

Theoretical Investigation of the Effect of Hydrogen Bonding on the Stereoselectivity of the Diels-Alder Reaction

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Optimized Structures of the MCs

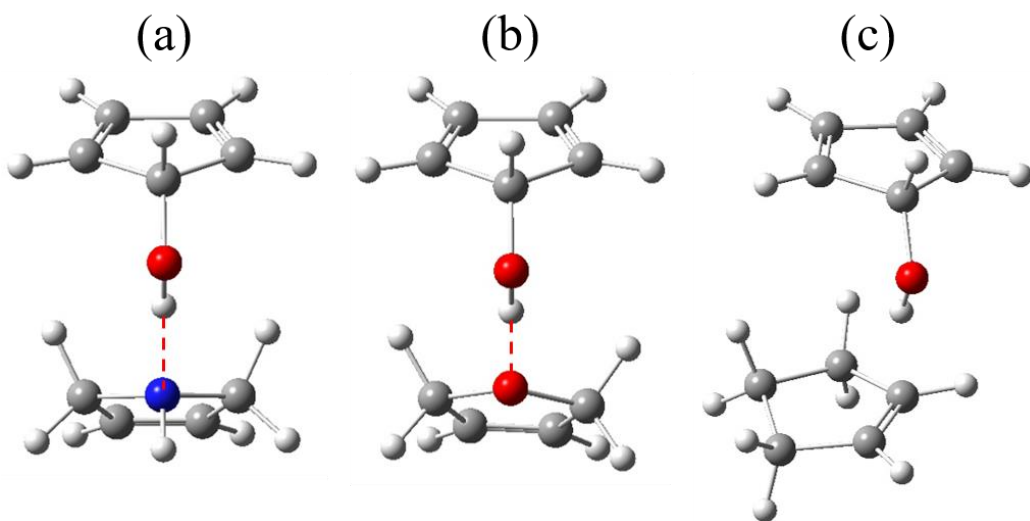


Figure S1. The optimized structures of the MCs for: (a) entry 1-1; (b) entry 1-2; and (c) entry 1-3. The red dashed lines indicate the HB interaction.

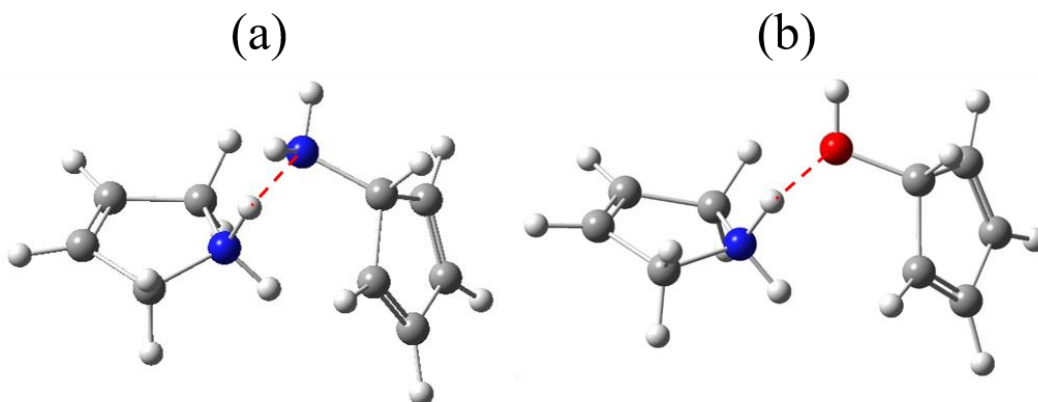


Figure S2. The optimized structures of the MCs for: (a) entry 2-1; and (b) entry 2-2. The red dashed lines indicate the HB interaction.

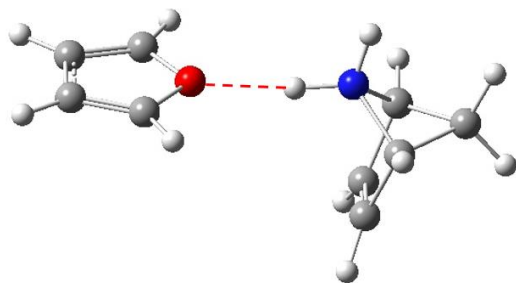


Figure S3. The optimized structure of the MC associated with the reactants of Scheme 3. The red dashed line indicates the HB interaction.

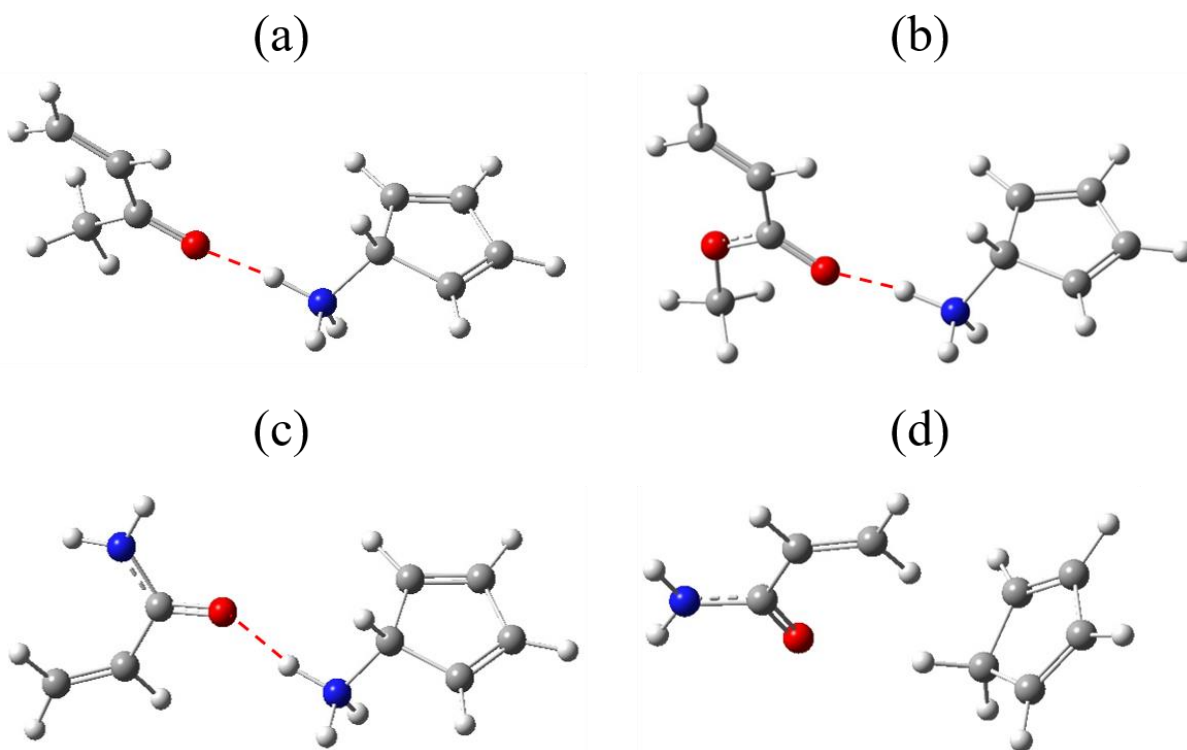


Figure S4. The optimized structures of the MCs for: (a) entry 3-1; (b) entry 3-2; (c) entry 3-3; and (d) entry 3-4. The red dashed lines indicate the HB interaction.

Results of the QTAIM Analysis

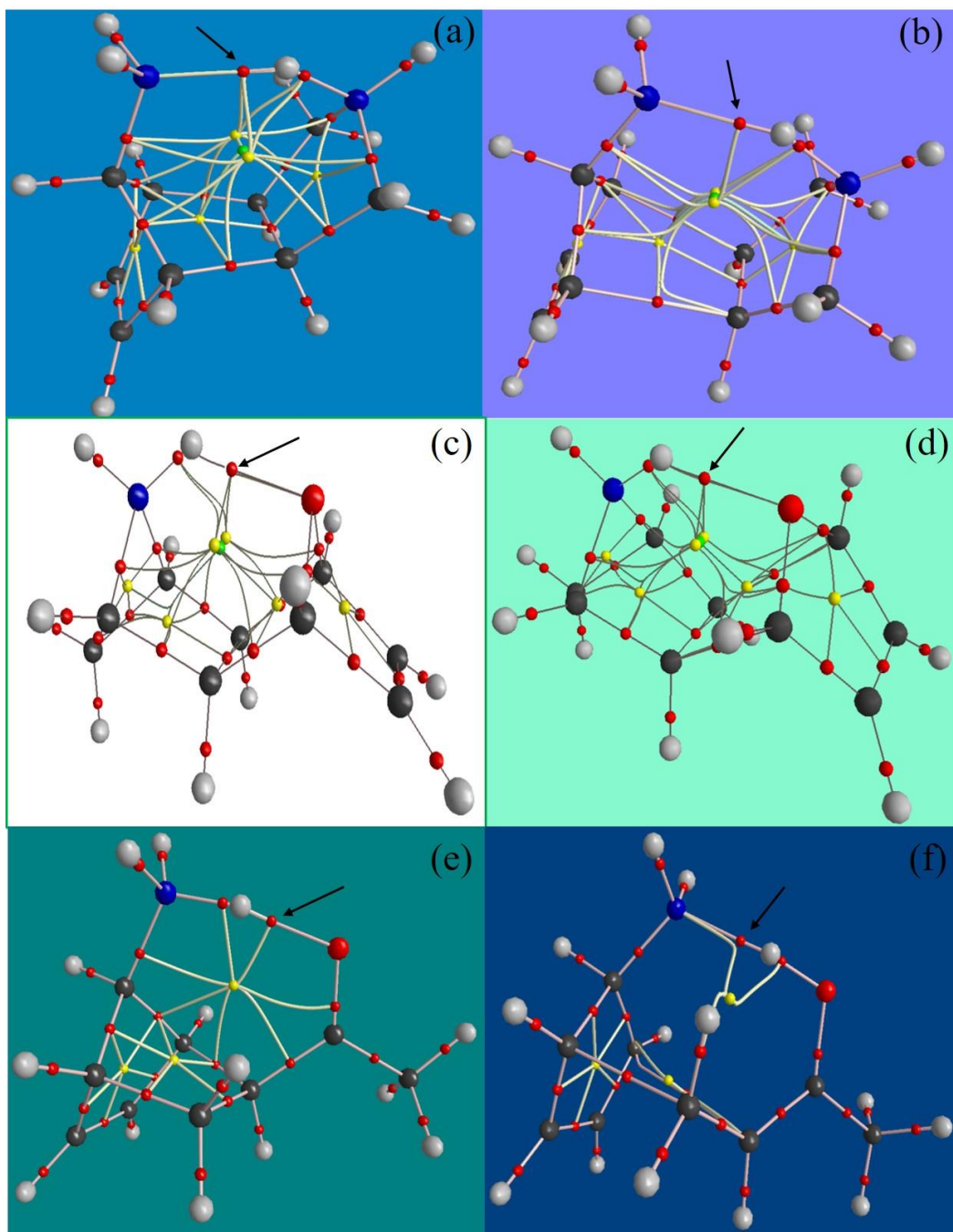


Figure S5. The results of the QTAIM analysis for: (a) exo cycloadduct corresponding to entry 2-1; (b) exo TS corresponding to entry 2-1; (c) exo1 cycloadduct corresponding to Scheme 3; (d) exo1 TS corresponding to Scheme 3; (e) exo cycloadduct corresponding to entry 3-1; and (f) exo TS corresponding to entry 3-1. Black arrows indicate the critical point corresponding to the HB interaction.

Cartesian Coordinates and Imaginary Frequencies of TS Structures

Name: 1-1 endo

Imaginary Frequency: 478.15 cm⁻¹

Coordinates:

	X	Y	Z
C	1.10196600	0.46035100	1.16107200
C	1.10198700	0.46039600	-1.16104400
C	1.90992400	-0.09112400	0.00001100
H	2.85752900	0.46812400	0.00003300
C	-0.56768600	-0.97099400	0.69704200
C	-0.56768900	-0.97094100	-0.69710500
H	1.34780400	0.24717500	2.19448500
H	1.34787000	0.24727200	-2.19445700
C	0.56316300	1.66402800	0.70384300
H	0.12940700	2.43550300	1.32765100
C	0.56316900	1.66406200	-0.70376700
H	0.12941600	2.43556300	-1.32754500
O	2.31151200	-1.44219000	-0.00001300
H	1.53107100	-2.00339200	-0.00020300
H	-0.08766200	-1.73817400	1.29469800
H	-0.08764600	-1.73804900	-1.29483600
C	-1.86811500	-0.34384700	1.18318800
H	-2.54401800	-1.13402800	1.53913600
H	-1.75154000	0.37084700	2.00217300
C	-1.86810900	-0.34372900	-1.18321400

H	-2.54401000	-1.13387000	-1.53925500
H	-1.75151500	0.37104700	-2.00212600
N	-2.44677500	0.32145900	0.00001800
H	-2.15304100	1.29007700	0.00007100

Name: 1-1 exo

Imaginary Frequency: 490.58 cm⁻¹

Coordinates:

	X	Y	Z
C	1.25101700	0.22427000	-1.15979400
C	1.25161300	0.22597600	1.15953500
C	0.99447200	1.17601500	-0.00082500
H	1.88024000	1.83356600	-0.00153500
C	-0.54482400	-1.07449500	-0.69839900
H	-0.12688600	-1.87530800	-1.28840200
C	-0.54491600	-1.07383800	0.69960400
H	-0.12669200	-1.87386100	1.29051700
H	1.11582700	0.51468100	-2.19534200
H	1.11656200	0.51797400	2.19466400
C	-1.80814700	-0.39315800	1.18826000
H	-2.54436900	-1.16003500	1.48469400
H	-1.66658600	0.27704300	2.04114700
C	-1.80813000	-0.39435900	-1.18773900
H	-1.66669600	0.27492300	-2.04136400
H	-2.54428700	-1.16163700	-1.48329000
C	2.22871700	-0.66571900	-0.70125700

H	2.81303100	-1.33257500	-1.32322600
C	2.22907600	-0.66478700	0.70183700
H	2.81373900	-1.33074800	1.32443600
N	-2.23618300	0.37275600	-0.00013500
H	-3.22324300	0.59868800	-0.00027500
O	-0.09177900	2.04918300	-0.00096600
H	-0.94639100	1.55510900	-0.00068300

Name: 1-2 endo

Imaginary Frequency: 478.64 cm⁻¹

Coordinates:

	X	Y	Z
C	1.10353600	0.46198500	1.16088900
C	1.10355100	0.46206700	-1.16085000
C	1.91088900	-0.08967700	0.00000500
H	2.86023700	0.46553900	0.00003200
C	-0.57417200	-0.96096500	0.69629100
C	-0.57416900	-0.96091600	-0.69636200
H	1.34864200	0.24824700	2.19445400
H	1.34866800	0.24840300	-2.19442600
C	0.55068300	1.65754500	0.70318200
H	0.09445000	2.41897200	1.32192800
C	0.55069200	1.65759500	-0.70306400
H	0.09446500	2.41906500	-1.32176200
O	2.30828600	-1.44333200	-0.00004000
H	1.52698300	-2.00294400	-0.00011400

H	-0.12094000	-1.73538700	1.30349100
H	-0.12094000	-1.73529800	-1.30361600
C	-1.85895600	-0.30759800	1.15994600
H	-2.56760200	-1.07138000	1.52096500
H	-1.74147400	0.44485600	1.94369000
C	-1.85894900	-0.30751400	-1.15997800
H	-2.56759400	-1.07126800	-1.52105800
H	-1.74146100	0.44499700	-1.94366600
O	-2.37479500	0.34971500	0.00000600

Name: 1-2 exo

Imaginary Frequency: 482.84 cm⁻¹

Coordinates:

	X	Y	Z
C	1.24586000	0.22176300	-1.16071200
C	1.24588500	0.22187500	1.16068800
C	0.98424500	1.16808000	-0.00005400
H	1.86112100	1.83615500	-0.00009600
C	-0.55709700	-1.07518700	-0.69749900
H	-0.15578000	-1.88053000	-1.29333300
C	-0.55710000	-1.07511700	0.69760900
H	-0.15577700	-1.88039300	1.29352900
H	1.11010400	0.51363900	-2.19558400
H	1.11013600	0.51384500	2.19553400
C	-1.81162800	-0.36776100	1.16074200
H	-2.57624300	-1.09616000	1.47147300

H	-1.68204900	0.35735800	1.96723500
C	-1.81163400	-0.36789200	-1.16070400
H	-1.68206700	0.35713500	-1.96728200
H	-2.57624600	-1.09633200	-1.47134600
C	2.22164700	-0.66796000	-0.70204100
H	2.80738100	-1.33310900	-1.32420800
C	2.22165900	-0.66789400	0.70208400
H	2.80740600	-1.33298300	1.32430300
O	-0.10921100	2.03874500	-0.00007900
H	-0.95302600	1.55209300	-0.00010500
O	-2.26653500	0.35498600	-0.00002100

Name: 1-3 endo

Imaginary Frequency: 491.29 cm⁻¹

Coordinates:

	X	Y	Z
C	1.11446900	0.46111800	1.15996000
C	1.11444500	0.46116100	-1.15995800
C	1.92348700	-0.09163600	-0.00001800
H	2.87337800	0.46338600	-0.00001700
C	-0.55351400	-0.95696900	0.69897800
C	-0.55352300	-0.95694300	-0.69900400
H	1.35911300	0.24686400	2.19360200
H	1.35907000	0.24694600	-2.19361300
C	0.58637700	1.67076900	0.70287300
H	0.14967100	2.44056200	1.32621700

C	0.58636300	1.67079500	-0.70281700
H	0.14964600	2.44061200	-1.32612300
O	2.32009300	-1.44520200	-0.00004700
H	1.53785700	-2.00375500	-0.00004000
H	-0.04977500	-1.71820100	1.28534200
H	-0.04979100	-1.71815400	-1.28540100
C	-1.85070700	-0.36609200	1.22856300
H	-2.49908200	-1.18213000	1.57420800
H	-1.71520200	0.30875500	2.07838500
C	-1.85072400	-0.36604900	-1.22854900
H	-2.49910500	-1.18207600	-1.57421200
H	-1.71523300	0.30882700	-2.07835100
C	-2.46917700	0.34259000	0.00002300
H	-3.56066700	0.30126700	0.00003000
H	-2.18559700	1.39623900	0.00004000

Name: 1-3 exo

Imaginary Frequency: 503.17 cm^{-1}

Coordinates:

	X	Y	Z
C	-1.07879500	-0.06416900	1.16100700
C	-1.07878600	-0.06420100	-1.16100700
C	-0.90667900	0.91103500	-0.00001200
C	0.93727400	-0.94482800	0.69979700
H	0.68141900	-1.82309700	1.27417500
C	0.93727600	-0.94485700	-0.69975900

H	0.68141700	-1.82314800	-1.27410200
H	-0.98616600	0.24751400	2.19406300
H	-0.98615100	0.24745500	-2.19407000
C	1.99993000	0.00319700	-1.23486600
H	2.82205100	-0.59168300	-1.65233300
H	1.64826000	0.64875700	-2.04573100
C	1.99992300	0.00325100	1.23486800
H	1.64824700	0.64884700	2.04570300
H	2.82204200	-0.59160900	1.65236800
C	-1.91607400	-1.07864800	0.70713400
H	-2.38754100	-1.83090600	1.32720000
C	-1.91606900	-1.07866700	-0.70711100
H	-2.38753200	-1.83094200	-1.32716000
C	2.48035500	0.81119200	-0.00001500
H	3.56358200	0.94861100	-0.00001500
H	2.04514800	1.81264300	-0.00003900
O	-1.89726300	1.95357200	-0.00003100
H	-2.76670100	1.53540300	-0.00002500
H	0.02989500	1.45375200	-0.00001500

Name: 2-1 endo

Imaginary Frequency: 471.26 cm⁻¹

Coordinates:

	X	Y	Z
C	1.10102300	0.50993900	1.15653500
C	1.09972300	0.51010300	-1.15617900

C	1.91494900	-0.02554800	-0.00016700
H	2.81727700	0.61930400	-0.00117700
C	-0.50371700	-0.99867200	0.69464300
H	0.02253900	-1.74909400	1.26445300
C	-0.50373500	-0.99688900	-0.69652500
H	0.02091400	-1.74711200	-1.26821400
H	1.35287500	0.31671900	2.19293700
H	1.35188100	0.31810200	-2.19276000
C	0.50466100	1.69424000	0.70386800
H	0.08678500	2.46744300	1.33760100
C	0.50417000	1.69446700	-0.70269300
H	0.08586600	2.46790000	-1.33585600
C	-1.80489200	-0.44585400	1.22048600
H	-2.52123500	-1.23165200	1.47790800
H	-1.73750100	0.25935700	2.04931900
C	-1.80542400	-0.44321700	-1.22041200
H	-1.73857500	0.26374200	-2.04782700
H	-2.52175300	-1.22858000	-1.47914600
N	-2.34221900	0.29253800	0.00091300
H	-3.35919600	0.38104400	0.00116700
H	-1.93866500	1.23362300	0.00188900
N	2.25552700	-1.43931900	-0.00020500
H	2.82056200	-1.66813500	-0.81304700
H	2.82451900	-1.66661200	0.81045400

Name: 2-1 exo

Imaginary Frequency: 484.00 cm⁻¹

Coordinates:

	X	Y	Z
C	-1.27138700	0.21126100	1.15905500
C	-1.27145000	0.21094000	-1.15903400
C	-1.03972400	1.15560400	-0.00011900
H	-1.93358800	1.80124200	-0.00018500
C	0.51838100	-1.10644400	0.69985400
H	0.09859500	-1.90610900	1.28885300
C	0.51834100	-1.10656400	-0.69967200
H	0.09858100	-1.90636500	-1.28850700
H	-1.15817600	0.50366000	2.19715800
H	-1.15832600	0.50307300	-2.19722200
C	1.79108700	-0.46552400	-1.20550000
H	2.55129700	-1.21486300	-1.44812200
H	1.68930200	0.21348800	-2.05361600
C	1.79117100	-0.46537100	1.20550900
H	1.68946900	0.21372700	2.05356600
H	2.55139000	-1.21469800	1.44814200
C	-2.24073100	-0.69137100	0.69962400
H	-2.81898700	-1.35657000	1.32683900
C	-2.24077600	-0.69156200	-0.69929700
H	-2.81907300	-1.35693000	-1.32629400
N	2.24113300	0.31976700	-0.00006000
H	3.23357000	0.54915900	-0.00010400
H	1.60996900	1.19073400	-0.00013000

N	0.16032300	2.02181700	-0.00025900
H	0.11314300	2.64167900	-0.80774200
H	0.11317300	2.64187500	0.80707700

Name: 2-2 endo

Imaginary Frequency: 463.38 cm⁻¹

Coordinates:

	X	Y	Z
C	1.14631000	0.49678300	1.15050300
C	1.09644400	0.44030300	-1.17538300
C	1.92683400	-0.07840500	-0.01411300
H	2.85130400	0.51993400	-0.05313500
C	-0.53379000	-0.98172400	0.72716500
H	-0.06564400	-1.72841800	1.35450200
C	-0.52773200	-1.01608100	-0.66601300
H	-0.04123700	-1.78970400	-1.24452600
H	1.41224900	0.31246000	2.18425600
H	1.33281800	0.21311100	-2.20792100
C	0.57074400	1.67864300	0.67549500
H	0.18763600	2.48204500	1.29379300
C	0.54430500	1.64750400	-0.73387700
H	0.14347100	2.42651000	-1.37213900
C	-1.81299400	-0.35933500	1.23255200
H	-2.55694100	-1.10696300	1.52244600
H	-1.71266100	0.37312500	2.03367700
C	-1.81472000	-0.44195600	-1.20743100

H	-1.72552300	0.23082400	-2.06037300
H	-2.55357400	-1.21516200	-1.43660400
N	-2.32506300	0.35126500	-0.01287300
H	-3.33929800	0.46894200	-0.01592500
H	-1.89594100	1.28047400	-0.04529300
O	2.37579100	-1.40292200	0.00229200
H	1.66004700	-2.01706300	0.18563400

Name: 2-2 exo

Imaginary Frequency: 481.45 cm⁻¹

Coordinates:

	X	Y	Z
C	-1.28193800	0.22286800	1.16355200
C	-1.28166900	0.22172000	-1.16380700
C	-1.02449400	1.15278000	-0.00056800
H	-1.85800900	1.86853200	-0.00100500
C	0.51233500	-1.08659600	0.69944700
H	0.09321200	-1.88711100	1.28795100
C	0.51221800	-1.08726000	-0.69827300
H	0.09315000	-1.88848800	-1.28586500
H	-1.15449900	0.52105300	2.19730200
H	-1.15399500	0.51884100	-2.19783500
C	1.77793800	-0.44411900	-1.21547800
H	2.52536000	-1.19296300	-1.49417500
H	1.66317000	0.26263700	-2.03780600
C	1.77796400	-0.44264900	1.21594400

H	1.66307500	0.26515600	2.03735200
H	2.52547000	-1.19103300	1.49564400
C	-2.26801100	-0.65446700	0.70200400
H	-2.86875900	-1.30306500	1.32568800
C	-2.26791500	-0.65518900	-0.70154100
H	-2.86856000	-1.30438900	-1.32469200
N	2.28302100	0.30818100	-0.00024300
H	3.29249600	0.44785000	-0.00035200
O	0.19437500	1.91194500	-0.00081700
H	1.78323700	1.21580900	-0.00071600
H	-0.01006900	2.85181800	-0.00093500

Name: 3 endo 1

Imaginary Frequency: 510.97 cm⁻¹

Coordinates:

	X	Y	Z
C	-1.63335600	-0.29024100	-1.08040800
C	-1.63285100	-0.29030700	1.08048500
C	0.42651700	-0.84497400	-0.70980400
C	0.42638200	-0.84474700	0.70984200
H	-1.87099800	-0.71419100	-2.04428600
H	-1.87037300	-0.71431100	2.04436500
C	-1.70304000	1.07524200	-0.68972100
H	-1.70945300	1.91948500	-1.36468500
C	-1.70279000	1.07521200	0.68989800
H	-1.70889200	1.91941500	1.36491200

O	-1.97179000	-1.05544500	0.00001400
C	1.60281500	0.08607900	-1.01699700
H	1.82052700	0.40619800	-2.03205400
C	1.60255300	0.08654100	1.01689200
H	1.82004100	0.40714300	2.03184600
H	0.31367100	-1.73446600	1.31285000
H	0.31349300	-1.73473600	-1.31267700
N	1.32601300	1.21543000	-0.00035100
H	2.04057600	1.94330500	-0.00039800
C	2.68829700	-0.40189300	0.00020400
H	3.60953900	0.19016400	0.00021200
H	2.90904100	-1.46578500	0.00047000
H	0.37789100	1.60785800	-0.00056500

Name: 3 endo 2

Imaginary Frequency: 465.97 cm⁻¹

Coordinates:

	X	Y	Z
C	1.65483200	-0.29031200	1.08028900
C	1.65657700	-0.29246700	-1.07926700
C	-0.40216400	-0.78580000	0.71446800
C	-0.40260100	-0.78700700	-0.71402400
H	1.87703100	-0.72161100	2.04465600
H	1.87892900	-0.72545100	-2.04283000
C	1.76047300	1.06963700	0.68667100
H	1.75720900	1.91719400	1.35586100

C	1.76123100	1.06827800	-0.68818200
H	1.75886200	1.91452300	-1.35903900
O	1.96730800	-1.07171400	0.00119700
C	-1.55920500	0.15582700	1.02159600
H	-1.92199800	0.28806200	2.03684800
C	-1.55961000	0.15399700	-1.02223400
H	-1.92313700	0.28434200	-2.03746100
H	-0.30532700	-1.69367200	-1.29702700
H	-0.30554500	-1.69178200	1.29869200
C	-1.42087700	1.30402700	-0.00137700
H	-0.49284300	1.85927000	-0.00209500
H	-2.27550700	1.98256600	-0.00180000
N	-2.63157100	-0.43136700	0.00067500
H	-2.75904700	-1.44573900	0.00165100
H	-3.53802300	0.04850100	0.00060700

Name: 3 exo 1

Imaginary Frequency: 501.54 cm⁻¹

Coordinates:

	X	Y	Z
C	1.45027900	1.08823900	0.41282200
C	1.45103100	-1.08823700	0.41260100
C	-0.36077500	0.70709400	-0.80273000
H	-0.09531700	1.33657600	-1.63774100
C	-0.36103100	-0.70709200	-0.80322800
H	-0.09572500	-1.33616400	-1.63859800

H	1.33192300	2.05230200	0.88498900
H	1.33335400	-2.05269500	0.88414000
C	-1.64898000	-1.01500700	-0.03164400
H	-1.90400800	-2.03202000	0.25311300
C	-1.64869100	1.01494800	-0.03110900
H	-1.90348100	2.03185300	0.25424700
C	2.39686400	0.68912300	-0.55588600
H	2.92725400	1.35214300	-1.22236600
C	2.39697800	-0.68867100	-0.55597300
H	2.92755500	-1.35144600	-1.22255500
N	-1.52103300	-0.00034800	1.12977700
O	1.17721600	-0.00025000	1.21347400
C	-2.66475300	0.00028400	-0.65273100
H	-3.65308400	0.00031300	-0.18125300
H	-2.74948700	0.00059000	-1.73582400
H	-0.62696700	-0.00072600	1.63936200
H	-2.32804300	-0.00037200	1.75352900

Name: 3 exo 2

Imaginary Frequency: 458.64 cm^{-1}

Coordinates:

	X	Y	Z
C	-1.49074400	-1.08168200	0.42943300
C	-1.49072700	1.08165000	0.42950800
C	0.33973400	-0.71155700	-0.73163500
H	0.08699600	-1.32040000	-1.58756200

C	0.33973400	0.71167800	-0.73150700
H	0.08705400	1.32066800	-1.58734800
H	-1.39134000	-2.04512200	0.90679100
H	-1.39136000	2.04504900	0.90695700
C	1.61422900	1.02014500	0.04456700
H	1.98868700	2.03684700	0.12280100
C	1.61421800	-1.02017200	0.04436700
H	1.98866700	-2.03689400	0.12237300
C	-2.38854200	-0.68723400	-0.59566800
H	-2.88134100	-1.35235500	-1.28843900
C	-2.38854200	0.68728200	-0.59561500
H	-2.88133500	1.35245500	-1.28833900
O	-1.25480400	-0.00005500	1.22800700
H	3.56207600	0.00003000	-0.32223400
H	2.59252000	0.00016400	-1.70034500
C	1.63428600	-0.00012500	1.20657200
H	2.58006900	-0.00018300	1.75108200
H	0.79388700	-0.00017400	1.88794900
N	2.60028100	0.00006300	-0.67826700

Name: 3-1 endo

Imaginary Frequency: 463.42 cm^{-1}

Coordinates:

	X	Y	Z
C	0.93065400	1.89813900	-0.01514100
C	1.62614700	0.88534300	0.66568000

C	0.63722100	0.00743200	-1.26171400
C	0.31946700	1.36030600	-1.15722800
C	1.87086100	-0.14834500	-0.41369400
H	2.74501200	0.16349700	-0.99890400
C	0.01475400	-0.19028800	1.59516400
H	0.63371600	-0.76452900	2.28027900
H	-0.44112800	0.66829700	2.06900500
C	-0.64043200	-0.83552700	0.54389600
H	2.33731700	1.08045100	1.46026400
H	0.37891700	-0.63593900	-2.09321700
H	-0.36620900	1.88369100	-1.80901400
H	0.79884900	2.90659200	0.35263600
N	2.19945300	-1.55599700	0.04795300
H	2.36774200	-2.17112400	-0.75402200
H	3.04080200	-1.56836200	0.63170700
H	1.42078000	-1.94918100	0.58460500
C	-1.98001500	-0.47219400	-0.02220700
C	-2.67556800	0.77544900	0.47233100
H	-2.01002000	1.64239200	0.49477200
H	-3.53382700	0.98284500	-0.16462700
H	-3.02963800	0.61257600	1.49596300
O	-2.49067200	-1.21976600	-0.83156300
H	-0.43164400	-1.88298800	0.32485900

Name: 3-1 exo

Imaginary Frequency: 304.67 cm^{-1}

Coordinates:

	X	Y	Z
C	-2.18682000	-1.18221900	0.21539500
C	-1.81519700	0.01330700	0.83378800
C	-1.16815400	0.01312400	-1.42526000
C	-1.72083800	-1.20231600	-1.12808200
C	-1.46116900	0.96617500	-0.30242400
H	-2.43856400	1.40678100	-0.57357500
C	0.03669700	-0.47305100	1.61349500
H	0.19041000	0.50629900	2.05409500
H	-0.35339600	-1.20625200	2.30759400
C	0.94353700	-0.93104800	0.64392200
H	0.97521500	-1.99365900	0.43653000
H	-2.28374200	0.36250800	1.74729600
H	-0.71794200	0.30117000	-2.36688600
C	1.95935500	-0.16805700	0.04932900
H	-1.78880500	-2.04754100	-1.79901200
H	-2.70512100	-1.99782600	0.70387100
N	-0.48551500	2.03532400	-0.03508600
H	-0.41675400	2.64535200	-0.84878300
H	-0.82370900	2.62886900	0.72059900
C	3.14580400	-0.80694200	-0.58911000
H	3.06948400	-1.89209600	-0.61137500
H	3.27981700	-0.41800500	-1.60215900
H	4.04075500	-0.52445800	-0.02461600
O	1.98919300	1.13460800	0.05549200

H 1.05812500 1.53089500 0.19177700

Name: 3-2 endo

Imaginary Frequency: 452.06 cm⁻¹

Coordinates:

	X	Y	Z
C	1.12324900	1.61945400	0.09673700
C	1.70926900	0.67236200	0.93868700
C	0.97728300	-0.36904900	-1.02560600
C	0.66617600	0.98096000	-1.07924700
C	2.02154400	-0.52657000	0.05656700
C	0.04026200	-0.40044500	1.76926400
H	-0.48685900	0.46379500	2.14775800
C	-0.48953900	-1.10024700	0.68807500
H	2.28681800	0.90811200	1.82431900
H	0.80218100	-1.10123700	-1.80256400
H	0.06276700	1.44954400	-1.84411400
H	0.92297300	2.64781200	0.36377200
H	0.64597300	-0.93406300	2.49343400
C	-1.74090900	-0.70870800	-0.01052700
O	-2.32126800	-1.42759000	-0.78820600
H	-0.22672200	-2.13791500	0.52007200
N	3.42312600	-0.29528700	-0.59057000
H	4.16914700	-0.28849200	0.11028500
H	3.64085200	-1.02183100	-1.27769900
H	3.41904100	0.61134900	-1.06980700

H	2.09941700	-1.49537700	0.54078700
C	-3.39059800	0.97554600	-0.26475200
H	-4.19860700	0.30258500	0.02087500
H	-3.56002500	1.97248400	0.13368400
H	-3.30716700	0.99854600	-1.35151400
O	-2.14524400	0.53157500	0.32689400

Name: 3-2 exo

Imaginary Frequency: 351.67 cm⁻¹

Coordinates:

	X	Y	Z
C	-2.22708400	-1.48294700	0.31788100
C	-2.09665400	-0.17217800	0.80565900
C	-1.30082200	-0.31393100	-1.39380500
C	-1.67143400	-1.57095300	-0.97933100
C	-0.26782700	-0.18218600	1.63075800
H	-0.49659700	-0.92874200	2.38036700
C	0.73920900	-0.50613500	0.70293900
H	0.98349500	-1.54792500	0.55188400
H	-2.68976900	0.18478100	1.64130200
H	-0.83769100	-0.05978500	-2.33887700
H	-1.54074900	-2.48435200	-1.54336800
H	-2.62310200	-2.31701600	0.88309600
O	1.36474800	1.70976400	0.03909900
H	-0.30161000	0.83172000	2.01655600
C	-1.88271500	0.68635400	-0.43784500

H	-2.90897100	0.85121700	-0.81233800
H	-1.24133700	2.49832800	-1.15824800
H	-1.69482200	2.55348300	0.39890800
H	0.34383100	1.87535100	0.03052400
C	1.61371000	0.44388900	0.12014300
O	2.78701400	0.14049900	-0.37414600
C	3.36300700	-1.17943900	-0.22953000
H	3.38409300	-1.47112600	0.82071400
H	2.80743700	-1.90232400	-0.82859200
H	4.37449400	-1.08232200	-0.61316600
N	-1.19844900	1.98025300	-0.28137200

Name: 3-3 endo

Imaginary Frequency: 464.60 cm⁻¹

Coordinates:

	X	Y	Z
C	-1.03964300	1.00009800	1.27497000
C	-1.46859400	1.14647300	-0.04574400
C	-0.60534400	-1.00460500	0.26100500
C	-0.50170600	-0.29505700	1.45058500
C	-1.61373400	-0.26514300	-0.59044900
C	0.39819600	1.32342500	-1.16101800
H	0.76865100	2.16130300	-0.58561200
C	0.97074100	0.05759900	-1.05319800
H	-2.05234300	1.97878400	-0.41969800
H	-0.32637900	-2.03825400	0.10673900

H	0.02644100	-0.63545800	2.33022300
H	-0.99576700	1.79620000	2.00566800
H	-0.08791700	1.60423500	-2.08861300
C	2.13114600	-0.33417700	-0.18429200
O	2.49615100	-1.49528200	-0.13468600
H	0.82504100	-0.65700400	-1.85567200
N	-3.03388600	-0.78608400	-0.21291700
H	-3.77227400	-0.25522100	-0.68257900
H	-3.14613600	-1.77282700	-0.46074100
H	-3.15931100	-0.69197500	0.80060900
H	-1.54962500	-0.39437900	-1.66673800
N	2.70415300	0.65481200	0.57209000
H	3.54413800	0.39166100	1.06984900
H	2.63803100	1.62241400	0.29869500

Name: 3-3 exo

Imaginary Frequency: 373.84 cm^{-1}

Coordinates:

	X	Y	Z
C	-2.30789600	-1.02019900	0.24631800
C	-1.79208800	0.15357700	0.82437700
C	-1.02938600	-0.07110100	-1.37370800
C	-1.78354100	-1.17948900	-1.05331100
C	-1.32742500	0.99505200	-0.35853800
H	-2.25769200	1.46553100	-0.72192800
C	-0.02375100	-0.44939100	1.56728200

H	-0.43939800	-1.17288300	2.25624200
C	0.81217900	-0.94234300	0.55277300
H	0.75595100	-1.99243800	0.29267600
H	-2.24903600	0.60957000	1.69657900
H	-0.50423900	0.09857700	-2.30502900
H	-1.92274100	-2.04793200	-1.68268200
H	-2.93879500	-1.73628900	0.75664200
C	1.94654400	-0.24315300	0.04413100
O	2.07617100	1.05170800	0.08020200
N	-0.31369100	2.03723200	-0.11620000
H	1.13973300	1.49953600	0.11391900
H	-0.23571000	2.63224400	-0.94009700
H	-0.62614000	2.65190500	0.63377300
H	0.24855900	0.48624200	2.04507500
N	2.97675000	-0.90459400	-0.48563600
H	3.04224500	-1.90880600	-0.43261500
H	3.76867600	-0.38511100	-0.83727600

Name: 3-4 endo

Imaginary Frequency: 480.05 cm^{-1}

Coordinates:

	X	Y	Z
C	1.60804500	1.26780500	0.24103200
C	1.97626500	-0.01637800	0.68511200
C	0.84529000	-0.19819100	-1.32484000
C	0.89928700	1.14726900	-0.96271200

C	0.17053800	-0.76661500	1.45153800
H	-0.06874600	0.00281400	2.17526100
C	-0.64958800	-0.95675700	0.33412200
H	2.68168000	-0.18314400	1.49076000
H	0.40770700	-0.57931200	-2.23765700
H	0.38185900	1.95078900	-1.46993100
H	1.73955000	2.18337600	0.80460300
H	0.64533700	-1.63590400	1.89217800
C	-1.83828400	-0.13929700	-0.00093000
O	-2.69285600	-0.53595800	-0.78400900
H	-0.68493700	-1.92769400	-0.14284800
N	-1.97203900	1.07333700	0.64276300
H	-1.17293300	1.52136400	1.06125600
H	-2.70086700	1.67563300	0.29110200
C	1.90853400	-0.91241900	-0.53484300
H	1.73603900	-1.97039300	-0.34535800
H	2.86190600	-0.81573000	-1.07750400

Name: 3-4 exo

Imaginary Frequency: 465.75 cm^{-1}

Coordinates:

	X	Y	Z
C	-2.45183900	0.14336500	-0.47673600
C	-1.77892000	-0.92129600	0.16054200
C	-0.77508100	1.07780900	0.74086300
C	-1.80961100	1.34468800	-0.15317500

C	-0.16153000	-1.18603700	-1.05652200
H	-0.68884600	-1.33284900	-1.98985400
C	0.64618300	-0.05108800	-0.91182900
H	0.57017100	0.75806800	-1.62801800
H	-2.19630400	-1.91938900	0.22978200
H	-0.12981300	1.81818200	1.19476500
H	-2.01806500	2.30735500	-0.60262900
H	-3.23720300	0.03254900	-1.21393300
C	1.85199600	-0.09097700	-0.06540500
O	2.07743900	-0.97072900	0.76204500
H	0.19143800	-2.09658700	-0.58419200
N	2.72901600	0.96392800	-0.22865500
H	2.67910800	1.54433400	-1.05028400
H	3.63051000	0.86622900	0.21278800
C	-0.98605300	-0.30089900	1.29163700
H	-1.65073400	-0.22282100	2.16662100
H	-0.08375600	-0.83013500	1.59291800

Name: 3-1 endo (DCM)

Imaginary Frequency: 447.14 cm^{-1}

Coordinates:

	X	Y	Z
C	1.04849200	1.48829200	-0.61495800
C	1.41767800	0.93435900	0.61544000
C	0.70040500	-0.75802900	-0.83015900
C	0.58588200	0.46172700	-1.47011600

C	1.62093700	-0.55378900	0.35509000
C	-0.38909000	0.58776200	1.59168500
H	-0.81191200	1.57891100	1.49662100
C	-0.98507300	-0.49391900	0.93511200
H	1.98596800	1.46390600	1.36948300
H	0.47224100	-1.72954200	-1.24516100
H	0.12061400	0.61800100	-2.43361600
H	1.00095500	2.54717300	-0.82903000
H	0.09714300	0.40312300	2.54296000
C	-2.16115800	-0.39954600	0.05143400
O	-2.76452600	-1.41764300	-0.27807400
H	-0.79180300	-1.50240700	1.28413400
C	-2.64582300	0.96327100	-0.39157800
H	-3.16514600	1.44967300	0.44094100
H	-1.82496700	1.62070700	-0.68670100
H	-3.34414400	0.84927500	-1.21969000
N	3.07026100	-0.79439900	-0.08368000
H	3.72637300	-0.57096400	0.66917000
H	3.21943300	-1.77420000	-0.33795800
H	3.30986000	-0.21759800	-0.89477700
H	1.47626200	-1.21489300	1.20228000

Name: 3-1 exo (DCM)

Imaginary Frequency: 322.03 cm^{-1}

Coordinates:

	X	Y	Z
C	-2.17620500	-1.17274400	0.20440100

C	-1.83109500	0.03146800	0.81138800
C	-1.13499800	0.00872000	-1.43378700
C	-1.68622000	-1.20439600	-1.13320200
C	-1.44037400	0.96848600	-0.32039200
H	-2.40060700	1.43044300	-0.61109300
C	0.03005500	-0.47967000	1.63832200
H	-0.39051200	-1.20919400	2.31701600
C	0.94192900	-0.93940000	0.67900000
H	0.97383000	-2.00136600	0.46996500
H	-2.29517700	0.39044500	1.72182600
H	-0.66289400	0.29258500	-2.36498800
H	-1.73311100	-2.05986000	-1.79218900
H	-2.68973100	-1.98887500	0.69555000
C	1.93681800	-0.16709700	0.06507600
O	1.95650000	1.13516200	0.07371100
N	-0.45271700	2.02325100	-0.03853100
H	0.98579300	1.53591500	0.16534000
H	-0.40308900	2.65783600	-0.83423700
H	-0.77409100	2.59096500	0.74363400
H	0.16399200	0.50565000	2.07004200
C	3.10843600	-0.80494800	-0.60674100
H	3.18655000	-0.44186000	-1.63515100
H	4.02250200	-0.49820500	-0.08864500
H	3.04347700	-1.89105000	-0.60142900

Name: 3-2 endo (DCM)

Imaginary Frequency: 450.83 cm⁻¹

Coordinates:

	X	Y	Z
C	1.08608200	1.59268100	0.25982900
C	1.67993400	0.55933400	0.98951000
C	1.00033600	-0.23828800	-1.10135400
C	0.65222600	1.09428000	-0.99002100
C	2.02875100	-0.52106200	-0.02742600
C	0.06265300	-0.54677400	1.71170100
H	-0.46902300	0.26710700	2.18335600
C	-0.49879200	-1.17199600	0.59807900
H	2.26838700	0.71013500	1.88566100
H	0.84637400	-0.87712500	-1.95956100
H	0.04963900	1.64269600	-1.70050300
H	0.87225400	2.58017900	0.64438200
H	0.68033600	-1.13939100	2.37643900
O	-2.37542900	-1.38555100	-0.84974000
H	-0.21331400	-2.18090500	0.32914000
N	3.42864200	-0.24576300	-0.59079300
H	4.14695000	-0.33188700	0.13277000
H	3.66365200	-0.90712900	-1.33519800
H	3.48193600	0.69969900	-0.97986300
H	2.07391400	-1.53801600	0.34673800
C	-1.74445900	-0.72643300	-0.04220300
O	-2.12975300	0.50047300	0.36727400
C	-3.34245200	1.02304600	-0.21335300

H	-4.18651700	0.37615200	0.02664800
H	-3.47712800	2.00538900	0.23271000
H	-3.24217900	1.10532300	-1.29601200

Name: 3-2 exo (DCM)

Imaginary Frequency: 426.76 cm⁻¹

Coordinates:

	X	Y	Z
C	-2.69068600	-1.02458900	0.12362900
C	-2.27600100	0.22738400	0.61271000
C	-1.08001300	-0.31526800	-1.32258600
C	-1.92932800	-1.36323600	-1.00840100
C	-1.62088100	0.88135600	-0.58910200
H	-2.44364700	1.27903700	-1.19627100
C	-0.58184500	-0.26245000	1.66136200
H	-1.09258000	-0.93279500	2.33811500
C	0.34361400	-0.80773900	0.76473300
H	0.35445600	-1.87238400	0.57930100
H	-2.85105300	0.80016800	1.33056200
H	-0.40665300	-0.26180600	-2.16697900
H	-1.94558100	-2.32098300	-1.50969900
H	-3.39655400	-1.67573400	0.62054700
C	1.54120700	-0.09445500	0.35440200
O	1.68656800	1.13594000	0.38012800
N	-0.70147800	2.03848100	-0.34985100
H	0.24030500	1.75716300	0.05785700

H	-0.50746700	2.51879300	-1.23129900
H	-1.13709100	2.72747000	0.26710000
H	-0.37015200	0.71166000	2.09152400
O	2.51339600	-0.90826700	-0.06198800
C	3.74747300	-0.29574000	-0.50341300
H	4.19734500	0.27392300	0.30901000
H	4.38854200	-1.12465300	-0.79073500
H	3.55953200	0.35780900	-1.35520700

Name: 3-3 endo (DCM)

Imaginary Frequency: 461.24 cm⁻¹

Coordinates:

	X	Y	Z
C	1.02808800	1.37944100	-0.81784900
C	1.44364700	1.01354500	0.46453700
C	0.65069400	-0.86852400	-0.67090300
C	0.52860500	0.24075900	-1.49003400
C	1.62255700	-0.49870300	0.42954200
C	-0.37590100	0.78948300	1.54113600
H	-0.76275200	1.78398500	1.36161900
C	-0.98823700	-0.33598900	0.99079700
H	2.02458300	1.64556900	1.12392200
H	0.41495200	-1.88998900	-0.93422400
H	0.02871800	0.25538000	-2.44820600
H	0.97549200	2.39441800	-1.18728200
H	0.12883500	0.68634400	2.49454200

C	-2.16674100	-0.33043600	0.08742400
O	-2.79075800	-1.37090500	-0.13781000
H	-0.84475100	-1.30122700	1.45995900
N	3.04908900	-0.82415500	-0.03314400
H	3.74375000	-0.50117800	0.64488000
H	3.17892100	-1.83281200	-0.14716100
H	3.24941800	-0.37628700	-0.93189800
H	1.51223500	-1.02166100	1.37351200
N	-2.52710800	0.85116600	-0.47959400
H	-2.08987400	1.72867200	-0.25441200
H	-3.34360400	0.86949600	-1.07151000

Name: 3-3 exo (DCM)

Imaginary Frequency: 442.01 cm^{-1}

Coordinates:

	X	Y	Z
C	-2.36514200	-0.93118000	0.26304200
C	-1.83540200	0.27614600	0.75265900
C	-0.84926400	-0.25201700	-1.29702900
C	-1.73264200	-1.26263000	-0.94666400
C	-1.25781600	0.94339200	-0.47960300
H	-2.11089100	1.40010800	-0.99733900
C	-0.05824300	-0.35554600	1.59830300
H	-0.53721900	-1.03737700	2.28644500
C	0.73207800	-0.88776500	0.57485400
H	0.65598300	-1.94315100	0.34780500

H	-2.29893200	0.84728200	1.54824900
H	-0.26045600	-0.19951800	-2.20278800
H	-1.85080700	-2.19615100	-1.47942500
H	-3.05620800	-1.56448100	0.80213600
C	1.93662100	-0.20844200	0.09155600
O	2.09074600	1.03726700	0.16562200
N	-0.26327500	2.04033300	-0.28070400
H	0.71863700	1.68208600	0.01002700
H	-0.13909300	2.56054700	-1.15143900
H	-0.60108300	2.70997900	0.41277900
H	0.24996000	0.58051200	2.05332900
N	2.90316100	-0.97581600	-0.44571900
H	2.84841900	-1.98186600	-0.44793100
H	3.75538100	-0.53947800	-0.76457700

Name: 3-4 endo (DCM)

Imaginary Frequency: 467.12 cm^{-1}

Coordinates:

	X	Y	Z
C	1.57416000	1.23875000	0.36613800
C	1.93308300	-0.08341000	0.70395900
C	0.89782000	-0.07011900	-1.36701400
C	0.91346800	1.23022700	-0.87111200
C	0.17645900	-0.87786500	1.37757600
H	-0.06849100	-0.17925300	2.16849700
C	-0.66601000	-0.99424600	0.26214300

H	2.62529200	-0.31396000	1.50523500
H	0.48804100	-0.37227600	-2.32135600
H	0.40800900	2.07682000	-1.31674000
H	1.67227300	2.09671900	1.01955500
H	0.64694800	-1.78283700	1.74528000
C	-1.83291100	-0.14308900	-0.01123500
O	-2.70080000	-0.47054600	-0.83269700
H	-0.68522800	-1.91971900	-0.29830100
N	-1.96314800	1.01507700	0.71126500
H	-1.17681700	1.40856700	1.20400700
H	-2.67130900	1.66462000	0.40298500
C	1.91724800	-0.86111300	-0.59790100
H	1.73407300	-1.93089100	-0.51790700
H	2.89573800	-0.72376800	-1.08386800

Name: 3-4 exo (DCM)

Imaginary Frequency: 456.17 cm^{-1}

Coordinates:

	X	Y	Z
C	-2.44357800	0.11993700	-0.48645400
C	-1.76813400	-0.92063600	0.18921200
C	-0.79109400	1.10768300	0.72222000
C	-1.81409200	1.33666900	-0.19392100
C	-0.16740400	-1.22992000	-1.00528200
H	-0.69453500	-1.40957000	-1.93300800
C	0.65202100	-0.09609200	-0.91214800

H	0.56844600	0.68800500	-1.65414900
H	-2.18448900	-1.91624100	0.29068800
H	-0.15642000	1.86820600	1.15757200
H	-2.02407400	2.28251900	-0.67689000
H	-3.21888500	-0.02069400	-1.22902600
C	1.86028500	-0.08913900	-0.07742700
O	2.12793800	-0.96627100	0.75657800
H	0.17838500	-2.12809000	-0.50496200
N	2.72437000	0.95273700	-0.29318300
H	2.46014200	1.74489600	-0.85655200
H	3.50947800	1.05916000	0.33042500
C	-0.99179800	-0.25723600	1.30845200
H	-1.66223100	-0.16571700	2.17734800
H	-0.08714800	-0.76906600	1.63030400