Electronic Supplementary Information For

DFT study on NHC-catalyzed intramolecular aldehyde-ketone crossed-benzoin reaction: mechanism, regioselectivity, stereoselectivity, and role of NHC

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List of the energies and Cartesian coordinates of all the structures involved in the reaction

React

Total Energy= -804.15665631
Sum of electronic and zero-point Energies= -803.919574
Sum of electronic and thermal Energies= -803.904777
Sum of electronic and thermal Enthalpies= -803.903833
Sum of electronic and thermal Free Energies= -803.963802

C	1.43336500	-1.68648300	0.33463600
C	1.41951000	-0.52169300	-0.43517300
C	2.23873500	0.56468300	-0.08557200
C	3.07268100	0.46540300	1.02787600
C	3.09991500	-0.69113700	1.79471900
C	2.27605000	-1.75726700	1.44167900
H	0.79845800	-2.53013200	0.09161100
H	3.68942500	1.32600800	1.26780700
H	3.74900300	-0.76290100	2.66009800
H	2.28155900	-2.66610600	2.03505400
C	2.22864900	1.82518900	-0.86701800
O	2.90798400	2.78514400	-0.57702500
H	1.55723500	1.84865400	-1.74367200
O	0.64805800	-0.35605000	-1.54802800
C	-0.31384700	-1.34665500	-1.84424600
H	-0.77158000	-1.03301000	-2.78775700
H	0.14306200	-2.33102900	-1.98875900
C	-1.41078900	-1.49572600	-0.78359100
O	-1.77020100	-2.61450600	-0.47968400
C	-2.02702900	-0.27791600	-0.18215600
C	-1.80113300	1.01048700	-0.67811900
C	-2.88846300	-0.46303300	0.90435600
C	-2.43083900	2.10078900	-0.08651800
H	-1.13321900	1.16572300	-1.51833800
C	-3.50927800	0.62783700	1.49608300
H	-3.05419500	-1.47314000	1.26427700
C	-3.27961900	1.91104900	1.00062300
H	-2.25608200	3.09928800	-0.47307500
H	-4.17374700	0.48195600	2.34135000
H	-3.76408700	2.76482100	1.46382300

Cat

Total Energy= -2355.60911444
Sum of electronic and zero-point Energies= -2355.240825

Sum of electronic and thermal Energies= -2355.218160
Sum of electronic and thermal Enthalpies= -2355.217215
Sum of electronic and thermal Free Energies= -2355.295042

C	-4.06572600	1.05029100	-1.16627900
C	-4.50294800	-0.12336500	-0.27383200
C	-2.92093300	0.92408900	0.97522200
C	-2.92430700	1.71895200	-0.34838300
H	-3.77227400	0.71431800	-2.16157300
H	-4.90558300	1.73518100	-1.31160800
H	-1.95219600	1.67278600	-0.84983200
H	-3.12621400	2.77656600	-0.16644100
C	-4.41152600	0.52131400	1.14797300
C	-3.32982300	-1.14019800	-0.22422100
H	-3.67772400	-2.06324500	0.24797700
C	-2.28352400	-0.45161300	0.71832700
H	-2.19888600	-1.00367400	1.65491600
H	-2.46618200	1.44903800	1.81944200
C	-0.67117400	-0.68005900	-1.15915500
C	-1.76790400	-0.96416300	-2.12787000
C	0.20057300	-0.15604400	0.85788300
H	-1.40993100	-1.65591500	-2.89259300
N	-0.94508700	-0.42496400	0.15588800
O	-2.86867600	-1.58916600	-1.49590400
H	-2.05259300	-0.03068900	-2.62763700
N	0.60247900	-0.59832500	-1.39365700
N	1.09906200	-0.27150300	-0.14514500
C	2.49415200	-0.08236400	-0.00955800
C	3.33611900	-1.15255800	0.29917300
C	3.06423300	1.17781300	-0.20329800
C	4.70880100	-0.98152000	0.42628400
C	4.43296100	1.38066500	-0.08232000
C	5.23460800	0.28998700	0.23227100
H	5.34878700	-1.82043200	0.66997000
H	4.86072700	2.36438700	-0.23050700
Cl	2.04225000	2.51978500	-0.60099500
Cl	6.95047000	0.52407800	0.38761900
Cl	2.65687100	-2.72856000	0.53274900
C	-5.81710400	-0.76462600	-0.67261300
H	-6.10598900	-1.54934500	0.03478000
H	-6.62172800	-0.02391900	-0.71277900
H	-5.72902200	-1.22102200	-1.66366100
C	-5.33577400	1.72548200	1.35446300
H	-6.38345900	1.41807500	1.27088700
H	-5.19079900	2.12845700	2.36191700

H	-5.16594800	2.53777900	0.64680600
C	-4.69091000	-0.45003400	2.30390200
H	-4.36371100	-0.00756500	3.25048300
H	-5.76751200	-0.63214300	2.38110700
H	-4.20733300	-1.42419700	2.20882600

Et_3N

Total Energy= -292.27369194

Sum of electronic and zero-point Energies= -292.065686

Sum of electronic and thermal Energies= -292.056565

Sum of electronic and thermal Enthalpies= -292.055621

Sum of electronic and thermal Free Energies= -292.099076

N	-0.00085100	-0.43032900	-0.29494700
C	-1.19377800	-0.84169500	0.44248800
H	-1.22307200	-0.40152400	1.45716800
H	-1.11666500	-1.92618500	0.58558300
C	1.19153600	-0.84410600	0.44200500
H	1.11291800	-1.92859800	0.58428000
H	1.22155300	-0.40471500	1.45700100
C	0.00065400	0.98759200	-0.65915600
H	-0.87167500	1.17058500	-1.29379000
H	0.87169100	1.16804300	-1.29634100
C	-2.49661400	-0.52987100	-0.28267900
H	-3.32761100	-1.03874900	0.21176200
H	-2.72091200	0.54023200	-0.28614600
H	-2.44686500	-0.87475300	-1.31945300
C	0.00390300	1.98591500	0.50238300
H	0.89009900	1.86770600	1.13362700
H	0.00424600	3.00879400	0.11644000
H	-0.88001800	1.86964600	1.13717300
C	2.49470000	-0.53341900	-0.28302900
H	2.71992600	0.53650000	-0.28626900
H	3.32518100	-1.04314800	0.21140100
H	2.44475200	-0.87803000	-1.31988100

$Et_3N{\cdot}H^+$

Total Energy= -292.72902425

Sum of electronic and zero-point Energies= -292.504679

Sum of electronic and thermal Energies= -292.495758

Sum of electronic and thermal Enthalpies= -292.494813

Sum of electronic and thermal Free Energies= -292.537339

N	0.02177000	-0.41868400	0.28124200
H	0.04521800	-0.94891700	1.15864200
C	1.26247100	-0.80268700	-0.48672600

H	1.19931200	-0.30265400	-1.45478800
H	1.17974100	-1.87795500	-0.65478100
C	-1.20691100	-0.87917500	-0.46467100
H	-1.09044700	-1.95859500	-0.57837000
H	-1.15838000	-0.42666100	-1.45666600
C	-0.01822000	1.03813300	0.67664600
H	0.87628800	1.21970500	1.27247000
H	-0.87925600	1.15291800	1.33518000
C	2.54516900	-0.46136900	0.24843900
H	3.37406800	-0.93725500	-0.27791800
H	2.73964300	0.61226100	0.27073500
H	2.53658500	-0.84548100	1.27250200
C	-0.09844500	1.97388900	-0.51363900
H	-1.00831600	1.82010000	-1.09803000
H	-0.11894600	2.99657900	-0.13348600
H	0.76826000	1.88504700	-1.17213600
C	-2.49998800	-0.54243300	0.25338700
H	-2.71479800	0.52764600	0.24174100
H	-3.31617000	-1.04986600	-0.26320800
H	-2.48965000	-0.89423700	1.28880200

Pre-Cat

Total Energy= -2356.07572596

Sum of electronic and zero-point Energies= -2355.693438

Sum of electronic and thermal Energies= -2355.670895

Sum of electronic and thermal Enthalpies= -2355.669950

Sum of electronic and thermal Free Energies= -2355.746127

C	-4.09811800	0.93777700	-1.25957500
C	-4.52073800	-0.16253800	-0.27286600
C	-2.95437000	1.01273300	0.88755300
C	-2.96530400	1.68728500	-0.50207200
H	-3.80571100	0.52938500	-2.22733600
H	-4.94571500	1.59851600	-1.45728900
H	-1.99327900	1.62328900	-1.00290100
H	-3.18126400	2.75255300	-0.40513500
C	-4.44100400	0.60010400	1.09083200
C	-3.34081400	-1.16028700	-0.13167700
H	-3.67646100	-2.04243600	0.41832400
C	-2.31414800	-0.37913000	0.76347300
H	-2.21761900	-0.85311900	1.74036600
H	-2.51526900	1.61663400	1.68623500
C	-0.67818200	-0.74084300	-1.10973100
C	-1.78028800	-1.10876700	-2.04447900
C	0.19504000	-0.11405500	0.77228500

H	-1.40877600	-1.84311400	-2.76069400
N	-0.96618400	-0.39837600	0.18373300
O	-2.84450700	-1.71452800	-1.34494200
H	-2.08267100	-0.21524900	-2.60040600
N	0.60372000	-0.67554700	-1.34034600
N	1.13036500	-0.27732300	-0.15217500
C	2.53405300	-0.07594100	-0.01022100
C	3.36491300	-1.15176800	0.30659800
C	3.08021900	1.19035000	-0.22587200
C	4.73530400	-0.96806700	0.42346100
C	4.44831400	1.39245900	-0.11141800
C	5.25463900	0.30547400	0.21261800
H	5.38091000	-1.80141100	0.67157500
H	4.87444100	2.37468300	-0.27411500
Cl	2.04456100	2.51103400	-0.64016800
Cl	6.96321100	0.54550000	0.35717900
Cl	2.68137600	-2.71798300	0.55429800
C	-5.82568900	-0.85236500	-0.61717600
H	-6.10013600	-1.58661600	0.14726800
H	-6.63911900	-0.12668300	-0.70712900
H	-5.73431200	-1.37748800	-1.57283900
C	-5.37621900	1.80845000	1.19519300
H	-6.41886700	1.48379300	1.12462900
H	-5.24594600	2.28470600	2.17172500
H	-5.20748200	2.56943100	0.43276100
C	-4.71191000	-0.27162900	2.32615600
H	-4.39386900	0.25484900	3.23156600
H	-5.78678300	-0.45497100	2.41433900
H	-4.22377900	-1.24852500	2.32042100
H	0.35273100	0.18590600	1.79890900

TS0

Total Energy= -2648.36364314

Sum of electronic and zero-point Energies= -2647.774982

Sum of electronic and thermal Energies= -2647.742421

Sum of electronic and thermal Enthalpies= -2647.741477

Sum of electronic and thermal Free Energies= -2647.837922

C	-4.36967800	-1.32736300	-1.47257500
C	-4.73303000	-0.82623300	-0.06493100
C	-3.09519800	0.60282900	-0.72613900
C	-3.18588900	-0.40756900	-1.88955300
H	-4.14245700	-2.39361900	-1.47840400
H	-5.22496500	-1.19679900	-2.14016200
H	-2.24581900	-0.94968400	-2.03821400

H	-3.38856000	0.10790400	-2.83023500
C	-4.56611200	0.71822100	-0.23632800
C	-3.54725900	-1.15523000	0.88091700
H	-3.85240900	-0.97545500	1.91481600
C	-2.45952400	-0.09229500	0.48930900
H	-2.31938900	0.61889900	1.30451300
H	-2.61549100	1.54962600	-0.98513200
C	-0.95499200	-2.03848600	0.05768800
C	-2.11283400	-2.97755900	0.04720000
C	0.04989200	-0.07986500	0.22965500
H	-1.78993200	-3.94656600	0.43108500
N	-1.14852400	-0.69793500	0.26426200
O	-3.13830500	-2.51722700	0.90250600
H	-2.45009100	-3.11830700	-0.98528200
N	0.30508400	-2.30830900	-0.11644500
N	0.89893100	-1.08246300	-0.01133100
C	2.30560100	-0.95940700	-0.15785500
C	3.15623000	-1.31688900	0.89102000
C	2.85222000	-0.46796300	-1.34542900
C	4.53238600	-1.17814500	0.76842100
C	4.22470100	-0.31087900	-1.48534200
C	5.04482900	-0.67035400	-0.42093200
H	5.18651700	-1.44965100	1.58776400
H	4.64222200	0.07781800	-2.40592300
Cl	1.81125500	-0.04558500	-2.66405100
Cl	6.75831600	-0.47189900	-0.57948800
Cl	2.48703800	-1.89091700	2.37683200
C	-6.05818900	-1.33499700	0.46616800
H	-6.29088200	-0.88809600	1.43841900
H	-6.87309500	-1.10222700	-0.22542300
H	-6.02250700	-2.42127600	0.59359200
C	-5.48847600	1.34340000	-1.28750200
H	-6.53513300	1.22014500	-0.99190700
H	-5.28962500	2.41777600	-1.35277600
H	-5.36860000	0.92423300	-2.28698100
C	-4.75769900	1.52930300	1.05449100
H	-4.36208400	2.54211800	0.92234500
H	-5.82555900	1.62227700	1.27347300
H	-4.28802800	1.10207100	1.94311800
H	0.40856400	1.20159700	0.42966000
N	0.71688900	2.52549100	0.61399100
C	1.99443900	2.88149700	-0.05912600
H	1.96223900	2.43110200	-1.05569500
H	2.02698900	3.97160900	-0.19475600

C	-0.42344800	3.21964600	-0.03353500
H	-1.33913800	2.81026300	0.40526800
H	-0.38706700	4.28615600	0.22808100
C	0.75833700	2.81438000	2.06877000
H	1.61212600	2.27404100	2.48086500
H	0.94133300	3.88868200	2.21193000
C	3.24918200	2.41411300	0.66539500
H	4.10012000	2.51835000	-0.01199900
H	3.46006800	3.00699700	1.55711300
H	3.18266200	1.36241000	0.95928400
C	-0.49316600	2.37483600	2.81764100
H	-0.33126200	2.52906500	3.88633600
H	-1.38356000	2.94135200	2.53731600
H	-0.68411700	1.30694700	2.67008500
C	-0.46942100	3.03879000	-1.54581700
H	-1.41670100	3.43406400	-1.92018100
H	0.33438500	3.57490900	-2.05274300
H	-0.41073600	1.98172800	-1.82830300

***Re*-TS1**

Total Energy= -3159.77995662

Sum of electronic and zero-point Energies= -3159.172815

Sum of electronic and thermal Energies= -3159.134880

Sum of electronic and thermal Enthalpies= -3159.133936

Sum of electronic and thermal Free Energies= -3159.244625

C	2.24947900	3.34498600	0.22842100
C	1.23961500	2.42311000	-0.02517900
C	1.36080200	1.48256400	-1.05025200
C	2.51099900	1.48888800	-1.83614200
C	3.53118300	2.40466800	-1.59233600
C	3.40141800	3.32991200	-0.55629900
H	2.12465200	4.05338300	1.04133000
H	2.58279600	0.75206600	-2.63155000
H	4.42954800	2.39480800	-2.20198600
H	4.19631100	4.04244800	-0.35910000
C	0.27186800	0.46563900	-1.31270000
O	0.31216700	-0.25613500	-2.33001200
H	-0.70301000	0.77260100	-0.88394100
O	0.10674600	2.40380600	0.76536900
C	-0.95357000	3.17615400	0.24855300
H	-0.87362800	4.22273500	0.57557400
H	-0.94526700	3.17460600	-0.85144600
C	-2.28049400	2.59343800	0.71174000
O	-2.31757200	1.56840100	1.36349900

C	-3.52796600	3.31579200	0.32138000
C	-3.51179000	4.44237000	-0.50786800
C	-4.74754000	2.82557600	0.80101100
C	-4.70544200	5.06765500	-0.85469100
H	-2.57702000	4.83790900	-0.89278600
C	-5.93751100	3.45187600	0.45461000
H	-4.73876400	1.95215600	1.44475700
C	-5.91653600	4.57343700	-0.37479200
H	-4.69037500	5.93976400	-1.49935800
H	-6.88118000	3.06946300	0.82905800
H	-6.84575500	5.06358900	-0.64705600
C	-2.87992100	-4.05348900	-0.84335200
C	-3.63323800	-3.11591300	0.11600100
C	-2.32492400	-1.69832600	-1.08866200
C	-1.92306900	-3.09457900	-1.60697400
H	-2.38114000	-4.86180200	-0.30680200
H	-3.58990500	-4.53202500	-1.52378600
H	-0.86284700	-3.30009300	-1.42661100
H	-2.06415300	-3.16082300	-2.68773700
C	-3.83952000	-1.85401800	-0.78517900
C	-2.60723600	-2.58694700	1.15315100
H	-3.14052900	-2.07509600	1.95891100
C	-1.78501300	-1.52904600	0.34252100
H	-1.99556000	-0.52593900	0.71336300
H	-2.03812900	-0.88293000	-1.75649900
C	0.24223600	-2.82668900	1.01463100
C	-0.59323400	-4.00041100	1.39938700
C	0.59644600	-0.78804600	0.20496400
H	-0.12106900	-4.52913100	2.22920000
N	-0.35013000	-1.70580400	0.50237400
O	-1.87215900	-3.59426600	1.84672700
H	-0.64844800	-4.68911400	0.54780300
N	1.53387600	-2.69299800	1.06729000
N	1.72197700	-1.42868100	0.54993200
C	3.02881800	-0.89422000	0.43828600
C	3.87948200	-1.30995600	-0.58698100
C	3.46906900	0.09280300	1.32326400
C	5.14174500	-0.75200400	-0.74361300
C	4.71985300	0.67768300	1.17729500
C	5.53589300	0.24434200	0.13993800
H	5.78931100	-1.07437600	-1.54941300
H	5.04533700	1.45541900	1.85701800
Cl	2.45000400	0.59631800	2.62790800
Cl	7.08967300	0.99181700	-0.07135600

Cl	3.33881800	-2.50407300	-1.71791100
C	-4.86031000	-3.72834600	0.76129300
H	-5.38463500	-2.99866000	1.38773400
H	-5.55943600	-4.09852600	0.00512400
H	-4.57317100	-4.57231400	1.39666500
C	-4.67692700	-2.11142800	-2.04109600
H	-5.69102600	-2.41933300	-1.76527100
H	-4.75993500	-1.18552400	-2.61916600
H	-4.25975900	-2.87349400	-2.70077900
C	-4.47390900	-0.65169100	-0.06945600
H	-4.35414900	0.25000500	-0.68128300
H	-5.54818200	-0.81989200	0.06087400
H	-4.05334000	-0.42768200	0.91318200

***Si*-TS1**

Total Energy= -3159.77757048

Sum of electronic and zero-point Energies=	-3159.171171
Sum of electronic and thermal Energies=	-3159.132995
Sum of electronic and thermal Enthalpies=	-3159.132051
Sum of electronic and thermal Free Energies=	-3159.244766

C	1.03379800	3.12869200	-0.10765600
C	0.82872200	1.85504900	-0.62507800
C	-0.28839700	1.56457300	-1.41288000
C	-1.18933500	2.58640200	-1.69900400
C	-0.99750700	3.86882700	-1.18795100
C	0.11197300	4.13711700	-0.38937300
H	1.90223100	3.31389100	0.51702700
H	-2.04118400	2.34008700	-2.32711300
H	-1.71099300	4.65593100	-1.41046800
H	0.26554800	5.13164400	0.01654100
C	-0.54897000	0.17270800	-1.95617600
O	-1.51770900	-0.02464600	-2.71444500
H	0.37756900	-0.42185500	-2.07461900
O	1.71499300	0.83383600	-0.31788900
C	2.72386400	0.63841900	-1.30033200
H	3.19379800	-0.32635800	-1.07209300
H	2.29983700	0.59955800	-2.30935100
C	3.78879100	1.73753200	-1.30464800
O	4.11232700	2.24226300	-2.36197300
C	4.43260600	2.13726100	-0.01923300
C	4.23786300	1.41593200	1.16278000
C	5.27579200	3.25346300	-0.02236200
C	4.88713200	1.80600000	2.32975600
H	3.57312400	0.55956800	1.17315600

C	5.91582300	3.64643900	1.14572600
H	5.41493500	3.79693800	-0.95113500
C	5.72304300	2.92112300	2.32207800
H	4.73579100	1.24308900	3.24519200
H	6.56525600	4.51545100	1.14327800
H	6.22452200	3.22740200	3.23467500
C	-5.79099500	-1.08599100	0.43650600
C	-5.52901400	0.37115200	0.85234100
C	-4.11693800	0.06569800	-0.90612400
C	-4.76535100	-1.32192700	-0.70874900
H	-5.69657800	-1.76983600	1.28091900
H	-6.81905200	-1.18823100	0.07860500
H	-4.01888600	-2.08707900	-0.47031700
H	-5.25573400	-1.65391700	-1.62611700
C	-5.26521300	1.04421500	-0.53346100
C	-4.11690700	0.43041100	1.49464300
H	-3.97824400	1.40591800	1.96901900
C	-3.15151400	0.32613800	0.26138500
H	-2.63040400	1.27213800	0.10870900
H	-3.63505000	0.21423400	-1.87393100
C	-2.12024000	-1.61179500	1.45268400
C	-3.31439200	-1.74452900	2.33363800
C	-0.91430600	-0.72041300	-0.18631900
H	-3.00620900	-2.13711600	3.30407800
N	-2.09683400	-0.66024800	0.46726500
O	-3.90344400	-0.48097900	2.56998300
H	-4.01554400	-2.45830100	1.88682500
N	-1.01787300	-2.29733200	1.47143300
N	-0.29539000	-1.72828100	0.44425200
C	1.02515200	-2.17515600	0.19288500
C	2.04643300	-1.89809000	1.10702200
C	1.33210400	-2.90100000	-0.96001900
C	3.34744300	-2.32967600	0.88322900
C	2.63066100	-3.33113500	-1.21316200
C	3.61929800	-3.04088600	-0.28194800
H	4.13021200	-2.11270600	1.60035300
H	2.85752400	-3.88983400	-2.11269600
Cl	0.08245800	-3.29012400	-2.09334200
Cl	5.24328900	-3.57816900	-0.57927600
Cl	1.69873200	-0.98467900	2.53403000
C	-6.60087000	0.97444300	1.73820200
H	-6.38996200	2.02667700	1.95716200
H	-7.58448600	0.91193500	1.26255200
H	-6.65166400	0.43651300	2.69024000

C	-6.44776500	0.96868400	-1.50426900
H	-7.30585600	1.51819100	-1.10294800
H	-6.16986100	1.43940300	-2.45254900
H	-6.77270100	-0.04864500	-1.72589400
C	-4.85944000	2.52341600	-0.45225500
H	-4.47669100	2.85893300	-1.42179500
H	-5.73705400	3.13391200	-0.21655800
H	-4.09907900	2.75166000	0.29793000

***Re*-M1**

Total Energy= -3159.78830730

Sum of electronic and zero-point Energies= -3159.180019

Sum of electronic and thermal Energies= -3159.141974

Sum of electronic and thermal Enthalpies= -3159.141030

Sum of electronic and thermal Free Energies= -3159.251172

C	2.19596300	3.34809100	0.02593800
C	1.27403300	2.31822100	-0.13093700
C	1.47110500	1.30322200	-1.06679100
C	2.60270100	1.34677100	-1.87501800
C	3.53872600	2.36798500	-1.72918800
C	3.33835900	3.36428500	-0.77294400
H	2.01808700	4.11203800	0.77677100
H	2.71882000	0.54897100	-2.60342800
H	4.42802100	2.38536800	-2.35210900
H	4.07014400	4.15629200	-0.64908700
C	0.47556100	0.14565100	-1.20953800
O	0.63135200	-0.66426200	-2.24418900
H	-0.54119300	0.59990100	-1.08120300
O	0.14296100	2.25725700	0.66905400
C	-0.92264800	3.02802700	0.15985800
H	-0.80209100	4.09071100	0.41558500
H	-0.96889500	2.95729300	-0.93728000
C	-2.23766300	2.51245100	0.72172000
O	-2.26614300	1.53689600	1.44796900
C	-3.48683400	3.22962900	0.32961900
C	-3.48586100	4.28262700	-0.59099400
C	-4.69220500	2.81086200	0.90313200
C	-4.68149900	4.90443800	-0.93704000
H	-2.56155800	4.62327900	-1.04705300
C	-5.88415400	3.43341700	0.55703100
H	-4.67109700	1.99751700	1.62130500
C	-5.87880200	4.48024900	-0.36500300
H	-4.67825400	5.71918600	-1.65312100
H	-6.81707400	3.10643200	1.00397000

H	-6.80966000	4.96735600	-0.63712200
C	-2.90690000	-4.05005700	-0.57518200
C	-3.70378500	-2.93532000	0.12532400
C	-2.27579100	-1.79732600	-1.23543000
C	-1.88164500	-3.27233000	-1.44825100
H	-2.46158200	-4.73927300	0.14415400
H	-3.57994500	-4.65130000	-1.19249800
H	-0.83824000	-3.45204100	-1.16913400
H	-1.96300000	-3.54380800	-2.50262600
C	-3.81203800	-1.86530200	-1.01392900
C	-2.74419100	-2.22623500	1.11504500
H	-3.31563100	-1.54371800	1.75079500
C	-1.83330900	-1.37332800	0.17261200
H	-2.02475600	-0.31598400	0.34171000
H	-1.90687300	-1.12549600	-2.01369100
C	0.09989200	-2.53709000	1.25943700
C	-0.80269900	-3.58625200	1.81426900
C	0.59030700	-0.79307400	0.02105700
H	-0.41162200	-3.93980000	2.76959900
N	-0.42028200	-1.55730900	0.46432000
O	-2.09714000	-3.07672600	2.05986400
H	-0.81243700	-4.43225900	1.11674200
N	1.39049100	-2.42449400	1.36641200
N	1.67729300	-1.33102500	0.58619500
C	3.00974400	-0.85797000	0.47359700
C	3.86998800	-1.38089900	-0.49102100
C	3.45954300	0.16384900	1.31328600
C	5.14466200	-0.85451400	-0.66278300
C	4.72289900	0.71310000	1.15112300
C	5.54073500	0.19929900	0.15114500
H	5.80490400	-1.25187300	-1.42361400
H	5.05630600	1.52420100	1.78635500
Cl	2.42517700	0.75634200	2.56627600
Cl	7.10924900	0.90340000	-0.08904900
Cl	3.34374700	-2.68198900	-1.49592900
C	-4.98886800	-3.40005300	0.78131100
H	-5.53617400	-2.56186300	1.22581600
H	-5.64370100	-3.89322000	0.05615300
H	-4.76841900	-4.11696300	1.57868400
C	-4.57476100	-2.34508100	-2.25192400
H	-5.62000500	-2.54984000	-1.99793100
H	-4.56845700	-1.55703500	-3.01152100
H	-4.15638000	-3.24393400	-2.70704000
C	-4.45434700	-0.53713000	-0.58487500

H	-4.30479400	0.21671300	-1.36582100
H	-5.53410200	-0.66887300	-0.46003800
H	-4.06732400	-0.11655800	0.34660900

***Si*-M1**

Total Energy= -3159.78563362

Sum of electronic and zero-point Energies= -3159.177383

Sum of electronic and thermal Energies= -3159.139484

Sum of electronic and thermal Enthalpies= -3159.138540

Sum of electronic and thermal Free Energies= -3159.249012

C	1.17194200	3.17798600	-0.22235500
C	0.88166200	1.86062000	-0.56116700
C	-0.29025400	1.52164400	-1.23765300
C	-1.16045200	2.54141400	-1.60943100
C	-0.88689300	3.86828100	-1.28069900
C	0.27515200	4.18437900	-0.57971500
H	2.08731600	3.40105100	0.31758700
H	-2.04264400	2.24736400	-2.17251500
H	-1.57567800	4.65486400	-1.57283000
H	0.49249300	5.21451100	-0.31655000
C	-0.64105300	0.06075300	-1.60800900
O	-1.66375600	-0.09771000	-2.42151700
H	0.32396400	-0.41710600	-1.91264100
O	1.76459600	0.84154800	-0.22123200
C	2.73847300	0.59954000	-1.23063200
H	3.20516700	-0.36341200	-0.98975800
H	2.27716000	0.53679700	-2.22197000
C	3.81835900	1.68108100	-1.30136300
O	4.09769400	2.16960700	-2.37851900
C	4.53395500	2.08121100	-0.05359600
C	4.36580300	1.39163300	1.15129100
C	5.41735500	3.16413600	-0.11762200
C	5.08197100	1.77921100	2.27948800
H	3.66904500	0.56312700	1.21193900
C	6.12455900	3.55471100	1.01202400
H	5.53512300	3.68368500	-1.06293800
C	5.95856700	2.86013000	2.21084100
H	4.95130600	1.24107600	3.21272300
H	6.80634200	4.39715000	0.96185400
H	6.51307100	3.16347000	3.09319100
C	-5.85045800	-1.06845600	0.63515400
C	-5.57572800	0.42303700	0.88670900
C	-4.27246700	-0.05378300	-0.92076100
C	-4.88600400	-1.41674700	-0.53443300

H	-5.71500000	-1.66558200	1.53842000
H	-6.89482500	-1.20092800	0.33942300
H	-4.11550100	-2.14566900	-0.26040600
H	-5.42198500	-1.85233700	-1.38022300
C	-5.40862000	0.95001300	-0.57530700
C	-4.12603300	0.55377900	1.42537700
H	-3.96884700	1.56640300	1.80706400
C	-3.24155600	0.35140400	0.14413100
H	-2.76933300	1.28994800	-0.14087100
H	-3.84244900	0.00033300	-1.91991700
C	-2.10197800	-1.45852600	1.43264000
C	-3.25168600	-1.54041800	2.37757100
C	-0.96231800	-0.66325800	-0.26477600
H	-2.88788600	-1.86617900	3.35323100
N	-2.13404300	-0.57128700	0.39316200
O	-3.83018600	-0.26398100	2.55594600
H	-3.96776600	-2.28450700	2.01457200
N	-0.98767100	-2.12466400	1.45881200
N	-0.29100600	-1.61683200	0.39103700
C	1.02136700	-2.09960100	0.14517400
C	2.03277000	-1.87182600	1.08476600
C	1.30729600	-2.85655600	-0.99358900
C	3.31280800	-2.37314600	0.88789400
C	2.58785800	-3.35133600	-1.21671600
C	3.57184300	-3.10393500	-0.26794900
H	4.08978000	-2.19491900	1.62151400
H	2.80289500	-3.93022100	-2.10633400
Cl	0.05813100	-3.20564300	-2.13609900
Cl	5.16925400	-3.72848700	-0.52630500
Cl	1.70945300	-0.94483800	2.50757900
C	-6.59307300	1.11032500	1.77542200
H	-6.38368600	2.18172200	1.86379300
H	-7.60562400	0.98888000	1.37877800
H	-6.57032900	0.67836500	2.78108500
C	-6.64551700	0.76736300	-1.46100700
H	-7.49585700	1.32123200	-1.04892800
H	-6.44020800	1.17278500	-2.45666200
H	-6.94853400	-0.27257100	-1.58757900
C	-5.02054500	2.43384400	-0.67122800
H	-4.67237000	2.66311600	-1.68395600
H	-5.89939700	3.05700300	-0.47660300
H	-4.24236600	2.75335200	0.02617400

***Re*-M01^{B}**

Total Energy= -3452.06946381
Sum of electronic and zero-point Energies= -3451.251827
Sum of electronic and thermal Energies= -3451.204089
Sum of electronic and thermal Enthalpies= -3451.203145
Sum of electronic and thermal Free Energies= -3451.333064

C	-3.44288100	0.96198800	1.46901900
C	-2.19546400	0.51075400	1.05042200
C	-1.50871300	-0.49450300	1.73799000
C	-2.07927300	-1.02723000	2.88358100
C	-3.33204400	-0.59211300	3.32310500
C	-4.00829000	0.39732200	2.61592500
H	-3.97249600	1.72751100	0.91019500
H	-1.50617800	-1.78844000	3.40346300
H	-3.77510000	-1.01805700	4.21767900
H	-4.98286600	0.73948000	2.95007500
C	-0.09703700	-0.92691400	1.31220900
O	0.46722700	-1.85989500	2.07009500
H	0.46120700	0.03681200	1.20055900
O	-1.55290300	0.94907400	-0.07507200
C	-1.74141600	2.27206900	-0.49639600
H	-2.59240500	2.36113200	-1.18964300
H	-1.93091900	2.93077200	0.36023300
C	-0.46330100	2.69872500	-1.21431400
O	0.38232600	1.87860800	-1.50375200
C	-0.29096000	4.14836500	-1.53560400
C	-1.26705600	5.10403300	-1.23586000
C	0.90455200	4.54682400	-2.14386800
C	-1.04521500	6.44443600	-1.53911800
H	-2.20475800	4.81622500	-0.77037400
C	1.12685600	5.88522800	-2.43914300
H	1.64610500	3.78878900	-2.37476000
C	0.15118900	6.83516500	-2.13584800
H	-1.80496600	7.18328400	-1.30764400
H	2.05724700	6.19124400	-2.90591900
H	0.32439800	7.88160200	-2.36558700
C	4.17930100	-3.68650100	-0.81877300
C	4.63427100	-2.22593300	-0.97832800
C	3.11103100	-2.12165400	0.71312800
C	3.07821500	-3.60207300	0.27539100
H	3.85497200	-4.12178800	-1.76463700
H	5.02608400	-4.29282900	-0.48529300
H	2.08523500	-3.89334200	-0.08065700
H	3.29892100	-4.25779500	1.11996600
C	4.60290100	-1.73614000	0.50536100

C	3.46196700	-1.41005200	-1.58371300
H	3.82039400	-0.40885300	-1.83657800
C	2.44058900	-1.28422200	-0.39277600
H	2.33832300	-0.23969700	-0.08438700
H	2.65975000	-1.93646500	1.68735300
C	0.80478600	-2.36851400	-1.94596200
C	1.89260500	-2.79984400	-2.86644100
C	-0.06984100	-1.45971500	-0.14788200
H	1.51290400	-2.80693400	-3.88951400
N	1.09279600	-1.69961200	-0.78980900
O	2.97037800	-1.89008400	-2.83079200
H	2.19072500	-3.82178700	-2.60882400
N	-0.47055100	-2.56717200	-2.07993600
N	-0.99924100	-1.99377200	-0.95186100
C	-2.40989200	-1.91017700	-0.81932400
C	-3.08075200	-2.67285600	0.13719800
C	-3.13615700	-1.03168000	-1.62830300
C	-4.44063000	-2.49734100	0.35991500
C	-4.49821400	-0.85225200	-1.43188200
C	-5.12235600	-1.57228500	-0.41958300
H	-4.94888300	-3.06608500	1.12839300
H	-5.05534600	-0.15660900	-2.04714300
Cl	-2.34464400	-0.13298800	-2.87831200
Cl	-6.81217700	-1.30339200	-0.11904200
Cl	-2.21104600	-3.84527000	1.05987200
C	5.92347800	-2.05555300	-1.75712800
H	6.23001900	-1.00516900	-1.80083400
H	6.73472300	-2.63220900	-1.30204800
H	5.79284200	-2.40968000	-2.78462500
C	5.54363600	-2.49987300	1.44387400
H	6.58620100	-2.34894900	1.14433100
H	5.43293400	-2.11077600	2.46089800
H	5.35554100	-3.57334900	1.48183700
C	4.94379500	-0.24890800	0.66969400
H	4.78232000	0.06546500	1.70630800
H	6.00245000	-0.08710200	0.44104300
H	4.36880200	0.42135600	0.02719200
N	1.64726800	2.17042400	1.76359600
C	0.41945500	2.85266200	2.12069400
H	0.21281000	3.58496500	1.32748300
H	-0.40093600	2.11876800	2.09753200
C	0.37910600	3.55955300	3.48111400
H	-0.58732500	4.05503900	3.61736800
H	0.49581700	2.83702600	4.29438500

H	1.16870600	4.30965600	3.57530200
C	2.14376100	1.17849200	2.70270000
H	2.58407200	0.34685600	2.13282400
H	1.27537400	0.73799000	3.20915200
C	3.17470700	1.65132400	3.73240500
H	2.78490500	2.45241100	4.36679600
H	3.47241700	0.81637000	4.37476000
H	4.07758900	2.02450500	3.23675100
C	2.62181700	2.92238300	0.99488400
H	2.21924900	3.07393200	-0.01728900
H	3.50616200	2.28400200	0.88224800
C	3.05036400	4.28634400	1.54864700
H	3.46211500	4.20297800	2.55824600
H	3.81113000	4.73162900	0.89976600
H	2.20201500	4.97745500	1.58100700

***Si*-M01^{B}**

Total Energy= -3452.07351575

Sum of electronic and zero-point Energies= -3451.256027

Sum of electronic and thermal Energies= -3451.207227

Sum of electronic and thermal Enthalpies= -3451.206283

Sum of electronic and thermal Free Energies= -3451.340456

C	0.60512400	-3.11730000	2.61560600
C	0.35950500	-1.94606500	1.90417200
C	1.40435800	-1.06731400	1.57751300
C	2.69760600	-1.40943200	1.95078000
C	2.96822500	-2.59466500	2.63778000
C	1.91681000	-3.43666300	2.97655000
H	-0.20409200	-3.78263800	2.89377700
H	3.50757800	-0.73242900	1.68535900
H	3.98673800	-2.84901200	2.91209000
H	2.10486400	-4.35411100	3.52518600
C	1.10169200	0.29911600	0.93446500
O	-0.86557700	-1.57645500	1.42924500
C	-1.94670700	-2.46472500	1.52410400
H	-1.63766700	-3.50715600	1.35414100
H	-2.41890400	-2.39983800	2.51080100
C	-2.91060000	-2.09658900	0.39837700
O	-2.47197600	-1.59199500	-0.61531000
C	-4.36560700	-2.37674400	0.55014500
C	-4.87783800	-3.16940900	1.58127300
C	-5.23082600	-1.81462300	-0.39684400
C	-6.24762100	-3.40221000	1.66086200
H	-4.21825100	-3.61916300	2.31701400

C	-6.59856000	-2.03609800	-0.30382600
H	-4.80582000	-1.20125300	-1.18779700
C	-7.10641900	-2.83230000	0.72339500
H	-6.64449800	-4.02463600	2.45561700
H	-7.27162800	-1.59273300	-1.03008700
H	-8.17503100	-3.00834400	0.79369700
C	-2.74294600	3.58422900	-1.87080100
C	-3.54465000	2.88555100	-0.75839300
C	-1.41949800	2.88583600	0.04862800
C	-1.27607400	3.50837400	-1.35662300
H	-2.90728500	3.11448100	-2.84232400
H	-3.07698600	4.62091100	-1.97038200
H	-0.62402900	2.90725500	-2.00004500
H	-0.81869400	4.49939200	-1.30612800
C	-2.80720800	3.39603300	0.51986700
C	-3.13878300	1.38572200	-0.77682800
H	-3.82087100	0.80568400	-0.14662000
C	-1.72183900	1.39095000	-0.10412700
H	-1.73310600	0.91837900	0.87582100
H	-0.58569600	3.04232900	0.73411700
C	-0.96064200	0.15814000	-2.13427100
C	-2.16444100	0.59333400	-2.89643600
C	0.38915900	0.04703100	-0.42054400
H	-2.42400200	-0.18613500	-3.61491100
N	-0.73913000	0.61790000	-0.86540600
O	-3.28406900	0.77830500	-2.05868500
H	-1.91812400	1.50516200	-3.45578300
N	-0.02352600	-0.65144800	-2.52763800
N	0.81255900	-0.70063300	-1.44430500
C	1.96600000	-1.52452600	-1.42694800
C	3.23622700	-0.96968700	-1.58836100
C	1.84328700	-2.89316100	-1.17264500
C	4.37571100	-1.75205200	-1.44465100
C	2.96689000	-3.69383400	-1.03051500
C	4.21912400	-3.10148500	-1.15349400
H	5.35968700	-1.31422800	-1.55734800
H	2.86602700	-4.75075000	-0.81792900
Cl	0.27142700	-3.59597300	-1.02345700
Cl	5.63602100	-4.08604500	-0.94735400
Cl	3.40001500	0.71044800	-1.96480800
C	-5.04482100	3.08582900	-0.83749000
H	-5.55196600	2.60733200	0.00744800
H	-5.30265000	4.14947200	-0.83598600
H	-5.43765900	2.64484200	-1.75936800

C	-2.84009600	4.91480300	0.71256500
H	-3.86953400	5.26374600	0.84617600
H	-2.28292400	5.17593800	1.61831800
H	-2.39919400	5.47268500	-0.11516300
C	-3.30573300	2.77026100	1.83093300
H	-4.23163900	3.26028500	2.14856400
H	-3.51230500	1.69965500	1.77081800
H	-2.56120200	2.91775100	2.61996200
N	3.45953800	2.96016100	0.66540300
C	4.72621600	3.47271200	0.18706700
H	5.51734000	2.95010300	0.73942000
H	4.84467900	3.17832200	-0.86758300
C	4.95788300	4.98776900	0.27598800
H	5.96209900	5.23746900	-0.08142400
H	4.24090700	5.52632800	-0.35141300
H	4.85429700	5.35593000	1.30008100
C	2.25559100	3.52155000	0.08120700
H	1.49432200	2.72984300	0.03079700
H	2.49701900	3.80423200	-0.95260900
C	1.62847600	4.71658700	0.81135100
H	2.33797300	5.53912500	0.93798500
H	0.76080400	5.09120000	0.25729800
H	1.27728400	4.41070200	1.80208200
C	3.38351600	2.53160800	2.05197000
H	4.02377000	1.64289800	2.17095000
H	2.35178200	2.19745200	2.22724500
C	3.80747200	3.54977300	3.11908200
H	3.67702900	3.12101900	4.11791400
H	4.86330000	3.81980300	3.01196600
H	3.21674300	4.46824300	3.06212100
O	0.42729000	1.13941600	1.70617300
H	2.10346100	0.66715200	0.57857500

***Re*-M01^{BA}**

Total Energy= -3452.56419892

Sum of electronic and zero-point Energies= -3451.732028

Sum of electronic and thermal Energies= -3451.683376

Sum of electronic and thermal Enthalpies= -3451.682432

Sum of electronic and thermal Free Energies= -3451.815123

C	-3.32974300	1.91985900	0.97233600
C	-2.20631000	1.15409800	0.68881600
C	-1.72382900	0.20259800	1.59133000
C	-2.36794500	0.04478900	2.81366500
C	-3.49806900	0.80599800	3.11222100

C	-3.97512100	1.73879800	2.19568400
H	-3.69736200	2.63180100	0.23989900
H	-1.97975800	-0.66087300	3.54070900
H	-3.99773900	0.67407500	4.06526200
H	-4.85614000	2.32752900	2.42754100
C	-0.44494800	-0.53783100	1.25000500
O	-0.01355400	-1.40793200	2.26656000
H	0.34620900	0.22394000	1.13471600
O	-1.55674600	1.19528100	-0.51484800
C	-1.03974600	2.41370100	-0.99658900
H	-1.57638000	2.71420500	-1.90540600
H	-1.14921700	3.21045000	-0.25237300
C	0.43534700	2.19608400	-1.33816600
O	0.93870400	1.09714700	-1.19654500
C	1.20948100	3.35510400	-1.86074000
C	0.67863200	4.64928200	-1.88729900
C	2.51045800	3.12764900	-2.32440300
C	1.44740200	5.70565500	-2.36631400
H	-0.32950200	4.84673700	-1.53607000
C	3.27399900	4.18266100	-2.80448600
H	2.90181400	2.11544200	-2.30196000
C	2.74227200	5.47290300	-2.82331200
H	1.03589400	6.70890800	-2.38278600
H	4.28097800	4.00426400	-3.16612600
H	3.33938800	6.29864700	-3.19630000
C	3.46507800	-4.25066200	-0.64608800
C	4.12579500	-2.86326100	-0.69287100
C	2.54365500	-2.63466200	0.92741400
C	2.32068800	-4.06759200	0.39194100
H	3.14223900	-4.58788500	-1.63092000
H	4.19532800	-4.98762600	-0.30207500
H	1.32134500	-4.19733500	-0.03650100
H	2.39472100	-4.79484300	1.20247900
C	4.08465200	-2.46169200	0.81517200
C	3.10897400	-1.86009900	-1.30210700
H	3.61084000	-0.91126000	-1.50866900
C	2.07505500	-1.62638900	-0.13867800
H	2.14189100	-0.59727800	0.22635300
H	2.11374000	-2.44102700	1.91053000
C	0.35016100	-2.39434400	-1.78126400
C	1.39555900	-2.97743400	-2.66717500
C	-0.43407900	-1.29569100	-0.06743000
H	1.05546800	-2.91058800	-3.70172500
N	0.69430800	-1.77890500	-0.61074500

O	2.58504800	-2.22433600	-2.57321200
H	1.53209700	-4.03544400	-2.42290500
N	-0.93403900	-2.35573000	-1.97700300
N	-1.41123200	-1.67762900	-0.89639400
C	-2.80546600	-1.40941500	-0.80511700
C	-3.55732800	-1.92845100	0.24983500
C	-3.42985400	-0.59141800	-1.75272200
C	-4.88479000	-1.56945400	0.42882800
C	-4.76426400	-0.23950200	-1.60265200
C	-5.46498400	-0.71282400	-0.49930600
H	-5.45055100	-1.95633900	1.26721400
H	-5.24049500	0.40791700	-2.32865100
Cl	-2.55870100	0.02423000	-3.11221800
Cl	-7.11234800	-0.22544100	-0.27607700
Cl	-2.84276000	-3.05585100	1.35842400
C	5.46774000	-2.82715900	-1.39640300
H	5.91921100	-1.83108900	-1.34006700
H	6.16221100	-3.54631500	-0.95229600
H	5.34662100	-3.08319600	-2.45348200
C	4.84932100	-3.40553800	1.74931600
H	5.91118300	-3.42058100	1.48380000
H	4.77233900	-3.03770600	2.77717300
H	4.48411300	-4.43278500	1.73968600
C	4.60845500	-1.04861100	1.09734400
H	4.30308700	-0.72669300	2.09970600
H	5.70239500	-1.04990300	1.07379900
H	4.27514400	-0.29126700	0.38469700
N	1.63689500	1.96688000	1.96831300
H	-0.69283500	-2.08263500	2.41313000
C	0.65710400	3.04558800	1.99540100
H	0.77349100	3.60618500	1.05796000
H	-0.34693500	2.59569800	1.97286400
C	0.69360600	4.02363900	3.17472700
H	-0.06264200	4.80062100	3.02874400
H	0.46147100	3.51100500	4.11240200
H	1.66737700	4.50670900	3.27967400
C	1.72914300	1.14802800	3.17216000
H	2.02110400	0.13124800	2.86708400
H	0.71341100	1.05156700	3.57907800
C	2.69488700	1.60971900	4.26887200
H	2.45201500	2.60737200	4.64157200
H	2.66025200	0.91159800	5.11048700
H	3.72505200	1.62787900	3.89895200
C	2.90119900	2.25774500	1.29879100

H	2.73769100	2.20754600	0.21405400
H	3.58454700	1.43862700	1.54315800
C	3.58907300	3.58890200	1.61580000
H	3.81817800	3.69102800	2.68019400
H	4.52634200	3.65488200	1.05515300
H	2.96843700	4.43858900	1.31399700

***Si*-M01^{BA}**

Total Energy= -3452.56669796

Sum of electronic and zero-point Energies= -3451.734015

Sum of electronic and thermal Energies= -3451.686075

Sum of electronic and thermal Enthalpies= -3451.685131

Sum of electronic and thermal Free Energies= -3451.816082

C	0.77053800	-2.84467400	2.50446400
C	0.44664500	-1.69588900	1.78546000
C	1.46141300	-0.85344800	1.30857800
C	2.79195600	-1.17666300	1.55191500
C	3.12761400	-2.33635100	2.24709600
C	2.11214200	-3.15905500	2.72167400
H	-0.00178000	-3.49404400	2.89820600
H	3.56624200	-0.51266400	1.17918200
H	4.16769700	-2.58742000	2.42175500
H	2.35645500	-4.05923600	3.27571300
C	1.10819600	0.42433300	0.57735300
O	-0.81730800	-1.31012300	1.46168500
C	-1.88447400	-2.19003400	1.72280100
H	-1.60742800	-3.23242300	1.51471000
H	-2.19673900	-2.12067400	2.77192300
C	-3.02418000	-1.81998700	0.78395300
O	-2.82332000	-1.05497600	-0.13800600
C	-4.35809700	-2.43655500	1.01134000
C	-4.57926300	-3.39478200	2.00602300
C	-5.41090400	-2.03170400	0.18281300
C	-5.84711000	-3.94395000	2.16867100
H	-3.77295100	-3.72430700	2.65416100
C	-6.67606400	-2.57798900	0.35204100
H	-5.21209100	-1.28733600	-0.58254100
C	-6.89340800	-3.53456800	1.34482500
H	-6.01807500	-4.68938100	2.93755300
H	-7.49428100	-2.26290900	-0.28659500
H	-7.88190700	-3.96274900	1.47580200
C	-2.84048900	3.80583100	-2.08976900
C	-3.58127500	3.26325600	-0.85599300
C	-1.39808800	3.19102600	-0.22868800

C	-1.34205500	3.67691700	-1.69326300
H	-3.11655700	3.26522100	-2.99648000
H	-3.11755000	4.84975100	-2.25860400
H	-0.78425400	2.98379000	-2.33255500
H	-0.82321000	4.63506100	-1.76268100
C	-2.70816300	3.83318100	0.30592300
C	-3.27156500	1.74443300	-0.76679900
H	-3.91900000	1.26686800	-0.02697100
C	-1.79979100	1.71028100	-0.21274100
H	-1.79287900	1.31059000	0.79898800
H	-0.50100800	3.38987800	0.35936600
C	-1.30650700	0.24770700	-2.17115800
C	-2.53911500	0.70823700	-2.86959900
C	0.19794300	0.18626900	-0.60282700
H	-2.90502600	-0.10344400	-3.50052500
N	-0.93000100	0.80220700	-0.97528200
O	-3.56462700	1.03433900	-1.96325200
H	-2.27462800	1.55250300	-3.51925000
N	-0.46202000	-0.65529900	-2.57207700
N	0.47459800	-0.67497400	-1.58337000
C	1.60497200	-1.53472100	-1.64296200
C	2.86084500	-1.02234000	-1.96835000
C	1.47594700	-2.88333200	-1.30210200
C	3.99312700	-1.82244100	-1.89407800
C	2.59354400	-3.70111900	-1.22619000
C	3.83998100	-3.14942900	-1.50693200
H	4.96897400	-1.41863000	-2.13470600
H	2.49388700	-4.74276100	-0.94719100
Cl	-0.08926900	-3.53562000	-0.96964200
Cl	5.24687200	-4.15205500	-1.38286900
Cl	3.01185800	0.63159100	-2.46527600
C	-5.06786000	3.55654400	-0.82920900
H	-5.52518700	3.19618800	0.09836700
H	-5.25817100	4.63072900	-0.91344000
H	-5.56613900	3.05852100	-1.66674000
C	-2.63566500	5.36225900	0.35501300
H	-3.63057300	5.78322700	0.53104000
H	-1.99689500	5.66957600	1.18906200
H	-2.23437200	5.81423300	-0.55285800
C	-3.13363500	3.36313400	1.70457800
H	-4.00697700	3.93463900	2.03310400
H	-3.40218000	2.30638100	1.76749300
H	-2.32905300	3.54668300	2.42410900
N	3.52360800	2.35013800	1.35357200

C	4.77460400	1.74651400	0.89653500
H	5.10814200	1.05998400	1.68422600
H	4.55032800	1.12385700	0.01697800
C	5.92392100	2.68348900	0.51355600
H	6.79757300	2.08949400	0.23037600
H	5.65532500	3.30175100	-0.34762800
H	6.21176700	3.34423900	1.33411000
C	2.97904600	3.39997500	0.49314400
H	1.88229700	3.34574500	0.55035600
H	3.23874200	3.13156500	-0.53824700
C	3.39474700	4.84672200	0.77185300
H	4.47665000	4.98369300	0.71293200
H	2.92528600	5.50872600	0.03853900
H	3.06302300	5.16730400	1.76364200
C	3.41841500	2.56647100	2.79653100
H	3.29965100	1.58254800	3.27299600
H	2.48331400	3.11600300	2.97502300
C	4.56518000	3.29869500	3.49986000
H	4.32605200	3.41813200	4.56027900
H	5.49355600	2.72445800	3.43440900
H	4.74254100	4.28859000	3.07378300
O	0.49562300	1.37304800	1.41402400
H	2.04021400	0.83962700	0.16449500
H	1.21571900	1.80156500	1.89916900

***Re*-TS2^{D}**

Total Energy= -3159.72343513

Sum of electronic and zero-point Energies= -3159.119805

Sum of electronic and thermal Energies= -3159.082196

Sum of electronic and thermal Enthalpies= -3159.081251

Sum of electronic and thermal Free Energies= -3159.188686

C	3.61209800	2.20502500	-0.90313100
C	2.34374300	1.68214800	-0.68361700
C	1.72608700	0.84457700	-1.62225200
C	2.37637300	0.62700500	-2.83957200
C	3.64348200	1.15316100	-3.07449600
C	4.27179100	1.92680800	-2.09904300
H	4.06017700	2.82824100	-0.13575100
H	1.86558200	0.01550100	-3.57626200
H	4.14452600	0.95646700	-4.01704000
H	5.26278400	2.33325500	-2.27413600
C	0.40485000	0.22016500	-1.35440800
O	-0.38751700	-0.14335400	-2.52017700
H	-0.56930600	0.82155500	-1.62195600

O	1.70315100	1.96707200	0.50819100
C	0.57141500	2.80622900	0.37130900
H	0.74029900	3.72840400	0.94579300
H	0.42965300	3.09906800	-0.67242600
C	-0.68744100	2.16682800	0.93416900
O	-0.63637200	1.23853200	1.71732800
C	-2.00372700	2.78958700	0.57692800
C	-2.23466700	3.44756000	-0.63619900
C	-3.04531600	2.66860600	1.50614400
C	-3.49380500	3.97511400	-0.91333300
H	-1.45138200	3.53708800	-1.38209500
C	-4.29617600	3.20857700	1.23284300
H	-2.84964600	2.15151600	2.44060700
C	-4.52099700	3.86230900	0.02066700
H	-3.67123100	4.47151100	-1.86131500
H	-5.09510500	3.12010800	1.96176500
H	-5.49863200	4.28061500	-0.19615600
C	-4.17435600	-3.04320000	0.07035000
C	-4.53439600	-1.55479600	0.21057100
C	-2.89660900	-1.54915500	-1.36910300
C	-2.99266100	-3.02883900	-0.94062600
H	-3.94130100	-3.49374100	1.03684000
H	-5.03160500	-3.59445100	-0.32594900
H	-2.04995600	-3.38098600	-0.50903700
H	-3.19256100	-3.67068300	-1.80133500
C	-4.36522400	-1.05422500	-1.26006600
C	-3.34130200	-0.85596300	0.91491400
H	-3.63080400	0.15667400	1.20947100
C	-2.26527100	-0.74741600	-0.22240800
H	-2.16960500	0.30136000	-0.51558300
H	-2.38247700	-1.36953600	-2.31304700
C	-0.70959600	-1.78276600	1.40923500
C	-1.85631200	-2.35614700	2.16359100
C	0.25051900	-0.63652700	-0.21003200
H	-1.56724100	-2.48994300	3.20686200
N	-0.93904600	-1.13902100	0.22475700
O	-2.95035000	-1.45963300	2.14429500
H	-2.11485900	-3.33701500	1.74760900
N	0.54070900	-1.77476700	1.73837400
N	1.14023700	-1.07461300	0.71774800
C	2.54894500	-0.98248500	0.67730500
C	3.26185200	-1.53973000	-0.39080300
C	3.25832500	-0.32485400	1.68828600
C	4.63204700	-1.36146200	-0.51395200

C	4.63446400	-0.15576000	1.59438500
C	5.29549300	-0.65235900	0.47913200
H	5.16505200	-1.77356600	-1.36174800
H	5.17202100	0.37128400	2.37280900
Cl	2.44452600	0.30797900	3.07513400
Cl	7.00656700	-0.38829300	0.32436500
Cl	2.43529500	-2.48908400	-1.58342200
C	-5.85649700	-1.27898000	0.89870800
H	-6.07375300	-0.20490500	0.91486500
H	-6.68090100	-1.78987100	0.39172300
H	-5.82593800	-1.63200800	1.93445500
C	-5.29542400	-1.73305500	-2.26939900
H	-6.34223600	-1.53146100	-2.01866200
H	-5.11131800	-1.32119100	-3.26677500
H	-5.16488200	-2.81446000	-2.33103800
C	-4.54523700	0.46163000	-1.43463300
H	-4.09961100	1.06850800	-0.64236100
H	-4.10624600	0.78440300	-2.38509400
H	-5.61151700	0.71025200	-1.46036000

***Si*-TS2^{D}**

Total Energy= -3159.71344623

Sum of electronic and zero-point Energies= -3159.110164

Sum of electronic and thermal Energies= -3159.071861

Sum of electronic and thermal Enthalpies= -3159.070917

Sum of electronic and thermal Free Energies= -3159.183128

C	3.21052500	0.05951800	1.49300303
C	2.01804900	0.44309500	0.88705400
C	0.77605600	0.12950200	1.45808700
C	0.76862000	-0.54484700	2.68128800
C	1.95589000	-0.92203100	3.30536200
C	3.17654900	-0.62787400	2.70505800
H	4.14937200	0.28919400	0.99877800
H	-0.18756800	-0.79867600	3.13170400
H	1.92500000	-1.45865100	4.24792100
H	4.10562700	-0.93373800	3.17524000
C	-0.50669200	0.47922500	0.77367400
O	-1.12329900	1.74799500	1.11421300
H	-0.54827300	1.35092200	-0.01731100
O	2.06150700	1.07472900	-0.34040700
C	1.89801600	2.48618100	-0.26798700
H	1.71240200	2.82718500	-1.29276500
H	1.04199600	2.75392100	0.36265000
C	3.13133900	3.20294200	0.28061700

O	2.98339600	4.12699400	1.05638100
C	4.49158000	2.77219000	-0.16549100
C	4.69179400	1.94179900	-1.27433600
C	5.59238900	3.23675600	0.56115800
C	5.98324500	1.57872300	-1.64405500
H	3.84317200	1.57025000	-1.83782900
C	6.88003100	2.86530600	0.19516700
H	5.41491500	3.88366900	1.41416000
C	7.07541100	2.03435900	-0.90775700
H	6.13767600	0.93418900	-2.50330000
H	7.73138700	3.21918900	0.76719100
H	8.08059300	1.74096300	-1.19339300
C	-5.71101400	0.61092500	-1.66114900
C	-5.97562400	0.81745000	-0.16105000
C	-3.84923500	1.57725100	-0.42712800
C	-4.22538300	1.04266400	-1.82538300
H	-5.92749400	-0.41130900	-1.97516100
H	-6.37732000	1.25420400	-2.24235700
H	-3.56986500	0.22125300	-2.13425100
H	-4.11491300	1.82111000	-2.58326700
C	-5.19467200	2.14471900	0.10598600
C	-5.11017200	-0.21103900	0.61799800
H	-5.42345000	-0.22610800	1.66557100
C	-3.66463800	0.38962700	0.53105300
H	-3.33495700	0.75900900	1.49864300
H	-2.99311300	2.25291700	-0.39453600
C	-2.99066900	-1.82456500	-0.42317700
C	-4.41189000	-2.14161200	-0.74021200
C	-1.32696900	-0.58769000	0.33766000
H	-4.55545100	-3.22223100	-0.69349400
N	-2.67717300	-0.61024700	0.13514800
O	-5.28286400	-1.56724300	0.21373600
H	-4.63366100	-1.81307800	-1.76166500
N	-1.95386400	-2.57618000	-0.60005600
N	-0.91034100	-1.80766200	-0.11868000
C	0.42943700	-2.13578800	-0.42296800
C	1.15855700	-3.01548100	0.38269100
C	1.06902600	-1.53040500	-1.50849000
C	2.51015300	-3.23671700	0.16101300
C	2.42246300	-1.72823600	-1.74734000
C	3.12445700	-2.56734000	-0.89258900
H	3.07373300	-3.89989000	0.80546500
H	2.91540100	-1.22923200	-2.57236400
Cl	0.16408300	-0.50140200	-2.56794800

Cl	4.83017000	-2.78550700	-1.14455400
Cl	0.36578700	-3.82827100	1.68687000
C	-7.43845800	0.76578700	0.23315100
H	-7.57057900	0.98485600	1.29824200
H	-8.02757800	1.48650000	-0.34226300
H	-7.84572900	-0.23206500	0.04165500
C	-5.69393100	3.34710000	-0.70131700
H	-6.73811400	3.56529600	-0.45371800
H	-5.10251300	4.23009500	-0.43936400
H	-5.62357500	3.21298300	-1.78157700
C	-5.17539400	2.57963100	1.57919500
H	-6.12352200	3.06425200	1.83221000
H	-5.03246700	1.76484200	2.29185300
H	-4.37518000	3.30830000	1.74408700

***Re*-TS2^{B}**

Total Energy= -3452.04173442

Sum of electronic and zero-point Energies= -3451.227747

Sum of electronic and thermal Energies= -3451.180283

Sum of electronic and thermal Enthalpies= -3451.179339

Sum of electronic and thermal Free Energies= -3451.307769

C	2.81091600	1.38210700	2.29396800
C	1.72933100	0.74757400	1.68040300
C	0.40950200	1.16310100	1.93856800
C	0.22194000	2.17516100	2.88028700
C	1.29159800	2.82057100	3.49513100
C	2.58916700	2.42853000	3.19022000
H	3.82953100	1.07977700	2.08433900
H	-0.81033800	2.43140000	3.09444600
H	1.11287300	3.61919000	4.20824100
H	3.43994600	2.91718300	3.65453900
C	-0.84634300	0.56110700	1.33120200
O	-1.96764000	0.71756800	2.03912100
H	-0.63175400	-0.80246900	1.40886400
O	1.88120000	-0.29477600	0.79301700
C	3.18372200	-0.79679200	0.65209500
H	3.85368300	-0.03983900	0.22065300
H	3.60287900	-1.08917900	1.62874900
C	3.17473400	-2.02330900	-0.24435200
O	2.13841400	-2.57005900	-0.56198800
C	4.49926100	-2.54268900	-0.70219700
C	5.71308400	-2.01768400	-0.24587100
C	4.50211500	-3.59888000	-1.61888500
C	6.91564800	-2.54747100	-0.70361600

H	5.73532900	-1.20235200	0.47062000
C	5.70342400	-4.12092100	-2.08016600
H	3.55031200	-3.99258000	-1.95944900
C	6.91144000	-3.59506600	-1.62181100
H	7.85519700	-2.14159000	-0.34433500
H	5.70156600	-4.93686800	-2.79520300
H	7.85082500	-4.00247600	-1.98147300
C	-5.55577000	0.82113300	-2.02461800
C	-5.55877400	-0.52204400	-1.27620400
C	-4.35384400	0.83851700	0.09206800
C	-4.65706700	1.72565200	-1.13320300
H	-5.21114200	0.70816700	-3.05391300
H	-6.57628300	1.20948700	-2.08517100
H	-3.73733500	2.04678100	-1.63391800
H	-5.17701600	2.63933800	-0.83633100
C	-5.62806100	-0.04136900	0.21140600
C	-4.11755200	-1.10041900	-1.34768800
H	-4.13250100	-2.14182900	-1.00829600
C	-3.33178700	-0.23396300	-0.30714900
H	-3.09401100	-0.82149100	0.57414200
H	-4.02157800	1.36322300	0.98890700
C	-1.73679400	0.26188200	-2.14513400
C	-2.74541500	-0.16418100	-3.15731100
C	-0.94945900	0.64051800	-0.10383000
H	-2.22809800	-0.56079800	-4.03252300
N	-2.05928500	0.23978300	-0.81834200
O	-3.57182600	-1.19879300	-2.66108600
H	-3.32235300	0.71239900	-3.47342000
N	-0.54255600	0.69885700	-2.37061100
N	-0.05151600	0.97641300	-1.09347300
C	0.96950200	1.93825600	-0.97092400
C	0.73027500	3.17415500	-0.35156400
C	2.26134800	1.69410400	-1.45034000
C	1.75988300	4.06466100	-0.07842700
C	3.30546200	2.57894300	-1.21180600
C	3.04380700	3.73848300	-0.49298800
H	1.55583000	4.99720100	0.43290900
H	4.30179800	2.36001500	-1.57674900
Cl	2.59069700	0.26033300	-2.36677500
Cl	4.35524900	4.82247800	-0.12875200
Cl	-0.89150600	3.64958600	0.04332900
C	-6.61105400	-1.50643000	-1.74630500
H	-6.60766000	-2.41217800	-1.13003500
H	-7.61158000	-1.06502000	-1.70227800

H	-6.41807000	-1.80273200	-2.78244100
C	-6.88299000	0.76740200	0.55648200
H	-7.78281800	0.15987200	0.41156800
H	-6.84830900	1.05707900	1.61164100
H	-6.99306000	1.67991100	-0.03092800
C	-5.53568300	-1.17371700	1.24710200
H	-5.25517100	-0.76379200	2.22359100
H	-6.51101600	-1.65848100	1.35698400
H	-4.81631400	-1.95839400	0.99927900
N	-0.72714100	-2.14340900	1.76776200
C	0.53662000	-2.44725400	2.47729500
H	1.31348300	-2.49836200	1.71252200
H	0.75464300	-1.57324600	3.10345100
C	0.55390800	-3.70245600	3.34660200
H	1.54424900	-3.79929200	3.79993000
H	-0.17400000	-3.64176500	4.15952700
H	0.35581900	-4.60981900	2.77234000
C	-1.93916100	-2.23613800	2.61799200
H	-2.60623700	-1.43020400	2.30396700
H	-1.62674400	-1.96228500	3.63015800
C	-2.66952300	-3.57583300	2.62756900
H	-2.04637900	-4.39691900	2.98939900
H	-3.53961500	-3.49409000	3.28540200
H	-3.03842300	-3.83928600	1.63113500
C	-0.83253300	-2.72554200	0.41031000
H	-0.16780500	-2.12649400	-0.22344800
H	-1.86048600	-2.55621000	0.07002800
C	-0.45637100	-4.19352100	0.24761100
H	-1.07171400	-4.85768200	0.85800600
H	-0.59040900	-4.47086100	-0.80161200
H	0.59606400	-4.35328800	0.49214100

***Si*-TS2^{B}**

Total Energy= -3452.02971057

Sum of electronic and zero-point Energies= -3451.216008

Sum of electronic and thermal Energies= -3451.168114

Sum of electronic and thermal Enthalpies= -3451.167170

Sum of electronic and thermal Free Energies= -3451.298062

C	-0.83251900	3.14376300	2.18845200
C	-0.42920200	1.88708400	1.74054400
C	-1.37947600	0.89391000	1.41838200
C	-2.72575300	1.21396600	1.56751100
C	-3.14556900	2.47821700	1.99016900
C	-2.19413400	3.43618100	2.30781800

H	-0.10203000	3.90263200	2.44522500
H	-3.47018700	0.46397800	1.31049200
H	-4.20426400	2.70299400	2.07291100
H	-2.49779700	4.42077200	2.64950100
C	-0.87232900	-0.46920200	0.97211100
O	0.87416700	1.54832500	1.52936000
C	1.82538800	2.57120200	1.51828800
H	1.45724600	3.46295800	0.98817000
H	2.10273800	2.87874700	2.53673100
C	3.05881100	2.07853300	0.77387000
O	3.06532700	1.00293700	0.21057200
C	4.24506200	2.98686900	0.73545600
C	4.22272200	4.26735800	1.29750800
C	5.40403900	2.52978200	0.10010600
C	5.34944700	5.08052400	1.22306500
H	3.33238300	4.64402700	1.79124200
C	6.52912800	3.34117100	0.03064900
H	5.40102400	1.53458400	-0.33244900
C	6.50184600	4.61770600	0.59220300
H	5.32720200	6.07424300	1.65747300
H	7.42757200	2.98234600	-0.46045100
H	7.38046200	5.25247200	0.53825400
C	2.51851200	-4.40330300	-1.55337100
C	3.42796400	-3.26401200	-1.05937700
C	1.64063800	-3.15315800	0.33839900
C	1.25840600	-4.27541100	-0.64830800
H	2.31857300	-4.32357000	-2.62333900
H	3.01796500	-5.36519100	-1.40601200
H	0.35210200	-4.01917000	-1.20990300
H	1.04454800	-5.21101000	-0.12445200
C	3.17766900	-3.31798500	0.48021100
C	2.73772600	-1.92674400	-1.44021400
H	3.42810400	-1.09138800	-1.28698200
C	1.57718100	-1.80250300	-0.38884800
H	1.79316100	-1.00483000	0.31747400
H	1.07791100	-3.12325800	1.27196500
C	0.12370800	-1.38188100	-2.36477500
C	1.08037000	-2.10846400	-3.24147200
C	-0.63558500	-0.57696000	-0.43815700
H	0.98098100	-1.73893000	-4.26329500
N	0.30259200	-1.41909800	-1.00573100
O	2.40674200	-1.83825400	-2.82799800
H	0.85366300	-3.18129200	-3.23751500
N	-0.84673700	-0.61758600	-2.73657600

N	-1.35257500	-0.11972900	-1.53790900
C	-2.11782500	1.06173700	-1.57158800
C	-3.50256500	1.02551800	-1.73866900
C	-1.51270800	2.31446500	-1.40200100
C	-4.28283400	2.16882900	-1.61374500
C	-2.26165600	3.47060000	-1.24876800
C	-3.64609800	3.36948500	-1.33079100
H	-5.35911900	2.11734200	-1.72216800
H	-1.77893200	4.42450000	-1.07545400
Cl	0.21771200	2.41598000	-1.41934600
Cl	-4.60764500	4.79988100	-1.09158400
Cl	-4.27472000	-0.48067600	-2.12592300
C	4.86194800	-3.34707700	-1.54288100
H	5.46792300	-2.54000900	-1.11679300
H	5.31744000	-4.30288000	-1.26491400
H	4.90153000	-3.25756400	-2.63334200
C	3.57859900	-4.64110200	1.14033600
H	4.65647300	-4.80855100	1.03845500
H	3.35376800	-4.59472100	2.21094900
H	3.06293300	-5.51260400	0.73379600
C	3.87211000	-2.20011000	1.27200400
H	4.93463200	-2.43722100	1.39241000
H	3.80369300	-1.21053500	0.81523300
H	3.43287400	-2.12994100	2.27283200
N	-2.70303300	-2.35504100	1.53284500
C	-4.12242300	-2.11845400	1.19572800
H	-4.52910200	-1.46918900	1.97785000
H	-4.12939900	-1.54039100	0.26631000
C	-5.01069200	-3.34466600	1.01348600
H	-6.02620300	-3.00858100	0.78739500
H	-4.67441400	-3.95925300	0.17429300
H	-5.05123300	-3.96972500	1.90766900
C	-2.01848400	-3.39330100	0.72814200
H	-0.97293700	-3.07204700	0.70059500
H	-2.41858100	-3.31322500	-0.28992800
C	-2.08534700	-4.83027600	1.23103300
H	-3.10576200	-5.20918100	1.31667400
H	-1.54539100	-5.46813000	0.52521800
H	-1.59314600	-4.92920400	2.20232100
C	-2.40436700	-2.37193300	2.98587300
H	-2.44420000	-1.32662800	3.31259500
H	-1.35860500	-2.66538300	3.07568500
C	-3.32686400	-3.21728100	3.85919500
H	-2.98378300	-3.14468200	4.89479300

H	-4.35908400	-2.85709000	3.83239600
H	-3.32223700	-4.27267900	3.57795600
O	-0.06066400	-1.10835100	1.80635000
H	-1.99674000	-1.31721600	1.05854600

***Re*-TS2^{BA}**

Total Energy= -3452.54423552

Sum of electronic and zero-point Energies= -3451.715102

Sum of electronic and thermal Energies= -3451.667516

Sum of electronic and thermal Enthalpies= -3451.666572

Sum of electronic and thermal Free Energies= -3451.795489

C	-2.97717000	-1.23106500	2.10392800
C	-1.81201700	-0.72049900	1.53761600
C	-0.55213200	-1.26628200	1.85366600
C	-0.50539000	-2.26810900	2.82317300
C	-1.66430300	-2.77908100	3.40512500
C	-2.90016700	-2.27245400	3.02975200
H	-3.94746800	-0.83188700	1.83555600
H	0.45779100	-2.65733200	3.13294900
H	-1.59302200	-3.56804100	4.14563600
H	-3.81407200	-2.66695900	3.46093200
C	0.70577900	-0.74028800	1.22533500
O	1.88418200	-1.15087900	1.90205200
H	0.72257400	0.65109600	1.56821300
O	-1.79826000	0.31716000	0.64111400
C	-3.01398400	1.00676300	0.47180900
H	-3.76359300	0.36756000	-0.01382700
H	-3.42344900	1.32141300	1.44445400
C	-2.77056200	2.24516500	-0.37636200
O	-1.64147700	2.60204800	-0.64608000
C	-3.96640400	3.00772100	-0.83470000
C	-5.26838500	2.65598500	-0.46240200
C	-3.75545300	4.11880700	-1.65805300
C	-6.34678700	3.41213600	-0.91018800
H	-5.45532200	1.80185900	0.18100500
C	-4.83389500	4.86835600	-2.10814700
H	-2.73818800	4.37632200	-1.93323100
C	-6.13039900	4.51506100	-1.73328300
H	-7.35514900	3.14028300	-0.61759800
H	-4.66747200	5.72747600	-2.74923800
H	-6.97414100	5.10146900	-2.08237900
C	5.58210200	-0.80790500	-2.04450900
C	5.42853800	0.56142400	-1.36196900
C	4.35402900	-0.85494700	0.05673900

C	4.76242600	-1.75912400	-1.12614500
H	5.25999800	-0.78297000	-3.08605400
H	6.63793600	-1.08935500	-2.06211100
H	3.88933000	-2.19751300	-1.62086500
H	5.36539400	-2.59991500	-0.77837300
C	5.52732500	0.16311600	0.14487600
C	3.93708700	0.98063800	-1.47223200
H	3.83180300	2.03298800	-1.18896100
C	3.22483700	0.08996200	-0.39115000
H	2.91427700	0.69423500	0.45880000
H	4.12062200	-1.38074800	0.98274400
C	1.73468200	-0.66184200	-2.23937400
C	2.73292700	-0.21140800	-3.24936300
C	0.88180500	-0.88926300	-0.21859100
H	2.20592800	0.06581000	-4.16333300
N	1.99471400	-0.50595500	-0.90326400
O	3.39969400	0.94694200	-2.78835300
H	3.41733800	-1.03183900	-3.48516600
N	0.56035900	-1.16305000	-2.44893000
N	0.04389800	-1.32535200	-1.18638700
C	-1.13202900	-2.09889100	-1.02615000
C	-1.07894900	-3.32415000	-0.35463500
C	-2.35821700	-1.65687400	-1.52945800
C	-2.23473400	-4.03682500	-0.06947200
C	-3.52617700	-2.36208500	-1.26958700
C	-3.44879100	-3.52683200	-0.51322200
H	-2.18475100	-4.96802900	0.48106500
H	-4.47624700	-2.00517400	-1.64874400
Cl	-2.44338900	-0.21495600	-2.48042900
Cl	-4.90812600	-4.37814100	-0.12554500
Cl	0.45398300	-3.99489600	0.11098700
C	6.37326900	1.63104800	-1.87260300
H	6.26235500	2.56229600	-1.30705400
H	7.41429900	1.30351000	-1.79688200
H	6.16367500	1.84869200	-2.92443400
C	6.85065800	-0.49624800	0.54446600
H	7.68274700	0.19538500	0.37849300
H	6.82929300	-0.73468200	1.61233200
H	7.06665200	-1.41982100	0.00618500
C	5.31078900	1.33037000	1.12072600
H	5.11588600	0.94827400	2.12892900
H	6.21797200	1.93989100	1.17144600
H	4.49440800	2.00766100	0.85360300
N	0.85086500	1.85778500	2.05540600

H	1.99086000	-2.10946100	1.80147700
C	-0.45146100	2.11831600	2.72653700
H	-1.16425400	2.32558200	1.92540100
H	-0.74893000	1.17128900	3.19043000
C	-0.48511900	3.21800300	3.78129700
H	-1.50888500	3.29703000	4.15589100
H	0.15523700	2.97970400	4.63389100
H	-0.19550000	4.19305100	3.38635200
C	2.01477700	1.76668700	2.97641000
H	2.71633900	1.05958100	2.52199200
H	1.65292200	1.28621600	3.89068600
C	2.74596900	3.06647400	3.29118800
H	2.11124200	3.80299700	3.78611900
H	3.58205400	2.83775000	3.95733700
H	3.16466500	3.52178000	2.38909800
C	1.08362500	2.65622700	0.82165400
H	0.50166000	2.16879400	0.03229100
H	2.14631700	2.56037500	0.57676700
C	0.70423500	4.13042400	0.86485300
H	1.26468000	4.68660500	1.61920600
H	0.92175600	4.56606300	-0.11349200
H	-0.36547000	4.25937600	1.04427200

***Si*-TS2^{BA}**

Total Energy= -3452.54488518

Sum of electronic and zero-point Energies= -3451.715139

Sum of electronic and thermal Energies= -3451.667378

Sum of electronic and thermal Enthalpies= -3451.666434

Sum of electronic and thermal Free Energies= -3451.796504

C	-1.22627900	3.56914300	1.28214300
C	-0.65563400	2.32950800	1.01346900
C	-1.38685900	1.13536500	1.14194400
C	-2.70526400	1.22814100	1.58231200
C	-3.29659800	2.46020300	1.85884400
C	-2.55405300	3.62581800	1.70583400
H	-0.66157400	4.48354700	1.13806900
H	-3.29048100	0.32022700	1.68328300
H	-4.33011800	2.50584600	2.18492200
H	-3.00506000	4.59190100	1.90737400
C	-0.69951900	-0.16873500	0.81094900
O	0.61963500	2.15595700	0.55822900
C	1.56619700	3.18304300	0.70161800
H	1.55978200	3.84488600	-0.17268500
H	1.37383300	3.78859800	1.59765800

C	2.92184200	2.50398700	0.87084400
O	2.96995600	1.29848800	1.04305300
C	4.14543700	3.34386500	0.85366400
C	4.08696700	4.73358800	0.70172100
C	5.38366100	2.70970300	1.00746400
C	5.25999900	5.48081100	0.70282400
H	3.13586000	5.24349400	0.58526100
C	6.55268000	3.45834700	1.00398600
H	5.40629500	1.63146700	1.12963500
C	6.49023800	4.84401400	0.85148400
H	5.21431900	6.55805600	0.58673200
H	7.51266900	2.96742900	1.12164600
H	7.40392700	5.42932900	0.84968400
C	2.71218000	-4.08636400	-1.76840300
C	3.64147300	-2.88267300	-1.54442200
C	2.07849000	-2.64459600	0.08777400
C	1.59122300	-3.87521000	-0.70954400
H	2.35947300	-4.14376400	-2.79900200
H	3.26104900	-5.01343900	-1.58382600
H	0.60660500	-3.70562400	-1.16045900
H	1.48420200	-4.74572600	-0.05794600
C	3.62584800	-2.76819500	0.01202800
C	2.86502500	-1.60298800	-1.95421200
H	3.55379900	-0.75391400	-1.97219000
C	1.85502800	-1.38559700	-0.76306600
H	2.15291700	-0.49877900	-0.20921800
H	1.67416600	-2.54463200	1.09731000
C	0.10456600	-1.30517900	-2.53529700
C	1.00421000	-2.01371700	-3.48518700
C	-0.54051700	-0.45990300	-0.59792000
H	0.73835600	-1.72855600	-4.50396900
N	0.48004000	-1.12304000	-1.22422800
O	2.34499100	-1.62793300	-3.27786700
H	0.85477100	-3.09470300	-3.38287700
N	-1.05536700	-0.79980300	-2.79220100
N	-1.45631200	-0.27905000	-1.58498400
C	-2.64537700	0.48629500	-1.52923400
C	-3.87587100	-0.12081600	-1.28464800
C	-2.59916300	1.87078000	-1.72376000
C	-5.02998100	0.63587900	-1.12640100
C	-3.73318200	2.65098100	-1.55993500
C	-4.93007100	2.01731300	-1.24085300
H	-5.98032600	0.15858300	-0.92165600
H	-3.68424300	3.72624700	-1.67971700

Cl	-1.10777400	2.61582700	-2.18798300
Cl	-6.34908500	2.98581300	-0.99434600
Cl	-3.96614400	-1.84969200	-1.19223900
C	4.98868800	-2.99048800	-2.23042100
H	5.62602600	-2.13356900	-1.98794200
H	5.51030300	-3.90403300	-1.92968100
H	4.85832700	-3.01777400	-3.31673800
C	4.15180000	-4.00587500	0.74600000
H	5.20256100	-4.17940200	0.49237400
H	4.09877200	-3.83631400	1.82613700
H	3.59738100	-4.91968700	0.52830100
C	4.39929900	-1.56365500	0.56614800
H	5.47163600	-1.78315400	0.55798800
H	4.25162400	-0.63121800	0.01899800
H	4.10617200	-1.37357300	1.60397900
N	-1.78250400	-2.22978000	2.20690300
H	1.10400200	0.36303500	1.39600000
C	-3.25667200	-2.17727000	2.40284700
H	-3.44216900	-1.44348000	3.19268700
H	-3.67533800	-1.77320800	1.47618000
C	-3.95606800	-3.49470700	2.71361800
H	-5.02186200	-3.29209400	2.84337900
H	-3.85620000	-4.20506900	1.88908100
H	-3.58808000	-3.96332300	3.62737400
C	-1.30992000	-3.33776100	1.33505000
H	-0.42295200	-2.94707100	0.82516500
H	-2.07757300	-3.48057900	0.56838600
C	-0.95404700	-4.65530800	2.00874200
H	-1.79310900	-5.09259800	2.55226100
H	-0.65020000	-5.36368100	1.23364200
H	-0.11238300	-4.53765100	2.69643700
C	-0.98985000	-2.01142400	3.45347200
H	-1.05060800	-0.93745500	3.65675200
H	0.05189000	-2.21416500	3.19690300
C	-1.42223200	-2.79303900	4.68680000
H	-0.74820200	-2.52942900	5.50553000
H	-2.43468100	-2.52945500	5.00186300
H	-1.36939300	-3.87384600	4.54517700
O	0.49443100	-0.38416000	1.54095200
H	-1.46437600	-1.26161700	1.48636500

***Re*-M02^{B}**

Total Energy= -3452.10016248

Sum of electronic and zero-point Energies= -3451.281461

Sum of electronic and thermal Energies= -3451.233195
Sum of electronic and thermal Enthalpies= -3451.232251
Sum of electronic and thermal Free Energies= -3451.364455

C	-3.12823200	-0.54233400	1.97102700
C	-1.90042000	-0.40142200	1.32510100
C	-0.76013400	-1.09848300	1.77202600
C	-0.87874000	-1.85541800	2.94194800
C	-2.09384000	-1.98626600	3.60834800
C	-3.22252200	-1.34427900	3.10851200
H	-4.01035700	-0.03378700	1.59870900
H	0.01092700	-2.35722000	3.31063000
H	-2.15990700	-2.59466300	4.50429000
H	-4.18224100	-1.45254500	3.60346600
C	0.54567600	-0.98794700	1.10023600
O	1.63301800	-0.73754900	1.92263900
H	1.43181200	0.14798000	2.35085100
O	-1.70705800	0.40929700	0.24277100
C	-2.69385100	1.35922400	-0.04226700
H	-3.58114900	0.89475600	-0.49852300
H	-3.01907800	1.88043200	0.87166300
C	-2.10364300	2.38267800	-1.00274000
O	-0.93940300	2.32635400	-1.33781700
C	-3.01004400	3.46677200	-1.48896500
C	-4.34348900	3.56654900	-1.07903100
C	-2.48551900	4.41203000	-2.37658900
C	-5.14228300	4.60250100	-1.55311300
H	-4.76947000	2.84490200	-0.38882600
C	-3.28488200	5.44395700	-2.85036900
H	-1.44883200	4.31776100	-2.68262100
C	-4.61409000	5.54006000	-2.43798100
H	-6.17559500	4.67769500	-1.23183400
H	-2.87572900	6.17415100	-3.54058000
H	-5.23919000	6.34696200	-2.80670900
C	5.55011800	-1.39926700	-1.76396800
C	5.30588700	0.10039000	-1.52432800
C	4.21075100	-0.89115300	0.20245400
C	4.73850300	-2.08145900	-0.62604600
H	5.25661400	-1.69928000	-2.77142100
H	6.61852500	-1.61786600	-1.68049900
H	3.91303600	-2.69672400	-0.99736300
H	5.36791800	-2.73598600	-0.01905100
C	5.33194300	0.17227800	0.03557100
C	3.81006200	0.38065600	-1.82294300
H	3.64195000	1.46211200	-1.83271700

C	3.06150100	-0.23017800	-0.58080200
H	2.63301700	0.57493600	0.01888300
H	3.92102600	-1.13397800	1.22601300
C	1.65736800	-1.41035600	-2.25067900
C	2.71968000	-1.26083100	-3.27904900
C	0.75668500	-1.24700200	-0.21334900
H	2.26418200	-1.25381600	-4.27034800
N	1.94129200	-1.08152300	-0.94977500
O	3.39781700	-0.02784600	-3.12329900
H	3.40502500	-2.11549300	-3.21915500
N	0.45884900	-1.83698200	-2.43986700
N	-0.11792100	-1.78512300	-1.16993500
C	-1.37515900	-2.34692500	-0.94835500
C	-1.55333200	-3.42073300	-0.06220100
C	-2.52544000	-1.82917600	-1.56489900
C	-2.81463100	-3.87626800	0.30082400
C	-3.79652800	-2.28964100	-1.24944200
C	-3.92305200	-3.28941200	-0.29170500
H	-2.92219000	-4.68130400	1.01716000
H	-4.66902900	-1.85919500	-1.72606400
Cl	-2.37993900	-0.55036400	-2.72760500
Cl	-5.51519900	-3.82550500	0.16748400
Cl	-0.16652300	-4.23970900	0.58367300
C	6.23865000	1.01796800	-2.28959600
H	6.04669100	2.06970900	-2.05099300
H	7.28592100	0.79789500	-2.05935200
H	6.09479400	0.88734200	-3.36693800
C	6.66284100	-0.25616500	0.66194100
H	7.46289400	0.43008000	0.36420900
H	6.58317600	-0.21433200	1.75312300
H	6.97083400	-1.26777900	0.39411100
C	5.01428900	1.56277100	0.60412900
H	4.89174400	1.50290700	1.69069500
H	5.85099400	2.24205600	0.40968100
H	4.11712700	2.03199900	0.19347800
N	1.04277400	1.74303000	2.83732900
C	-0.15275800	1.67172300	3.68305700
H	-1.01000800	1.53881500	3.01234500
H	-0.08899500	0.74596700	4.27085100
C	-0.40796900	2.83993000	4.63724300
H	-1.34143400	2.66629100	5.18053700
H	0.39125300	2.92774700	5.37893400
H	-0.49172700	3.79363700	4.11091000
C	2.29900800	2.04817400	3.52889600

H	3.09693700	1.50665000	3.00152800
H	2.23302900	1.60061100	4.52699700
C	2.71362100	3.51634000	3.63728600
H	1.97253200	4.11820100	4.16837600
H	3.66269000	3.58637400	4.17663500
H	2.86458800	3.95426400	2.64620300
C	0.86247300	2.38271400	1.52534600
H	0.29495800	1.69282700	0.88802600
H	1.86134100	2.47139600	1.07851100
C	0.16527900	3.74413000	1.49074100
H	0.67549000	4.49630400	2.09774700
H	0.12745100	4.09809200	0.45660500
H	-0.86791100	3.66331400	1.84520400

***Si*-M02^{B}**

Total Energy= -3452.09003104

Sum of electronic and zero-point Energies= -3451.272158

Sum of electronic and thermal Energies= -3451.223507

Sum of electronic and thermal Enthalpies= -3451.222563

Sum of electronic and thermal Free Energies= -3451.357103

C	-3.07186800	-1.01388700	2.42784600
C	-1.86873000	-0.54863000	1.90363600
C	-0.92273900	-1.44055200	1.35655200
C	-1.21958600	-2.80201600	1.36329000
C	-2.43047900	-3.27890900	1.86923400
C	-3.34968000	-2.38257100	2.40067200
H	-3.79303900	-0.32207600	2.84976300
H	-0.49513500	-3.49257700	0.93553600
H	-2.65013800	-4.34117500	1.84534800
H	-4.29251300	-2.74095700	2.80173700
C	0.29954400	-0.86186000	0.75321400
O	-1.52842900	0.76971300	1.84560000
C	-2.55282900	1.72219100	1.85740000
H	-3.45084400	1.35301800	1.33904100
H	-2.84201200	1.99138000	2.88266700
C	-2.06910900	2.96357700	1.11396300
O	-1.00633300	2.97342500	0.52770900
C	-2.97471600	4.15313800	1.11088200
C	-4.23514600	4.13353400	1.71664800
C	-2.53433900	5.31404300	0.46727000
C	-5.04421100	5.26519200	1.67882300
H	-4.59991600	3.24223400	2.21748200
C	-3.34177900	6.44366700	0.43336800
H	-1.55492600	5.30845600	0.00034100

C	-4.59755400	6.41954800	1.04001800
H	-6.02188800	5.24513300	2.14836500
H	-2.99585200	7.34326800	-0.06484000
H	-5.22870200	7.30199000	1.01435500
C	4.56720400	1.91600100	-2.02516100
C	3.49975600	2.93851600	-1.59946300
C	3.29086800	1.29460500	-0.04992400
C	4.37341800	0.75430900	-1.00920400
H	4.44588900	1.62160900	-3.06942900
H	5.56296900	2.36055700	-1.94194800
H	4.04798100	-0.17555200	-1.48760000
H	5.30003100	0.52314800	-0.47612000
C	3.55782300	2.82359700	-0.04377100
C	2.11592700	2.30774900	-1.90745200
H	1.33569400	3.06772900	-1.79448100
C	1.93237900	1.24008100	-0.76675100
H	1.14178500	1.57509400	-0.09226500
H	3.26225400	0.81803500	0.93171300
C	1.31362000	-0.29743000	-2.59478000
C	2.10609800	0.50480800	-3.56388200
C	0.52109300	-0.83491600	-0.57892100
H	1.70411700	0.35855400	-4.56728400
N	1.50009400	-0.07457200	-1.24788500
O	1.97999900	1.88335000	-3.26154100
H	3.15315600	0.17717800	-3.55331100
N	0.40005600	-1.15321200	-2.87705100
N	-0.08533600	-1.57697800	-1.62560300
C	-1.42283700	-2.02055000	-1.61015600
C	-1.72049600	-3.37652600	-1.77256900
C	-2.49423900	-1.14319500	-1.40411400
C	-3.01890900	-3.86069900	-1.68059300
C	-3.79906200	-1.59642900	-1.26831400
C	-4.03734600	-2.95874300	-1.40239500
H	-3.22392200	-4.91769000	-1.79609200
H	-4.60830000	-0.90244000	-1.07581700
Cl	-2.17934500	0.56073100	-1.31490300
Cl	-5.66289300	-3.55340800	-1.21726300
Cl	-0.42732600	-4.50234100	-2.04310000
C	3.66803500	4.31509700	-2.21179500
H	2.91144400	5.01158000	-1.83450900
H	4.65698000	4.72801600	-1.98887600
H	3.56202700	4.26035500	-3.30007100
C	4.91478800	3.19072500	0.56494800
H	5.14591300	4.24483900	0.37750500

H	4.87605100	3.05113900	1.65040500
H	5.74444200	2.59213900	0.18574700
C	2.50142900	3.65929000	0.69365600
H	2.78979200	4.71587000	0.67616900
H	1.49134700	3.58671100	0.28625900
H	2.45103900	3.34879200	1.74277100
N	3.06347800	-1.97792700	2.11095500
C	3.24440600	-2.48568500	0.74645100
H	2.34698700	-3.06547300	0.50022600
H	3.23447000	-1.61822500	0.07209200
C	4.50183900	-3.30715000	0.45954000
H	4.48480000	-3.64096300	-0.58199800
H	5.40583400	-2.70577700	0.59629000
H	4.57567100	-4.18913300	1.10016400
C	4.21467900	-1.28112300	2.69356700
H	3.82513100	-0.49861700	3.35877500
H	4.72254000	-0.76299500	1.87106500
C	5.22409300	-2.11915400	3.48111400
H	5.66236800	-2.91599700	2.87641100
H	6.03331800	-1.47366400	3.83458100
H	4.75777100	-2.57224800	4.36057200
C	2.30634800	-2.83991200	3.02458900
H	1.25224300	-2.79869400	2.71730200
H	2.35443700	-2.37316000	4.01510000
C	2.72295500	-4.30862900	3.11664900
H	2.08409300	-4.82122300	3.84158600
H	2.59696600	-4.81278800	2.15390700
H	3.76193500	-4.42837900	3.43278000
O	1.13045700	-0.15105700	1.60259800
H	1.88079800	-0.77292000	1.84577300

***Re*-M02^{BA}**

Total Energy= -3452.55260580

Sum of electronic and zero-point Energies= -3451.718426

Sum of electronic and thermal Energies= -3451.670197

Sum of electronic and thermal Enthalpies= -3451.669253

Sum of electronic and thermal Free Energies= -3451.799685

C	-2.93675300	-1.10389800	2.23613800
C	-1.76367400	-0.69021000	1.60600400
C	-0.53560300	-1.33716700	1.86644600
C	-0.52671900	-2.32982300	2.85411500
C	-1.68920000	-2.73425500	3.50144900
C	-2.89909500	-2.13559400	3.17341300
H	-3.88558400	-0.63308300	2.01156700

H	0.41599800	-2.80644500	3.10155200
H	-1.64740500	-3.52040400	4.24751600
H	-3.81993400	-2.45089700	3.65233500
C	0.71478700	-0.99464200	1.16377500
O	1.89489500	-1.15062600	1.91363700
H	0.65238900	0.98040900	1.69979500
O	-1.71384400	0.35858700	0.71873100
C	-2.91550900	1.06972400	0.53758200
H	-3.67891700	0.43173300	0.07467100
H	-3.31480700	1.42218100	1.50208300
C	-2.65134600	2.28546400	-0.33605800
O	-1.51473200	2.66487000	-0.54289000
C	-3.83125800	3.01232100	-0.88224400
C	-5.14570600	2.66205200	-0.55376800
C	-3.59334600	4.09112200	-1.74092100
C	-6.20924600	3.38777500	-1.07969400
H	-5.35384000	1.83396800	0.11642100
C	-4.65719800	4.80876400	-2.27034800
H	-2.56713600	4.34770200	-1.98154400
C	-5.96596500	4.45731800	-1.93882200
H	-7.22733200	3.11792900	-0.82088400
H	-4.47022700	5.64102500	-2.94044800
H	-6.79819600	5.01825300	-2.35169600
C	5.58205200	-0.88605500	-2.08712900
C	5.41365700	0.47545100	-1.39159100
C	4.37544600	-0.96763500	0.02284200
C	4.79214000	-1.85905300	-1.16594200
H	5.23764900	-0.85643700	-3.12176000
H	6.64218700	-1.14949400	-2.12646900
H	3.91918300	-2.30577400	-1.65275800
H	5.41529300	-2.69031100	-0.83031700
C	5.52893400	0.06909600	0.11216300
C	3.91472300	0.86699100	-1.49213900
H	3.79366500	1.91264900	-1.18850400
C	3.21998400	-0.05359800	-0.42364400
H	2.89891400	0.54498800	0.42965900
H	4.16350500	-1.50601000	0.94780700
C	1.67959300	-0.71890900	-2.26246200
C	2.69013600	-0.29641500	-3.26983100
C	0.86760900	-1.00032300	-0.21301900
H	2.17921100	-0.01260100	-4.19052500
N	2.00847100	-0.67757000	-0.92876900
O	3.38549800	0.84916700	-2.81110900
H	3.36262400	-1.13177100	-3.49233900

N	0.46770100	-1.09870000	-2.47602500
N	-0.04254800	-1.31243900	-1.20009100
C	-1.21753500	-2.06735500	-1.03738600
C	-1.20152700	-3.30427400	-0.37891800
C	-2.45027200	-1.58883000	-1.49879000
C	-2.37551800	-3.97462600	-0.06095700
C	-3.63651800	-2.25411300	-1.21877400
C	-3.58257900	-3.42362100	-0.46845000
H	-2.34227900	-4.91228700	0.48003900
H	-4.58175700	-1.86080600	-1.57354900
Cl	-2.51759100	-0.13193100	-2.43417000
Cl	-5.06351500	-4.22877300	-0.04858700
Cl	0.31041600	-4.06101600	0.02042600
C	6.33759300	1.56365600	-1.90069600
H	6.21581500	2.48903100	-1.32734600
H	7.38462800	1.25314500	-1.83495800
H	6.11654400	1.78560700	-2.94933400
C	6.86849500	-0.56452900	0.49804900
H	7.68431200	0.14847700	0.34145400
H	6.85652000	-0.82216500	1.56187200
H	7.10312300	-1.47336300	-0.05732700
C	5.29071500	1.22147900	1.10108000
H	5.09714500	0.82330100	2.10378600
H	6.18638200	1.84676000	1.16414900
H	4.46392300	1.88708600	0.83636300
N	0.83391700	1.93557700	2.08279900
H	2.17685700	-2.07649100	1.86386700
C	-0.48385500	2.32440400	2.71018800
H	-1.12811100	2.60101800	1.87531400
H	-0.87347000	1.40046600	3.14708300
C	-0.42985700	3.41259500	3.76748900
H	-1.45428700	3.58545900	4.10514500
H	0.15187600	3.10652300	4.63919900
H	-0.04007000	4.35833000	3.38995100
C	1.96499900	1.73877300	3.06197300
H	2.60730200	0.97787300	2.61180000
H	1.51980000	1.29034600	3.95383300
C	2.77498500	2.98109200	3.39239200
H	2.18765500	3.76910800	3.86392500
H	3.55911600	2.68248600	4.09204700
H	3.26946300	3.39131600	2.50847400
C	1.20703500	2.72087200	0.84585700
H	0.62666600	2.26985200	0.03851300
H	2.26910100	2.52870900	0.67386000

C	0.93232500	4.21208600	0.89729000
H	1.47972400	4.71986300	1.69282100
H	1.25493200	4.63396200	-0.05715900
H	-0.13532900	4.41730100	0.99731700

***Si*-M02^{BA}**

Total Energy= -3452.55085920

Sum of electronic and zero-point Energies= -3451.716995

Sum of electronic and thermal Energies= -3451.668423

Sum of electronic and thermal Enthalpies= -3451.667479

Sum of electronic and thermal Free Energies= -3451.800982

C	-1.18739700	3.77331300	0.83991500
C	-0.56009700	2.55920500	0.58580500
C	-1.21268000	1.33017800	0.80649400
C	-2.51325800	1.36847900	1.31296500
C	-3.16119800	2.57750800	1.56392200
C	-2.49455700	3.77485000	1.32818400
H	-0.67836900	4.70887900	0.63500000
H	-3.03866700	0.43352200	1.49374500
H	-4.17790400	2.57962400	1.94140600
H	-2.98947500	4.72156300	1.51696500
C	-0.45764000	0.09146500	0.50061300
O	0.69258100	2.44255700	0.06089700
C	1.62981200	3.47420000	0.22613200
H	1.60486200	4.16955700	-0.62118500
H	1.44750900	4.04432900	1.14772000
C	2.99757100	2.80327000	0.33334600
O	3.06514500	1.59319900	0.46329100
C	4.21109400	3.65728400	0.29614600
C	4.12942600	5.05328300	0.24978300
C	5.46283800	3.03229100	0.32089800
C	5.29256700	5.81569800	0.23062800
H	3.16775400	5.55665500	0.23339500
C	6.62178900	3.79614900	0.29544600
H	5.50533600	1.94863300	0.35677700
C	6.53615600	5.18808800	0.25137300
H	5.22841800	6.89775000	0.19766600
H	7.59193400	3.31119200	0.31087600
H	7.44201000	5.78519800	0.23328900
C	2.50821200	-4.65947700	-1.04776800
C	3.17112900	-3.46812900	-1.75916000
C	2.27248200	-2.52917000	0.10234300
C	1.82549500	-4.00455800	0.18705400
H	1.82472200	-5.19465700	-1.70926900

H	3.27106500	-5.38163100	-0.74487500
H	0.73342200	-4.09351700	0.16364900
H	2.15890000	-4.46415700	1.12107700
C	3.67867000	-2.62409600	-0.54997900
C	2.03228900	-2.56943700	-2.30860400
H	2.45683200	-1.81216800	-2.97401800
C	1.47596500	-1.84387000	-1.02216200
H	1.74617900	-0.78693800	-1.06706800
H	2.23834900	-1.97650300	1.04346600
C	-0.75029600	-2.55216500	-1.86086300
C	-0.12878100	-3.67884100	-2.60397100
C	-0.78680900	-0.81954100	-0.46281600
H	-0.76796000	-3.95330300	-3.44377700
N	0.00942400	-1.86881300	-0.93178000
O	1.11244000	-3.26538600	-3.14230400
H	-0.02637400	-4.54887800	-1.94400600
N	-1.93326600	-2.07956200	-2.02106000
N	-1.99599100	-1.00176900	-1.13415600
C	-2.97548100	-0.01748400	-1.36425500
C	-4.27908100	-0.19316600	-0.89176900
C	-2.67887500	1.17409100	-2.03741400
C	-5.25088800	0.78712500	-1.03864100
C	-3.62023400	2.18496900	-2.17641500
C	-4.89601300	1.97493300	-1.66660000
H	-6.25135300	0.63550800	-0.65275500
H	-3.36528500	3.10917100	-2.68021500
Cl	-1.09810900	1.40457700	-2.70785000
Cl	-6.08098000	3.23547600	-1.81530300
Cl	-4.68088400	-1.65084600	-0.03892400
C	4.17959400	-3.84945200	-2.82424800
H	4.65948300	-2.96145200	-3.24938300
H	4.95877200	-4.49891900	-2.41382100
H	3.68474700	-4.38796400	-3.63842100
C	4.69637100	-3.34412000	0.34009300
H	5.60469500	-3.57043500	-0.22783100
H	4.98289600	-2.68979700	1.16982700
H	4.32681600	-4.27699200	0.76801200
C	4.30473300	-1.27521400	-0.93381800
H	5.32445900	-1.43438900	-1.29872000
H	3.76802100	-0.72913300	-1.71270500
H	4.35791000	-0.62085500	-0.05797600
N	-1.11921500	-1.43732800	2.99613600
H	1.40563600	0.60875800	0.82505300
C	-2.57398300	-1.56351500	3.37354100

H	-2.85759800	-0.60269300	3.81110900
H	-3.10850800	-1.67168900	2.42505900
C	-2.93209200	-2.72482000	4.28532200
H	-4.00481300	-2.66441900	4.48109000
H	-2.74230500	-3.68726800	3.80591100
H	-2.41490900	-2.69489100	5.24457700
C	-0.47367800	-2.72141600	2.53417800
H	0.28115200	-2.40169000	1.81212700
H	-1.24934700	-3.26851300	1.99010800
C	0.16788800	-3.57227400	3.61513900
H	-0.53445100	-3.89031200	4.38597800
H	0.56267600	-4.46944800	3.13259000
H	1.00796900	-3.05794600	4.08712700
C	-0.28305200	-0.60029100	3.93558200
H	-0.55620400	0.43414100	3.70956200
H	0.74975400	-0.73771100	3.61231400
C	-0.47080800	-0.88243400	5.41528500
H	0.20771100	-0.22327300	5.96113500
H	-1.48506900	-0.65410700	5.74939800
H	-0.22832700	-1.91003200	5.68833700
O	0.77390000	-0.06921700	1.13851700
H	-1.12581100	-0.87967900	2.11959000

***Re*-M2**

Total Energy= -3159.81818386

Sum of electronic and zero-point Energies= -3159.210340

Sum of electronic and thermal Energies= -3159.172525

Sum of electronic and thermal Enthalpies= -3159.171580

Sum of electronic and thermal Free Energies= -3159.278184

C	-3.94094500	1.43834700	1.70446300
C	-2.64467000	1.45721000	1.17169300
C	-1.68036200	0.55018500	1.64571500
C	-2.03740800	-0.26497400	2.73561300
C	-3.31046300	-0.26699400	3.28060100
C	-4.27803000	0.58183700	2.73849600
H	-4.66303200	2.13324100	1.28886600
H	-1.27449100	-0.93199300	3.12621500
H	-3.55168700	-0.92501300	4.10838500
H	-5.28939700	0.58907900	3.13233400
C	-0.29435200	0.40814400	1.13539300
O	0.70786400	0.61068400	2.07515100
O	-2.49824300	2.40279500	0.19463500
C	-1.26745300	2.73824600	-0.40155200
H	-1.47189400	3.64131000	-0.98940000

H	-0.95507100	1.96046800	-1.09975000
C	-0.15512000	3.04581200	0.58028200
C	1.24829700	3.06639000	0.06399600
C	1.57791400	2.79733200	-1.27009300
C	2.26471300	3.37107100	0.97705900
C	2.90886400	2.83611800	-1.67920900
H	0.80983400	2.56105300	-2.00134300
C	3.59224700	3.39590600	0.56986000
H	1.99245400	3.59305800	2.00374300
C	3.91622800	3.12724100	-0.76084200
H	3.15982700	2.64684300	-2.71814300
H	4.37585700	3.62416200	1.28497300
H	4.95275000	3.15019500	-1.08318400
O	-0.39670700	3.29154400	1.75230200
H	0.56723200	1.50518100	2.43036100
C	3.78559800	-3.08449800	-0.16766600
C	4.57625900	-1.76162900	-0.19067400
C	2.80686500	-1.28781100	1.15399000
C	2.52231900	-2.72176600	0.65906500
H	3.55226600	-3.43732800	-1.17141500
H	4.38479100	-3.85539000	0.32519100
H	1.61067800	-2.75345000	0.05393000
H	2.37116200	-3.40600600	1.49762500
C	4.35607200	-1.24813100	1.26412400
C	3.72681600	-0.75696600	-1.01755100
H	4.31379600	0.12168900	-1.32528300
C	2.59572900	-0.31199200	-0.01787900
H	2.78374700	0.71037000	0.31823900
H	2.26479600	-0.99470800	2.05254700
C	1.07763200	-0.59800500	-1.98199000
C	2.26517400	-0.72030800	-2.87530100
C	0.02856100	-0.11018700	-0.07721900
H	2.60928400	0.28351400	-3.16716200
N	1.28197200	-0.32688200	-0.65184100
O	3.27218000	-1.41998600	-2.18663400
H	2.00576400	-1.28302500	-3.77239500
N	-0.16048200	-0.68593600	-2.31978100
N	-0.85301300	-0.40670500	-1.13496200
C	-2.20251800	-0.77245600	-1.02160400
C	-3.20091400	-0.10148600	-1.74319600
C	-2.61670900	-1.79490600	-0.15414300
C	-4.54945400	-0.36471500	-1.54509500
C	-3.95805100	-2.05270900	0.09272500
C	-4.90925600	-1.31707900	-0.60084000

H	-5.30163900	0.18101200	-2.10105000
H	-4.24904800	-2.82338100	0.79605800
Cl	-1.42977100	-2.79777300	0.61865200
Cl	-6.59609900	-1.60938300	-0.29168700
Cl	-2.76865700	1.10571900	-2.91441100
C	6.00385900	-1.88116700	-0.68877800
H	6.52540200	-0.91936300	-0.63415400
H	6.56511600	-2.61055400	-0.09656100
H	6.01658500	-2.21389400	-1.73142600
C	4.89044600	-2.17733500	2.35836900
H	5.97041300	-2.32210300	2.24567600
H	4.72201700	-1.71769300	3.33770700
H	4.41597500	-3.15978200	2.37010500
C	4.96093800	0.13977300	1.52158100
H	4.47945600	0.61232000	2.38527000
H	6.02738800	0.04056300	1.74826100
H	4.87357500	0.82941800	0.67843200

***Si*-M2**

Total Energy= -3159.81766004

Sum of electronic and zero-point Energies= -3159.209872

Sum of electronic and thermal Energies= -3159.171988

Sum of electronic and thermal Enthalpies= -3159.171044

Sum of electronic and thermal Free Energies= -3159.279428

C	2.35207900	-1.42720600	3.45980900
C	1.42853500	-0.59809200	2.82305400
C	0.32449300	-1.13484900	2.14669400
C	0.14119300	-2.52394900	2.19508700
C	1.05043000	-3.35911000	2.83369000
C	2.17140200	-2.80544500	3.45211300
H	3.20086000	-0.96882900	3.95659200
H	-0.71916100	-2.94190600	1.67974700
H	0.89599600	-4.43266200	2.83703500
H	2.89743200	-3.44474000	3.94409000
C	-0.64750400	-0.31737100	1.38020200
O	-1.87247900	-0.10281700	2.00535200
O	1.70336600	0.74799500	2.85040300
C	0.63685800	1.60421500	3.23148600
H	-0.15549200	1.05101000	3.74466200
H	1.05246300	2.34289800	3.92844400
C	-0.01082200	2.36490400	2.08322400
C	0.81574400	2.91378100	0.97267600
C	2.21050800	3.01051800	1.04861400
C	0.14248900	3.39177200	-0.15682000

C	2.92236800	3.58702200	-0.00030300
H	2.73957700	2.63432000	1.91802400
C	0.85794700	3.96281500	-1.20265000
H	-0.93877900	3.29319100	-0.20008300
C	2.24773700	4.06329000	-1.12398200
H	4.00284300	3.66952700	0.06219500
H	0.33400700	4.32783000	-2.08069100
H	2.80520200	4.51236400	-1.94029000
C	3.23625200	-2.18395200	-2.43865000
C	3.89758700	-0.92745400	-1.84081700
C	2.45793100	-1.57831900	-0.21107300
C	2.15467000	-2.53531600	-1.38340300
H	2.82218500	-1.99929100	-3.42883000
H	3.98631200	-2.97437700	-2.53327100
H	1.14315100	-2.36333800	-1.76548900
H	2.20815800	-3.57958000	-1.06580400
C	3.98420600	-1.31501700	-0.33594400
C	2.80314200	0.17550600	-1.81743500
H	3.23001700	1.18466700	-1.71027200
C	1.92646500	-0.17622900	-0.55877500
H	2.15764700	0.50900700	0.26301800
H	2.15328400	-1.95880300	0.76002800
C	0.03819000	0.62985700	-1.98242600
C	0.99093800	0.98113200	-3.07919400
C	-0.55808200	0.00344600	0.06438800
H	1.30912700	2.02644200	-2.95431200
N	0.50333300	-0.00209300	-0.84635800
O	2.09122300	0.11091000	-3.04106900
H	0.50114000	0.87396300	-4.04829600
N	-1.20781300	0.93623400	-1.95485500
N	-1.62802900	0.57544300	-0.65404400
C	-2.93462100	0.02257400	-0.59564800
C	-3.19371200	-1.31168500	-0.92958000
C	-4.02776300	0.82049800	-0.24561100
C	-4.47342200	-1.84965000	-0.88550800
C	-5.32231500	0.31753800	-0.20049800
C	-5.52296800	-1.01951500	-0.51525900
H	-4.64540300	-2.88713900	-1.14433700
H	-6.15147800	0.95565600	0.07846600
Cl	-3.77196000	2.48639500	0.15576700
Cl	-7.13557800	-1.67122200	-0.45110200
Cl	-1.89021000	-2.34060900	-1.44149200
C	5.17299600	-0.48688800	-2.53286000
H	5.62424200	0.37400400	-2.02784000

H	5.90815900	-1.29766800	-2.55106900
H	4.96398700	-0.19953700	-3.56820300
C	4.80624200	-2.56907700	-0.02793300
H	5.84428200	-2.44268500	-0.35376800
H	4.81643700	-2.73130900	1.05551200
H	4.41125900	-3.47479300	-0.49109800
C	4.53455100	-0.18831400	0.55387400
H	4.22258000	-0.33820500	1.59369000
H	5.62900500	-0.20170400	0.52881000
H	4.22000400	0.81530900	0.25327700
O	-1.20785900	2.60923500	2.15442300
H	-1.97625200	0.86053600	2.13678700

TS3*RR*

Total Energy= -3159.79182365

Sum of electronic and zero-point Energies= -3159.183600

Sum of electronic and thermal Energies= -3159.147111

Sum of electronic and thermal Enthalpies= -3159.146167

Sum of electronic and thermal Free Energies= -3159.250438

C	-2.61380300	-2.03301400	3.31904500
C	-1.69307000	-1.12633500	2.77498100
C	-0.91704300	-1.47859100	1.66167300
C	-1.10176800	-2.76856100	1.13518900
C	-2.02008100	-3.66722300	1.65683700
C	-2.77659200	-3.29317700	2.76980700
H	-3.19438000	-1.70909700	4.17624700
H	-0.48784900	-3.05936800	0.28868300
H	-2.13797200	-4.64941800	1.21214200
H	-3.49658900	-3.98038800	3.20258800
C	0.22176200	-0.64808900	1.11489300
O	-1.67312800	0.08130900	3.39908000
C	-1.08642400	1.17941800	2.73708000
H	-1.63042400	1.42228100	1.81812700
H	-1.19617300	2.02240100	3.42819400
C	0.39493200	0.99945900	2.45419900
C	0.97675200	2.19231300	1.73235500
C	2.09737700	2.79541500	2.31132600
C	0.35463400	2.82441500	0.65109200
C	2.57161900	4.01386000	1.83538700
H	2.56454700	2.30235200	3.15703000
C	0.83039800	4.03947800	0.16864800
H	-0.50810500	2.36641500	0.17907500
C	1.93591500	4.64293800	0.76638800
H	3.43511100	4.47717300	2.30254000

H	0.33635800	4.51610700	-0.67218600
H	2.30050200	5.59692700	0.39870400
C	-4.34039500	1.87885700	-1.39303000
C	-4.49380700	0.40055100	-1.78836700
C	-3.21838800	0.29207200	0.08672400
C	-3.33519800	1.80646800	-0.21372500
H	-3.98117000	2.49341300	-2.21699300
H	-5.31039400	2.27447100	-1.08105500
H	-2.36884600	2.22488200	-0.50993600
H	-3.67460200	2.36357300	0.66284900
C	-4.58597100	-0.27576700	-0.38913300
C	-3.09232600	-0.06582000	-2.28015900
H	-3.15327000	-0.97441700	-2.89684500
C	-2.29967200	-0.36082800	-0.95364200
H	-2.26922200	-1.43611500	-0.78037200
H	-2.98370300	0.04229000	1.11862900
C	-0.34659200	0.43614000	-2.28480600
C	-1.21843600	0.67281500	-3.47689400
C	0.18855500	-0.24238000	-0.24585600
H	-1.20208400	-0.22443500	-4.11277300
N	-0.88146800	0.05601600	-1.06903200
O	-2.52035600	0.97278300	-3.05337000
H	-0.84000000	1.51776300	-4.05386300
N	0.94057000	0.44559000	-2.28541000
N	1.28715600	0.02535900	-1.01688900
C	2.62490600	-0.44130800	-0.88025000
C	2.91806100	-1.80625400	-0.98005500
C	3.69270400	0.45243600	-0.80435000
C	4.21667500	-2.28180500	-0.89500500
C	5.00812200	0.00397200	-0.72699400
C	5.24888800	-1.36067800	-0.75482500
H	4.41800900	-3.34403100	-0.95443700
H	5.82157100	0.71485800	-0.65270700
Cl	3.39843900	2.15126700	-0.82844600
Cl	6.88509800	-1.93779200	-0.64761100
Cl	1.64148300	-2.94145000	-1.26658700
C	-5.60102500	0.11245100	-2.78347400
H	-5.69598200	-0.96199400	-2.97239800
H	-6.56150500	0.48207300	-2.41187800
H	-5.39641300	0.60809600	-3.73748900
C	-5.73900500	0.20920300	0.49458700
H	-5.66569700	1.26092600	0.77524600
H	-6.69965900	0.05497400	-0.00779700
H	-5.75160100	-0.37782800	1.41858000

C	-4.68016400	-1.80847000	-0.44440000
H	-5.72449000	-2.10550600	-0.58244600
H	-4.11234200	-2.26457100	-1.26001600
H	-4.32902800	-2.24616500	0.49734500
O	1.45447400	-1.18213100	1.45563200
O	1.10833900	0.40771500	3.31331500
H	1.66237400	-0.72197700	2.32275900

TS3*RS*

Total Energy= -3159.79341304

Sum of electronic and zero-point Energies= -3159.184529

Sum of electronic and thermal Energies= -3159.148218

Sum of electronic and thermal Enthalpies= -3159.147273

Sum of electronic and thermal Free Energies= -3159.250152

C	-3.78194800	2.00068500	0.20720100
C	-2.49570300	1.60987300	-0.14856200
C	-1.50058100	1.40739200	0.81282900
C	-1.80084500	1.67617400	2.14965700
C	-3.08448200	2.06976900	2.51925900
C	-4.07787200	2.21633800	1.55065700
H	-4.52507000	2.13198000	-0.57258700
H	-1.02123300	1.54479800	2.89226600
H	-3.31171900	2.25741600	3.56348100
H	-5.08075500	2.51515300	1.83889300
C	-0.14536200	0.93154900	0.37230200
O	0.83453800	1.19802800	1.34918000
O	-2.19446500	1.38540800	-1.46154200
C	-1.04935900	2.13722500	-1.88129300
H	-1.23877400	3.19327700	-1.65869500
H	-0.98716500	1.99978000	-2.96203800
C	0.32088700	1.65297500	-1.32624000
O	0.91349400	0.77042100	-2.04919300
C	1.18246600	2.85762700	-0.90373500
C	2.49466600	2.91321300	-1.37532400
C	0.72440100	3.89125500	-0.07407200
C	3.33734200	3.96618300	-1.02733500
H	2.81865700	2.10753600	-2.02817500
C	1.56712000	4.94296500	0.28266200
H	-0.29447300	3.86934600	0.30840800
C	2.87613000	4.98355000	-0.19430500
H	4.35516600	3.99330100	-1.40566500
H	1.19926800	5.73140800	0.93179100
H	3.53001300	5.80479400	0.08107800
H	1.22381700	2.06302200	1.14508600

C	4.33255200	-2.84681200	0.93807000
C	4.73505000	-1.67552100	0.02567800
C	3.15911400	-0.76104000	1.38491000
C	3.18607600	-2.24753100	1.80142700
H	4.05891900	-3.73301900	0.36393500
H	5.18524600	-3.13632500	1.55821100
H	2.21786700	-2.73227900	1.63687600
H	3.39350300	-2.34797500	2.86893200
C	4.64230300	-0.47392300	1.01930700
C	3.53795400	-1.39095500	-0.92452200
H	3.84692500	-0.71658800	-1.72836800
C	2.52090900	-0.62774100	-0.00630300
H	2.47255000	0.41032200	-0.31879500
H	2.70911200	-0.08918500	2.11618000
C	0.87618200	-2.35226900	-0.70232200
C	1.97506900	-3.27011900	-1.11211600
C	-0.02320800	-0.49498700	0.03377800
H	1.61103200	-3.91124300	-1.91666100
N	1.15370700	-1.12946000	-0.16169800
O	3.06651500	-2.53779600	-1.62542200
H	2.25375700	-3.90979300	-0.26781000
N	-0.39894200	-2.55051600	-0.82259900
N	-0.95152200	-1.38971900	-0.35491100
C	-2.36033200	-1.34077000	-0.20498000
C	-2.93267300	-1.40304200	1.06830100
C	-3.18824800	-1.26359200	-1.32628300
C	-4.30325500	-1.28019300	1.24012000
C	-4.56455800	-1.15187900	-1.17650600
C	-5.09580400	-1.13707700	0.10751900
H	-4.73772500	-1.29805700	2.23170900
H	-5.20449900	-1.06783300	-2.04623300
Cl	-2.50729200	-1.29197100	-2.91322700
Cl	-6.80896100	-0.93248100	0.30716700
Cl	-1.92247100	-1.65333300	2.45458000
C	6.04018700	-1.87373900	-0.71859600
H	6.30764500	-0.98028300	-1.29278400
H	6.85805900	-2.09645500	-0.02645400
H	5.95382600	-2.71044900	-1.41916200
C	5.57726400	-0.57081100	2.22982000
H	6.62203600	-0.59912900	1.90296000
H	5.45319500	0.31972000	2.85450000
H	5.39603600	-1.44211400	2.86024500
C	4.89807000	0.89508800	0.37231500
H	4.47630300	1.69452600	0.99206000

H	5.97574100	1.06989400	0.29260100
H	4.48061600	1.00701600	-0.63024300

TS3*SR*

Total Energy= -3159.78401498

Sum of electronic and zero-point Energies= -3159.176132

Sum of electronic and thermal Energies= -3159.139397

Sum of electronic and thermal Enthalpies= -3159.138453

Sum of electronic and thermal Free Energies= -3159.245006

C	-2.42798100	3.25923000	0.28354900
C	-1.39819200	2.34084800	0.46918800
C	-0.72054600	1.79683100	-0.63140800
C	-1.01677500	2.26805100	-1.91011100
C	-2.03030500	3.20352900	-2.10121700
C	-2.74471800	3.68414700	-1.00390700
H	-2.94312300	3.65036100	1.15500200
H	-0.44319700	1.88383600	-2.74829000
H	-2.26241700	3.55604200	-3.10046400
H	-3.54029300	4.40839100	-1.14636500
C	0.38193500	0.86256100	-0.33112800
O	1.43143900	0.78799500	-1.23442100
O	-1.11883300	1.95717300	1.75689100
C	0.23370800	1.65971700	2.17818000
H	0.44539400	2.33371700	3.01561400
H	0.25512100	0.63038700	2.55059500
C	1.31225700	1.80049900	1.10953500
O	2.38697000	1.11733800	1.20936300
C	1.50352200	3.22653900	0.58905000
C	0.71835300	4.30684500	1.00601200
C	2.58890100	3.48550700	-0.25523500
C	0.98289100	5.59873000	0.55661400
H	-0.10559300	4.15333000	1.69575900
C	2.84831200	4.77122000	-0.71582300
H	3.25402600	2.67303400	-0.52464900
C	2.04009300	5.83433500	-0.31675800
H	0.36127000	6.42185500	0.89505800
H	3.69090300	4.94717800	-1.37744500
H	2.24315700	6.83995000	-0.67146500
C	-3.90882600	-2.99412000	-0.60808900
C	-4.57033700	-1.82326300	0.13767000
C	-2.91854600	-0.81797400	-1.06043800
C	-2.72596600	-2.32059600	-1.36231900
H	-3.61740700	-3.79710700	0.06956900
H	-4.62488200	-3.43455700	-1.30672700

H	-1.74546600	-2.68782800	-1.04114800
H	-2.77681700	-2.50626300	-2.43719000
C	-4.46076900	-0.68263100	-0.92801400
C	-3.57853300	-1.32257700	1.22125900
H	-4.09409900	-0.60912200	1.86920300
C	-2.50101800	-0.54079900	0.39452700
H	-2.59989200	0.51161600	0.62386000
H	-2.44448900	-0.13895500	-1.77493000
C	-0.85286000	-2.13450100	1.31705400
C	-1.92630200	-3.00816000	1.87934000
C	0.05630500	-0.43654800	0.23487500
H	-1.58162400	-3.41701000	2.83146600
N	-1.12631200	-0.93322500	0.71925600
O	-3.11396300	-2.30073800	2.14106500
H	-2.07628200	-3.84820800	1.19207800
N	0.40037800	-2.44258800	1.24258500
N	0.96769200	-1.38722200	0.57482900
C	2.29578100	-1.59453500	0.11307000
C	2.52206500	-1.91951000	-1.22781900
C	3.36700600	-1.63601000	1.00925500
C	3.80681600	-2.14739000	-1.70285900
C	4.65815800	-1.87586600	0.55695600
C	4.85998000	-2.10533800	-0.79863000
H	3.97476800	-2.37372600	-2.74821400
H	5.48723500	-1.88757000	1.25330900
Cl	3.10402000	-1.44364600	2.70458000
Cl	6.47589100	-2.38768400	-1.37537800
Cl	1.18402300	-2.09828300	-2.31604600
C	-5.94352600	-2.12661300	0.70183400
H	-6.38872500	-1.23504900	1.15594200
H	-6.61846200	-2.48903500	-0.07926600
H	-5.87400100	-2.89929100	1.47408600
C	-5.19394400	-0.97264900	-2.24240900
H	-6.27105400	-1.05929400	-2.06600000
H	-5.04048900	-0.13812600	-2.93394200
H	-4.86019100	-1.88150100	-2.74404700
C	-4.94717400	0.69439100	-0.45225200
H	-4.58452600	1.47063500	-1.13459400
H	-6.04136400	0.72234400	-0.46352000
H	-4.62941300	0.97572700	0.55433500
H	2.22926900	0.87135100	-0.65842400

TS3*SS*

Total Energy= -3159.79530949

Sum of electronic and zero-point Energies= -3159.186720
Sum of electronic and thermal Energies= -3159.150127
Sum of electronic and thermal Enthalpies= -3159.149182
Sum of electronic and thermal Free Energies= -3159.253467

C	2.72906900	0.13532500	3.61354300
C	1.79014300	0.66064200	2.71411200
C	0.75419300	-0.14469900	2.23186900
C	0.65207300	-1.45463000	2.72680900
C	1.57996900	-1.98270500	3.61077000
C	2.63323300	-1.17560100	4.04892100
H	3.52171100	0.79131100	3.95815000
H	-0.18999000	-2.05296200	2.39236600
H	1.48333300	-3.00390100	3.96276900
H	3.37138900	-1.56472800	4.74292100
C	-0.32753100	0.32691100	1.30073000
O	-1.60247300	0.07181500	1.78923800
O	2.02019300	1.95715200	2.37082500
C	1.14803100	2.66299900	1.50643600
H	1.28166100	3.71877600	1.76635500
H	1.47292200	2.54243000	0.46697100
C	-0.33374600	2.35283500	1.65346300
C	-1.15378400	2.99240600	0.54843300
C	-0.76279900	3.05160200	-0.79585500
C	-2.31130700	3.66967600	0.93994900
C	-1.50906100	3.77606200	-1.71936500
H	0.13179000	2.53905800	-1.14079100
C	-3.05702800	4.39893500	0.01862100
H	-2.59533300	3.62694800	1.98587000
C	-2.65632000	4.45708500	-1.31445200
H	-1.19303100	3.80879600	-2.75727200
H	-3.94855600	4.92775000	0.34157000
H	-3.23212000	5.03007300	-2.03449700
C	3.83934800	-1.74195200	-2.32819900
C	4.35882000	-0.42121000	-1.73845700
C	2.96367900	-1.20656000	-0.12023600
C	2.81015000	-2.22797700	-1.26826300
H	3.43563200	-1.60865700	-3.33216800
H	4.66817200	-2.44761100	-2.42777700
H	1.78333100	-2.26036800	-1.64762100
H	3.03548500	-3.23832700	-0.92054300
C	4.45815200	-0.78510100	-0.22108400
C	3.18504800	0.59574400	-1.73026500
H	3.57618100	1.59145400	-1.50160300
C	2.29328000	0.11607800	-0.53210000

H	2.38043000	0.82346200	0.28711600
H	2.63890200	-1.56403500	0.86072500
C	0.43113700	-0.05259900	-2.18457900
C	1.40155300	0.00634700	-3.31602800
C	-0.22363200	0.04106200	-0.08015900
H	0.92068200	0.49322500	-4.16593200
N	0.87980000	0.06069300	-0.89082200
O	2.52677100	0.79109500	-2.97691900
H	1.66701100	-1.01209600	-3.61710000
N	-0.85016300	-0.19188200	-2.25785900
N	-1.27091500	-0.14840700	-0.93601000
C	-2.45814000	-0.87341700	-0.63123200
C	-2.37628100	-2.23168400	-0.31000600
C	-3.71981700	-0.28803000	-0.71939900
C	-3.50885600	-2.98486800	-0.03714800
C	-4.87241100	-1.02057700	-0.45987200
C	-4.74720300	-2.35915500	-0.11361200
H	-3.42611200	-4.03406500	0.21761600
H	-5.84516000	-0.54941800	-0.52680500
Cl	-3.85247900	1.37690200	-1.14418100
Cl	-6.17938100	-3.28459300	0.22100700
Cl	-0.82489200	-3.01432900	-0.26900100
C	5.60033600	0.12463000	-2.41528900
H	5.95436400	1.03548500	-1.92122600
H	6.40979800	-0.61156400	-2.40209900
H	5.38450500	0.37064700	-3.45979400
C	5.41321400	-1.94100000	0.09462300
H	6.43956600	-1.67160900	-0.17507700
H	5.39601400	-2.13754300	1.17144200
H	5.16471100	-2.87361600	-0.41341900
C	4.87596400	0.38204400	0.68556600
H	4.70962500	0.11296900	1.73327800
H	5.94506400	0.57901600	0.55745800
H	4.35213100	1.32383100	0.50401300
O	-0.83214500	2.30185100	2.81447400
H	-1.73600400	0.81976500	2.42450900

M3*RR*

Total Energy= -3159.80291718

Sum of electronic and zero-point Energies= -3159.192915

Sum of electronic and thermal Energies= -3159.156584

Sum of electronic and thermal Enthalpies= -3159.155640

Sum of electronic and thermal Free Energies= -3159.259084

C	-2.45136400	-2.40041400	3.22889700

C	-1.52545400	-1.42235400	2.84442200
C	-0.72575600	-1.60081800	1.71275700
C	-0.86665900	-2.79465700	0.99391600
C	-1.79785000	-3.75940100	1.34937900
C	-2.59107500	-3.55951600	2.48340500
H	-3.05070100	-2.21545000	4.11430000
H	-0.22284900	-2.95202300	0.13313200
H	-1.89433400	-4.66735500	0.76374800
H	-3.31842600	-4.30729800	2.78294300
C	0.39739600	-0.62389700	1.30561100
O	-1.45635800	-0.31992000	3.63639100
C	-0.95784400	0.84246100	3.00420900
H	-1.69822500	1.20507100	2.28277500
H	-0.84693000	1.59257600	3.79057400
C	0.39782900	0.64056300	2.33033500
C	0.80054400	1.99257200	1.73979800
C	1.92656900	2.64546100	2.24646200
C	0.00033200	2.67159400	0.81342900
C	2.24228300	3.93985100	1.84229500
H	2.53274100	2.12607300	2.97911400
C	0.31470400	3.96475500	0.40372100
H	-0.89048100	2.20175200	0.40804600
C	1.43715400	4.60686600	0.92203300
H	3.11936100	4.43130600	2.25248900
H	-0.32458700	4.47145000	-0.31334000
H	1.67980100	5.61875200	0.61319200
C	-4.10691800	1.52364200	-2.32646000
C	-4.48086400	0.14930700	-1.74370300
C	-3.12343100	1.04258700	-0.15812400
C	-3.10069000	2.09493700	-1.28544800
H	-3.71775100	1.44328400	-3.34223700
H	-5.00145100	2.14820500	-2.39217100
H	-2.09138500	2.24178500	-1.68639300
H	-3.41881700	3.06942000	-0.90885200
C	-4.57116900	0.47618200	-0.22082000
C	-3.21062100	-0.74136700	-1.79520800
H	-3.47681400	-1.78368100	-1.59718100
C	-2.34721100	-0.21316700	-0.58932000
H	-2.37886600	-0.94315200	0.21389200
H	-2.84331300	1.42503700	0.82307500
C	-0.51680400	0.01576200	-2.24877800
C	-1.51137200	0.07569300	-3.35548100
C	0.19260100	-0.25623400	-0.18396800
H	-1.03643000	-0.28586500	-4.26854800

N	-0.92305900	-0.09639600	-0.94347400
O	-2.58500900	-0.79740700	-3.07091400
H	-1.83237300	1.10796600	-3.52283900
N	0.77336500	-0.04647300	-2.35156800
N	1.20137800	-0.21356600	-1.06851000
C	2.61070900	-0.41008500	-0.90876100
C	3.15455000	-1.69676800	-0.95678200
C	3.47194800	0.68308700	-0.91926400
C	4.52294200	-1.89536400	-0.88472700
C	4.85141300	0.50872900	-0.84439200
C	5.35446000	-0.78153400	-0.80888300
H	4.93172300	-2.89785400	-0.89970200
H	5.50903500	1.36873700	-0.83286700
Cl	2.84016900	2.28215100	-1.07183300
Cl	7.07354700	-1.02079400	-0.71245600
Cl	2.12326100	-3.06956400	-1.15666900
C	-5.68121000	-0.50890400	-2.39406200
H	-5.93544300	-1.44799700	-1.89137400
H	-6.55510000	0.14838700	-2.36054400
H	-5.46742400	-0.73399100	-3.44351500
C	-5.62415000	1.52689400	0.14441200
H	-5.46554900	2.49625600	-0.32923700
H	-6.62213100	1.17287300	-0.13322300
H	-5.62023500	1.68342000	1.22756600
C	-4.82951700	-0.74130100	0.68152400
H	-5.89662500	-0.98271900	0.67241500
H	-4.29474000	-1.65078500	0.39657200
H	-4.55211700	-0.50810800	1.71555900
O	1.60733500	-1.19950700	1.39459800
O	1.30490900	0.21469400	3.29313100
H	1.79016000	-0.49535300	2.73358500

M3*RS*

Total Energy= -3159.79921488

Sum of electronic and zero-point Energies= -3159.189151

Sum of electronic and thermal Energies= -3159.152624

Sum of electronic and thermal Enthalpies= -3159.151680

Sum of electronic and thermal Free Energies= -3159.255334

C	-3.79918500	1.93369300	0.96590600
C	-2.52386500	1.77952900	0.42898900
C	-1.47994200	1.22782600	1.17269400
C	-1.72071100	0.88152100	2.49898800
C	-2.99055200	1.02255500	3.05374000
C	-4.03127700	1.53766200	2.28043500

H	-4.58192500	2.36540300	0.35007100
H	-0.88259200	0.48978000	3.06624900
H	-3.17045500	0.73364400	4.08433400
H	-5.02444100	1.64888200	2.70523700
C	-0.07056600	0.98220000	0.58799300
O	0.87402900	0.99851900	1.49910700
O	-2.28570900	2.18937300	-0.85683400
C	-1.04144200	2.88159800	-0.93735400
H	-1.03495800	3.69157500	-0.19843800
H	-0.98075800	3.30139500	-1.94380300
C	0.16752700	1.97191500	-0.71948300
O	0.26498100	1.22398600	-1.92976400
C	1.39157100	2.84384800	-0.51472500
C	2.33119200	3.01796600	-1.53356400
C	1.57546100	3.52658600	0.69516600
C	3.44887700	3.83244600	-1.34241200
H	2.18469900	2.53996900	-2.49733100
C	2.68310900	4.34439800	0.88114600
H	0.86093900	3.37934300	1.49619000
C	3.63011100	4.49420600	-0.13383100
H	4.16852400	3.95436600	-2.14592800
H	2.81474900	4.86208400	1.82621300
H	4.49702100	5.12973300	0.01773600
C	4.23344600	-3.00006500	0.64398100
C	4.66217400	-1.73176700	-0.11266500
C	3.06110600	-0.97443000	1.31639600
C	3.07275800	-2.49888800	1.54999200
H	3.96819300	-3.80945800	-0.03827300
H	5.07135300	-3.37055700	1.24060500
H	2.10495700	-2.95383900	1.31300000
H	3.25963800	-2.72458500	2.60190300
C	4.55133200	-0.65231800	1.01390100
C	3.48520500	-1.32871300	-1.04583700
H	3.82903500	-0.58046100	-1.76752500
C	2.46428400	-0.66246800	-0.06264400
H	2.44899700	0.41950300	-0.17831600
H	2.57636000	-0.38197200	2.08999700
C	0.79280600	-2.27235400	-0.96580800
C	1.88944800	-3.15708400	-1.45447000
C	-0.06568400	-0.45277300	-0.08326800
H	1.53552000	-3.70799900	-2.32723200
N	1.09150100	-1.10649300	-0.31765900
O	2.99180400	-2.37803900	-1.87761300
H	2.15518900	-3.88192500	-0.67882800

N	-0.48889200	-2.41881700	-1.11502800
N	-1.00653400	-1.28157700	-0.55093200
C	-2.42183400	-1.15958100	-0.47424500
C	-3.08628600	-1.60074900	0.67351700
C	-3.16111800	-0.66708100	-1.54924300
C	-4.45900800	-1.45521800	0.79964300
C	-4.53861200	-0.51471700	-1.44330700
C	-5.16008800	-0.89148500	-0.26021200
H	-4.96528900	-1.76806600	1.70431100
H	-5.10840200	-0.10703000	-2.26917400
Cl	-2.37613600	-0.25822600	-3.03011200
Cl	-6.87168600	-0.64846300	-0.09336800
Cl	-2.18943200	-2.36009100	1.94337500
C	5.98086900	-1.84962700	-0.85021800
H	6.26132100	-0.89723100	-1.31291100
H	6.78453800	-2.15226000	-0.17206800
H	5.90713600	-2.60168900	-1.64229200
C	5.46528600	-0.89623700	2.21798300
H	6.51541100	-0.88633700	1.90769400
H	5.32922900	-0.08834100	2.94373300
H	5.27506700	-1.83794900	2.73514600
C	4.81133500	0.78864500	0.54252800
H	4.35424200	1.49984400	1.23991500
H	5.88794100	0.98431200	0.52109100
H	4.42530700	1.02221800	-0.45279900
H	1.14703600	0.83419400	-1.98882500

M3*SR*

Total Energy= -3159.80173266

Sum of electronic and zero-point Energies= -3159.190882

Sum of electronic and thermal Energies= -3159.154156

Sum of electronic and thermal Enthalpies= -3159.153212

Sum of electronic and thermal Free Energies= -3159.257993

C	2.48091400	3.00588600	1.19815800
C	1.51258000	2.37178000	0.41584500
C	0.55050400	1.55390700	1.01415300
C	0.56776700	1.38199300	2.39700900
C	1.54698500	1.98078600	3.18134100
C	2.50284000	2.79791900	2.57246900
H	3.19695700	3.66085500	0.71245900
H	-0.22954000	0.78280700	2.82822900
H	1.55875300	1.83238500	4.25579900
H	3.26277000	3.28951900	3.17174500
C	-0.59266500	0.94767200	0.19172900

O	-1.75406400	0.78932600	0.79620100
O	1.58016000	2.60316600	-0.93336200
C	0.60511700	2.00359300	-1.78642200
H	0.51960800	2.66094500	-2.65363900
H	0.95791000	1.02839300	-2.14694600
C	-0.73865000	1.83056300	-1.09438200
O	-1.57707000	1.13749300	-1.99494300
C	-1.34565200	3.20830500	-0.79056200
C	-1.68634900	3.99304000	-1.89882600
C	-1.59203700	3.71905900	0.48605800
C	-2.22833200	5.26433600	-1.74392900
H	-1.54232900	3.58855300	-2.89702000
C	-2.13274600	4.99509200	0.64282500
H	-1.39328100	3.10757100	1.35604800
C	-2.44657800	5.77483100	-0.46600200
H	-2.48405900	5.85290300	-2.61951000
H	-2.31611600	5.37588000	1.64296300
H	-2.86841000	6.76670800	-0.33694500
C	4.32243800	-2.66225500	0.55127200
C	4.66926800	-1.60662500	-0.51035700
C	3.16121800	-0.53636500	0.81655800
C	3.21779400	-1.96685400	1.39623600
H	4.03177400	-3.61327300	0.10428800
H	5.20836600	-2.87423700	1.15565300
H	2.24509100	-2.46724500	1.34070900
H	3.47977100	-1.93869900	2.45566400
C	4.62332700	-0.29579200	0.33591400
C	3.42997100	-1.41896000	-1.42714800
H	3.71280800	-0.82721000	-2.30188300
C	2.44367600	-0.56347700	-0.54545400
H	2.39443600	0.44477700	-0.94440100
H	2.76516800	0.21141300	1.50380100
C	0.81825100	-2.40462200	-0.88862700
C	1.90113800	-3.32699500	-1.33092300
C	-0.12003500	-0.51233400	-0.26483000
H	1.48137700	-4.03439600	-2.04802100
N	1.07017900	-1.09558600	-0.56921700
O	2.91786600	-2.61505400	-1.99963000
H	2.26818800	-3.89625200	-0.47173200
N	-0.44057800	-2.68876500	-0.76976500
N	-1.00413100	-1.51430700	-0.36998300
C	-2.38505600	-1.58541100	-0.01204600
C	-2.74235200	-1.79676500	1.32346900
C	-3.36595900	-1.67228600	-0.99491800

C	-4.06494600	-1.97859700	1.68647400
C	-4.70433300	-1.85263600	-0.65366500
C	-5.03335300	-1.98924900	0.68506100
H	-4.33483600	-2.12028700	2.72557700
H	-5.46272600	-1.90169500	-1.42507500
Cl	-2.93722300	-1.58835500	-2.67225300
Cl	-6.69911800	-2.22042600	1.12758200
Cl	-1.51298600	-1.86289500	2.53928000
C	5.93391800	-1.89773200	-1.29376400
H	6.15458400	-1.09611400	-2.00624100
H	6.79144100	-2.00897300	-0.62302500
H	5.82293400	-2.82873900	-1.85842100
C	5.61217000	-0.24705800	1.50464900
H	6.64218000	-0.26985500	1.13454300
H	5.47625800	0.69469100	2.04638500
H	5.49269200	-1.05870400	2.22321000
C	4.86279000	0.98037100	-0.48442700
H	4.63786200	1.86061400	0.12312600
H	5.91887700	1.03330000	-0.76787200
H	4.28038700	1.05851300	-1.40518700
H	-2.34549900	0.90479600	-1.44363700

M3*SS*

Total Energy= -3159.80878086

Sum of electronic and zero-point Energies= -3159.198269

Sum of electronic and thermal Energies= -3159.161949

Sum of electronic and thermal Enthalpies= -3159.161005

Sum of electronic and thermal Free Energies= -3159.265553

C	2.73234300	-0.59751100	3.48963800
C	1.79898800	0.13864100	2.74859800
C	0.70002600	-0.49476000	2.16619200
C	0.53256300	-1.86447000	2.38460400
C	1.46532600	-2.61104500	3.09100900
C	2.57554300	-1.96693300	3.64338600
H	3.56548100	-0.06698900	3.93954000
H	-0.36899700	-2.32028200	1.99053300
H	1.32264800	-3.67732800	3.23023500
H	3.31056000	-2.52882600	4.21106200
C	-0.40070100	0.24732200	1.38729600
O	-1.63344600	-0.15302400	1.71656300
O	2.06508500	1.46884500	2.64161400
C	1.16718100	2.31810800	1.93963400
H	1.11826100	3.25030600	2.51016900
H	1.60559300	2.56001600	0.96438200

C	-0.26138300	1.80824600	1.78059400
C	-0.97531200	2.77947300	0.83887600
C	-0.49520900	3.07307200	-0.44499700
C	-2.09496900	3.47414200	1.30030300
C	-1.12543500	4.02112700	-1.24595500
H	0.38905700	2.57715800	-0.83913400
C	-2.72565900	4.42527900	0.50289600
H	-2.45528200	3.26598300	2.30031500
C	-2.24597600	4.70191400	-0.77484500
H	-0.73541400	4.22960500	-2.23731700
H	-3.59553100	4.95266400	0.88254800
H	-2.73499000	5.44552100	-1.39617100
C	3.99278000	-1.54147600	-2.34971600
C	4.40486000	-0.19437600	-1.73631600
C	3.04689100	-1.09933200	-0.14846800
C	2.98291300	-2.11070400	-1.31298200
H	3.60117400	-1.42785300	-3.36101600
H	4.87252900	-2.18437300	-2.43742200
H	1.96638000	-2.21889300	-1.70643800
H	3.27635000	-3.10450600	-0.96944500
C	4.50768300	-0.56728700	-0.22234300
C	3.15763800	0.73302100	-1.73508800
H	3.46647500	1.75720600	-1.50924300
C	2.29843600	0.18797600	-0.54009300
H	2.33603100	0.88398500	0.29252800
H	2.74245300	-1.50383200	0.81792700
C	0.46563700	-0.11137700	-2.19796500
C	1.43412000	-0.00380800	-3.32694000
C	-0.20985300	0.00698600	-0.11458400
H	0.92308100	0.43805200	-4.18391300
N	0.88532400	0.05160300	-0.90410800
O	2.49047200	0.87028400	-2.98490700
H	1.77780500	-1.00162800	-3.61496300
N	-0.81503100	-0.31321400	-2.25746800
N	-1.22189900	-0.25297200	-0.95424800
C	-2.52487400	-0.77642600	-0.67548600
C	-2.65523800	-2.14760600	-0.44644700
C	-3.67347000	-0.00342200	-0.80971700
C	-3.89883300	-2.72974100	-0.25642600
C	-4.93226800	-0.56358400	-0.62304500
C	-5.02483800	-1.91805200	-0.33582200
H	-3.98572600	-3.79159600	-0.06351900
H	-5.81979100	0.05109700	-0.70804600
Cl	-3.54295200	1.66610100	-1.21568200

Cl	-6.59257600	-2.62751300	-0.09775300
Cl	-1.24396400	-3.15389300	-0.43738100
C	5.61206400	0.45334700	-2.38461700
H	5.89004500	1.37767000	-1.86747600
H	6.47274000	-0.22195500	-2.37008600
H	5.39498200	0.70212900	-3.42814100
C	5.53499200	-1.65569900	0.10418100
H	6.54321900	-1.31814200	-0.15683600
H	5.51943000	-1.84938700	1.18172100
H	5.35419100	-2.60445700	-0.40267000
C	4.82543800	0.62233400	0.69717900
H	4.59253800	0.36556500	1.73486500
H	5.89440000	0.84969200	0.64042800
H	4.29228500	1.54627100	0.46048900
O	-0.85601300	1.79992900	3.04945500
H	-1.49658000	1.04087100	2.93274000

TS4*RR*

Total Energy= -3159.79538657

Sum of electronic and zero-point Energies= -3159.186153

Sum of electronic and thermal Energies= -3159.149665

Sum of electronic and thermal Enthalpies= -3159.148721

Sum of electronic and thermal Free Energies= -3159.252719

C	-3.07869600	3.31248000	0.53877200
C	-1.84766200	2.77548000	0.15681600
C	-1.02409600	2.16240400	1.10445500
C	-1.44354000	2.09825400	2.43145600
C	-2.68350100	2.59597700	2.81581900
C	-3.49681200	3.20991100	1.86008100
H	-3.69207000	3.79460400	-0.21537600
H	-0.76169700	1.64331700	3.14408500
H	-3.00917100	2.52514800	3.84799800
H	-4.46332400	3.61394200	2.14521100
C	0.34734400	1.61537100	0.73517300
O	-1.52106600	2.88768500	-1.16026900
C	-0.34901700	2.22909400	-1.62302800
H	-0.58647300	1.18651400	-1.87692000
H	-0.06104500	2.75753200	-2.53433100
C	0.78897000	2.25841000	-0.61752800
C	2.09632900	1.74374600	-1.20662400
C	3.28134500	1.93976300	-0.47943800
C	2.19247900	1.23340500	-2.50178100
C	4.51837300	1.66538700	-1.04655500
H	3.21905500	2.30943800	0.53742500

C	3.43584500	0.94492500	-3.06852300
H	1.30246600	1.05274700	-3.09622600
C	4.60275900	1.17495600	-2.35071500
H	5.42353700	1.83171800	-0.46926100
H	3.48390800	0.55239600	-4.07959800
H	5.57140700	0.96680800	-2.79534700
C	-3.71796000	-2.44709900	-1.55888100
C	-4.59877900	-1.70629600	-0.53265400
C	-3.04744300	-0.15603900	-1.13478700
C	-2.63875400	-1.39837100	-1.95152800
H	-3.31229300	-3.37713300	-1.16145900
H	-4.32524200	-2.73385300	-2.42169000
H	-1.61934900	-1.72724500	-1.72680800
H	-2.66376700	-1.17864000	-3.02095700
C	-4.60043200	-0.25691100	-1.11618100
C	-3.78739300	-1.47727800	0.76300300
H	-4.44744300	-1.00039400	1.49189100
C	-2.70182500	-0.41639800	0.34822300
H	-2.82929800	0.48359900	0.94681100
H	-2.65960400	0.79416500	-1.50839700
C	-1.05713800	-2.18372200	0.94391100
C	-2.11406600	-3.21676300	1.14508100
C	-0.14222500	-0.21771200	0.44498900
H	-1.83116400	-3.84050300	1.99564300
N	-1.32759700	-0.88805200	0.58492600
O	-3.35805400	-2.63769600	1.45510200
H	-2.15393600	-3.86227800	0.26126600
N	0.21799500	-2.38900100	1.04816600
N	0.75579900	-1.17039400	0.74109100
C	2.16917700	-1.12760700	0.61256800
C	2.99575300	-0.90233100	1.71192000
C	2.73929300	-1.49709500	-0.60802000
C	4.37859100	-0.92460200	1.56776100
C	4.11471100	-1.54808300	-0.76951000
C	4.91227600	-1.23268500	0.32359800
H	5.02081800	-0.72501600	2.41677500
H	4.54997500	-1.81552800	-1.72408100
Cl	1.71312800	-1.96587600	-1.92562300
Cl	6.63865900	-1.22547900	0.11836100
Cl	2.31664400	-0.68881300	3.28383100
C	-5.93658400	-2.36877500	-0.27030500
H	-6.54733400	-1.77763400	0.41999400
H	-6.49766200	-2.50169600	-1.20040800
H	-5.78537700	-3.35554600	0.17821800

C	-5.22146400	-0.14591400	-2.51283000
H	-4.82246800	-0.85786600	-3.23558500
H	-6.30374500	-0.29960400	-2.45280800
H	-5.05374900	0.86047500	-2.90933900
C	-5.30881300	0.79020000	-0.24680700
H	-6.37697900	0.55705500	-0.18450900
H	-4.92640300	0.88304600	0.77098800
H	-5.21358700	1.77631400	-0.71090200
O	1.21904800	1.59040900	1.64797900
O	0.96579600	3.63158800	-0.26900800
H	1.37725700	3.62673400	0.60873200

TS4*RS*

Total Energy= -3159.79489557

Sum of electronic and zero-point Energies= -3159.186051

Sum of electronic and thermal Energies= -3159.149444

Sum of electronic and thermal Enthalpies= -3159.148500

Sum of electronic and thermal Free Energies= -3159.254100

C	3.79394300	1.70724000	-2.16926800
C	2.53955100	1.93226600	-1.59450600
C	1.52528200	0.97463500	-1.70618400
C	1.74247800	-0.13041600	-2.52686800
C	2.97494200	-0.35490800	-3.12604700
C	4.01173500	0.55899000	-2.91797800
H	4.56646800	2.45766900	-2.03849000
H	0.91879200	-0.82560100	-2.66617500
H	3.13336100	-1.23498500	-3.74107600
H	4.98642700	0.39054800	-3.36564100
C	0.15913900	1.19665800	-1.07009000
O	-0.83870200	1.15670500	-1.82899000
O	2.35591600	3.12486400	-0.96252500
C	1.00064100	3.48474700	-0.74008400
H	0.50778300	3.69574300	-1.69742700
H	1.02171100	4.38617400	-0.12559600
C	0.25944300	2.36009300	-0.00579600
O	1.12232300	2.04731400	1.06295500
C	-1.11441000	2.79928000	0.45793500
C	-1.51054400	2.61950200	1.78532100
C	-2.03342200	3.34723400	-0.44745000
C	-2.80205300	2.94719200	2.19693000
H	-0.81144200	2.23657100	2.52236700
C	-3.31487100	3.69372700	-0.03176700
H	-1.75483700	3.46583400	-1.48748300
C	-3.70955100	3.48447600	1.28932100

H	-3.09103800	2.79089800	3.23143400
H	-4.01566000	4.11150700	-0.74813800
H	-4.71415100	3.74431500	1.60756100
C	-4.14362800	-2.89834600	-0.35166800
C	-4.69372300	-1.49625100	-0.04204300
C	-2.87623100	-1.07038700	-1.34089200
C	-2.84790100	-2.60339700	-1.16070400
H	-3.99462100	-3.48873000	0.55343600
H	-4.87057600	-3.44828900	-0.95569200
H	-1.93535000	-2.94094900	-0.65714600
H	-2.85852200	-3.10668900	-2.12995300
C	-4.39711800	-0.75449600	-1.38594500
C	-3.69698900	-0.79619000	0.92410600
H	-4.15169600	0.11527000	1.32390000
C	-2.50881800	-0.39214300	-0.01200200
H	-2.47539600	0.68621800	-0.15546800
H	-2.27775600	-0.68007500	-2.16542400
C	-1.06150400	-1.71568700	1.51958200
C	-2.24931800	-2.38260900	2.12695900
C	0.01625600	-0.31008200	0.17843200
H	-2.03630100	-2.59632600	3.17605300
N	-1.20631700	-0.76807000	0.54101200
O	-3.37907100	-1.53626500	2.10131000
H	-2.42404100	-3.33752800	1.61989400
N	0.18981500	-1.91176100	1.80701600
N	0.83408900	-1.03493700	0.97077200
C	2.25418600	-1.06213400	0.90565000
C	2.88237500	-1.84457300	-0.06668600
C	3.04726100	-0.36444900	1.81872500
C	4.25748100	-1.79690800	-0.24678500
C	4.42612500	-0.30739500	1.66727900
C	5.00490700	-0.99640900	0.60811400
H	4.73035900	-2.37681600	-1.02956000
H	5.03170900	0.25865700	2.36402000
Cl	2.32896300	0.37318600	3.21325400
Cl	6.72224900	-0.89183000	0.37208800
Cl	1.94254300	-2.94706200	-1.01509400
C	-6.11829400	-1.47743400	0.47530200
H	-6.47707800	-0.45122800	0.60973200
H	-6.79486100	-1.99108500	-0.21468400
H	-6.17568500	-1.98409200	1.44406400
C	-5.09125300	-1.35620500	-2.61199900
H	-6.17902000	-1.31198500	-2.49314900
H	-4.83305300	-0.76668100	-3.49743400

H	-4.81553300	-2.39181700	-2.81558400
C	-4.74310700	0.74093400	-1.37053900
H	-4.19179600	1.25930800	-2.16241800
H	-5.81255600	0.87525600	-1.56181800
H	-4.51570100	1.25026300	-0.43204100
H	0.71134500	1.36876000	1.60999600

TS4*SR*

Total Energy= -3159.79830185

Sum of electronic and zero-point Energies= -3159.188759

Sum of electronic and thermal Energies= -3159.152374

Sum of electronic and thermal Enthalpies= -3159.151430

Sum of electronic and thermal Free Energies= -3159.255968

C	2.41527900	3.17865900	0.49907300
C	1.37350000	2.39545100	0.00236000
C	0.49554900	1.75360900	0.88276500
C	0.68705100	1.88294500	2.25540300
C	1.75387300	2.61922800	2.75995200
C	2.61058600	3.27439600	1.87314900
H	3.05470800	3.70295100	-0.20321700
H	-0.03487500	1.40094300	2.90798600
H	1.90447000	2.70605000	3.83052700
H	3.43039000	3.87700600	2.25161900
C	-0.72556200	1.05949500	0.33311300
O	-1.71689500	0.80714800	1.07531700
O	1.28459300	2.29826300	-1.36112400
C	0.13742500	1.67654000	-1.95659600
H	-0.06164700	2.22312800	-2.88200300
H	0.37574600	0.63991300	-2.21814100
C	-1.07822600	1.69347900	-1.04585400
O	-2.08023200	0.90009600	-1.63818000
C	-1.60706400	3.11693400	-0.80693700
C	-2.82718700	3.27535900	-0.13792400
C	-0.95026700	4.26076700	-1.26822300
C	-3.37336600	4.53795300	0.06196500
H	-3.33759800	2.39984100	0.24728700
C	-1.49886400	5.52781500	-1.06982500
H	0.00315400	4.17946200	-1.77923000
C	-2.71176200	5.67207400	-0.40625100
H	-4.32052700	4.63681900	0.58318300
H	-0.97133000	6.40198400	-1.43868100
H	-3.13964400	6.65795700	-0.25410200
C	4.58489600	-2.32354600	0.89363100
C	4.79972000	-1.49613700	-0.38329100

C	3.27148000	-0.27443800	0.77739500
C	3.46722600	-1.54181200	1.63890100
H	4.34917700	-3.36464300	0.67190600
H	5.51030900	-2.34378900	1.47535300
H	2.53572700	-2.10839200	1.74287600
H	3.77104000	-1.27240200	2.65252600
C	4.68797400	-0.04156000	0.17235700
C	3.50967600	-1.58966100	-1.24211200
H	3.70820900	-1.17327000	-2.23372600
C	2.49204900	-0.64472800	-0.49814300
H	2.31469000	0.24794900	-1.09599900
H	2.84725200	0.57009300	1.32020900
C	1.00310100	-2.62766500	-0.39340300
C	2.14348300	-3.54303900	-0.67432000
C	-0.03421400	-0.67848700	-0.13297500
H	1.76735100	-4.41942200	-1.20493500
N	1.17839900	-1.27014200	-0.32154900
O	3.07760900	-2.91447600	-1.52754900
H	2.58651800	-3.88233100	0.26689900
N	-0.24183800	-2.94946000	-0.23494900
N	-0.85765400	-1.73785800	-0.06192100
C	-2.26973800	-1.77679200	0.10240400
C	-2.83621800	-1.80229300	1.37848100
C	-3.09516200	-1.93086700	-1.01173600
C	-4.21138100	-1.86981200	1.54338200
C	-4.47780600	-1.99644600	-0.87099400
C	-5.01310800	-1.94870700	0.40899800
H	-4.64600000	-1.86972900	2.53509400
H	-5.11430500	-2.09557900	-1.74151400
Cl	-2.40386800	-2.07656800	-2.59092100
Cl	-6.73845800	-2.02169300	0.60478500
Cl	-1.81654500	-1.79359000	2.77208700
C	6.04679300	-1.86550000	-1.16205200
H	6.17665800	-1.22203500	-2.03825900
H	6.93959600	-1.77956700	-0.53497100
H	5.97910900	-2.90007900	-1.51303300
C	5.72291900	0.31934500	1.24240500
H	6.73186400	0.30807900	0.81702100
H	5.52590400	1.33486000	1.60176900
H	5.71476200	-0.34150000	2.10985000
C	4.79402600	1.04168000	-0.91071700
H	4.61317300	2.02493700	-0.47062700
H	5.81037700	1.04654500	-1.31789000
H	4.10764300	0.92737900	-1.75243600

H	-2.62410700	0.61684200	-0.88155800

TS4*SS*

Total Energy= -3159.80420653

Sum of electronic and zero-point Energies= -3159.195060

Sum of electronic and thermal Energies= -3159.158672

Sum of electronic and thermal Enthalpies= -3159.157728

Sum of electronic and thermal Free Energies= -3159.261580

C	1.69908100	1.83639200	3.55012300
C	0.87424400	2.15636800	2.46597900
C	-0.03957100	1.22109700	1.97321500
C	-0.18886000	0.00728100	2.64577500
C	0.60432100	-0.31243500	3.73741100
C	1.56814000	0.60301700	4.17349300
H	2.41225600	2.57650700	3.89720400
H	-0.93071300	-0.69250300	2.27285800
H	0.48537400	-1.26667200	4.23917700
H	2.20744100	0.36083800	5.01644900
C	-0.90836200	1.55547500	0.78786100
O	-2.14768500	1.46236400	0.89218600
O	0.99778300	3.40543500	1.93810800
C	-0.06679900	3.81963600	1.08635800
H	-0.97606200	3.97299200	1.68198800
H	0.24102800	4.77003900	0.64636900
C	-0.40199600	2.80741400	-0.02672000
C	0.73953800	2.61997300	-1.01367800
C	2.03830600	3.08555200	-0.78800500
C	0.45605000	2.01348400	-2.24440200
C	3.03059700	2.91955700	-1.75752200
H	2.29343700	3.57425400	0.14474300
C	1.44965200	1.81763200	-3.19540500
H	-0.55895800	1.68844100	-2.44265000
C	2.74807400	2.27066800	-2.95437300
H	4.03163200	3.29255300	-1.56324300
H	1.20962400	1.32393800	-4.13193100
H	3.52464600	2.13018700	-3.69973500
C	3.33885500	-3.05182500	0.35652400
C	4.06613200	-1.95265100	-0.43930500
C	2.58607200	-0.79329700	0.83600200
C	2.27356500	-2.26517200	1.17477700
H	2.93299000	-3.82691500	-0.29399500
H	4.05214600	-3.55407500	1.01612300
H	1.24310600	-2.53575500	0.91862400
H	2.37422100	-2.44153500	2.24820900

C	4.12199900	-0.80435000	0.61758400
C	3.06908900	-1.36034700	-1.47175800
H	3.60705300	-0.68144000	-2.13975100
C	2.09073800	-0.50290600	-0.59292400
H	2.21131400	0.55189700	-0.83521200
H	2.23091000	-0.06924400	1.56974800
C	0.28096800	-1.93520000	-1.52198600
C	1.26125200	-2.91140400	-2.07703600
C	-0.40554900	-0.13764000	-0.39655600
H	0.87277100	-3.31853700	-3.01250200
N	0.68537600	-0.82249100	-0.83585800
O	2.49581900	-2.29830700	-2.37574800
H	1.36350000	-3.74173500	-1.36871300
N	-1.01228300	-2.02584600	-1.55180200
N	-1.41195000	-0.91415300	-0.84342000
C	-2.79521800	-0.84472600	-0.51434900
C	-3.30436500	-1.68635700	0.47738400
C	-3.68133000	-0.01124800	-1.19419000
C	-4.64948800	-1.67384600	0.82067200
C	-5.03045300	0.02687600	-0.86896700
C	-5.49347800	-0.80443500	0.14281200
H	-5.02547700	-2.32923900	1.59623700
H	-5.70313700	0.68893100	-1.39982800
Cl	-3.10848200	1.00073500	-2.47364100
Cl	-7.17944800	-0.76782400	0.56031100
Cl	-2.24962900	-2.79209600	1.30302700
C	5.37086500	-2.39236900	-1.07293300
H	5.87477000	-1.55358700	-1.56528400
H	6.05083000	-2.80998500	-0.32400900
H	5.18531200	-3.16308400	-1.82769200
C	4.89332800	-1.15062900	1.89565000
H	5.94636100	-1.34104000	1.66373100
H	4.85405300	-0.29817600	2.58217500
H	4.50245300	-2.01886400	2.42705300
C	4.70360200	0.51590700	0.09675500
H	4.41604800	1.33818000	0.76237800
H	5.79688600	0.46190100	0.08663700
H	4.38046100	0.78556200	-0.90968200
O	-1.51132900	3.31090300	-0.72523900
H	-2.26647400	2.81362900	-0.34683700

M4*RR*

Total Energy= -3159.81109914

Sum of electronic and zero-point Energies= -3159.202738

Sum of electronic and thermal Energies= -3159.164602
Sum of electronic and thermal Enthalpies= -3159.163658
Sum of electronic and thermal Free Energies= -3159.273494

C	-2.66136200	3.34442200	0.80392600
C	-1.37477100	2.95983900	0.41675400
C	-0.51706200	2.34978300	1.34142800
C	-0.97713300	2.08175700	2.63403600
C	-2.26311000	2.43351600	3.01585000
C	-3.09570500	3.08186600	2.09608000
H	-3.30113500	3.83044700	0.07533300
H	-0.29173600	1.59874500	3.32381300
H	-2.61628900	2.22287200	4.01905600
H	-4.09998900	3.37481500	2.38695500
C	0.88073800	2.02622700	0.96778600
O	-1.01276200	3.21352300	-0.86300600
C	0.12757600	2.51407600	-1.35678100
H	-0.13126300	1.46127800	-1.51275900
H	0.37692800	3.00289100	-2.29978500
C	1.31070500	2.59595800	-0.40179400
C	2.57294400	1.96688100	-0.96941200
C	3.75832000	2.03442200	-0.22359300
C	2.62677200	1.43006100	-2.25723900
C	4.96516700	1.60384000	-0.76237000
H	3.73614100	2.42048200	0.79040200
C	3.83745300	0.99963900	-2.79946800
H	1.72982100	1.34419800	-2.86136900
C	5.01111500	1.09479300	-2.05914100
H	5.87190200	1.66332500	-0.16850100
H	3.85691400	0.59110200	-3.80515900
H	5.95423500	0.76124700	-2.48122600
C	-4.02508100	-2.14387500	-1.68653100
C	-4.85658200	-1.32999400	-0.66815600
C	-3.12853300	0.04518700	-1.21154400
C	-2.86757300	-1.18795900	-2.09191600
H	-3.67982300	-3.08864100	-1.26450900
H	-4.64559100	-2.41023000	-2.54693100
H	-1.87591600	-1.61692500	-1.92946500
H	-2.92466900	-0.91757300	-3.14854000
C	-4.68121600	0.12775300	-1.21127800
C	-4.06295400	-1.21769700	0.65095300
H	-4.67162400	-0.64942200	1.35880500
C	-2.82824500	-0.33912400	0.25782200
H	-2.76683600	0.54910000	0.89175100
H	-2.60704700	0.95628600	-1.52323700

C	-1.46830100	-2.35533000	0.84579600
C	-2.66689600	-3.19927900	1.12482000
C	-0.33600600	-0.53290000	0.16176200
H	-2.48973700	-3.78587000	2.02957300
N	-1.57174400	-1.05620600	0.42662600
O	-3.81944500	-2.42146200	1.36605000
H	-2.81121200	-3.90604600	0.29932300
N	-0.22593100	-2.72816300	0.90258300
N	0.43395600	-1.59181800	0.48152900
C	1.84584700	-1.60422100	0.41088100
C	2.62109200	-1.52344800	1.56965100
C	2.49418500	-1.71478400	-0.82070800
C	4.00882800	-1.52245000	1.50895200
C	3.87905300	-1.72425500	-0.90977500
C	4.61458200	-1.61758500	0.26295000
H	4.59912300	-1.44928800	2.41394000
H	4.36867800	-1.80728800	-1.87151000
Cl	1.56094800	-1.87172700	-2.27474600
Cl	6.35116200	-1.60253900	0.16370800
Cl	1.84708800	-1.42438300	3.11537600
C	-6.26885900	-1.84280800	-0.47060700
H	-6.82754600	-1.21523800	0.23178600
H	-6.81256400	-1.86606900	-1.42028600
H	-6.24854100	-2.85956900	-0.06584200
C	-5.28764600	0.33568800	-2.60308000
H	-5.05884500	-0.46326100	-3.30954500
H	-6.37741400	0.40941300	-2.52673900
H	-4.92284900	1.27602500	-3.02931700
C	-5.25519800	1.23497400	-0.31695600
H	-6.33361500	1.09479400	-0.18662900
H	-4.80168500	1.30427200	0.67334700
H	-5.10804000	2.20551800	-0.80166300
O	1.66086100	1.50907700	1.74135800
O	1.50258700	3.99245500	-0.16263200
H	2.30709400	4.10038400	0.36126700

M4*RS*

Total Energy= -3159.82926356

Sum of electronic and zero-point Energies= -3159.220563

Sum of electronic and thermal Energies= -3159.182917

Sum of electronic and thermal Enthalpies= -3159.181973

Sum of electronic and thermal Free Energies= -3159.289994

C	4.75231300	1.96507400	-0.86997500
C	3.40712400	2.14343900	-0.53051100

C	2.40028500	1.57638900	-1.32761300
C	2.75379200	0.90679300	-2.50691300
C	4.08188600	0.76007200	-2.86666500
C	5.07936300	1.27559600	-2.02744600
H	5.51341200	2.39080600	-0.22534500
H	1.95290600	0.49795600	-3.11426400
H	4.35064500	0.23957100	-3.77946300
H	6.12530600	1.14838100	-2.28926000
C	0.98512500	1.63338200	-0.89801000
O	0.08388800	1.12425800	-1.53769400
O	3.13575500	2.88367400	0.56769000
C	1.80856900	3.39217500	0.65267200
H	1.66615500	4.17056800	-0.10956200
H	1.71414900	3.83109300	1.64717800
C	0.76425800	2.29125500	0.48261000
O	1.05720700	1.32445100	1.45621600
C	-0.63042400	2.87565500	0.62090700
C	-1.33613000	2.69491400	1.81050700
C	-1.21161600	3.61439100	-0.41338100
C	-2.61226500	3.23314700	1.96162200
H	-0.87768400	2.12151600	2.60919500
C	-2.48656500	4.15296200	-0.26320300
H	-0.67852000	3.75160100	-1.35018300
C	-3.19092600	3.96182600	0.92459800
H	-3.15597800	3.08015100	2.88906500
H	-2.93350100	4.71703700	-1.07591200
H	-4.18672500	4.37964100	1.03948300
C	-4.11536500	-1.29989500	-1.93178100
C	-4.94421700	-1.11688700	-0.64666800
C	-3.16907500	0.27544100	-0.34714300
C	-2.88312500	-0.37835400	-1.71333700
H	-3.86789800	-2.34712600	-2.11072000
H	-4.70525400	-0.98109000	-2.79612800
H	-1.92837300	-0.91208300	-1.72166500
H	-2.80561100	0.38683800	-2.48845500
C	-4.71790000	0.40232400	-0.34307700
C	-4.17326900	-1.75615300	0.53481100
H	-4.81174200	-1.71410500	1.42097700
C	-2.96167700	-0.78743300	0.75000500
H	-3.00206800	-0.32842100	1.73968500
H	-2.60452300	1.19249300	-0.16136200
C	-1.51934400	-2.77121700	0.25815000
C	-2.68594300	-3.60928600	-0.14524900
C	-0.47515500	-0.90485200	0.90723700

H	-2.53963200	-4.63104400	0.21198500
N	-1.68228500	-1.47610000	0.67249200
O	-3.89103500	-3.14763300	0.42832500
H	-2.73203300	-3.64454500	-1.23982600
N	-0.26215900	-3.09460600	0.21815000
N	0.35145600	-1.92676700	0.61171900
C	1.76267000	-1.81047800	0.59744900
C	2.47206800	-1.92679500	-0.60181500
C	2.47324100	-1.50664900	1.76331400
C	3.84924000	-1.75134700	-0.64785900
C	3.84652100	-1.30271200	1.73734700
C	4.51494200	-1.42916900	0.52671700
H	4.38137800	-1.83933200	-1.58651000
H	4.38007100	-1.05737900	2.64698500
Cl	1.65306100	-1.38872400	3.28524200
Cl	6.23622500	-1.18771800	0.48198200
Cl	1.63315300	-2.26197700	-2.08000200
C	-6.37261600	-1.61264900	-0.75190300
H	-6.93046600	-1.42724800	0.17236700
H	-6.89818000	-1.12012700	-1.57607300
H	-6.38498300	-2.69116900	-0.93884600
C	-5.23976400	1.34833000	-1.42891300
H	-6.33480200	1.34615400	-1.44123800
H	-4.91036200	2.36852100	-1.20258600
H	-4.89207500	1.10371800	-2.43335300
C	-5.32914200	0.88695900	0.97946300
H	-5.04427400	1.92863400	1.15249400
H	-6.42174000	0.84683500	0.91807500
H	-5.03087000	0.31806600	1.86233500
H	0.39494200	0.57404000	1.33966100

M4*SR*

Total Energy= -3159.81702519

Sum of electronic and zero-point Energies= -3159.208013

Sum of electronic and thermal Energies= -3159.169973

Sum of electronic and thermal Enthalpies= -3159.169029

Sum of electronic and thermal Free Energies= -3159.279513

C	1.44151100	3.82493700	-0.11970000
C	0.36819800	2.94764500	-0.30636700
C	-0.11698800	2.19880300	0.77803300
C	0.50106300	2.30817600	2.03037600
C	1.56749800	3.17191700	2.21643900
C	2.02440300	3.93654700	1.13464400
H	1.79465500	4.40324300	-0.96659900

H	0.10762700	1.70668400	2.84418400
H	2.03953900	3.26365800	3.18810600
H	2.85022300	4.62751800	1.27343400
C	-1.29413200	1.33730900	0.58852500
O	-1.70346400	0.52982900	1.40417600
O	-0.16488300	2.88289100	-1.54827200
C	-1.04626500	1.78787800	-1.82279600
H	-1.54256700	2.02575600	-2.76556400
H	-0.46363700	0.86647300	-1.91330300
C	-2.06874800	1.56759400	-0.71202400
O	-2.79833700	0.40533800	-1.02456600
C	-3.01564200	2.74712500	-0.47389100
C	-4.02289500	2.58482000	0.48374500
C	-2.93819900	3.94791200	-1.18000700
C	-4.94029000	3.59946100	0.72631600
H	-4.08371400	1.65243400	1.03859000
C	-3.86064700	4.96583600	-0.93699300
H	-2.15902300	4.10210100	-1.91811300
C	-4.86191300	4.79555400	0.01318000
H	-5.71725200	3.45819000	1.47069600
H	-3.79377900	5.89336600	-1.49665400
H	-5.57882200	5.58891000	0.19855400
C	4.93875600	-0.90026300	1.30712100
C	5.23372000	-0.43481700	-0.12924800
C	3.22075000	0.51247900	0.32643200
C	3.52300200	-0.32016100	1.59005600
H	5.01372000	-1.98422600	1.40483500
H	5.68395500	-0.48045200	1.98852500
H	2.76554300	-1.09268600	1.75794700
H	3.51576600	0.31405300	2.47966300
C	4.62524700	1.00551700	-0.11369300
C	4.24954400	-1.17156000	-1.07877700
H	4.55718800	-0.99693000	-2.11381500
C	2.88435700	-0.44683300	-0.82591500
H	2.58586500	0.12199800	-1.70812400
H	2.46451200	1.28696700	0.46323100
C	1.97139000	-2.68864500	-0.25093700
C	3.34128500	-3.26744100	-0.14065800
C	0.46934100	-1.03825100	-0.56335600
H	3.32683000	-4.30999600	-0.46388200
N	1.79542100	-1.36846900	-0.56107200
O	4.25973700	-2.59356000	-0.98027000
H	3.65028500	-3.24727400	0.91108700
N	0.83149900	-3.27420200	-0.04473900

N	-0.05997300	-2.23647800	-0.23754700
C	-1.44051000	-2.47602500	-0.05159100
C	-1.97123200	-2.58343400	1.23706800
C	-2.30478400	-2.59816000	-1.14191800
C	-3.32950300	-2.78768800	1.44437000
C	-3.66876400	-2.79687800	-0.96338000
C	-4.15893100	-2.88914400	0.33350200
H	-3.72856900	-2.86054300	2.44829700
H	-4.32933600	-2.87554200	-1.81772100
Cl	-1.68143800	-2.48610000	-2.75193200
Cl	-5.86225200	-3.13874500	0.57567300
Cl	-0.92170800	-2.44316100	2.60583500
C	6.68093800	-0.58568900	-0.55348200
H	6.84468500	-0.18389700	-1.55932000
H	7.35080900	-0.06542500	0.13820300
H	6.96301400	-1.64335000	-0.56420000
C	5.27140800	1.95406400	0.90085400
H	6.33218400	2.09665100	0.66854500
H	4.78587100	2.93329900	0.83826000
H	5.19368600	1.61525200	1.93483300
C	4.65570200	1.72751000	-1.46802000
H	3.97499200	2.58578400	-1.44272600
H	5.66287400	2.10962800	-1.66248400
H	4.37700900	1.10736100	-2.32209500
H	-2.81741600	-0.12142400	-0.20766300

M4*SS*

Total Energy= -3159.81841095

Sum of electronic and zero-point Energies= -3159.209892

Sum of electronic and thermal Energies= -3159.171935

Sum of electronic and thermal Enthalpies= -3159.170990

Sum of electronic and thermal Free Energies= -3159.280821

C	2.78327700	2.63400400	2.41730500
C	1.93853800	2.91775500	1.33926300
C	0.59842000	2.50584200	1.37129200
C	0.10881000	1.81977500	2.49082400
C	0.93914300	1.54643700	3.56347500
C	2.27937400	1.95534400	3.51709500
H	3.81155400	2.97708900	2.38033900
H	-0.92706400	1.49982500	2.47106400
H	0.56129300	1.01453900	4.42942400
H	2.93653100	1.74537800	4.35542000
C	-0.28794400	2.83629700	0.24464300
O	-1.50119200	2.73717100	0.26642300

O	2.46486300	3.61188800	0.29654200
C	1.52384000	4.30258000	-0.52270400
H	1.07203300	5.12434100	0.04698600
H	2.08389200	4.71977800	-1.36122100
C	0.40136600	3.39011900	-1.01046300
C	0.87379000	2.22213700	-1.87456000
C	2.19407400	2.07828600	-2.30704000
C	-0.08276900	1.28853000	-2.28599400
C	2.54862900	1.01368600	-3.13651000
H	2.95907800	2.77940700	-1.99019600
C	0.27467000	0.21784900	-3.09857100
H	-1.10905700	1.38959300	-1.94315400
C	1.59366800	0.07812400	-3.52717900
H	3.57767600	0.91292900	-3.46891500
H	-0.47448500	-0.51483900	-3.38501200
H	1.87805800	-0.76383200	-4.15039700
C	3.13626900	-3.33863800	0.96702500
C	3.80130100	-2.33747300	0.00597800
C	2.40460900	-1.03875800	1.24179300
C	2.13974000	-2.46165100	1.77653100
H	2.67174400	-4.16694300	0.42969400
H	3.89366300	-3.78640600	1.61713700
H	1.09603200	-2.75888200	1.63549400
H	2.33628200	-2.51707300	2.84955300
C	3.92140700	-1.06668000	0.91157600
C	2.73536400	-1.86180700	-1.01345700
H	3.23108800	-1.24996400	-1.77157100
C	1.80167500	-0.93138200	-0.16803500
H	1.86456400	0.09732600	-0.53036700
H	2.07212400	-0.23390600	1.90159700
C	-0.05891200	-2.42446900	-0.87455900
C	0.89024700	-3.45610600	-1.38257200
C	-0.63526900	-0.51793000	0.18332300
H	0.46326700	-3.94736600	-2.25923600
N	0.39940200	-1.29378600	-0.25964100
O	2.11693100	-2.88303800	-1.79115200
H	1.02994300	-4.21873900	-0.60675200
N	-1.35681500	-2.46429200	-0.87361800
N	-1.67378000	-1.28720100	-0.21784600
C	-3.03215300	-0.98768500	0.03102700
C	-3.55511000	-1.05802500	1.32640400
C	-3.89461800	-0.62345800	-1.00630100
C	-4.88618500	-0.75880700	1.58957400
C	-5.23225700	-0.32975800	-0.77457800

C	-5.70707900	-0.39932800	0.52852300
H	-5.27254100	-0.81649700	2.59961900
H	-5.88213900	-0.04647000	-1.59305500
Cl	-3.29274400	-0.51298000	-2.62875900
Cl	-7.37689900	-0.02988900	0.84007800
Cl	-2.54192700	-1.54806500	2.64533900
C	5.06306900	-2.85044400	-0.65844700
H	5.52088700	-2.08070600	-1.28905000
H	5.79925600	-3.16851200	0.08665800
H	4.83216100	-3.71113700	-1.29429700
C	4.79905200	-1.25519400	2.15207400
H	5.84452100	-1.40068700	1.86020200
H	4.75158800	-0.35143000	2.76962400
H	4.50584100	-2.09863400	2.77903500
C	4.44911700	0.18137700	0.18966100
H	4.36001500	1.05216800	0.84699500
H	5.51112800	0.05248600	-0.04517400
H	3.93390600	0.42754900	-0.74156700
O	-0.51628300	4.18794300	-1.71882300
H	-1.39524900	3.92743200	-1.39675300

P1*R*

Total Energy= -804.18148197

Sum of electronic and zero-point Energies= -803.942923

Sum of electronic and thermal Energies= -803.928949

Sum of electronic and thermal Enthalpies= -803.928005

Sum of electronic and thermal Free Energies= -803.984634

C	3.64737400	-1.04880800	0.03999500
C	2.27484400	-0.78555000	0.02408200
C	1.81073000	0.51929200	-0.19545200
C	2.73399400	1.54967600	-0.42133300
C	4.09299000	1.29222700	-0.41685500
C	4.54252400	-0.01306500	-0.17654600
H	3.98159500	-2.06563200	0.21315700
H	2.34496600	2.54999400	-0.58305200
H	4.80538500	2.09106700	-0.58839100
H	5.60732500	-0.22312400	-0.16649500
C	0.36625900	0.82339500	-0.10802200
O	-0.10106600	1.91523100	-0.35025300
H	-0.76507100	-1.01788200	2.21935700
O	1.44020500	-1.83359300	0.22471100
C	0.09531800	-1.63707200	-0.18753700
H	0.06424000	-1.59620100	-1.28430000
H	-0.46023600	-2.51414800	0.15364100

C	-0.49304600	-0.35540900	0.40645400
O	-0.24653100	-0.31471600	1.80446800
C	-1.96277900	-0.16784600	0.08808000
C	-2.60937900	-0.84816200	-0.94567900
C	-2.69086400	0.73869000	0.86470600
C	-3.96410000	-0.63043300	-1.19271300
H	-2.07373300	-1.55590600	-1.57027900
C	-4.04072300	0.95768100	0.61606200
H	-2.18530200	1.26315300	1.66843200
C	-4.68207700	0.27174600	-0.41445700
H	-4.45593600	-1.16968900	-1.99574500
H	-4.59414700	1.66423900	1.22627700
H	-5.73633200	0.44056200	-0.60872000

P1S

Total Energy= -804.18910320

Sum of electronic and zero-point Energies= -803.949840

Sum of electronic and thermal Energies= -803.936187

Sum of electronic and thermal Enthalpies= -803.935242

Sum of electronic and thermal Free Energies= -803.990663

C	-2.74861500	-1.41604200	0.69191800
C	-1.72404200	-0.46650100	0.71418600
C	-1.55980700	0.41143400	-0.36861600
C	-2.44325100	0.34862200	-1.45501800
C	-3.46025500	-0.58761300	-1.47785900
C	-3.60170900	-1.47171800	-0.39957600
H	-2.85917100	-2.08526400	1.53768400
H	-2.29247900	1.04550700	-2.27334800
H	-4.13983100	-0.64177500	-2.32046000
H	-4.39720900	-2.21014800	-0.41055300
C	-0.44769100	1.37066900	-0.36013200
O	-0.32553500	2.29840400	-1.14128800
H	1.08520600	2.92813300	0.22947400
O	-0.92238100	-0.44145700	1.80744200
C	-0.11957200	0.72280800	1.98592200
H	-0.75350700	1.56217500	2.29753400
H	0.58606400	0.49333900	2.78634800
C	0.61756100	1.13392600	0.71316300
O	1.28102000	2.34431500	0.98065400
C	1.59195000	0.08430800	0.17639000
C	2.32556300	0.41144700	-0.96928300
C	1.80219100	-1.15139800	0.78858800
C	3.25784600	-0.47706600	-1.49055900
H	2.16216500	1.37217100	-1.45032000

C	2.73993800	-2.04196200	0.26566500
H	1.23500300	-1.43395200	1.66841400
C	3.46863500	-1.70881600	-0.87111900
H	3.82126700	-0.20943800	-2.37854300
H	2.89838500	-2.99884500	0.75246800
H	4.19682000	-2.40458300	-1.27518100

***Re*-TS5^{D}**

Total Energy= -3159.76362710

Sum of electronic and zero-point Energies= -3159.160595

Sum of electronic and thermal Energies= -3159.122746

Sum of electronic and thermal Enthalpies= -3159.121802

Sum of electronic and thermal Free Energies= -3159.235213

C	-0.07849000	3.67054800	2.12154200
C	0.11392500	2.78563500	1.06123200
C	-0.25652000	1.43564200	1.20076400
C	-0.76697000	0.99849200	2.42447300
C	-0.96031100	1.88329200	3.48178000
C	-0.62228000	3.22527600	3.32096400
H	0.23007500	4.69996100	1.98020600
H	-1.03193100	-0.04921100	2.55554800
H	-1.36573700	1.52511100	4.42183000
H	-0.76551800	3.92548700	4.13775300
C	-0.01887300	0.51483800	0.00433800
O	1.30515400	0.18555200	-0.17532300
H	-0.44236300	1.03799300	-0.87888800
O	0.59210000	3.28470900	-0.11190200
C	1.80434100	2.68777800	-0.61807200
H	1.79160800	2.76983000	-1.70682100
C	2.99294000	3.22690200	0.00868900
O	2.98731800	3.90308900	1.04044700
C	4.31171000	2.84205700	-0.61874000
C	4.44051500	1.79081100	-1.53293800
C	5.44365900	3.58069400	-0.26554500
C	5.68105900	1.49719700	-2.09316300
H	3.57569900	1.18592100	-1.79022700
C	6.68199900	3.29086200	-0.82773800
H	5.32555400	4.38100200	0.45784400
C	6.80248200	2.24865700	-1.74596400
H	5.77470300	0.67627400	-2.79724800
H	7.55448400	3.87468000	-0.55105000
H	7.76835500	2.01891000	-2.18520300
C	-5.27267000	-0.62434600	-1.89111600
C	-5.50159200	0.27418400	-0.66516400

C	-3.40465500	0.83453100	-1.34781900
C	-3.80760500	-0.30769700	-2.30520500
H	-5.46745000	-1.67398400	-1.66830800
H	-5.97515400	-0.34899200	-2.68172300
H	-3.13793500	-1.17047100	-2.22090100
H	-3.74485900	0.02197900	-3.34370200
C	-4.74809100	1.57609600	-1.09199800
C	-4.59124200	-0.23700100	0.48208100
H	-4.86226900	0.27236300	1.41007800
C	-3.16137200	0.24574800	0.05189400
H	-2.79794300	1.01334200	0.73584400
H	-2.58660800	1.46583200	-1.70420300
C	-2.49046900	-2.16449400	0.22685100
C	-3.91723500	-2.59613000	0.22934700
C	-0.83920400	-0.73870300	0.11741900
H	-4.01747500	-3.50101700	0.83072500
N	-2.17907800	-0.83727800	0.12208700
O	-4.73748500	-1.61188500	0.82149100
H	-4.21254300	-2.83706000	-0.79780700
N	-1.41777900	-2.89714700	0.28366000
N	-0.39689700	-1.99049200	0.21145600
C	0.94399400	-2.47479300	0.18875100
C	1.59242700	-2.67082200	-1.02986800
C	1.58430500	-2.81658700	1.37529500
C	2.87613000	-3.19099700	-1.07047400
C	2.87050900	-3.34151400	1.35922700
C	3.49567800	-3.51922900	0.13171000
H	3.38199900	-3.33299300	-2.01718900
H	3.37039100	-3.59966900	2.28442500
Cl	0.78063500	-2.56909600	2.88723600
Cl	5.10473600	-4.17075200	0.09306400
Cl	0.79103900	-2.23654700	-2.49977000
C	-6.95059200	0.40687500	-0.24111600
H	-7.05807900	1.11685100	0.58561700
H	-7.57272900	0.74881100	-1.07337300
H	-7.33654700	-0.56110700	0.09329600
C	-5.30383200	2.24136000	-2.35494700
H	-6.33646000	2.56344400	-2.18692600
H	-4.71469400	3.13438300	-2.58509900
H	-5.28926500	1.60131800	-3.23777800
C	-4.68780000	2.66595500	-0.01100800
H	-3.93745700	3.41653100	-0.27972300
H	-5.65485500	3.17422500	0.05065700
H	-4.45141800	2.30819800	0.99347000

H	1.73179100	1.27676900	-0.37114900

***Re*-TS5^{B}**

Total Energy= -3452.04392507

Sum of electronic and zero-point Energies= -3451.228947

Sum of electronic and thermal Energies= -3451.181259

Sum of electronic and thermal Enthalpies= -3451.180315

Sum of electronic and thermal Free Energies= -3451.309633

C	-1.43739600	0.48809500	2.84217300
C	-0.96884200	0.34491400	1.53048000
C	0.39104600	0.55110400	1.24032900
C	1.25298000	0.88643100	2.27959800
C	0.80366400	1.00608900	3.59218700
C	-0.54785100	0.81319500	3.86448600
H	-2.48792600	0.34194100	3.06431600
H	2.29794700	1.06604800	2.03970800
H	1.49411100	1.26018200	4.38969200
H	-0.92129300	0.91351300	4.87916500
C	0.93531300	0.55218500	-0.21203500
O	1.61398400	1.64330000	-0.54724000
O	-1.76005100	-0.02458000	0.49455000
C	-3.14420300	0.28394200	0.52633200
H	-3.66073300	-0.10798200	1.40209200
C	-3.76421300	0.01034000	-0.73818800
O	-3.14077200	-0.09025800	-1.80779700
C	-5.27508500	-0.05407700	-0.76937000
C	-6.08990100	0.33462000	0.30096700
C	-5.87469700	-0.54148500	-1.93259200
C	-7.47413100	0.22888300	0.20746700
H	-5.64654300	0.74209700	1.20491800
C	-7.25865500	-0.65592700	-2.02440700
H	-5.23029900	-0.82644500	-2.75766200
C	-8.06253800	-0.27154900	-0.95350400
H	-8.09556200	0.53933300	1.04152500
H	-7.71058900	-1.04340400	-2.93225100
H	-9.14243200	-0.35666900	-1.02320500
C	6.56529800	-0.25018800	0.69498400
C	6.49820100	0.43297000	-0.68195300
C	4.57109300	1.09012000	0.33071100
C	5.21089000	0.13374500	1.35842900
H	6.74120400	-1.32312000	0.60602900
H	7.41143500	0.14924600	1.26062300
H	4.57202100	-0.73311100	1.56141500
H	5.36010700	0.63198400	2.31885900

C	5.80050200	1.78356400	-0.31920600
C	5.38698400	-0.26922900	-1.50700100
H	5.43480100	0.07856800	-2.54251000
C	4.06377800	0.27092300	-0.86191500
H	3.50417500	0.92386800	-1.52708800
H	3.78844700	1.75450000	0.69951800
C	3.45674200	-2.14131200	-0.55815200
C	4.87452700	-2.55373300	-0.75209500
C	1.80225400	-0.73038300	-0.31051900
H	4.90155600	-3.54928800	-1.19820700
N	3.12315300	-0.81092200	-0.54156600
O	5.53964600	-1.68102100	-1.63911000
H	5.36056900	-2.60855500	0.22923600
N	2.41979500	-2.90031900	-0.36209500
N	1.40189800	-2.00166900	-0.20429300
C	0.05895000	-2.42306200	-0.01426200
C	-0.41298300	-2.72893400	1.26266000
C	-0.81939200	-2.46683200	-1.09779200
C	-1.74700800	-3.05039200	1.46626700
C	-2.15650100	-2.79017200	-0.92017700
C	-2.59852400	-3.06514400	0.36668600
H	-2.11341600	-3.27184900	2.46103000
H	-2.83903400	-2.78242400	-1.76005000
Cl	-0.24052100	-2.08912600	-2.68434200
Cl	-4.28041700	-3.42804000	0.61438800
Cl	0.66789900	-2.67039300	2.61192200
C	7.82143700	0.49793000	-1.41801200
H	7.72324600	1.04599200	-2.36116800
H	8.58609800	0.99245900	-0.81105500
H	8.17591600	-0.51129500	-1.65096000
C	6.58491800	2.65275600	0.66836900
H	7.53711500	2.96389900	0.22616900
H	6.01270000	3.55958700	0.88851500
H	6.79929600	2.16053800	1.61785500
C	5.46809800	2.67617300	-1.52363800
H	4.75032500	3.44688600	-1.22585600
H	6.37468300	3.18144600	-1.87195100
H	5.04498600	2.14656100	-2.37910800
N	-2.73998800	2.94337600	0.03110000
C	-2.67141900	3.68348600	1.31837800
H	-3.70522500	3.86827100	1.62775700
H	-2.23720100	2.98252500	2.04076200
C	-1.86155600	4.97290000	1.32273400
H	-1.91663900	5.41007000	2.32289600

H	-0.80881100	4.77886900	1.10537100
H	-2.23687000	5.70979700	0.61050300
C	-1.43388700	2.75735600	-0.67287100
H	-1.52931200	1.80469300	-1.20282300
H	-0.66674200	2.62132000	0.09324700
C	-0.99775300	3.83979500	-1.64856300
H	-0.93169200	4.82950900	-1.19191200
H	0.00135600	3.55270100	-1.98627500
H	-1.65284700	3.89675500	-2.52208700
C	-3.87889900	3.30370500	-0.85516900
H	-4.77149400	2.86688300	-0.39167900
H	-3.71513400	2.76173200	-1.79189400
C	-4.11304200	4.78718900	-1.10340900
H	-3.24784100	5.27839300	-1.55112400
H	-4.95554500	4.89214700	-1.79139600
H	-4.37577400	5.31115500	-0.18093800
H	0.06682300	0.28731400	-0.86064300
H	-3.04393700	1.81913600	0.35148500

***Re*-M03^{B}**

Total Energy= -3452.04545589

Sum of electronic and zero-point Energies= -3451.225632

Sum of electronic and thermal Energies= -3451.177628

Sum of electronic and thermal Enthalpies= -3451.176684

Sum of electronic and thermal Free Energies= -3451.307406

C	-1.49085600	0.39195400	2.94596100
C	-0.99108600	0.27337900	1.64284300
C	0.37946800	0.46926000	1.39003500
C	1.22184900	0.74557000	2.46139000
C	0.74388200	0.82619800	3.76743200
C	-0.61883100	0.66282600	3.99912400
H	-2.55065600	0.27392200	3.13547200
H	2.27463400	0.91626800	2.25006600
H	1.42059500	1.03434000	4.58957600
H	-1.01571200	0.74416900	5.00659300
C	0.94862800	0.56490200	-0.04888800
O	1.63841800	1.67673900	-0.28764200
O	-1.75912700	-0.04635000	0.57465500
C	-3.15807000	0.08651700	0.62592900
H	-3.64937300	-0.34648900	1.49022800
C	-3.77856800	0.09869900	-0.62410500
O	-3.17912700	0.22830400	-1.73009200
C	-5.28791500	0.01896700	-0.63483700
C	-6.09061700	0.32019900	0.47276100

C	-5.90610500	-0.37043900	-1.82548600
C	-7.47566300	0.21077200	0.39427000
H	-5.62884800	0.66641100	1.39333500
C	-7.29119800	-0.48577300	-1.90462000
H	-5.27298200	-0.57596200	-2.68252400
C	-8.08131600	-0.19782000	-0.79364200
H	-8.08501400	0.45478100	1.25919900
H	-7.75618100	-0.79749100	-2.83523700
H	-9.16192400	-0.28165300	-0.85418500
C	6.61144800	-0.39207500	0.61112700
C	6.49687600	0.44478800	-0.67491900
C	4.61787700	0.99271200	0.48245100
C	5.28729500	-0.07764100	1.36890700
H	6.77201800	-1.44930000	0.39451000
H	7.48302700	-0.06584100	1.18518400
H	4.64689200	-0.95744000	1.49854500
H	5.48072200	0.30827800	2.37221000
C	5.82801200	1.74825800	-0.13205100
C	5.34774200	-0.15459600	-1.52801400
H	5.36004200	0.30231600	-2.52150100
C	4.05818400	0.32160900	-0.77626400
H	3.48659300	1.05417500	-1.34139900
H	3.85645300	1.61457700	0.95600100
C	3.42460700	-2.10060800	-0.72656500
C	4.82985700	-2.50450800	-1.01132100
C	1.79872500	-0.70747500	-0.27509300
H	4.82741900	-3.44388300	-1.56656700
N	3.11232400	-0.77743500	-0.54773900
O	5.47900900	-1.54513000	-1.81740200
H	5.34672000	-2.67394400	-0.05929800
N	2.38080100	-2.86379000	-0.59306100
N	1.38065600	-1.97684900	-0.30709400
C	0.03358000	-2.39855400	-0.15252200
C	-0.43092000	-2.84708400	1.08394300
C	-0.85657800	-2.30228200	-1.22407300
C	-1.76587000	-3.18103100	1.26051600
C	-2.19593100	-2.62662100	-1.07174900
C	-2.62728500	-3.05727200	0.17578000
H	-2.12497100	-3.52088900	2.22399000
H	-2.88824200	-2.50073000	-1.89422400
Cl	-0.28917000	-1.75016800	-2.76185200
Cl	-4.30666900	-3.44627300	0.39297800
Cl	0.66238700	-2.95923600	2.42105500
C	7.78969700	0.58944500	-1.45245600

H	7.65628800	1.24586800	-2.31912000
H	8.58276800	1.00620800	-0.82399200
H	8.12452800	-0.38672600	-1.81713600
C	6.65955800	2.49420500	0.91644200
H	7.60323800	2.83545700	0.47825700
H	6.11173800	3.38169000	1.24860900
H	6.89428600	1.90128100	1.80154300
C	5.46322000	2.77636300	-1.21322200
H	4.75951400	3.50841000	-0.80451000
H	6.36152900	3.31779900	-1.52636600
H	5.01217500	2.35441200	-2.11330200
N	-2.68109400	2.91401400	-0.01164400
C	-2.59327000	3.68197100	1.27462000
H	-3.62262800	3.89716200	1.57511700
H	-2.17665700	2.97648100	2.00095600
C	-1.74631000	4.94356700	1.24704800
H	-1.79190000	5.39737700	2.23980300
H	-0.69947100	4.71564000	1.03631000
H	-2.10243800	5.67878600	0.52420400
C	-1.36428200	2.68785600	-0.71098400
H	-1.50258600	1.73686400	-1.23038900
H	-0.60548900	2.54763100	0.06308300
C	-0.91496500	3.75639500	-1.69211400
H	-0.83178000	4.75063700	-1.24950700
H	0.08197800	3.45033800	-2.01967100
H	-1.56270000	3.80957500	-2.57077300
C	-3.81557700	3.30172200	-0.91681900
H	-4.71534400	2.89873600	-0.43997600
H	-3.66093600	2.72847800	-1.83423800
C	-3.98990900	4.78896900	-1.17184300
H	-3.10813400	5.24785000	-1.62039300
H	-4.82342600	4.91286700	-1.86706000
H	-4.24415200	5.33027400	-0.25735200
H	0.08320900	0.36837400	-0.72323900
H	-2.97461700	1.93940500	0.30874200

***Re*-M04^{B}**

Total Energy= -3452.08081311

Sum of electronic and zero-point Energies= -3451.261857

Sum of electronic and thermal Energies= -3451.213762

Sum of electronic and thermal Enthalpies= -3451.212818

Sum of electronic and thermal Free Energies= -3451.345242

C	0.45921700	-1.27627700	3.32645100
C	0.24948100	-0.40479500	2.25867400

C	1.28101100	-0.15442200	1.34443600
C	2.53240900	-0.73236000	1.53907500
C	2.75509500	-1.58639000	2.61634400
C	1.70945000	-1.86428300	3.49601700
H	-0.36233400	-1.48084700	4.00406100
H	3.32044500	-0.52133800	0.82039800
H	3.72981600	-2.04155000	2.75794900
H	1.86987800	-2.53986000	4.33075500
C	1.00578200	0.73597200	0.14070900
O	2.16619100	1.18250500	-0.49494400
O	-0.90210400	0.29428200	2.07562500
C	-2.12707300	-0.33824800	2.38448200
H	-2.61492400	0.01236100	3.28313300
C	-2.60619800	-1.25135600	1.47713500
O	-2.02110400	-1.57751100	0.38956200
C	-3.96167200	-1.84869100	1.76597000
C	-4.46038100	-2.04568700	3.05844000
C	-4.75339800	-2.22700400	0.67592800
C	-5.73092300	-2.58103000	3.25584900
H	-3.83879500	-1.79678600	3.91373900
C	-6.02536500	-2.75777700	0.87148700
H	-4.34343200	-2.08408900	-0.32056000
C	-6.52035900	-2.93577200	2.16281400
H	-6.10215300	-2.73308700	4.26521000
H	-6.63268400	-3.03761900	0.01533600
H	-7.50905700	-3.35720900	2.31694000
C	-3.63329500	2.27858700	-2.98162000
C	-4.15347800	1.96350500	-1.56796900
C	-1.98745000	2.55288800	-1.21523100
C	-2.13058500	2.60623400	-2.75052400
H	-3.81274100	1.45053000	-3.66925500
H	-4.16862200	3.13927300	-3.39168000
H	-1.45401600	1.89985500	-3.24329400
H	-1.87023700	3.59570800	-3.13213300
C	-3.38242600	3.01701000	-0.70899100
C	-3.48373700	0.64101900	-1.11301000
H	-3.94847500	0.26969500	-0.19519700
C	-2.02302500	1.08748700	-0.76102300
H	-1.87863800	0.99380900	0.31257400
H	-1.13441500	3.11267300	-0.81833900
C	-1.29776200	-0.74668900	-2.27922000
C	-2.63398800	-0.77977000	-2.93401600
C	0.22205000	-0.02864100	-0.90420100
H	-2.83276700	-1.79652600	-3.27633300

N	-1.01425700	0.20812000	-1.34778700
O	-3.65946200	-0.43154700	-2.03342000
H	-2.61301500	-0.12135700	-3.81246400
N	-0.28215400	-1.53370000	-2.48220300
N	0.66346800	-1.06256400	-1.62044200
C	1.92715900	-1.70741600	-1.53100100
C	3.01135700	-1.25331700	-2.28297800
C	2.07280800	-2.82286900	-0.70335800
C	4.25274800	-1.86467400	-2.16786600
C	3.30623500	-3.45072300	-0.57987900
C	4.37909400	-2.95028200	-1.30675600
H	5.09651200	-1.50962200	-2.74626900
H	3.42232100	-4.30432500	0.07638200
Cl	0.71697300	-3.39334000	0.18921600
Cl	5.93040500	-3.71409400	-1.14722600
Cl	2.80569000	0.04969500	-3.39910500
C	-5.66349700	1.92619300	-1.44386200
H	-5.96961300	1.74599000	-0.40801700
H	-6.11080800	2.86722300	-1.77889300
H	-6.07207300	1.11849500	-2.05949400
C	-3.69031200	4.47291600	-1.07019800
H	-4.74134300	4.69987200	-0.86432500
H	-3.08304900	5.13883300	-0.44872000
H	-3.49070900	4.72103300	-2.11372300
C	-3.59671300	2.87639800	0.80602400
H	-2.85687400	3.48065500	1.34255700
H	-4.58705800	3.25957500	1.07232800
H	-3.52557600	1.85463000	1.18886900
N	3.38365100	2.85317100	1.17746100
C	2.45215500	3.07928400	2.29226500
H	1.62966600	3.68896800	1.89927900
H	2.02250100	2.10503000	2.56096100
C	3.01466400	3.71299700	3.56561200
H	2.20461200	3.84599800	4.28794300
H	3.76183200	3.06214200	4.02821200
H	3.47267200	4.68736300	3.38325600
C	4.62516500	2.14549400	1.51904200
H	4.91487600	1.55533500	0.63853500
H	4.36973300	1.42363700	2.30345300
C	5.82608500	2.99079200	1.94578500
H	5.60658500	3.61541000	2.81424900
H	6.65855400	2.32981400	2.20246200
H	6.16088500	3.63909800	1.13115100
C	3.52028600	3.96361900	0.22396700

H	2.59025300	4.00261200	-0.35844500
H	4.31136400	3.67891100	-0.47909200
C	3.79481600	5.35801000	0.78762000
H	4.70719700	5.39394500	1.38682100
H	3.90266500	6.06427100	-0.04029600
H	2.96225300	5.70351400	1.40668000
H	0.35614200	1.56476700	0.45737000
H	2.64479000	1.78812800	0.16854100

***Re*-M5**

Total Energy= -3159.76642678

Sum of electronic and zero-point Energies= -3159.158406

Sum of electronic and thermal Energies= -3159.120220

Sum of electronic and thermal Enthalpies= -3159.119275

Sum of electronic and thermal Free Energies= -3159.231524

C	-1.29411500	3.38246100	2.04073500
C	-0.66218200	2.59126300	1.08053200
C	-0.42909000	1.23502800	1.34904200
C	-0.75683400	0.71028300	2.60098800
C	-1.37760800	1.50139000	3.56058200
C	-1.66038500	2.83687100	3.26446800
H	-1.46393200	4.42776200	1.80798000
H	-0.55108900	-0.33865600	2.80919100
H	-1.64083400	1.08397400	4.52612200
H	-2.14944700	3.46318900	4.00379700
C	0.14415400	0.36465100	0.25340500
O	1.52574400	0.15530800	0.35608200
H	-0.10507400	0.83415400	-0.71179400
O	-0.36139100	3.14530300	-0.12495000
C	0.99158800	2.98897600	-0.55337600
H	1.06279200	2.73409400	-1.60294000
C	1.97608400	3.64769100	0.17196800
O	1.79408700	4.25514000	1.26191200
C	3.38566700	3.57955800	-0.38830300
C	3.80643000	2.67556900	-1.37231900
C	4.31630800	4.49109500	0.11761600
C	5.11343800	2.70209300	-1.85137800
H	3.11521800	1.92914700	-1.75499900
C	5.62373900	4.52029800	-0.35818400
H	3.98047100	5.16873600	0.89551200
C	6.02737300	3.62767100	-1.34906600
H	5.42338400	1.99132700	-2.61186200
H	6.33132200	5.23897400	0.04501200
H	7.04719600	3.64526300	-1.72080900

C	-4.66496600	-0.68922200	-2.19118400
C	-5.15329900	-0.11372700	-0.84952200
C	-3.05534200	0.74483500	-1.07069300
C	-3.20749200	-0.15837500	-2.31254700
H	-4.75522300	-1.77571300	-2.22241500
H	-5.29165900	-0.31154100	-3.00295100
H	-2.45899400	-0.95841800	-2.34055400
H	-3.06471400	0.41975200	-3.22718700
C	-4.49087700	1.30377000	-0.86009600
C	-4.35813300	-0.80538500	0.28447900
H	-4.78740900	-0.51525500	1.24639400
C	-2.93824600	-0.15276200	0.17307400
H	-2.73535900	0.44302100	1.06111100
H	-2.27022000	1.50560400	-1.13474900
C	-2.07642900	-2.49509700	-0.06933100
C	-3.45220000	-3.02003900	-0.30790100
C	-0.54047100	-0.96853700	0.19461300
H	-3.53134700	-4.02409600	0.11199900
N	-1.86874500	-1.15598300	0.11165600
O	-4.42789500	-2.22601700	0.32589700
H	-3.60208900	-3.09336700	-1.39154200
N	-0.95349700	-3.15052700	-0.08558200
N	-0.00381600	-2.18182500	0.07907600
C	1.36877700	-2.56571600	0.04703400
C	2.12486300	-2.36408200	-1.10671500
C	1.94217700	-3.18721600	1.15286300
C	3.44522100	-2.78182000	-1.16601400
C	3.26225300	-3.61754900	1.11396200
C	3.99171800	-3.40872300	-0.05009200
H	4.03386900	-2.61872300	-2.06020300
H	3.70860100	-4.09833300	1.97537200
Cl	1.00915500	-3.40480200	2.59378600
Cl	5.64093400	-3.94205500	-0.11307500
Cl	1.41343500	-1.55983600	-2.46236900
C	-6.65285200	-0.18969500	-0.64139600
H	-6.94802800	0.27818900	0.30372400
H	-7.18599100	0.31054600	-1.45511100
H	-6.97792100	-1.23440900	-0.61580000
C	-4.95008900	2.20031100	-2.01392300
H	-6.01233000	2.43986700	-1.90316200
H	-4.39466000	3.14266600	-1.98565500
H	-4.80558700	1.76017700	-3.00120500
C	-4.67023600	2.12008800	0.42850600
H	-3.99744700	2.98387300	0.41364300

H	-5.69513200	2.49907000	0.48549100
H	-4.47609900	1.57604200	1.35563800
H	1.88222200	1.05158100	0.17158100

TS6*RR*

Total Energy= -3159.71537157

Sum of electronic and zero-point Energies= -3159.110078

Sum of electronic and thermal Energies= -3159.071902

Sum of electronic and thermal Enthalpies= -3159.070957

Sum of electronic and thermal Free Energies= -3159.181902

C	-1.95722600	3.84485300	1.43750700
C	-1.01992400	3.10812000	0.70951100
C	-0.62963900	1.83157200	1.14397000
C	-1.11526900	1.36663300	2.36911400
C	-2.02714500	2.10503800	3.11373200
C	-2.45826600	3.34169500	2.63071600
H	-2.24830700	4.82027300	1.06412800
H	-0.77778100	0.39325800	2.71574800
H	-2.39737000	1.72148500	4.05777100
H	-3.17685000	3.92666800	3.19623900
C	0.36059200	1.03720900	0.36642100
O	1.52226800	0.84421400	1.00556000
H	0.27624900	0.81490700	-0.68462300
O	-0.51703700	3.65552900	-0.41908800
C	0.66032900	3.04180900	-0.87613900
H	0.58213300	2.66237200	-1.88630500
C	1.86727600	3.35339000	-0.23703800
O	1.96444600	3.98639500	0.83546600
C	3.09224900	2.65281100	-0.79040200
C	3.23191800	2.23577700	-2.12017300
C	4.13239900	2.38668500	0.10886900
C	4.38569600	1.57558000	-2.53776000
H	2.45365300	2.44910400	-2.84621600
C	5.28148100	1.71817600	-0.30396700
H	4.01008700	2.72734900	1.13193400
C	5.41320900	1.31412800	-1.63190100
H	4.48503700	1.27061500	-3.57526200
H	6.07682500	1.51515600	0.40678300
H	6.31172500	0.79926900	-1.95920900
C	-4.56511700	-1.19573000	-2.12682200
C	-5.15210100	-0.84213300	-0.75056400
C	-3.22976400	0.36750700	-0.82788600
C	-3.20681100	-0.43847600	-2.14517100
H	-4.48668200	-2.27405000	-2.27111800

H	-5.23180900	-0.83268200	-2.91346700
H	-2.34208400	-1.10857400	-2.19861800
H	-3.12952400	0.22838900	-3.00616200
C	-4.74108800	0.66139000	-0.61877700
C	-4.25472300	-1.49896100	0.33291500
H	-4.75122100	-1.42012500	1.30383900
C	-2.97742700	-0.59212100	0.34672200
H	-2.91996400	-0.03255000	1.27986900
H	-2.57406600	1.24347000	-0.81374800
C	-1.68504600	-2.67218300	-0.13053900
C	-2.92960100	-3.40547900	-0.50325100
C	-0.49216800	-0.90905800	0.52236000
H	-2.82982000	-4.45611300	-0.22466900
N	-1.74354800	-1.36209700	0.26556100
O	-4.05177000	-2.90226000	0.19291100
H	-3.05400900	-3.35604000	-1.59100900
N	-0.45873400	-3.10078600	-0.15723100
N	0.25047300	-1.99062200	0.24145700
C	1.66755800	-2.01591500	0.23884200
C	2.36889600	-1.63147700	-0.90809400
C	2.38245100	-2.35458400	1.38762900
C	3.75602000	-1.56923100	-0.91526600
C	3.77108500	-2.30870300	1.40463300
C	4.43573200	-1.91073100	0.25031000
H	4.29048000	-1.25285100	-1.80243000
H	4.31868900	-2.56694800	2.30237800
Cl	1.52370300	-2.80758600	2.81778900
Cl	6.16886800	-1.84129800	0.25965600
Cl	1.49142300	-1.18963300	-2.33844300
C	-6.61839300	-1.18856900	-0.58524000
H	-6.99822300	-0.85474200	0.38623500
H	-7.22295500	-0.72358900	-1.36990400
H	-6.75974600	-2.27223100	-0.64795100
C	-5.32272600	1.57595800	-1.70113200
H	-6.41550700	1.59202600	-1.63660400
H	-4.96834500	2.59882000	-1.53847900
H	-5.04845700	1.29064100	-2.71740400
C	-5.08541600	1.30664800	0.73173600
H	-4.52488900	2.24040900	0.84957600
H	-6.15199900	1.55046500	0.76225400
H	-4.87200400	0.68650500	1.60522700
H	2.23400900	0.62785300	0.38167800

M6*RR*

Total Energy= -3159.79748026
Sum of electronic and zero-point Energies= -3159.189591
Sum of electronic and thermal Energies= -3159.150824
Sum of electronic and thermal Enthalpies= -3159.149880
Sum of electronic and thermal Free Energies= -3159.264644

C	-2.65815300	3.66516700	2.25377700
C	-1.55932000	3.26546600	1.50338700
C	-0.93986300	2.03601600	1.69475400
C	-1.40468200	1.15657500	2.66445500
C	-2.51277900	1.53187100	3.42743300
C	-3.12189200	2.77315100	3.22208200
H	-3.12191300	4.63170600	2.09400800
H	-0.91210300	0.19870100	2.80243400
H	-2.89981100	0.86150500	4.18723600
H	-3.97932000	3.05294200	3.82610200
C	0.27012800	1.95662400	0.80376200
O	1.48686100	1.86429400	1.51858400
H	0.24894400	1.07352300	0.16045600
O	-0.98072300	4.01804600	0.52748700
C	0.11812000	3.28194400	-0.02091800
H	-0.11503700	3.06925300	-1.06973300
C	1.38679000	4.13145100	0.07966200
O	1.42887700	5.07354600	0.84247700
C	2.54974100	3.76174100	-0.77785300
C	2.60555500	2.55206400	-1.47507800
C	3.61713000	4.66067800	-0.86019500
C	3.71978300	2.24717400	-2.25052500
H	1.79513900	1.83242900	-1.40508200
C	4.72486800	4.35933000	-1.64237800
H	3.55804400	5.59070100	-0.30440200
C	4.77625600	3.15148100	-2.33810500
H	3.76258300	1.30359300	-2.78475600
H	5.54896000	5.06174000	-1.70991200
H	5.64238900	2.91335100	-2.94721100
C	-4.02425000	-1.19324100	-2.53655600
C	-4.76633300	-1.02557400	-1.19964000
C	-2.83387900	0.12154300	-0.87541400
C	-2.66734500	-0.47320200	-2.28993100
H	-3.93426400	-2.24272600	-2.81915200
H	-4.59081200	-0.70991800	-3.33738400
H	-1.80618200	-1.14655800	-2.34946500
H	-2.49210100	0.31467600	-3.02556200
C	-4.35304500	0.42878300	-0.79809500
C	-4.00996900	-1.86137300	-0.13116100

H	-4.61551900	-1.90399300	0.77839700
C	-2.72435000	-1.01546100	0.15471000
H	-2.75427800	-0.60193600	1.16370500
H	-2.16996200	0.96189400	-0.64815900
C	-1.42681300	-3.03838300	-0.49349400
C	-2.63719600	-3.68694700	-1.07661600
C	-0.27505600	-1.36926000	0.49090600
H	-2.58759300	-4.76587800	-0.91715300
N	-1.50458900	-1.79701700	0.07493100
O	-3.82428400	-3.23804600	-0.45147000
H	-2.64612000	-3.50964300	-2.15863400
N	-0.20556900	-3.47986800	-0.48128900
N	0.46735700	-2.43540000	0.12484700
C	1.87694600	-2.49041000	0.22015300
C	2.67053700	-1.85675100	-0.73900400
C	2.50878100	-3.16896500	1.26301200
C	4.05653700	-1.87557500	-0.66223400
C	3.89385900	-3.21214200	1.36285200
C	4.64647100	-2.55872100	0.39485400
H	4.65802900	-1.37303600	-1.40963800
H	4.37146800	-3.73796400	2.18016600
Cl	1.54818700	-3.95978400	2.46827400
Cl	6.38051600	-2.59701500	0.50743700
Cl	1.90906900	-1.03450300	-2.06315400
C	-6.24705800	-1.34298700	-1.25504500
H	-6.72977200	-1.14451100	-0.29213300
H	-6.74941200	-0.74500200	-2.02164800
H	-6.39998300	-2.39964200	-1.49666100
C	-4.79528000	1.50920600	-1.78950400
H	-5.88821100	1.56091400	-1.83336000
H	-4.43312100	2.48413900	-1.44668600
H	-4.42396200	1.35780500	-2.80368600
C	-4.84269700	0.87891400	0.58542300
H	-4.29655300	1.77585300	0.89683400
H	-5.90620400	1.13491200	0.53683800
H	-4.72548700	0.13705200	1.37818900
H	1.43454900	2.45842300	2.27967500

P2*RR*

Total Energy= -804.17513686

Sum of electronic and zero-point Energies=	-803.936380
Sum of electronic and thermal Energies=	-803.922380
Sum of electronic and thermal Enthalpies=	-803.921436
Sum of electronic and thermal Free Energies=	-803.978155

C	2.48942800	-1.37812900	-1.20834900
C	1.76156100	-0.26421200	-0.81316400
C	2.14020000	0.52669100	0.26482000
C	3.27581500	0.21284700	0.99777400
C	4.03072300	-0.89712000	0.61731300
C	3.63592800	-1.67781200	-0.47235300
H	2.17301000	-1.98118900	-2.05133900
H	3.56527800	0.81939400	1.85025600
H	4.92574700	-1.15880900	1.17064400
H	4.23184400	-2.53963300	-0.75520100
C	1.11068600	1.60428300	0.46548300
O	0.42234000	1.37391800	1.68133800
O	0.61020400	0.15577700	-1.41468200
C	0.22200500	1.39244300	-0.80409200
H	-0.07587700	2.17087500	1.90513300
H	1.54063900	2.61085300	0.45671400
C	-1.26115600	1.43266600	-0.44847300
O	-1.79753200	2.52459100	-0.42296400
H	0.39421500	2.19758400	-1.52447100
C	-2.01150500	0.18723400	-0.12816300
C	-3.39361600	0.19345100	-0.34001600
C	-1.39314400	-0.94235500	0.41696300
C	-4.15202500	-0.92942400	-0.03195500
H	-3.85540400	1.08557100	-0.75074000
C	-2.15872000	-2.05737100	0.74156000
H	-0.32853800	-0.93623600	0.62427700
C	-3.53319400	-2.05562400	0.50917300
H	-5.22251600	-0.92699800	-0.20805600
H	-1.68261500	-2.92901400	1.17799800
H	-4.12381300	-2.93208200	0.75612300