Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Mechanistic Insights into Challenges of Organocatalytic Beckmann Rearrangement Reactions

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The XYZ Coordinates, Energies Of The Structures Along The Reaction Paths

Reactant

O	-3.29864500	-0.64310300	-0.22786100
N	-1.92624900	-0.85914500	-0.26908500
C	-1.26292000	0.18630200	0.06111000
C	-1.90928100	1.49205100	0.43247500
H	-1.23173800	2.10912100	1.02253900
H	-2.19261100	2.04661300	-0.46868300
H	-2.82022500	1.30572500	1.00313300
C	0.21832700	0.05397300	0.03725200
H	-3.67206900	-1.49675100	-0.48113300
C	0.83356500	-1.18763100	0.24939000
H	0.21627500	-2.05471200	0.46044900
C	2.21954000	-1.30439400	0.20383500
H	2.68390300	-2.27032700	0.37673400
C	3.01154300	-0.18359900	-0.05414100
H	4.09258700	-0.27575100	-0.08740600
C	2.40726300	1.05505500	-0.26289100
H	3.01475600	1.93118000	-0.46691900
C	1.01899000	1.17483400	-0.21204900
H	0.55986000	2.14419200	-0.38211800

Sum of electronic and zero-point Energies= -439.877621
Sum of electronic and thermal Energies= -439.865306
Sum of electronic and thermal Enthalpies= -439.864188
Sum of electronic and thermal Free Energies= -439.920736

Acetonitrile

C	0.00000000	0.00000000	-1.18175300
H	0.00000000	1.02792200	-1.54698600
H	-0.89020700	-0.51396100	-1.54698600
H	0.89020700	-0.51396100	-1.54698600
C	0.00000000	0.00000000	0.27966700
N	0.00000000	0.00000000	1.43621000

Sum of electronic and zero-point Energies= -132.663473
Sum of electronic and thermal Energies= -132.658935
Sum of electronic and thermal Enthalpies= -132.657817
Sum of electronic and thermal Free Energies= -132.691593

DCP

C	0.00000900	1.37638800	0.00024200
C	0.66261700	0.09197700	-0.00015700
C	-0.66263500	0.09200400	0.00045600
C	-1.96775900	-0.52766600	-0.00180800
C	-3.10556900	0.29110000	0.02977800
C	-2.10722400	-1.92235200	-0.03694800
C	-4.37289800	-0.28357600	0.02883000
H	-2.98619500	1.37074400	0.05546600
C	-3.37651200	-2.48994100	-0.03821300
H	-1.22449200	-2.55278300	-0.06536700
H	-5.25371400	0.34935800	0.05336700
H	-3.48547900	-3.56910400	-0.06580700
C	1.96775900	-0.52765200	0.00188400
C	2.10723300	-1.92232300	0.03774100
C	3.10555200	0.29108700	-0.03075800
H	1.22449500	-2.55270800	0.06704400
C	4.37287200	-0.28360900	-0.03011200
H	2.98618800	1.37072100	-0.05689900
H	5.25368400	0.34930800	-0.05533500
Cl	-0.00253200	2.43922700	-1.46391100
Cl	0.00255400	2.43927000	1.46431700
C	3.37651400	-2.48992800	0.03873100
H	3.48547300	-3.56907600	0.06698100
C	-4.50876800	-1.67218700	-0.00457100
H	-5.49803700	-2.11881000	-0.00531200
C	4.50875300	-1.67220200	0.00399900
H	5.49802500	-2.11881900	0.00440400

Sum of electronic and zero-point Energies= -1497.484254
Sum of electronic and thermal Energies= -1497.464575
Sum of electronic and thermal Enthalpies= -1497.463457
Sum of electronic and thermal Free Energies= -1497.540249

M_TS1

C	0.00027900	1.27908500	-0.43166000
C	-0.68546300	0.09304200	-0.26727300
C	0.68703500	0.09374400	-0.26504600
C	1.96962100	-0.54169300	-0.15585300
C	3.11780600	0.25720300	-0.27479500
C	2.07900800	-1.92071700	0.07634700
C	4.37308300	-0.32780400	-0.16466800
H	3.01396900	1.32458300	-0.44631400
C	3.33852500	-2.49680700	0.18237700
H	1.18562000	-2.52806600	0.17318600
H	5.26551300	0.28221600	-0.25191100
H	3.43291100	-3.56227600	0.36126800
C	-1.96830100	-0.54354400	-0.16460200
C	-2.07972100	-1.93417200	-0.01847500
C	-3.11466300	0.26609400	-0.20398600
H	-1.18870300	-2.55187300	0.00688100
C	-4.36994200	-0.31912900	-0.09347300
H	-3.00903800	1.34166400	-0.31180500

H	-5.26044000	0.29925400	-0.11711200
Cl	-0.00291200	2.30140700	1.87710500
Cl	-0.00053600	2.71973200	-1.31150500
C	-3.33941000	-2.51037300	0.08498500
H	-3.43543500	-3.58495400	0.19584000
C	4.48111900	-1.70173500	0.06164500
H	5.46274100	-2.15658900	0.14808700
C	-4.48011200	-1.70393400	0.04960000
H	-5.46169000	-2.15888000	0.13594500

Sum of electronic and zero-point Energies= -1497.463802
Sum of electronic and thermal Energies= -1497.444214
Sum of electronic and thermal Enthalpies= -1497.443097
Sum of electronic and thermal Free Energies= -1497.520086

DCP Ion

C	0.01388000	1.41941500	-0.67525000
C	-0.67789900	0.25812600	-0.50229600
C	0.71707700	0.26678800	-0.49308800
C	1.98665100	-0.37992200	-0.35044900
C	3.14879900	0.40283700	-0.45220300
C	2.06820000	-1.75853100	-0.10311500
C	4.39090200	-0.20004900	-0.30831000
H	3.06778500	1.46898800	-0.64039400
C	3.31561900	-2.35138700	0.03989800
H	1.16402900	-2.35143700	-0.02255600
H	5.29461800	0.39443500	-0.38326300
H	3.39037400	-3.41575200	0.23270400
C	-1.94330700	-0.40124800	-0.38349300
C	-2.01942100	-1.78925900	-0.19458100
C	-3.10825800	0.38140500	-0.44633000
H	-1.11412600	-2.38407400	-0.14858400
C	-4.34783900	-0.23004600	-0.31851500
H	-3.03049800	1.45507400	-0.58754200
H	-5.25326100	0.36493900	-0.36134100
Cl	-0.13410400	1.15699800	2.56492700
Cl	0.00452500	3.06724000	-0.88706500
C	-3.26456000	-2.39116900	-0.06974000
H	-3.33544100	-3.46316000	0.07692200
C	4.47151100	-1.57320800	-0.06350600
H	5.44414500	-2.04120000	0.04986500
C	-4.42319200	-1.61248400	-0.13072000
H	-5.39377200	-2.08746000	-0.02927600

Sum of electronic and zero-point Energies= -1497.469191
Sum of electronic and thermal Energies= -1497.448555
Sum of electronic and thermal Enthalpies= -1497.447437
Sum of electronic and thermal Free Energies= -1497.528520

M_TS2

O	0.85269200	-1.06575900	1.74063900
N	0.19955200	0.16866200	1.64022000
C	-1.08184300	0.04831800	1.66784700
C	-1.83663300	-1.21830500	1.94991200
H	-2.21613100	-1.17924900	2.97693100
H	-2.69382200	-1.30489100	1.27766100

H	-1.20110100	-2.09719400	1.85653800
C	-1.83760200	1.29935900	1.40171500
C	1.19444700	-1.63726200	-0.04462300
C	0.12666400	-1.28672600	-0.87307400
C	1.25251000	-0.53189000	-0.89736300
C	2.03450300	0.58178600	-1.36485400
C	-1.22465500	-1.56630700	-1.29740600
Cl	2.11807300	-3.02462300	0.33434400
H	1.79669900	-0.82550000	2.09956000
C	-1.27246800	2.30614200	0.60593900
H	-0.27927600	2.16049000	0.19084600
C	-1.98599000	3.46942900	0.33536600
H	-1.54381100	4.23928900	-0.28902600
C	-3.27043700	3.64002300	0.85538300
H	-3.82770400	4.54639100	0.64075900
C	-3.84001600	2.63973300	1.64234300
H	-4.83835400	2.76697100	2.04812700
C	-3.13124900	1.47006100	1.90891500
H	-3.58666400	0.69770900	2.52089200
C	1.55017000	1.42608800	-2.37572200
H	0.58271400	1.23299500	-2.82869800
C	2.32275600	2.50279600	-2.79293700
H	1.95750600	3.16045800	-3.57426600
C	4.04725800	1.89909700	-1.19526400
H	5.01234000	2.09058600	-0.73848400
C	3.28464800	0.81547800	-0.77353300
H	3.63249700	0.16397800	0.02409700
C	-1.76928700	-2.83880500	-1.07247600
H	-1.15990800	-3.61377600	-0.61635300
C	-3.08769600	-3.09269600	-1.43222400
H	-3.51417000	-4.07612900	-1.26653700
C	-3.32506300	-0.80691000	-2.20912600
H	-3.93579500	-0.02004400	-2.63862100
C	-2.00169100	-0.54894500	-1.86905900
H	-1.57688000	0.43971500	-2.01539600
Cl	3.45834800	-0.37171900	2.71714300
C	3.56741100	2.73884100	-2.20187300
H	4.16467900	3.58460900	-2.52749400
C	-3.86459100	-2.07715900	-1.99450900
H	-4.89725300	-2.27602500	-2.26273300

Sum of electronic and zero-point Energies= -1937.354091
Sum of electronic and thermal Energies= -1937.321035
Sum of electronic and thermal Enthalpies= -1937.319917
Sum of electronic and thermal Free Energies= -1937.428109

M1+HCl

O	-0.03585400	-1.32926400	0.11528500
N	-1.33840500	-0.82330500	0.18094500
C	-2.19856600	-1.64279700	-0.29975400
C	-1.85891400	-2.98787100	-0.87758000
H	-2.68091400	-3.68812300	-0.72352100
H	-1.68285000	-2.89843800	-1.95519100
H	-0.95230100	-3.38280300	-0.42107200
C	-3.60952100	-1.16973200	-0.29066700
C	-4.52708900	-1.68875100	-1.21153700
C	-4.03764900	-0.19739400	0.62443200
C	-5.84504600	-1.23361200	-1.22839600

H	-4.21334000	-2.44046600	-1.92944600
C	-5.35431000	0.25156900	0.60889800
H	-3.33328300	0.19346600	1.35171600
C	-6.26228200	-0.26361300	-0.31934400
H	-6.54424500	-1.63912900	-1.95270200
H	-5.67677800	0.99906700	1.32703700
H	-7.28985100	0.08594100	-0.32833000
C	0.84390700	-0.44055000	0.71870100
C	2.12905800	-0.13749600	0.12435800
C	1.23710300	0.84170000	0.16404900
C	0.80175200	2.20639800	-0.04145200
C	-0.51723200	2.55924900	0.27977100
C	1.68269200	3.17596900	-0.54234100
C	-0.94715800	3.87081500	0.09941400
H	-1.18916500	1.79338200	0.65721300
C	1.24630500	4.48416600	-0.72066300
H	2.70450500	2.90297600	-0.78567500
H	-1.96816700	4.14270300	0.34742200
H	1.92973600	5.23272800	-1.10799000
C	3.41886900	-0.71890700	-0.17794500
C	4.43460100	0.03088800	-0.78821000
C	3.64194400	-2.06517900	0.14375400
C	5.65893000	-0.56457600	-1.07305500
H	4.26028300	1.07207500	-1.03948200
C	4.86989600	-2.65474900	-0.14087100
H	2.84734100	-2.63748300	0.61460900
H	6.44383500	0.01530800	-1.54763000
H	5.04119500	-3.69665200	0.10912500
Cl	0.69575100	-0.62609500	2.54693700
C	5.87787200	-1.90569500	-0.74988000
H	6.83497800	-2.36649700	-0.97288200
C	-0.06800800	4.83311600	-0.40007000
H	-0.40598400	5.85512900	-0.53967900

Sum of electronic and zero-point Energies= -1476.610692
Sum of electronic and thermal Energies= -1476.580807
Sum of electronic and thermal Enthalpies= -1476.579690
Sum of electronic and thermal Free Energies= -1476.681014

M_TS3

O	-0.15022600	-1.34259400	-0.23151000
N	-1.42962300	-0.72444300	-0.19770500
C	-2.35449900	-1.61052900	-0.25886200
C	-2.10933100	-3.08854700	-0.36044100
H	-2.99443700	-3.64602300	-0.05720900
H	-1.86023100	-3.35549800	-1.39277200
H	-1.26539200	-3.37206900	0.26950300
C	-3.73829500	-1.06891200	-0.24222400
C	-4.76059400	-1.74308400	-0.91964100
C	-4.02917800	0.12020200	0.43952400
C	-6.05335700	-1.22288000	-0.93218300
H	-4.54749500	-2.66514500	-1.45211300
C	-5.32300800	0.63183100	0.43214100
H	-3.24021500	0.62661100	0.98654800
C	-6.33687900	-0.03639700	-0.25702000
H	-6.83867800	-1.74630700	-1.46775100
H	-5.54306100	1.54761900	0.97130800
H	-7.34612300	0.36298500	-0.26082000

C	0.78515600	-0.49031100	0.12700600
C	2.13246900	-0.24905000	-0.12882000
C	1.26831800	0.80003200	-0.09226300
C	0.95317200	2.20560800	-0.14595000
C	-0.38945300	2.59358100	-0.02582100
C	1.96081900	3.16888700	-0.29942400
C	-0.71983800	3.94369400	-0.06332400
H	-1.14958400	1.82680700	0.09075100
C	1.62094500	4.51617700	-0.33694500
H	2.99802100	2.86200400	-0.38270300
H	-1.75643200	4.25026700	0.02881800
H	2.39561300	5.26610600	-0.45522000
C	3.44022900	-0.83935900	-0.26605300
C	4.56453400	-0.06149900	-0.57713500
C	3.56583700	-2.22301700	-0.07370200
C	5.80785900	-0.67155700	-0.69675300
H	4.46095600	1.00769100	-0.72884600
C	4.81414000	-2.82438400	-0.18869100
H	2.68531900	-2.81052300	0.16976500
H	6.68051800	-0.07564900	-0.94142900
H	4.91661200	-3.89355600	-0.03695100
Cl	0.51731300	-0.70768600	2.48598500
C	5.93251200	-2.04912600	-0.50116700
H	6.90619100	-2.51950300	-0.59421300
C	0.28344800	4.90216300	-0.21959500
H	0.02322200	5.95554400	-0.24833600

Sum of electronic and zero-point Energies= -1476.600724
Sum of electronic and thermal Energies= -1476.570054
Sum of electronic and thermal Enthalpies= -1476.568936
Sum of electronic and thermal Free Energies= -1476.672403

M2

O	-0.16520800	-1.42239600	-0.47695600
N	-1.44737300	-0.76893500	-0.45064000
C	-2.36660200	-1.64266800	-0.26599100
C	-2.11919100	-3.11670000	-0.12976000
H	-1.34891400	-3.28620900	0.62630200
H	-3.02981600	-3.63604700	0.16262300
H	-1.75265400	-3.52781500	-1.07480000
C	-3.73856900	-1.07965200	-0.19444300
C	-4.81362000	-1.79189900	-0.73721500
C	-3.96146900	0.16739000	0.40310200
C	-6.09596400	-1.24913700	-0.70435400
H	-4.64940700	-2.75959000	-1.20189500
C	-5.24654900	0.70027300	0.44386900
H	-3.12873800	0.69970400	0.85255200
C	-6.31431500	-0.00434100	-0.11390800
H	-6.92437400	-1.79963600	-1.13816900
H	-5.41545200	1.66180000	0.91776900
H	-7.31601900	0.41226100	-0.08071600
C	0.78667800	-0.55687300	-0.41639500
C	2.13680600	-0.32685400	-0.39364200
C	1.24972700	0.73341900	-0.38578900
C	0.94687600	2.13857600	-0.32847900
C	-0.40089300	2.52963600	-0.34481900
C	1.96940500	3.09424600	-0.24605300
C	-0.72031900	3.88014800	-0.27992200

H	-1.17109000	1.76681100	-0.40882900
C	1.63917200	4.44241300	-0.18080600
H	3.00767600	2.78165300	-0.23010900
H	-1.75908000	4.19223200	-0.29166300
H	2.42321700	5.18875400	-0.11403400
C	3.46249400	-0.88282600	-0.34072700
C	4.59638500	-0.05793000	-0.35330300
C	3.59370300	-2.27815700	-0.26825300
C	5.85921800	-0.63422900	-0.29371300
H	4.48696700	1.01940300	-0.41261200
C	4.86045400	-2.84493200	-0.20568800
H	2.70457700	-2.90121900	-0.25705800
H	6.74184100	-0.00436900	-0.30354200
H	4.97005300	-3.92221100	-0.14596600
Cl	0.40734700	-0.39535500	2.64171300
C	0.29789700	4.83270700	-0.19824900
H	0.04551100	5.88712000	-0.14729400
C	5.98959400	-2.02302500	-0.21909600
H	6.97856700	-2.46739300	-0.16975900

Sum of electronic and zero-point Energies= -1476.607552
Sum of electronic and thermal Energies= -1476.575889
Sum of electronic and thermal Enthalpies= -1476.574771
Sum of electronic and thermal Free Energies= -1476.681653

M_TS4

O	0.37548400	-1.99059000	-1.14379800
N	-1.58262500	-1.33668200	-0.97969600
C	-2.05313500	-2.04250800	-0.09737100
C	-1.79643000	-3.22795900	0.74431400
H	-1.92717500	-2.93641500	1.78749200
H	-2.52350400	-4.00040700	0.48013900
H	-0.77599900	-3.56404900	0.56384100
C	-3.30045200	-1.13053200	-0.17519600
C	-4.38378900	-1.51468800	-0.97913000
C	-3.35680100	-0.02337600	0.68384900
C	-5.57076900	-0.80444900	-0.86856600
H	-4.28689500	-2.35204800	-1.66274800
C	-4.55443500	0.67519100	0.77833300
H	-2.47311900	0.24499300	1.25948100
C	-5.65199100	0.28475600	0.00656900
H	-6.42787800	-1.08545500	-1.47005500
H	-4.62898200	1.53092100	1.44036200
H	-6.58029400	0.84280100	0.07622500
C	1.01877200	-0.96793400	-0.86379000
C	2.23166200	-0.33754900	-0.56149800
C	1.08679000	0.40827100	-0.60235800
C	0.44517400	1.69661200	-0.43059900
C	-0.85333100	1.89313700	-0.91848400
C	1.10590100	2.73268600	0.24373200
C	-1.48318600	3.12086200	-0.73768100
H	-1.35698600	1.08194400	-1.43336800
C	0.46773400	3.95427800	0.43020900
H	2.10321300	2.57102100	0.64054400
H	-2.48809100	3.27268400	-1.11837900
H	0.97522100	4.75349000	0.96002400
C	3.65890000	-0.43502000	-0.34063800
C	4.44877300	0.71444100	-0.20070800

C	4.24723100	-1.70614500	-0.27754300
C	5.81797700	0.58964700	0.00736300
H	3.99205700	1.69649400	-0.27036300
C	5.61613600	-1.82435800	-0.06134000
H	3.62510500	-2.58883200	-0.39244200
H	6.43193000	1.47807400	0.11138000
H	6.07253600	-2.80694600	-0.00464400
Cl	-0.24134300	-0.60900900	2.34838700
C	-0.82453700	4.14971300	-0.06246200
H	-1.31829700	5.10532800	0.08286800
C	6.39984100	-0.67792200	0.08098300
H	7.46829900	-0.77189000	0.24738800

Sum of electronic and zero-point Energies= -1476.571168
Sum of electronic and thermal Energies= -1476.538973
Sum of electronic and thermal Enthalpies= -1476.537855
Sum of electronic and thermal Free Energies= -1476.644252

M3

O	0.28298900	-2.02190400	-0.30043300
N	-1.65656700	-0.93868800	-0.79142000
C	-1.13496900	-1.96166400	-0.28806400
C	-1.68233700	-3.21913200	0.28731100
H	-1.49081100	-3.21825100	1.36435200
H	-2.75277200	-3.28887600	0.09833100
H	-1.16543300	-4.07122100	-0.16064500
C	-3.05362800	-0.73308300	-0.71236800
C	-3.76444200	-0.43406600	-1.87767500
C	-3.70034900	-0.73160100	0.52866600
C	-5.13145200	-0.17609500	-1.80284400
H	-3.24158800	-0.41342700	-2.82882500
C	-5.06517100	-0.45675100	0.59383000
H	-3.11865000	-0.92861600	1.42751800
C	-5.78550300	-0.18516900	-0.56965100
H	-5.68492000	0.04316900	-2.71051200
H	-5.56465500	-0.45312500	1.55773200
H	-6.84837700	0.02689500	-0.51577000
C	0.92688000	-0.90122100	-0.23087100
C	2.15804700	-0.30395900	-0.24440400
C	1.01064700	0.46143500	-0.09953500
C	0.40378400	1.76104800	0.03034800
C	-0.91461500	1.87601800	0.49616900
C	1.13870700	2.90189700	-0.32661900
C	-1.49293400	3.13591100	0.59503000
H	-1.44708100	0.98326100	0.80350700
C	0.54704000	4.15548700	-0.23370600
H	2.15295200	2.80148500	-0.69918400
H	-2.50894000	3.23438200	0.96251400
H	1.10630700	5.04005800	-0.51794200
C	3.58967200	-0.42814700	-0.31684700
C	4.41144800	0.69316100	-0.13190500
C	4.14800300	-1.69356600	-0.55548300
C	5.79139100	0.54564700	-0.19089800
H	3.97029800	1.66377600	0.06842300
C	5.52906000	-1.83011200	-0.61758500
H	3.49733600	-2.55239300	-0.68938800
H	6.43448500	1.40664100	-0.04512300
H	5.96974800	-2.80360800	-0.80246400

Cl	-0.42552900	-0.90348000	2.70970200
C	-0.76650100	4.27076600	0.22741000
H	-1.22454400	5.25181200	0.30494100
C	6.34677400	-0.71243600	-0.43622900
H	7.42540100	-0.82296600	-0.48348500

Sum of electronic and zero-point Energies= -1476.657011
Sum of electronic and thermal Energies= -1476.625687
Sum of electronic and thermal Enthalpies= -1476.624570
Sum of electronic and thermal Free Energies= -1476.728802

M_TS5

O	-0.11624900	-0.61837600	-1.29575900
N	0.82524800	1.39863900	-0.81344200
C	0.91400700	0.30881500	-1.43337500
C	1.96314000	-0.23889000	-2.34361900
H	1.48596300	-0.68139500	-3.22059100
H	2.65314700	0.54761500	-2.64651000
H	2.52263300	-1.02697900	-1.82744600
C	1.89446700	2.31880100	-0.80268600
C	3.14218800	1.95444400	-0.28376400
C	1.67190500	3.63092500	-1.23094800
C	4.16795400	2.89469500	-0.22069800
H	3.28798700	0.93975100	0.07897000
C	2.70714000	4.56192300	-1.17337300
H	0.69351600	3.90703900	-1.61368400
C	3.95678300	4.19911800	-0.66900200
H	5.13373400	2.60549900	0.18258300
H	2.53364400	5.57636100	-1.51887500
H	4.75753000	4.92969200	-0.61754600
C	-1.08170400	-0.38248100	-0.39576400
C	-2.41342300	-0.81271100	-0.29693600
C	-2.15271300	0.50493900	-0.15600700
C	-2.68151100	1.84645100	-0.01306700
C	-1.83596100	2.94444500	0.18964100
C	-4.06961800	2.02929000	-0.09729300
C	-2.38377400	4.21801200	0.30678400
H	-0.76825300	2.77794000	0.26682100
C	-4.60847400	3.30601000	0.01519600
H	-4.71869100	1.17542400	-0.26599000
H	-1.73188700	5.07019100	0.47041900
H	-5.68163600	3.44837100	-0.05502500
C	-3.34079000	-1.92184100	-0.36853600
C	-4.60928200	-1.81837900	0.21900800
C	-2.96134400	-3.10058500	-1.02530900
C	-5.49085500	-2.89145600	0.14848600
H	-4.88945600	-0.91123300	0.74523000
C	-3.85279500	-4.16527800	-1.10198900
H	-1.97918600	-3.16991300	-1.48315600
H	-6.46988000	-2.81589800	0.60957700
H	-3.56425400	-5.07501900	-1.61761200
Cl	-0.54777300	1.31971000	3.04195100
O	-0.20241300	-0.78582200	1.14727000
N	1.18630900	-0.98329000	1.11334300
C	1.51350500	-2.14412000	0.66838400
C	0.55009800	-3.20702200	0.23114700
H	0.50253200	-3.23788000	-0.86310000
H	0.88921600	-4.18381400	0.58166600

H	-0.44830700	-3.01111000	0.62142600
C	2.97803300	-2.39516700	0.58017000
H	-0.32950500	0.02475500	1.79070500
C	3.88807600	-1.61021200	1.30427000
H	3.51492300	-0.83561500	1.96611600
C	5.25558300	-1.83154600	1.18448400
H	5.94976000	-1.22219900	1.75448000
C	5.73430900	-2.83735700	0.34139400
H	6.80224800	-3.00808200	0.24939200
C	4.83626300	-3.62426800	-0.37601100
H	5.19987800	-4.40769900	-1.03292900
C	3.46395000	-3.40825200	-0.25475000
H	2.77784900	-4.02526500	-0.82643900
C	-5.11486900	-4.06167700	-0.51396000
H	-5.80688600	-4.89572900	-0.57082200
C	-3.76518300	4.40007200	0.21915100
H	-4.18669100	5.39608900	0.31161700

Sum of electronic and zero-point Energies= -1916.535707
Sum of electronic and thermal Energies= -1916.491835
Sum of electronic and thermal Enthalpies= -1916.490717
Sum of electronic and thermal Free Energies= -1916.623450

Meisenheimer Complex-HCl Intermediate

O	-0.10275300	-0.54335900	-1.24000600
N	0.80921600	1.47344700	-0.72578500
C	0.87675200	0.41140500	-1.40307100
C	1.88898600	-0.05098700	-2.40146100
H	1.37854700	-0.50139300	-3.25509500
H	2.51448500	0.77843900	-2.72941500
H	2.52433400	-0.81771800	-1.94319000
C	1.85177900	2.42019100	-0.74603100
C	3.13853600	2.07746600	-0.31257300
C	1.57120400	3.74095200	-1.11196500
C	4.13971700	3.04540300	-0.27217200
H	3.33506800	1.05505700	0.00204000
C	2.58083900	4.70068300	-1.07699800
H	0.56480000	4.00072800	-1.42773200
C	3.86718600	4.35863500	-0.65732500
H	5.13501700	2.77150800	0.06449100
H	2.35873800	5.72158100	-1.37242800
H	4.64873300	5.11081600	-0.62283200
C	-0.96645300	-0.39584600	-0.17127600
C	-2.33521600	-0.83895800	-0.18353100
C	-2.11909400	0.46452500	-0.03469900
C	-2.68710600	1.79997000	0.04504900
C	-1.89221200	2.92314200	0.30494600
C	-4.06526700	1.95066600	-0.16962300
C	-2.47810700	4.18555300	0.35059800
H	-0.83014600	2.78652400	0.47257100
C	-4.64256900	3.21515400	-0.12819800
H	-4.67514400	1.07730000	-0.38270600
H	-1.86320600	5.05593500	0.55738300
H	-5.70789700	3.32945900	-0.29984800
C	-3.25450700	-1.95836200	-0.30410900
C	-4.50553600	-1.89607100	0.32469800
C	-2.90343400	-3.09137700	-1.04982600

C	-5.39380000	-2.96087800	0.21091600
H	-4.76745400	-1.02286800	0.91477300
C	-3.80086800	-4.14857300	-1.16959800
H	-1.93951300	-3.13086000	-1.54796200
H	-6.35827100	-2.91316900	0.70585100
H	-3.53040300	-5.02101700	-1.75518300
Cl	-0.28120700	1.30598600	3.00492700
O	-0.18215600	-0.69330500	1.10970100
N	1.22437800	-0.95748000	1.02088900
C	1.47430800	-2.15687300	0.63527700
C	0.45490000	-3.19224800	0.27502600
H	0.34313700	-3.22360300	-0.81439100
H	0.78589900	-4.17585700	0.61153300
H	-0.51276600	-2.96389800	0.72152400
C	2.92417700	-2.47315200	0.52119700
H	-0.24454800	0.18113900	1.85163400
C	3.87921900	-1.72278400	1.22293900
H	3.55271000	-0.92717600	1.88459300
C	5.23260300	-2.00713600	1.07994000
H	5.96506200	-1.42790600	1.63289700
C	5.64831600	-3.03745700	0.23337200
H	6.70557600	-3.25673500	0.12296900
C	4.70354600	-3.78715000	-0.46430000
H	5.02038200	-4.58934900	-1.12260300
C	3.34496100	-3.51117900	-0.31772600
H	2.61916400	-4.09949100	-0.87022800
C	-5.04376300	-4.08617200	-0.53768900
H	-5.73994800	-4.91375200	-0.62842700
C	-3.84879700	4.33398400	0.13371200
H	-4.29953700	5.32093700	0.16972300

Sum of electronic and zero-point Energies= -1916.540206
Sum of electronic and thermal Energies= -1916.496174
Sum of electronic and thermal Enthalpies= -1916.495056
Sum of electronic and thermal Free Energies= -1916.627128

Meisenheimer Complex

O	0.90553300	-0.07636100	1.82159400
N	-0.48126100	1.50284500	0.93508400
C	0.04890500	0.96574300	1.95326100
C	-0.12651100	1.30252000	3.40653600
H	-0.95117100	1.99942000	3.55051100
H	-0.31297400	0.38327900	3.96593100
H	0.79273500	1.75066900	3.79429500
C	-1.31197000	2.62942900	1.02531600
C	-2.59670400	2.56166500	0.46890700
C	-0.86475100	3.84591600	1.56038700
C	-3.43096500	3.67696200	0.48520400
H	-2.92885100	1.62517800	0.02967000
C	-1.70077200	4.96133200	1.56378800
H	0.14270200	3.91189300	1.96229000
C	-2.98829600	4.88281800	1.03218900
H	-4.42801100	3.60474700	0.06099700
H	-1.34068900	5.89670600	1.98183300
H	-3.63594900	5.75346600	1.03649600
C	1.23968000	-0.60283200	0.54188000
C	2.55253800	-0.33984200	-0.02839300

C	1.51369800	0.18862400	-0.65504900
C	0.93454400	0.89192800	-1.78570000
C	-0.44306900	0.79588300	-2.02987600
C	1.74355100	1.63507300	-2.65499500
C	-0.99890000	1.43568300	-3.13312400
H	-1.05314200	0.22271800	-1.33809300
C	1.18070100	2.28176600	-3.75284100
H	2.80913700	1.71555000	-2.46367100
H	-2.06564500	1.35834600	-3.32027300
H	1.81076200	2.86377300	-4.41787400
C	3.96495600	-0.61749000	0.13973400
C	4.92175100	-0.08100100	-0.73395600
C	4.37675000	-1.44207200	1.19629800
C	6.27079600	-0.36760200	-0.55104600
H	4.60551700	0.55649900	-1.55317600
C	5.72748200	-1.72692400	1.37494800
H	3.63076600	-1.85416600	1.87021500
H	7.00733700	0.04934700	-1.23029800
H	6.04097100	-2.36556500	2.19443400
O	0.71822500	-1.90670300	0.46556600
N	-0.66199900	-1.82972900	0.29131600
C	-1.22256400	-2.97976900	0.22700000
C	-0.49537500	-4.29212100	0.31511500
H	-1.10254100	-5.02768300	0.84621700
H	-0.29735600	-4.68019000	-0.69006600
H	0.45878400	-4.16928000	0.82493800
C	-2.69682500	-2.95801600	0.01803200
C	-3.34442100	-4.06258800	-0.54625800
C	-3.45526000	-1.83148800	0.37011100
C	-4.72105800	-4.03662700	-0.77094400
H	-2.77587100	-4.94411500	-0.82607600
C	-4.82823400	-1.80871700	0.14817100
H	-2.95789700	-0.98171500	0.82692100
C	-5.46634400	-2.91105100	-0.42573200
H	-5.20837000	-4.89763700	-1.21746300
H	-5.40407000	-0.93252400	0.43016500
H	-6.53807300	-2.89299800	-0.59681700
C	-0.19009400	2.18163200	-3.99426900
H	-0.62845700	2.68460200	-4.85070000
C	6.67577500	-1.18992500	0.50262100
H	7.72902500	-1.41107900	0.64363700

Sum of electronic and zero-point Energies= -1455.780800
Sum of electronic and thermal Energies= -1455.738947
Sum of electronic and thermal Enthalpies= -1455.737829
Sum of electronic and thermal Free Energies= -1455.867652

M_TS6

O	-0.11753300	-0.92556200	1.49559900
N	1.67837800	0.43826200	1.36264200
C	1.09895900	-0.65536300	1.79960100
C	1.77856900	-1.67169100	2.71015100
H	2.67515800	-1.28031800	3.19339500
H	1.05683500	-1.98678000	3.46701500
H	2.05692700	-2.55900600	2.13084700
C	3.04448800	0.67237200	1.49674400
C	3.47303000	1.95333000	1.89712800

C	4.03848600	-0.26544700	1.14974300
C	4.82573200	2.27096000	1.98224100
H	2.71628700	2.69413600	2.14218500
C	5.39145700	0.05787000	1.23076200
H	3.74072700	-1.24988500	0.79616500
C	5.79891100	1.32496900	1.65141500
H	5.12252600	3.26554900	2.30380000
H	6.13274900	-0.68730000	0.95288700
H	6.85375800	1.57394000	1.71034000
C	-0.50899900	-0.82255100	-0.64517000
C	0.76127900	-0.76801300	-1.18240200
C	0.02813500	0.37753700	-1.07592300
C	-0.11110400	1.80598600	-1.21843400
C	-1.36752300	2.39490000	-1.02116400
C	1.00530500	2.59542700	-1.52583800
C	-1.50453500	3.77390900	-1.14497900
H	-2.21469300	1.76208700	-0.77316100
C	0.86085700	3.97245900	-1.64312500
H	1.97828900	2.13069900	-1.64896900
H	-2.47453900	4.23662700	-0.99662300
H	1.72219200	4.58907400	-1.87692800
C	1.99175200	-1.46948800	-1.44947400
C	3.06093400	-0.83292800	-2.09288200
C	2.12238100	-2.78673200	-0.98645200
C	4.25985100	-1.51392000	-2.26738600
H	2.95064700	0.18596200	-2.44907400
C	3.33041500	-3.45613300	-1.15090300
H	1.28452300	-3.26509700	-0.48674000
H	5.09169300	-1.02512200	-2.76319600
H	3.44216700	-4.47011000	-0.78196300
O	-1.57466200	-1.56605600	-0.51947800
N	-2.71344600	-0.75213000	-0.25868400
C	-3.72757300	-1.48131900	0.02829400
C	-3.71323100	-2.98232600	0.07057000
H	-4.54112000	-3.35471400	0.67278600
H	-3.80697000	-3.38450000	-0.94356000
H	-2.77060500	-3.33982900	0.48562000
C	-4.97829700	-0.72701200	0.30400600
C	-6.21764000	-1.29920300	-0.00323200
C	-4.93025200	0.55915700	0.85763700
C	-7.39360500	-0.58635100	0.22295400
H	-6.26921400	-2.29467900	-0.43396700
C	-6.10723800	1.26407800	1.09044300
H	-3.96952000	0.99218800	1.11779200
C	-7.34099700	0.69451400	0.77072200
H	-8.34999400	-1.03432300	-0.02681400
H	-6.06161300	2.25589500	1.52883100
H	-8.25822400	1.24477400	0.95519700
C	-0.39342900	4.55984600	-1.45611800
H	-0.50332900	5.63570300	-1.54992300
C	4.39702900	-2.81926500	-1.78983800
H	5.33949600	-3.34238100	-1.91716700

Sum of electronic and zero-point Energies= -1455.744988
Sum of electronic and thermal Energies= -1455.703160
Sum of electronic and thermal Enthalpies= -1455.702042
Sum of electronic and thermal Free Energies= -1455.830134

M2-Product+HCl

O	0.00503200	-1.43212000	1.64080200
N	1.45845300	0.28695900	1.45435300
C	1.13941600	-0.92423700	1.88724000
C	2.07442200	-1.77310100	2.75016500
H	2.88074700	-1.19861800	3.20996600
H	1.47288300	-2.25244000	3.52588800
H	2.52201200	-2.56764700	2.14244300
C	2.74730200	0.79306700	1.48163000
C	2.92343400	2.16741300	1.75493600
C	3.90279200	0.05919600	1.13006700
C	4.17822700	2.76640600	1.71000700
H	2.04100200	2.75457300	1.99658100
C	5.15817700	0.66270700	1.08568900
H	3.80533600	-0.99132500	0.86659400
C	5.31221400	2.01910600	1.37773500
H	4.27279000	3.82639300	1.93136200
H	6.02317100	0.06572400	0.80704400
H	6.29111000	2.48624500	1.33611100
C	-0.57653700	-1.00290000	-0.91850000
C	0.76252600	-0.99491800	-1.19377100
C	0.05967100	0.18862800	-1.15737400
C	0.03311600	1.62526500	-1.25418900
C	-1.20027100	2.28743600	-1.32168100
C	1.23634200	2.34403100	-1.25699200
C	-1.22471300	3.67519000	-1.40914600
H	-2.11764200	1.70652300	-1.30373100
C	1.20082600	3.73102500	-1.33484600
H	2.18140600	1.81751100	-1.15852200
H	-2.17363800	4.19768100	-1.46753300
H	2.12638500	4.29705500	-1.32468800
C	2.02250600	-1.68157200	-1.31856100
C	3.10181300	-1.05167000	-1.95221500
C	2.16441500	-2.95910600	-0.75914900
C	4.32620900	-1.70435200	-2.02704800
H	2.97558600	-0.06404400	-2.38459400
C	3.40069900	-3.59328900	-0.81584200
H	1.31682900	-3.42519100	-0.26525200
H	5.16550900	-1.22537100	-2.51964600
H	3.52672600	-4.57420000	-0.37008100
O	-1.65353800	-1.67862000	-0.69061500
N	-2.75663100	-0.78451600	-0.48180700
C	-3.76220100	-1.43224100	-0.02016900
C	-3.77325900	-2.91161000	0.23423200
H	-4.61295800	-3.18702600	0.86980600
H	-3.85059900	-3.45195300	-0.71461100
H	-2.84089600	-3.21297200	0.71424500
C	-4.96333300	-0.59803600	0.24326900
C	-6.24114400	-1.15383600	0.11533600
C	-4.82774000	0.74754200	0.61044500
C	-7.37049800	-0.36795400	0.33539200
H	-6.35958700	-2.19409100	-0.17226200
C	-5.95796100	1.52602400	0.83782200
H	-3.83570200	1.17018600	0.73322900
C	-7.23135500	0.97093400	0.69834600
H	-8.35797800	-0.80399800	0.22513400
H	-5.84561100	2.56417500	1.13345100
H	-8.11198900	1.57890400	0.88012500
C	-0.02685700	4.39320300	-1.41622200

H	-0.04978800	5.47659500	-1.47971400
C	4.47700300	-2.96754500	-1.45051900
H	5.43874000	-3.46871000	-1.49717800

Sum of electronic and zero-point Energies= -1455.746587
Sum of electronic and thermal Energies= -1455.704277
Sum of electronic and thermal Enthalpies= -1455.703160
Sum of electronic and thermal Free Energies= -1455.831184

M2+Product+Cl-

O	-1.30302800	0.57155900	-0.78966700
N	-3.32065900	-0.32230600	-0.52125600
C	-2.12731200	-0.47205700	-0.95350200
C	-1.53113400	-1.67401300	-1.63862300
H	-2.30122300	-2.37234700	-1.96329100
H	-0.93417100	-1.34782000	-2.49347600
H	-0.85485800	-2.18860300	-0.94435000
C	-4.27071300	-1.35568700	-0.58734900
C	-5.52175500	-1.07157800	-1.15480400
C	-4.05871700	-2.62546400	-0.02995900
C	-6.51918500	-2.04234400	-1.19613200
H	-5.69437600	-0.08083200	-1.56472500
C	-5.06350300	-3.59125100	-0.06445300
H	-3.10238300	-2.84863000	0.43303300
C	-6.29712300	-3.30855900	-0.65071000
H	-7.47697600	-1.80633700	-1.65016500
H	-4.87874500	-4.56854700	0.37173600
H	-7.07779400	-4.06184600	-0.67643600
C	3.50949600	-0.29468400	0.41918700
C	2.21813700	-0.55746600	0.83597900
C	1.16684100	-1.45841300	1.23006700
C	-0.05349900	-0.91597900	1.66374100
C	1.35544800	-2.84740000	1.17240100
C	-1.07754000	-1.77125400	2.05396700
H	-0.18177200	0.16218500	1.67636300
C	0.32212000	-3.69306600	1.55667300
H	2.29599100	-3.25649400	0.82015000
C	-0.88762300	-3.15444900	2.00321300
H	-2.02494100	-1.36139400	2.38934400
H	0.45698300	-4.76804000	1.51211600
C	4.83439800	-0.71155800	0.04481300
C	5.24544700	-2.04072700	0.21998900
C	5.70840200	0.24231900	-0.49937600
C	6.53092700	-2.41257000	-0.15331900
H	4.56709400	-2.76774800	0.65274200
C	6.99016700	-0.14049800	-0.87493200
H	5.37400300	1.26751500	-0.62630800
C	7.39878300	-1.46479000	-0.70132100
H	6.85779500	-3.43772800	-0.01896900
H	7.67043900	0.58874700	-1.30067900
O	2.35241200	1.98397100	0.46034000
N	0.97471900	2.23839000	0.82518000
C	0.52688100	3.22670300	0.14119200
C	1.30927700	3.93541300	-0.92436200
H	1.45862100	3.24671800	-1.76315500
H	0.79149900	4.83102700	-1.26125600
H	2.29334900	4.21338900	-0.54221700

C	-0.87077700	3.60832500	0.46391800
C	-1.69575500	4.13536900	-0.53578500
C	-1.38307500	3.41534800	1.75369700
C	-3.02273400	4.45069700	-0.25245900
H	-1.31509100	4.27605300	-1.54247900
C	-2.70643800	3.74093300	2.03488000
H	-0.73719300	3.02235100	2.53206800
C	-3.52949500	4.25649500	1.03214500
H	-3.65959800	4.84761500	-1.03614100
H	-3.09439100	3.59757300	3.03812200
H	-4.56141700	4.50992400	1.25315400
Cl	1.36744900	0.39927200	-2.27157500
H	-0.42640100	0.43418800	-1.22795500
C	2.60387200	0.72642300	0.54783700
H	-1.68851300	-3.82012000	2.31104400
H	8.40103800	-1.76055800	-0.99400800

Sum of electronic and zero-point Energies= -1916.557048
Sum of electronic and thermal Energies= -1916.511113
Sum of electronic and thermal Enthalpies= -1916.509995
Sum of electronic and thermal Free Energies= -1916.650698

M_TS7

O	-1.49471000	0.64340400	-1.02979600
N	-3.46787100	-0.34126700	-0.74649300
C	-2.25591900	-0.46255900	-1.12380900
C	-1.57104300	-1.68115200	-1.68399500
H	-2.29257500	-2.44777900	-1.96266900
H	-0.97536700	-1.39895500	-2.55549000
H	-0.88556700	-2.09413900	-0.93427000
C	-4.35115300	-1.43596700	-0.74526400
C	-5.58222900	-1.30261300	-1.40264400
C	-4.08723500	-2.61747700	-0.03739200
C	-6.51062000	-2.34053900	-1.38204600
H	-5.79458300	-0.37797000	-1.93096100
C	-5.02432300	-3.64913500	-0.01064600
H	-3.14593100	-2.71834500	0.49507500
C	-6.23833900	-3.51965700	-0.68540200
H	-7.45426400	-2.22471700	-1.90664500
H	-4.80226800	-4.55696400	0.54246000
H	-6.96627000	-4.32412500	-0.66345600
C	3.23425700	-0.64261400	0.17558400
C	1.97670500	-0.74781500	0.66330300
C	0.90727900	-1.45709200	1.32316200
C	-0.28770200	-0.77241000	1.59468600
C	1.04062500	-2.81321400	1.65542100
C	-1.34249200	-1.44766200	2.19969300
H	-0.37228600	0.27455200	1.31788300
C	-0.02066300	-3.48050500	2.25700200
H	1.96274900	-3.33920700	1.43122000
C	-1.20905300	-2.79833500	2.52997700
H	-2.27108000	-0.92434300	2.40557200
H	0.07510000	-4.53063100	2.51106400
C	4.56821800	-1.13355500	-0.06794000
C	4.98636100	-2.37684600	0.42741800
C	5.44572000	-0.33884800	-0.82002500
C	6.27895900	-2.81869200	0.17012300
H	4.30419200	-2.98477800	1.01219400

C	6.73556500	-0.79029700	-1.07738700
H	5.10660100	0.62147000	-1.19762100
C	7.15116800	-2.02777300	-0.58204700
H	6.60789700	-3.77872200	0.55309100
H	7.41620600	-0.18014700	-1.66125500
O	2.34443800	1.72655800	0.09945100
N	1.04494900	2.17904000	0.46187000
C	0.88161500	3.39740100	0.09686000
C	1.90720900	4.18502100	-0.66794100
H	2.04071900	3.74811600	-1.66219400
H	1.61151800	5.22793400	-0.76358800
H	2.87029900	4.13389100	-0.15588000
C	-0.42853000	3.98898600	0.47024200
C	-1.03166700	4.93640200	-0.36498500
C	-1.08514200	3.58425500	1.64036800
C	-2.28209100	5.46003000	-0.04229900
H	-0.53886600	5.25230800	-1.27922000
C	-2.32953300	4.11646800	1.96415000
H	-0.60847500	2.86255700	2.29588200
C	-2.93197800	5.05322100	1.12238700
H	-2.74705300	6.18563400	-0.70160800
H	-2.82736800	3.80453000	2.87658700
H	-3.90219900	5.46787500	1.37654900
Cl	1.46669100	0.28392800	-2.12825600
H	-0.58455400	0.48984600	-1.35645400
C	2.33596300	0.41014900	-0.04433300
H	-2.03590600	-3.32380800	2.99813000
H	8.15863100	-2.37803800	-0.78223700

Sum of electronic and zero-point Energies= -1916.545687
Sum of electronic and thermal Energies= -1916.500628
Sum of electronic and thermal Enthalpies= -1916.499510
Sum of electronic and thermal Free Energies= -1916.638088

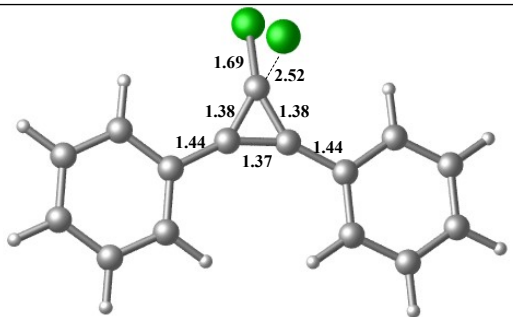
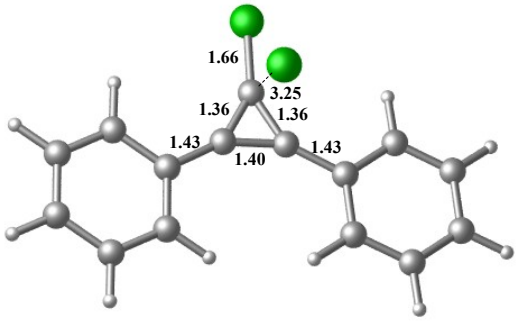
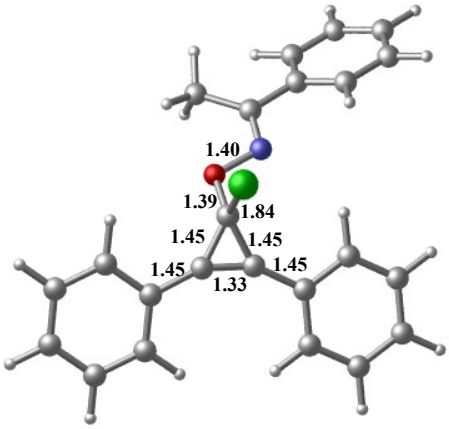
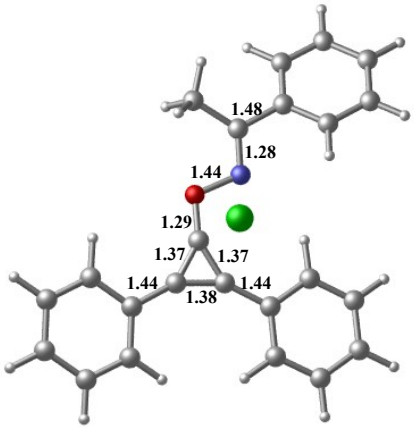
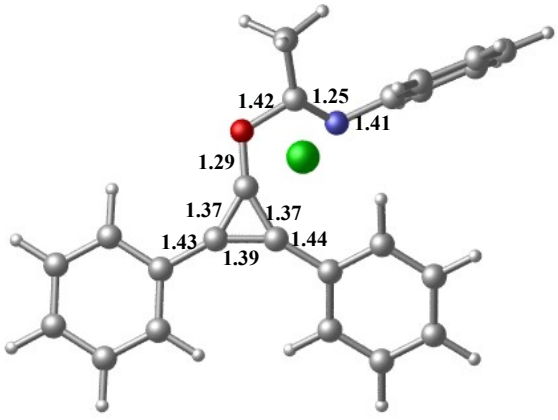
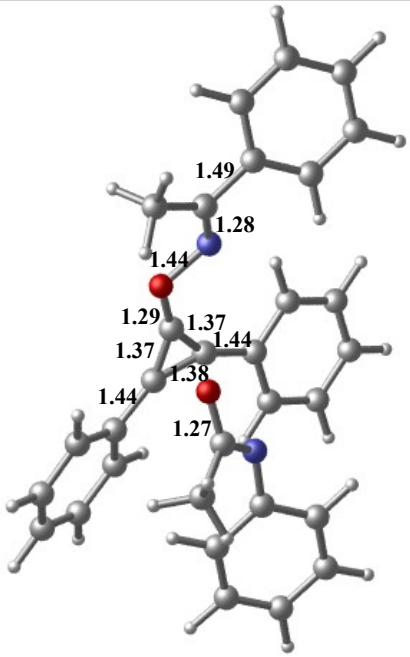
M1+Product

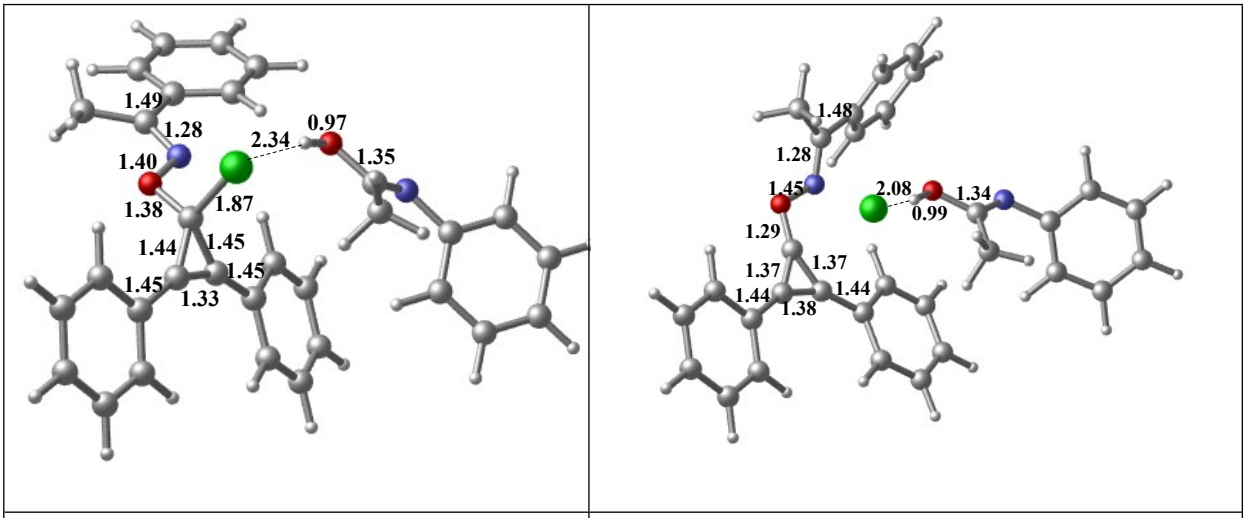
O	-1.54673100	0.86862900	-1.68581700
N	-3.40771700	-0.11708000	-0.97046600
C	-2.28173700	-0.25773400	-1.54569400
C	-1.67274700	-1.50658900	-2.12470500
H	-2.41542800	-2.29744600	-2.21862600
H	-1.24809800	-1.28574700	-3.10722400
H	-0.85924300	-1.86092400	-1.48136700
C	-4.22346300	-1.22572000	-0.68193600
C	-5.58143600	-1.16682900	-1.02354000
C	-3.74753400	-2.34371900	0.01927500
C	-6.43609500	-2.21849200	-0.70225600
H	-5.95155300	-0.28946900	-1.54547300
C	-4.61002000	-3.38755000	0.34933200
H	-2.70326300	-2.38141800	0.31837800
C	-5.95622900	-3.33403900	-0.01290800
H	-7.48314600	-2.16253100	-0.98419200
H	-4.22554000	-4.24381700	0.89586800
H	-6.62576600	-4.14803800	0.24540300
C	2.61744400	-1.23907700	0.02602000
C	1.37784700	-0.94610900	0.39866500
C	0.19935600	-1.16650200	1.21425000
C	-0.76559700	-0.15407700	1.32694400

C	0.04503800	-2.36220000	1.93393800
C	-1.85908000	-0.33056900	2.17119800
H	-0.63638600	0.76338700	0.75945200
C	-1.05209700	-2.53179400	2.77180500
H	0.78472000	-3.15021600	1.83523400
C	-1.99987500	-1.51254100	2.89845600
H	-2.60559400	0.45294700	2.25348300
H	-1.16857600	-3.45643500	3.32762800
C	3.83422600	-2.02057000	0.03932100
C	3.94732500	-3.18146600	0.81771900
C	4.91594100	-1.59624900	-0.74562400
C	5.13361400	-3.90725300	0.80902000
H	3.11006400	-3.50824300	1.42554100
C	6.09963800	-2.32780000	-0.75152500
H	4.81823900	-0.69501800	-1.34442500
C	6.20923200	-3.48223700	0.02540200
H	5.22115600	-4.80482000	1.41221500
H	6.93573600	-1.99857800	-1.35948100
O	2.46149300	1.21843000	-0.28698900
N	1.35084000	2.05900800	-0.13200700
C	1.67947100	3.28236500	0.06179600
C	3.09205400	3.79052200	0.11752600
H	3.16697100	4.74935500	-0.39896300
H	3.39087200	3.94512600	1.15963900
H	3.77979600	3.07944400	-0.33520200
C	0.54193100	4.22167700	0.26860500
C	0.76678500	5.48217700	0.83331400
C	-0.76643200	3.85540400	-0.08519700
C	-0.29588900	6.35984000	1.05040700
H	1.76943000	5.78475800	1.11764600
C	-1.82238500	4.73458000	0.13014900
H	-0.94923800	2.88449300	-0.53561200
C	-1.59208800	5.98960000	0.69970500
H	-0.10652400	7.33208700	1.49392200
H	-2.82894400	4.44210600	-0.15258600
H	-2.41839500	6.67380900	0.86457500
Cl	1.51935800	-0.10612200	-2.35668700
H	-0.66526500	0.66768300	-2.04352600
C	2.01737300	-0.06343100	-0.55824000
H	-2.85528000	-1.64800000	3.55285400
H	7.13280100	-4.05209900	0.02098500

Sum of electronic and zero-point Energies= -1916.550688
Sum of electronic and thermal Energies= -1916.505588
Sum of electronic and thermal Enthalpies= -1916.504470
Sum of electronic and thermal Free Energies= -1916.641840

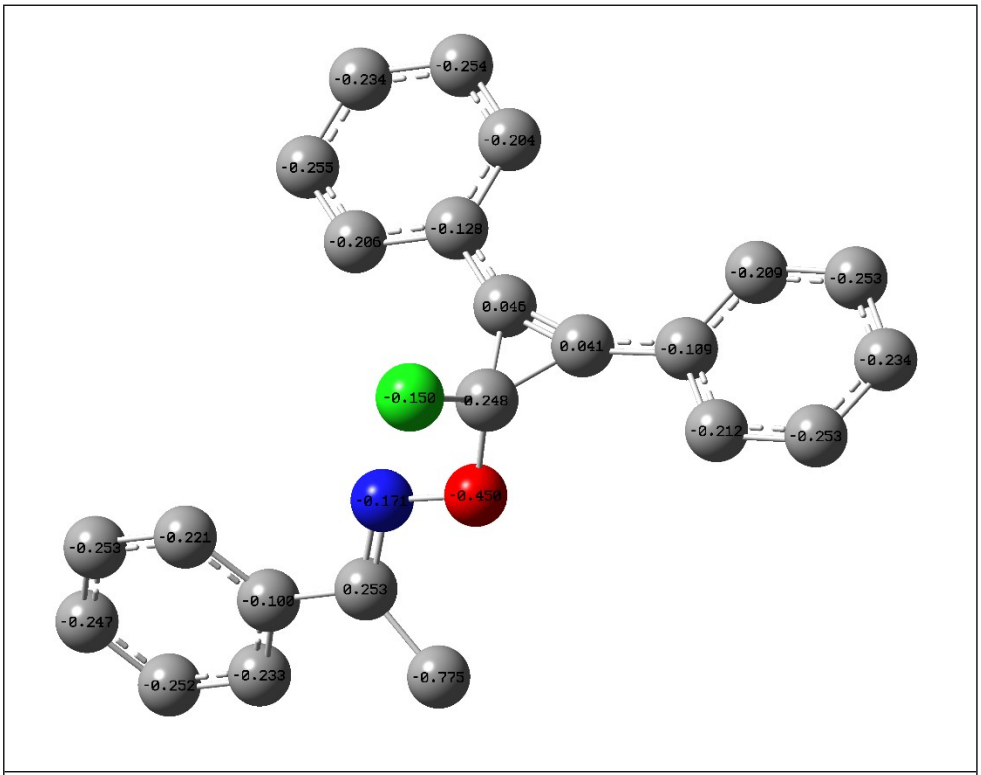
FIGURES

	
TS1	**DCP ion**
	
M1	**M2**
	
M3	**M2+Product+HCl**

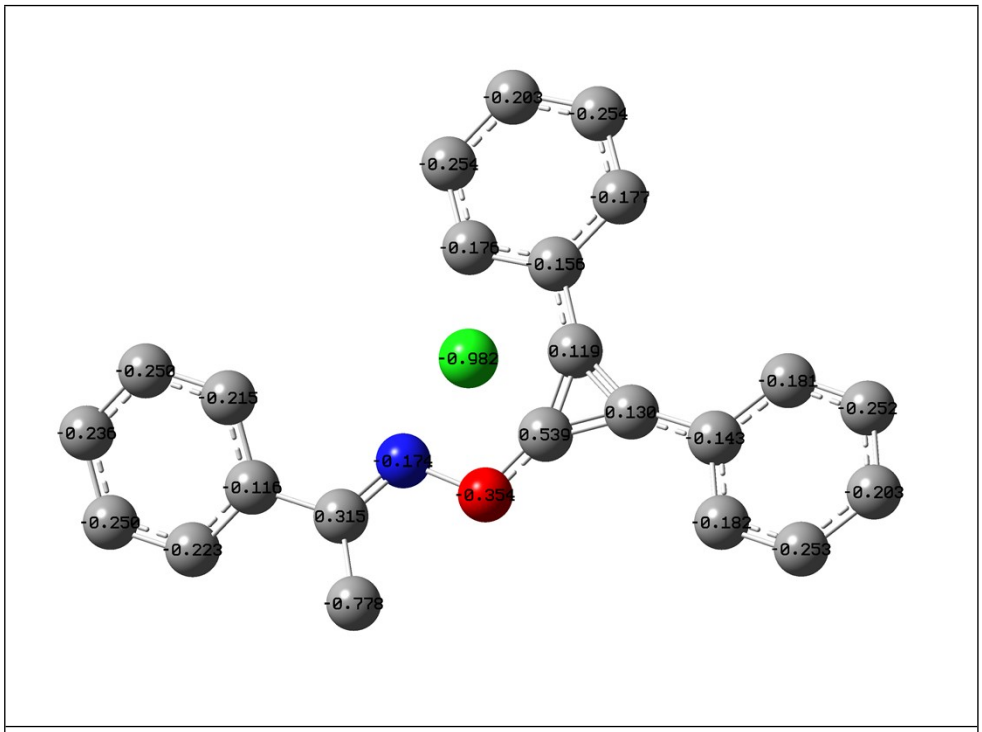


M2+Product+Cl-	M1+Product

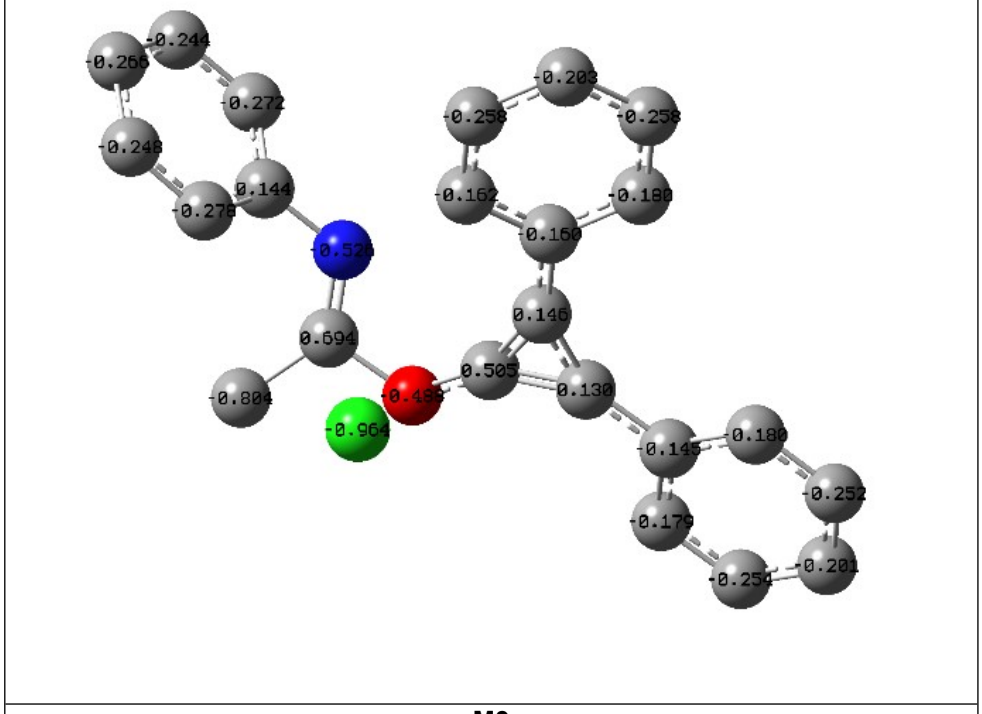
Figure SI.1. Key geometrical parameters and 3D Structures of Intermediates along the reaction coordinate



M1



M2



M3

Figure SI.2. NBO charges on heavy atoms of M1, M2 and M3 Structures.

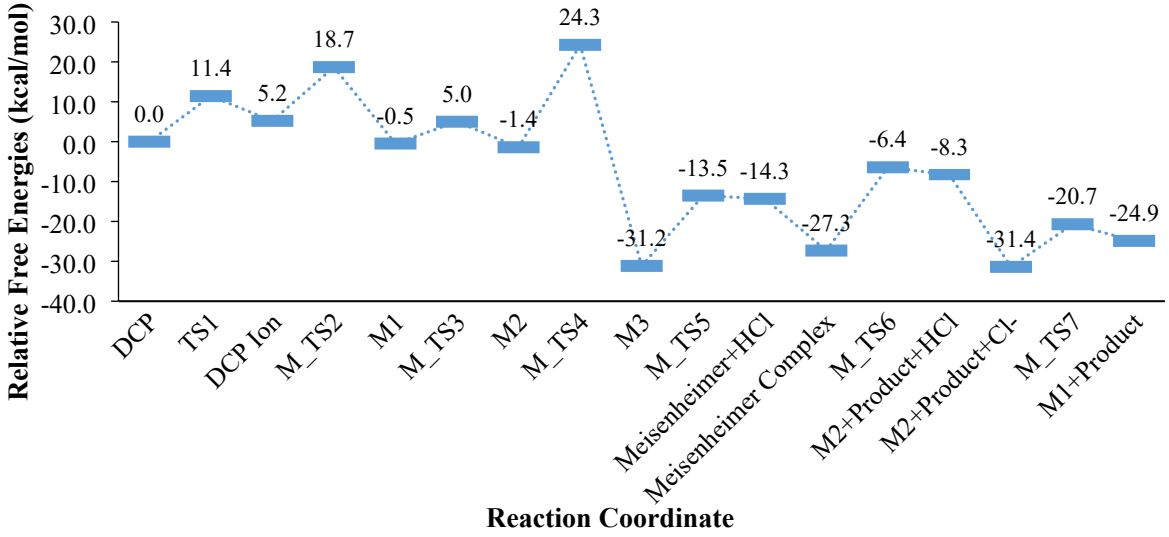


Figure SI.3. Reaction Energy Profile of Beckmann Rearrangement with 1,1-dichloro-2,3-p-Metoxy diphenylcyclopropene at 80℃.

TABLES

Table SI.1. : Second Order Perturbation Analysis of Fock Matrix Energies in NBO Basis (kcal/mol) for DCP Ion.

Donor (i)	Acceptor (j)	E(2) kcal/mol
BD (1) C 1 - C 2	BD*(1) C 1 - C 3	13.59
BD (1) C 1 - C 2	BD*(1) C 2 - C 3	7.45
BD (1) C 1 - C 2	BD*(1) C 2 - C 6	7.52
BD (1) C 1 - C 2	BD*(1) C 3 - C 7	31.31
BD (1) C 1 - C 3	BD*(1) C 1 - C 2	12.11
BD (1) C 1 - C 3	BD*(1) C 2 - C 3	5.45
BD (1) C 1 - C 3	BD*(1) C 2 - C 6	34.50
BD (1) C 1 - C 3	BD*(1) C 3 - C 7	6.95
BD (1) C 2 - C 3	BD*(1) C 1 - C 2	8.10
BD (1) C 2 - C 3	BD*(1) C 1 - C 3	7.41
BD (1) C 2 - C 3	BD*(1) C 7 - C 7'	2.31
BD (1) C 2 - C 3	BD*(1) C 6 - C 6'	2.36
BD (1) C 2 - C 3	BD*(1) C 3 - C 7	5.19
BD (1) C 2 - C 3	BD*(1) C 2 - C 6	6.00

Table SI.2 NBO Charge (eV) variations among reaction coordinate structures M_TS5, Meisenheimer-HCl Complex Intermediate, Meisenheimer Complex

	M_TS5	Meisenheimer-HCl Complex Intermediate	Meisenheimer Complex
N9	-0.522	-0.539	-0.556
O8	-0.542	-0.573	-0.580
C10	0.647	0.650	0.654
C1	0.505	0.516	0.520
O12	-0.580	-0.517	-0.455
H13	0.521	0.468	-
N14	-0.166	-0.167	-0.163
C15	0.276	0.307	0.241
Cl	-0.811	-0.675	-

Table SI.3. The NBO Second Order Perturbation Energy Interactions for structure M_TS5

Donor (i)	**Acceptor (j)**	**E(2) kcal/mol**
LP (1) O8	LP* (1) C1	2.0
LP (2) O8	LP* (1) C1	71.60
LP (1) Cl	LP* (1) H13	5.98
LP (2) Cl	LP* (1) H13	0.16
LP (3) Cl	LP* (1) H13	0.13
LP (4) Cl	LP* (1) H13	117.81
LP (1) O12	LP* (1) C1	12.27
LP (2) O12	LP* (1) C1	30.86
LP (3) O12	LP* (1) C1	177.44
LP (1) O12	LP* (1) H13	7.02
LP (2) O12	LP* (1) H13	295.0
LP (3) O12	LP* (1) H13	4.74