2.40536600

H 0.33419200 -3.66550300 1.10339700

O 0.24777900 -3.86560500 -0.96508000

H 0.69273500 -4.72425600 -1.04279200

O 0.21630500 2.52829000 2.42914900

**TS-4 DCM**

E(RB3LYP) = -1630.66550639 A.U.

1 imaginary frequency -341.4635 cm-1

Sum of electronic and zero-point Energies= -1630.155926

Sum of electronic and thermal Energies= -1630.123058

Sum of electronic and thermal Enthalpies= -1630.122113

Sum of electronic and thermal Free Energies= -1630.222452

E (Thermal) CV S

KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin

Total 340.392 124.717 211.179

C 3.85039600 -0.26325800 -0.89803000

C 2.63046300 0.25264100 -0.22072400

C 2.09343600 -0.16051200 1.13856400

C 0.70572300 -0.88529300 1.21696600

C 3.95131600 -0.06803300 -2.40033600

O 1.90104400 1.08432800 1.88538600

C 0.58548400 1.38428000 2.05403500

C -0.23130600 0.23603400 1.60763100

O 3.87844200 0.97604900 -0.15617400

N -0.57655100 1.57788800 -0.66186500

N -1.83323200 1.32288900 -0.58522800

C -2.64322300 0.68815700 0.05265500

C -1.57495200 0.14771100 1.85898300

C -3.95450000 0.10710000 -0.11487200

C -4.77212900 -0.14779800 1.00084100

C -6.03907800 -0.69619000 0.83393100

C -6.47417600 -0.98777900 -0.45534700

C -5.68987500 -0.74988000 -1.58175100

C -4.42485200 -0.20276000 -1.40835500

C -0.30203800 2.95154600 -0.80036900

O -1.10914500 3.84970300 -0.96411500

O 1.02940900 3.10829800 -0.72503200

C 2.89745300 4.46964600 -0.11274200

C 1.53641100 4.46438400 -0.78244900

H 1.88781700 0.73906500 -0.85005000

H 2.85514200 -0.70928900 1.69174200

H 0.75978900 -1.53568500 2.10315400

H 3.59370800 -0.94808800 -2.94546400

H 3.35966900 0.79578000 -2.71641500

H 4.99525200 0.10447700 -2.68842000

H -2.03816000 0.94013000 2.44053800

H -2.05849400 -0.82477300 1.87695900

H -4.42024300 0.09079100 1.99824500

H -6.68625400 -0.89609400 1.68063700

H -6.07142200 -0.99393500 -2.56713800

H -3.79410000 -0.00888400 -2.26924100

H 3.34518100 5.46558100 -0.19747500

H 2.80302300 4.21811400 0.94835800

H 1.59651500 4.75829600 -1.83621400

H 0.82690100 5.12782000 -0.28286300

C 0.24589700 -1.76163700 0.03385900

H 0.59248300 -1.34155400 -0.91524500

C 0.69217500 -3.23499100 0.10550600

C 2.20864500 -3.36748300 0.22355000

C 2.95551700 -3.03441200 -0.83820300

C 4.43889900 -2.78000200 -0.86721500

C 4.73788400 -1.35854700 -0.31897100

H -0.84946200 -1.75864000 -0.00485900

H 2.41788200 -2.77267700 -1.74921300

H 4.99854800 -3.50496900 -0.26559900

H 5.78203700 -1.09395500 -0.53497200

H 4.63814900 -1.36385700 0.77042300

F -7.69794700 -1.52042300 -0.62089400

H 3.56582100 3.73963400 -0.57876700

H 4.81398300 -2.86960300 -1.89291000

C 2.74857300 -3.79331800 1.56603700

H 2.31811400 -4.75973600 1.86149300

H 3.83698500 -3.89418500 1.56729300

H 2.48083900 -3.08529400 2.36229500

H 0.22468500 -3.69936800 0.98974200

O 0.16734200 -3.83426700 -1.08455100

H 0.56350800 -4.71763400 -1.15760300

O 0.23031300 2.43079700 2.55949800

**TS-5 GAS**

E(RB3LYP) = -1630.61667422 A.U.

1 imaginary frequency -348.7065 cm-1

Sum of electronic and zero-point Energies= -1630.105619

Sum of electronic and thermal Energies= -1630.073339

Sum of electronic and thermal Enthalpies= -1630.072394

Sum of electronic and thermal Free Energies= -1630.169664

E (Thermal) CV S

KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin

Total 340.948 124.438 204.720

C 1.74471000 -2.19941400 1.04732700

C 0.56693300 -2.58900100 0.14824300

C -0.71289000 -2.93584900 0.79617500

C -0.25363300 0.76309000 2.03820100

C 1.04568100 0.25903900 1.96929200

C 1.47216000 -1.19975300 2.20533400

C -2.09593700 -2.59247900 0.26447100

C -2.30001100 -1.07185300 0.01025500

C -2.60153400 -0.20608300 1.23706400

C -1.48864800 -0.11219300 2.30712400

N -0.40874600 1.50712500 -0.41263300

N 0.87477600 1.45190100 -0.56112500

C 1.82668600 0.99252500 0.04044800

C 3.22253200 0.73765200 -0.24988000

C -0.41846300 2.23002800 2.38345700

C 0.65232300 -2.14398700 -1.29899200

O -2.38486100 -3.23311800 -0.99455500

C -3.25427900 -2.45842200 -1.72183800

C -3.36204100 -1.12062200 -1.06164600

C -4.26097500 -0.21710100 -1.45151600

O -3.78986900 -2.85767700 -2.72447600

O -2.07099000 0.31926900 3.54841200

C 4.17686200 0.58436400 0.77085000

C 5.51916100 0.38290800 0.46490800

C 5.90366400 0.34309700 -0.87123600

C 4.98700000 0.49632300 -1.90831600

C 3.64714700 0.68796300 -1.59537100

C -0.98066900 2.66310500 -0.94143500

O -0.45425600 3.50504900 -1.64295400

O -2.28187100 2.72481700 -0.53740000

C -4.34126900 3.92877600 -0.30506500

C -3.00484200 3.87839500 -1.02200700

H 2.11037200 -3.12240000 1.51362900

H 2.56224900 -1.82436500 0.42426000

H -0.71744600 -2.94395100 1.88775800

H 1.78370000 0.97364300 2.33456500

H 0.75507100 -1.66249800 2.89347700

H 2.40766200 -1.15153300 2.77646400

H -2.84453800 -2.95378800 0.98437400

H -1.38875800 -0.68119900 -0.45464600

H -2.84565100 0.80455600 0.89331500

H -3.48183700 -0.60717300 1.75644200

H -1.14710900 -1.12042400 2.53679800

H -0.42350900 2.35378400 3.47405800

H 0.40861400 2.82263500 1.98230200

H -1.35003000 2.64961400 1.99142700

H 1.57874000 -2.53765900 -1.73540200

H -0.18528900 -2.53538300 -1.87724900

H 0.67671700 -1.05466100 -1.39306800

H -4.93821700 -0.45031000 -2.26839500

H -4.33556800 0.76140200 -0.98908700

H 3.87087300 0.62501100 1.80994000

H 6.26626800 0.26310400 1.24201700

H 5.32859500 0.46118200 -2.93732400

H 2.91562400 0.81397300 -2.38634100

H -4.90826000 4.80247200 -0.64436400

H -4.94158700 3.03620000 -0.50974400

H -4.20278300 4.01138000 0.77821300

H -2.40861100 4.77544200 -0.83323100

H -3.12757400 3.78688500 -2.10656700

H -2.60420500 1.10944500 3.36456700

F 7.19933800 0.15062500 -1.17054400

O 0.10587600 -3.96799600 0.26446600

**TS-5 DCM**

E(RB3LYP) = -1630.63803125 A.U.

1 imaginary frequency -367.9845 cm-1

Sum of electronic and zero-point Energies= -1630.127373

Sum of electronic and thermal Energies= -1630.095058

Sum of electronic and thermal Enthalpies= -1630.094114

Sum of electronic and thermal Free Energies= -1630.191514

E (Thermal) CV S

KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin

Total 340.721 124.588 204.995

C 1.75319500 -2.18579100 0.98271400

C 0.55115800 -2.56397000 0.11270700

C -0.70676100 -2.92073700 0.79511700

C -0.21995100 0.77422500 2.01920600

C 1.07768800 0.27312900 1.92180100

C 1.51548900 -1.18369400 2.14671500

C -2.10671900 -2.57446500 0.31334100

C -2.32479200 -1.05856100 0.05135600

C -2.59038400 -0.18550800 1.28106200

C -1.44583900 -0.10280200 2.31802900

N -0.39802000 1.51277500 -0.47158200

N 0.89479300 1.47008700 -0.61325100

C 1.83905800 1.00737700 -0.00186200

C 3.23676300 0.73426100 -0.26833200

C -0.38529300 2.24472000 2.34432100

C 0.59347400 -2.09606000 -1.32862300

O -2.43954800 -3.22740800 -0.93820100

C -3.32431000 -2.45747100 -1.63968500

C -3.42320100 -1.12141300 -0.98424500

C -4.35108700 -0.23076900 -1.33700800

O -3.88238100 -2.87123900 -2.63076400

O -1.98938000 0.31972300 3.58155000

C 4.19300600 0.70135300 0.76251200

C 5.53527200 0.47343000 0.47652100

C 5.91346600 0.28275500 -0.84841600

C 4.99608200 0.31270800 -1.89542200

C 3.65617000 0.53402600 -1.60160600

C -0.96631200 2.67275900 -0.97741800

O -0.42681500 3.54626500 -1.64166000

O -2.27404100 2.71380200 -0.61039100

C -4.34045200 3.90264500 -0.33913500

C -2.99682200 3.89094600 -1.04256700

H 2.12346600 -3.10933600 1.44354700

H 2.55835900 -1.81942500 0.33925800

H -0.67544900 -2.95069700 1.88453400

H 1.81817700 0.99080300 2.27463800

H 0.82383400 -1.64718000 2.85959000

H 2.47018000 -1.13139200 2.68257600

H -2.83167400 -2.93515600 1.05430200

H -1.43148600 -0.66613000 -0.44615600

H -2.83556700 0.82549400 0.94027700

H -3.45996500 -0.57771800 1.82333900

H -1.09822400 -1.11288400 2.52903000

H -0.37268000 2.38524500 3.43275600

H 0.43428500 2.83407100 1.92433500

H -1.32648400 2.65382100 1.96530300

H 1.50496900 -2.48352100 -1.79988300

H -0.26433000 -2.46759500 -1.89074600

H 0.62075600 -1.00607600 -1.40341400

H -5.06050000 -0.46702000 -2.12513100

H -4.42602100 0.74282200 -0.86522700

H 3.89416400 0.86067200 1.79202600

H 6.28346200 0.44736900 1.26100700

H 5.33338800 0.16118100 -2.91503700

H 2.92452600 0.56240000 -2.40164200

H -4.89709900 4.79883900 -0.63331000

H -4.94223900 3.02813000 -0.60645300

H -4.21285600 3.91930400 0.74818900

H -2.40624100 4.77744400 -0.79632800

H -3.10903300 3.85458800 -2.13134900

H -2.52016800 1.11859300 3.42708100

F 7.21114700 0.06167500 -1.12850800

O 0.09083000 -3.95118400 0.21656600

**TS-6 GAS**

E(RB3LYP) = -1630.62079132 A.U.

1 imaginary frequency -373.4779 cm-1

Sum of electronic and zero-point Energies= -1630.109959

Sum of electronic and thermal Energies= -1630.077432

Sum of electronic and thermal Enthalpies= -1630.076488

Sum of electronic and thermal Free Energies= -1630.175420

E (Thermal) CV S

KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin

Total 340.963 124.514 208.221

C -2.40858700 1.88701000 -0.05250100

C -3.98944200 0.15924200 -1.35458400

C 0.28675600 -0.20269800 0.26566100

C 0.01860200 1.16922400 0.35549400

C -0.91891700 1.98680800 -0.51339700

C -3.83334700 -1.14833400 -0.59615700

C -2.63426700 -1.50214900 0.32652600

C -1.38566700 -2.05351600 -0.38344600

C -0.36137400 -1.00073900 -0.86879000

C 2.55393200 -0.09026200 -0.33600100

N 2.64545700 1.11316600 -0.46907500

N 1.85417000 2.13072300 -0.43709300

C 3.53496000 -1.16250000 -0.26501200

C 3.23869600 -2.51042400 -0.51178800

C 4.25044700 -3.44997800 -0.36812600

C 5.54273000 -3.11524200 0.01511200

C 5.82676800 -1.77008200 0.26553300

C 4.84093700 -0.79796100 0.13608300

O -5.01949700 -1.27856600 0.23085200

C -4.78127100 -2.13328200 1.27193200

C -3.32134600 -2.44956400 1.29114000

C -2.82989500 -3.41293800 2.07072200

O -5.65377900 -2.51609900 2.00959600

O 0.65771000 -1.68811900 -1.62233800

C 2.35870400 3.21549600 0.28415300

O 3.48033500 3.34913900 0.73578000

O 1.37778000 4.14625800 0.39460300

C 0.54350100 6.26173200 1.11965600

C 1.75411600 5.34717000 1.10025800

C 0.61483000 -0.94371600 1.56143100

H -2.73251100 2.86114900 0.33007900

H -4.95126400 0.15284900 -1.87617400

H 0.20749600 1.61941700 1.33019400

H -0.59669500 3.02706500 -0.46165500

H -2.34836700 -0.61994600 0.90748300

H -0.86408800 -2.75284800 0.27734000

H -0.87359100 -0.31194100 -1.54084100

H 2.24837000 -2.80681500 -0.82932100

H 6.29509500 -3.89069200 0.11266500

H 6.82896600 -1.47922900 0.56679400

H 5.05858400 0.24529900 0.33834000

H -3.50143900 -3.97363300 2.71472400

H -1.77516000 -3.67015800 2.09664000

H 0.78929900 7.19179400 1.64360800

H 0.22692300 6.51308800 0.10221700

H -0.29789800 5.78862300 1.63675400

H 2.08258300 5.08085100 2.11034300

H 2.60551200 5.80661000 0.58800200

H -0.29554200 -1.22671400 2.10956900

H 1.18845800 -1.86014600 1.39283000

H 1.20465600 -0.30673800 2.22810900

H -2.50276300 1.20867800 0.79684800

H -0.83179400 1.69155000 -1.56071800

F 3.95944700 -4.74582500 -0.61438300

O -2.89250100 0.56929500 -2.17814600

C -3.38209500 1.49788500 -1.17120300

C -4.12371800 2.67359300 -1.78262700

H -3.40953700 3.42650100 -2.13669000

H -4.73502700 2.35582300 -2.63223000

H -4.77465700 3.14839400 -1.03939300

H -3.89394600 -1.93678700 -1.36309600

H 0.24845500 -2.01447500 -2.44010100

H -1.70323700 -2.64629200 -1.25286700

**TS-6 DCM**

E(RB3LYP) = -1630.63830737 A.U.

1 imaginary frequency -373.3561 cm-1

Sum of electronic and zero-point Energies= -1630.128054

Sum of electronic and thermal Energies= -1630.095454

Sum of electronic and thermal Enthalpies= -1630.094510

Sum of electronic and thermal Free Energies= -1630.194172

E (Thermal) CV S

KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin

Total 340.645 124.702 209.756

C -2.31595100 1.97001500 0.12356100

C -3.98819900 0.39574400 -1.25571000

C 0.28972400 -0.20498000 0.28591300

C 0.08951600 1.17159200 0.42683000

C -0.83943700 2.05582900 -0.38053600

C -3.85212400 -0.97785700 -0.61627300

C -2.68637300 -1.42997600 0.30713500

C -1.44479800 -1.98119100 -0.41711400

C -0.40795100 -0.92932800 -0.87130000

C 2.55821600 -0.17651200 -0.31957300

N 2.72124200 1.01835400 -0.46095300

N 1.97925000 2.07960500 -0.43965100

C 3.45781600 -1.31647300 -0.23940800

C 3.07929700 -2.63032400 -0.55175600

C 4.01780000 -3.64197400 -0.40343000

C 5.31273100 -3.41497100 0.04480300

C 5.67825800 -2.10310700 0.35948800

C 4.76713100 -1.06006800 0.22843900

O -5.06871700 -1.16641400 0.16820300

C -4.86545800 -2.08442600 1.15060100

C -3.41596700 -2.42305100 1.19289900

C -2.95859400 -3.43913900 1.92610300

O -5.77199700 -2.50061800 1.83721800

O 0.58132900 -1.58806200 -1.68711400

C 2.54626700 3.15241700 0.24066300

O 3.67614600 3.23061800 0.69995300

O 1.63334200 4.14849000 0.30542200

C 0.90383000 6.32468800 0.96964900

C 2.06155600 5.34524300 0.99548200

C 0.59689800 -1.00448800 1.55212500

H -2.59228000 2.92006300 0.59228900

H -4.96296000 0.45638100 -1.74826300

H 0.34575900 1.58426100 1.40244600

H -0.48813900 3.08420000 -0.29247100

H -2.38705700 -0.59978100 0.95348200

H -0.93879700 -2.70904500 0.22416200

H -0.92238800 -0.19542300 -1.49283800

H 2.08360000 -2.84173700 -0.91836500

H 6.00637400 -4.24308300 0.14338200

H 6.68390900 -1.89538900 0.71221500

H 5.05084100 -0.04394500 0.47961700

H -3.65106700 -4.03233400 2.51656800

H -1.90879100 -3.71256700 1.96509400

H 1.19402800 7.24877200 1.48062100

H 0.62384400 6.57365600 -0.05903900

H 0.02771300 5.91061900 1.47930100

H 2.34970800 5.08187300 2.01805900

H 2.94548200 5.74645000 0.48994000

H -0.32233500 -1.25501800 2.09936400

H 1.11595400 -1.94510600 1.34692300

H 1.22523900 -0.41978900 2.23122100

H -2.40386500 1.22823600 0.91755300

H -0.79387100 1.80325900 -1.44136700

F 3.64850000 -4.90596000 -0.71366100

O -2.90432700 0.83900900 -2.08095900

C -3.33705700 1.69982600 -0.98671900

C -4.06422700 2.93884800 -1.47755200

H -3.34130100 3.69693500 -1.80129100

H -4.72031600 2.70411300 -2.32087200

H -4.66867200 3.37226700 -0.67277600

H -3.90875800 -1.69326500 -1.44957500

H 0.12816500 -1.93957400 -2.47193600

H -1.77361200 -2.53930400 -1.30397700