Electronic Supplementary Information

A Simple Topology-based Model for Predicting Activation Barriers of Reactive Processes at 0 K

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Optimized Cartesian coordinates for minima and transition state structures associated with reactions listed in Table 1 of the manuscript.

System 1 (UωB97X-D/6-311+G(d,p))

Reactant

C	0.10204700	-0.76956400	-0.79893300
C	1.39761900	-0.60432500	-0.56983900
H	-0.42651100	-0.17521900	-1.53684400
H	-0.48292100	-1.50585500	-0.25781300
H	1.92501000	-1.19811200	0.16963500
H	1.98148800	0.13355200	-1.11037400

C	-1.39981500	1.28297500	1.27822000
H	-0.86746700	2.07029900	0.76359800
H	-2.40989600	1.03072900	0.98573900
H	-0.90862600	0.72709100	2.06424700

Product

C	-0.29083200	-0.32977500	-0.35991700
C	1.19552300	-0.40503900	-0.36755900
H	-0.65456700	-0.04375600	-1.35282000
H	-0.71279000	-1.31641400	-0.13971400
H	1.72254700	-1.04874200	0.32778400
H	1.78394100	0.29218100	-0.95342900
C	-0.83833700	0.67779800	0.67085700
H	-0.46956300	1.68601200	0.46482400
H	-1.93152000	0.70218100	0.64392200
H	-0.52811600	0.40741500	1.68357600

Transition state

C	0.48981100	0.64583900	0.00003700
C	1.38508200	-0.36927100	-0.00001100
H	0.24590600	1.16492000	0.92016400
H	0.24606200	1.16523600	-0.91995500
H	1.73486000	-0.81448400	-0.92491500
H	1.73469000	-0.81470200	0.92485300
C	-1.62981400	-0.23785000	-0.00002800
H	-1.61132100	-0.80675200	0.92140900
H	-2.20912800	0.67917000	0.00057900
H	-1.61154200	-0.80569600	-0.92212000

System 2 (B3LYP/6-31G(d,p))

Reactant

C	-1.18972800	0.33737500	-0.47836500
C	-0.07409800	1.18308700	-1.02852500
C	0.62062500	0.92230000	-2.13583400
C	-0.90604800	-0.19998000	0.94725800
C	0.22286000	-1.19285200	0.99524400
C	1.34831900	-1.05136900	1.69532200
H	-1.38738200	-0.50367900	-1.15610300
H	-2.11390600	0.93276500	-0.43856800
H	0.17224800	2.07404200	-0.44727500
H	1.41917200	1.57480600	-2.47892500
H	0.41705600	0.04334600	-2.74463100
H	-0.69114200	0.63989000	1.62120400
H	-1.82589400	-0.67449800	1.31994400
H	0.08633400	-2.09098600	0.38939200
H	2.12902900	-1.80736900	1.68510300
H	1.53336000	-0.17116900	2.30821900

Product

C	-1.34838700	1.05097500	-1.69552300
C	-0.22293200	1.19264200	-0.99547700
C	0.90602300	0.19983200	-0.94731000
C	-0.62054600	-0.92190400	2.13603600
C	0.07416100	-1.18287700	1.02876000
C	1.18974800	-0.33722900	0.47841500
H	-1.53339000	0.17065100	-2.30825400
H	-2.12913200	1.80694100	-1.68544300
H	-0.08644400	2.09089600	-0.38979500
H	1.82584200	0.67432000	-1.32010200
H	0.69114800	-0.64018100	-1.62108800
H	-0.41699500	-0.04282600	2.74466100
H	-1.41906000	-1.57437400	2.47927000

H	-0.17216500	-2.07395200	0.44768700
H	2.11394900	-0.93259000	0.43872000
H	1.38737900	0.50396700	1.15598200

Transition state

C	0.95080100	1.21801500	-0.25476600
C	1.43198800	-0.00041000	0.25999400
C	0.94984600	-1.21898300	-0.25373300
C	-0.94978500	1.21885700	0.25482700
C	-1.43195400	0.00083100	-0.26012000
C	-0.95104700	-1.21813600	0.25376200
H	0.81392500	1.29909900	-1.33164100
H	1.31286200	2.14470800	0.19025700
H	1.82458400	-0.00001600	1.27738700
H	1.30979900	-2.14559800	0.19318000
H	0.81426800	-1.30145800	-1.33068800
H	-0.81303800	1.29965600	1.33173600
H	-1.31044200	2.14606900	-0.19022600
H	-1.82416200	0.00161600	-1.27766400
H	-1.31132700	-2.14473700	-0.19287300
H	-0.81556100	-1.30037600	1.33075100

System 3 (M06-2X/6-31+G(d))

Reactant

C	-2.81962200	-0.79453500	0.57670300
C	-2.71986300	-1.05959200	-0.74069000
C	-2.57391800	0.20321500	-1.47648900
C	-2.58620600	1.22895700	-0.60226200
H	-2.93571200	-1.51651900	1.37716500
H	-2.73941100	-2.04196100	-1.20083800

H	-2.47598000	0.28048000	-2.55407600
H	-2.50627500	2.28388900	-0.83930600
C	0.57982600	-0.61795300	0.68572500
C	0.65245900	0.51073500	-0.01963300
C	-2.75174600	0.69063400	0.79035500
H	-3.66202700	1.07663700	1.27094800
H	-1.91074800	0.96875200	1.44195700
C	0.52026300	-1.98773400	0.06825600
O	2.11701300	2.35490500	0.64193500
O	1.68828100	-2.74408900	0.32891600
C	2.69315500	2.50939500	-0.63277400
C	2.83760800	-2.22905200	-0.30349100
H	2.86881100	1.54068900	-1.12036400
H	2.05469900	3.12533000	-1.28500500
H	3.65057100	3.01323200	-0.49102500
H	3.64617300	-2.93710100	-0.11562600
H	2.67976500	-2.14050700	-1.38959500
H	3.11636600	-1.24449300	0.09345100
C	0.78447000	1.87412500	0.60712300
H	-0.30388400	-2.56903400	0.49055000
H	0.35797300	-1.89877000	-1.01928800
H	0.62352500	0.45609200	-1.10930100
H	0.61313300	-0.58052500	1.77669800
H	0.14870800	2.59925500	0.07197400
H	0.46496400	1.84023400	1.65291600

Product

C	-1.87590600	-0.78036400	0.71012000
C	-2.40636500	-1.07160700	-0.68698700
C	-2.26909700	0.05134300	-1.40254500
C	-1.66206100	1.10010000	-0.48994500

H	-2.18033900	-1.47462000	1.49671600
H	-2.72343500	-2.04425200	-1.04753200
H	-2.44909000	0.18262000	-2.46485800
H	-1.78436200	2.13878200	-0.80777200
C	-0.31674600	-0.64613800	0.56803600
C	-0.16803500	0.68363000	-0.24277200
C	-2.29779900	0.68949400	0.85564100
H	-3.38388600	0.81840600	0.86072100
H	-1.86128200	1.18539700	1.72911700
C	0.25850800	-1.93326600	-0.04728100
O	1.95253200	1.67781400	0.59821300
O	1.56504800	-2.27426200	0.34932200
C	2.64241900	2.04761400	-0.57197900
C	2.56469200	-1.45340300	-0.20915000
H	2.38766100	1.40341200	-1.42514500
H	2.42553400	3.09098600	-0.84027600
H	3.70892600	1.94570800	-0.36111600
H	3.52583500	-1.91340900	0.03030900
H	2.45815900	-1.40140300	-1.30522700
H	2.53084000	-0.44213800	0.20954100
C	0.55061900	1.81832200	0.49836400
H	-0.35777000	-2.77988900	0.27695600
H	0.20256400	-1.88282200	-1.14790600
H	0.33392200	0.50758900	-1.20351400
H	0.12779500	-0.52845600	1.56589200
H	0.32024600	2.77664500	0.00319200
H	0.19041800	1.88298000	1.52988600

Transition state

C	-2.32648800	0.50000100	-0.73100600
C	-2.66633400	0.70880700	0.60649100

C	-2.37786500	-0.45993800	1.33274400
C	-1.86153400	-1.41681800	0.46122000
H	-2.54334400	1.19681200	-1.53505200
H	-2.97258100	1.65628700	1.03683100
H	-2.42464700	-0.55587800	2.41223600
H	-1.65575900	-2.44711400	0.73457200
C	-0.12333900	0.61492400	-0.59551200
C	0.18996000	-0.51205800	0.15227000
C	-2.23971500	-0.98768000	-0.93135500
H	-3.25705100	-1.36163400	-1.13305200
H	-1.58905600	-1.32312100	-1.73929400
C	-0.00328300	2.00865700	-0.02290300
O	2.25957500	-1.57248200	-0.60451000
O	1.24905100	2.61438400	-0.27995200
C	2.94901700	-1.69713300	0.61576500
C	2.34415200	1.95351500	0.31104300
H	2.69449300	-0.89138500	1.31882200
H	2.73239900	-2.66431200	1.09383900
H	4.01534400	-1.64208000	0.38823500
H	3.21051200	2.60593600	0.18480600
H	2.17085600	1.79181700	1.38753700
H	2.54069400	0.98618400	-0.16765100
C	0.85265000	-1.71701200	-0.47377900
H	-0.73417100	2.69046900	-0.46704300
H	-0.18539200	1.96689600	1.06520900
H	0.36768200	-0.37565300	1.21845200
H	0.00565700	0.55473600	-1.67809500
H	0.64491400	-2.63381600	0.10048600
H	0.48712100	-1.86095200	-1.49500800

System 4 (M06-2X/6-31+G(d))

Reactant

C	2.16900000	-0.89348300	0.09866300
C	2.34487600	0.41808800	-0.18356500
C	1.73366800	0.71717300	-1.47882200
C	1.18636800	-0.41269000	-1.98351400
H	2.51659100	-1.41874600	0.98145300
H	2.84558700	1.14650800	0.44478200
H	1.71921900	1.69767600	-1.94203200
H	0.66999500	-0.51522500	-2.93162500
C	-0.59972000	0.04382400	1.06123900
C	-1.17243600	1.65734100	-0.67243700
C	-1.82722200	-0.69745500	-0.90889300
N	-1.19603800	2.73509100	-1.09107200
N	-2.36730600	-1.51937200	-1.51774300
C	-1.16744700	0.32267700	-0.14294500
C	1.45461900	-1.55446500	-1.04524000
H	2.10634200	-2.30039100	-1.52502700
H	0.55247500	-2.10670200	-0.74706100
C	0.01664900	1.07324200	1.85007900
C	-0.63804700	-1.28146900	1.61322700
N	-0.68062500	-2.34773400	2.05955200
N	0.49512300	1.90404700	2.49674800

Product

C	1.61577700	-0.67685900	0.35135600
C	2.29753900	0.55935200	-0.20016400
C	1.73894600	0.83247800	-1.38391900
C	0.67600600	-0.21713800	-1.63938200
H	2.11638400	-1.21192900	1.15814300
H	3.02080000	1.15565700	0.34356500
H	1.90936000	1.69917700	-2.01171600

H	0.31333000	-0.33011700	-2.66091300
C	0.15712900	-0.21452000	0.78729600
C	-0.94624200	1.51419300	-0.76818700
C	-1.65855800	-0.76202300	-0.93519900
N	-1.25047200	2.61847600	-0.91485000
N	-2.51950200	-1.47328400	-1.22959700
C	-0.51646400	0.11566800	-0.64016700
C	1.27984600	-1.44351600	-0.93735900
H	2.17815800	-1.80031500	-1.44391000
H	0.57644200	-2.27092500	-0.79646600
C	0.21056500	0.94645200	1.68519100
C	-0.51825500	-1.32144600	1.48031800
N	-0.98323200	-2.22735900	2.02520800
N	0.30924800	1.85259500	2.39418400

Transition state

C	0.40891600	1.15013100	1.51942400
C	1.72653600	0.69790400	1.36484400
C	1.72637500	-0.70045400	1.36430400
C	0.40869100	-1.15248100	1.51863400
H	0.11977400	2.19098400	1.62554300
H	2.58172900	1.32732800	1.14736500
H	2.58142600	-1.32990200	1.14636700
H	0.11918000	-2.19336600	1.62345300
C	-0.29113900	0.71368100	-0.56259200
C	0.73246800	-1.40968200	-1.30106000
C	-1.54098200	-1.41385200	-0.42185600
N	1.57234300	-1.96804400	-1.86808900
N	-2.53890700	-1.97841400	-0.26452200
C	-0.29073800	-0.71295500	-0.56394400
C	-0.40919000	-0.00127600	2.02788100

H	-0.33676500	-0.00165800	3.12690300
H	-1.47021500	-0.00111200	1.77073400
C	0.73117900	1.41267200	-1.29880200
C	-1.54195300	1.41340400	-0.41907800
N	-2.54027700	1.97692200	-0.26058000
N	1.57025500	1.97313000	-1.86493700

System 5 (M06-2X/6-31+G(d))

Reactant

C	0.22166100	0.66689700	-1.64460000
C	0.22165600	-0.66692800	-1.64458800
C	2.50670100	-1.17699800	0.51896600
C	1.60098300	-0.73336700	1.41510400
C	1.60098800	0.73337900	1.41509200
H	2.73424400	-2.21188000	0.29008600
H	0.95641600	-1.35251300	2.03054800
H	0.95642400	1.35253900	2.03052500
C	2.50670900	1.17698800	0.51894700
H	2.73425900	2.21186500	0.29004900
C	-0.75366200	1.14479200	-0.60500100
C	-0.75367000	-1.14479800	-0.60498100
O	-1.05853400	-2.28104000	-0.32539400
O	-1.05851700	2.28104100	-0.32543400
H	0.78930300	1.36077000	-2.25130500
H	0.78929200	-1.36081700	-2.25128200
C	3.19601200	-0.00001200	-0.11298600
H	3.11460600	-0.00002100	-1.20848300
H	4.27163100	-0.00001400	0.11688200
N	-1.27282100	0.00000400	-0.00802000
C	-2.31831000	0.00001700	1.00026100

H	-2.16535200	-0.88928200	1.61799300
H	-2.16534200	0.88932200	1.61798200
C	-3.70895500	0.00002200	0.37358400
H	-4.47737300	0.00003200	1.15239200
H	-3.84639800	0.89038900	-0.24689200
H	-3.84640900	-0.89035100	-0.24688100

Product

C	0.71715400	0.77162500	-0.93341100
C	0.71714900	-0.77164800	-0.93339700
C	1.98540600	-1.12924900	-0.07976700
C	1.70294600	-0.66960800	1.34063600
C	1.70295100	0.66961900	1.34062400
H	2.31798000	-2.15988700	-0.20223300
H	1.43674600	-1.32830000	2.16039200
H	1.43675500	1.32832800	2.16036800
C	1.98541400	1.12923200	-0.07978700
H	2.31799500	2.15986600	-0.20227200
C	-0.59682000	1.16352800	-0.28579700
C	-0.59682800	-1.16353100	-0.28577700
O	-1.00400000	-2.28183600	-0.06291500
O	-1.00398400	2.28184000	-0.06295500
H	0.78284300	1.21933400	-1.92872000
H	0.78283500	-1.21937500	-1.92869800
C	2.92633000	-0.00001600	-0.55274800
H	3.09414900	-0.00002600	-1.63600300
H	3.88309300	-0.00001500	-0.02399800
N	-1.27777000	0.00000400	0.05329800
C	-2.54614600	0.00001600	0.76808600
H	-2.55188300	-0.89148000	1.40044300
H	-2.55187200	0.89151800	1.40043500

C	-3.73360300	0.00001900	-0.18743800
H	-4.67075800	0.00002800	0.37695200
H	-3.71303900	0.89077400	-0.82195300
H	-3.71305100	-0.89074300	-0.82194500

Transition state

C	0.55688000	0.69292600	-1.26301900
C	0.55688200	-0.69292800	-1.26301900
C	2.17686000	-1.15559300	0.22408900
C	1.54809000	-0.70388500	1.38128300
C	1.54808800	0.70389000	1.38128200
H	2.38652300	-2.19704800	0.00534000
H	1.02622800	-1.33269900	2.09446000
H	1.02622400	1.33270300	2.09445800
C	2.17685600	1.15559800	0.22408700
H	2.38651700	2.19705300	0.00533700
C	-0.61878300	1.15202000	-0.46817200
C	-0.61878000	-1.15202500	-0.46817100
O	-1.01697700	-2.28026900	-0.27174700
O	-1.01698300	2.28026300	-0.27174800
H	1.00562400	1.34868400	-1.99781600
H	1.00562800	-1.34868500	-1.99781500
C	2.96393700	0.00000300	-0.33785300
H	3.10730100	0.00000300	-1.41964200
H	3.95676200	0.00000500	0.13942500
N	-1.20243400	-0.00000300	0.05869200
C	-2.38588200	-0.00000400	0.90085700
H	-2.32749200	-0.89027400	1.53306800
H	-2.32748700	0.89025900	1.53307900
C	-3.66896900	0.00000500	0.07634400
H	-4.54313800	0.00000400	0.73452600

H	-3.71251800	0.89090100	-0.55676700
H	-3.71252400	-0.89088400	-0.55677700

System 6 (M06-2X/6-31+G(d))

Reactant

C	0.44347200	-0.76499100	-1.70825400
C	0.40360200	0.56662500	-1.75094700
C	-1.91966100	1.45877500	0.81057700
C	-0.95531100	0.72461900	1.38629300
C	-1.04411100	-0.74024700	1.40449500
H	-1.85366800	2.54407100	0.80077800
H	-0.09266200	1.20668700	1.84122800
H	-0.35342400	-1.30414100	2.02743000
C	-1.92778100	-1.37924600	0.62105300
C	1.36280000	-1.18082900	-0.59454400
C	1.29992100	1.10792600	-0.67067700
O	1.53669700	2.26188800	-0.40244000
O	1.66544900	-2.29710500	-0.24392100
H	-0.15148700	1.22358000	-2.40818900
C	-3.15673300	0.79136500	0.26026700
C	-2.85252600	-0.60676800	-0.28792200
H	-1.95100600	-2.46620100	0.59290700
H	-0.07197900	-1.49354400	-2.32106200
H	-3.78513300	-1.15808900	-0.44571700
H	-2.37565000	-0.51797600	-1.27717200
H	-3.62081300	1.40750300	-0.51629000
H	-3.89266500	0.71294400	1.07630900
N	1.83340500	-0.00358200	-0.02282900
C	2.72123300	0.04494400	1.11735900
H	3.62359100	-0.53630800	0.91507800

H	2.98044800	1.09094000	1.28874900
H	2.22715900	-0.36478400	2.00371900

Product

C	-0.27198400	-0.77193600	-0.82565800
C	-0.27219100	0.76840300	-0.82912600
C	-1.37010000	1.29390500	0.13170900
C	-1.14140700	0.67127300	1.48805900
C	-1.14198300	-0.66688100	1.49040500
H	-1.34171800	2.38556100	0.16120000
H	-0.98674000	1.27948500	2.37454400
H	-0.98785700	-1.27213400	2.37902200
C	-1.37052900	-1.29399800	0.13618400
C	1.11545900	-1.15723500	-0.33974000
C	1.11521800	1.16227900	-0.34758600
O	1.53432000	2.28471800	-0.17772400
O	1.54498300	-2.27394300	-0.15537100
H	-0.42572500	1.19386900	-1.82672500
C	-2.72165800	0.77449600	-0.41603300
C	-2.72175700	-0.77621900	-0.41390200
H	-1.34230300	-2.38556100	0.16950700
H	-0.42381400	-1.20129400	-1.82185100
H	-3.53332300	-1.16375900	0.20835700
H	-2.87405700	-1.17001300	-1.42549200
H	-2.87478400	1.16558900	-1.42854400
H	-3.53264500	1.16379300	0.20588900
N	1.83893200	0.00203200	-0.10550300
C	3.18388700	-0.01582800	0.43408000
H	3.83443900	-0.60422000	-0.21624300
H	3.53179800	1.01602300	0.48970700
H	3.17823000	-0.46676800	1.42964900

Transition state

C	-0.05109100	-0.68642400	-1.21773300
C	-0.05458400	0.69473200	-1.21318600
C	-1.51610000	1.36261400	0.41759900
C	-0.92384000	0.69798100	1.47178700
C	-0.92069400	-0.71385600	1.46569400
H	-1.36986200	2.43654000	0.32039500
H	-0.26709100	1.23437100	2.15192000
H	-0.26145600	-1.25333900	2.14112700
C	-1.51036400	-1.37260200	0.40642400
C	1.17099600	-1.14544600	-0.49626300
C	1.16475200	1.15932200	-0.49006000
O	1.56668600	2.29002100	-0.31947900
O	1.58702800	-2.27170400	-0.32703500
H	-0.56265700	1.35295100	-1.90575600
C	-2.71663200	0.77069300	-0.28454100
C	-2.71335300	-0.78016500	-0.29099400
H	-1.35934700	-2.44506300	0.30067800
H	-0.55545600	-1.34220700	-1.91531600
H	-3.60074400	-1.14623800	0.23902900
H	-2.79168700	-1.17147100	-1.31023700
H	-2.79695000	1.17012000	-1.30046500
H	-3.60543200	1.12849900	0.24876300
N	1.78459900	0.00576200	-0.00673000
C	2.99623300	-0.00848900	0.78293800
H	3.77706900	-0.56796200	0.26199200
H	3.30817300	1.02725500	0.92516000
H	2.81160300	-0.48048900	1.75194400

System 7 (ωB97X-D/6-31+G(d,p))

Reactant

C	-0.74146800	-0.64082000	-0.05480300
C	0.74429400	-0.63709800	0.05958100
C	1.37800000	0.65718000	0.32257700
C	0.69746800	1.81152700	0.18684100
C	-0.70548600	1.80696400	-0.20038300
C	-1.38090200	0.64863100	-0.32747000
H	2.43548100	0.66095900	0.57165800
H	1.19570300	2.76304600	0.34396700
H	-1.20793900	2.75506000	-0.36461600
H	-2.43838500	0.64586900	-0.57655300
C	-1.48800500	-1.74359500	0.14522800
C	1.49573100	-1.73801100	-0.13218900
H	-2.56660500	-1.71307400	0.02422100
H	-1.05147200	-2.68670900	0.45602000
H	1.06341400	-2.68536100	-0.43591000
H	2.57418400	-1.70178200	-0.01142900

Product

C	-0.68796100	-0.47798100	-0.09285700
C	0.69011400	-0.47404100	0.09640200
C	1.42140100	0.69758800	0.19676000
C	0.68859800	1.88777800	0.09115800
C	-0.69732500	1.88381000	-0.10528300
C	-1.42463700	0.68948900	-0.20196200
H	2.49669100	0.71530800	0.34729200
H	1.20549300	2.84035700	0.16172700
H	-1.21863700	2.83342200	-0.18296800
H	-2.49999400	0.70115300	-0.35260400
C	-0.77652900	-1.99416100	-0.09374500

C	0.78581100	-1.98972800	0.10868600
H	-1.11534500	-2.44800900	-1.02966200
H	-1.33959200	-2.43022200	0.73669600
H	1.35092600	-2.42938000	-0.71846100
H	1.12673400	-2.43492500	1.04798700

Transition state

C	0.51657300	-0.70672000	0.01699700
C	0.51663700	0.70661800	-0.01713000
C	-0.68638200	1.42366200	0.17312000
C	-1.86003600	0.70259300	0.10968700
C	-1.86012100	-0.70241100	-0.10965700
C	-0.68655900	-1.42362500	-0.17317900
H	-0.69380900	2.50493600	0.27572100
H	-2.81248800	1.21772400	0.19003200
H	-2.81264100	-1.21743800	-0.18987800
H	-0.69412800	-2.50490800	-0.27569200
C	1.84754700	-1.09920600	0.31449000
C	1.84777900	1.09911000	-0.31451200
H	2.28299100	-2.03196600	-0.04757800
H	2.31682300	-0.68148400	1.19480300
H	2.31751200	0.68139400	-1.19458200
H	2.28311000	2.03162900	0.04827500

System 8 (ωB97X-D/6-31+G(d,p))

Reactant

C	1.03470900	-1.53078300	0.09942700
C	1.31407800	-0.26030600	-0.21443400
C	0.51001600	0.92543600	0.11319400
C	-0.82766600	1.02575800	0.15679700

C	-1.83295600	-0.04713400	-0.14104800
H	2.24530300	-0.05687600	-0.74276100
H	1.08367500	1.83046700	0.30681100
H	-1.23866700	1.99916300	0.41963900
H	-2.71975800	0.38049200	-0.61809200
H	-2.17026800	-0.54053700	0.77891500
H	0.15604300	-1.80319900	0.67555100
H	-1.41938800	-0.81899700	-0.79669600
H	1.70335900	-2.33564300	-0.18929900

Product

C	0.88495300	-1.59690900	-0.21886100
C	1.30982600	-0.19268100	0.09422300
C	0.54158200	0.90774100	0.11161000
C	-0.90150500	1.00315100	-0.14942100
C	-1.83784200	0.10642700	0.18209500
H	2.36762000	-0.05636900	0.31332900
H	1.03702300	1.85760600	0.30637500
H	-1.22381200	1.92190200	-0.63898400
H	-2.88284500	0.27878700	-0.05560800
H	-1.59935400	-0.80380900	0.72319100
H	0.67178500	-2.16016900	0.69813400
H	-0.01761500	-1.61887200	-0.83660200
H	1.68274700	-2.13061700	-0.74376500

Transition state

C	1.30250500	-0.90531000	-0.02158700
C	1.20705400	0.50535700	-0.01460800
C	0.00010300	1.18420500	0.15619300
C	-1.20685500	0.50563800	-0.01453800
C	-1.30268600	-0.90529700	-0.02179100

H	2.03927800	1.08904000	-0.40446900
H	0.00019100	2.26821700	0.08922000
H	-2.03914900	1.08964600	-0.40379400
H	-2.17149000	-1.32827400	-0.52731100
H	-1.05619100	-1.45353900	0.88497000
H	1.05550700	-1.45384700	0.88481100
H	-0.00016600	-1.19021600	-0.49850500
H	2.17129000	-1.32857700	-0.52693800

System 9 (ωB97X-D/6-31+G(d,p))

Reactant

C	1.34969500	-0.53231600	0.68263200
C	1.54105800	0.73229900	0.25933400
C	1.00468500	0.87137300	-1.09998800
C	0.49038300	-0.30949100	-1.49512000
H	1.63518900	-0.94390100	1.64296300
H	2.01400200	1.53076200	0.81946500
H	1.02743600	1.78656000	-1.68040300
H	0.02117100	-0.52531000	-2.44716600
C	-2.11722300	0.24713100	1.57978500
H	-1.08930700	0.51381400	1.80836300
H	-2.72717800	-0.12786000	2.39740400
C	-2.60278300	0.37289000	0.34675000
C	0.65425800	-1.31503300	-0.39289500
H	1.23887200	-2.18806600	-0.71283800
H	-0.31809300	-1.69308600	-0.04785500
H	-1.98437700	0.74549000	-0.46487800
H	-3.62876200	0.10558700	0.10782500

Product

C	0.54573700	-0.39342000	0.95908100

C	1.24306700	0.79031800	0.31181200
C	0.75406700	0.91508900	-0.92795400
C	-0.27573400	-0.18361200	-1.12362600
H	1.03973200	-0.82767100	1.82983500
H	1.91998900	1.46738700	0.82096800
H	0.95177800	1.71446800	-1.63350900
H	-0.53261000	-0.42613900	-2.15610400
C	-0.92961700	0.05329700	1.21198200
H	-0.98057400	0.98266200	1.78486600
H	-1.46703100	-0.71663100	1.77484200
C	-1.49795500	0.19866400	-0.22894000
C	0.35243100	-1.30377400	-0.27037100
H	1.29621000	-1.67376300	-0.67990300
H	-0.32868300	-2.14252600	-0.08624200
H	-1.85933900	1.20753900	-0.44363000
H	-2.32552600	-0.49694200	-0.40126500

Transition state

C	0.45955300	1.15362400	0.36036200
C	1.17788000	0.70082700	-0.74582200
C	1.17712400	-0.70266400	-0.74488600
C	0.45796300	-1.15319600	0.36173500
H	0.39833300	2.19166800	0.66814600
H	1.55432300	1.32716900	-1.54630400
H	1.55287200	-1.33046500	-1.54455200
H	0.39626700	-2.19074200	0.67113700
C	-1.61447900	0.69240600	-0.33197500
H	-1.55087300	1.23992700	-1.26500700
H	-2.05791100	1.23807500	0.49552700
C	-1.61425600	-0.69200800	-0.33141000
C	0.37410400	0.00087200	1.32476500

H	1.29211300	0.00050400	1.93398700
H	-0.48312600	0.00189000	1.99864000
H	-1.55078800	-1.24000200	-1.26430600
H	-2.05854700	-1.23719600	0.49611900

System 10 (B3LYP/6-31+G(d,p))

Reactant

H	1.17259400	2.09524800	-1.04580300
C	0.75386200	1.31877400	-0.41063300
C	0.00000000	-1.85263600	0.77567100
C	1.60457200	0.92659800	0.77516300
H	2.40103400	-0.03249900	-1.04524900
H	1.10858100	0.64068600	1.69790400
H	2.53561900	1.46411300	0.93289800
C	1.51905100	-0.00667800	-0.41032200
C	0.76520600	-1.31242100	-0.41013600
H	-2.40103400	-0.03249900	-1.04524900
C	-1.51905100	-0.00667800	-0.41032200
H	0.00000000	-2.92760900	0.93400300
C	-1.60457200	0.92659700	0.77516300
H	-1.17259400	2.09524800	-1.04580300
H	-1.10858100	0.64068600	1.69790400
H	-2.53561900	1.46411200	0.93289800
C	-0.75386300	1.31877400	-0.41063300
H	1.22846200	-2.06347400	-1.04496200
H	0.00000000	-1.27945100	1.69796400
C	-0.76520600	-1.31242100	-0.41013600
H	-1.22846100	-2.06347400	-1.04496200

Product

H	1.18107200	2.52290400	-0.94966100

C	0.67067000	1.83372900	-0.27642900
C	0.00000000	-1.80643500	0.52407000
C	1.56421500	0.90320200	0.52366800
H	2.77500700	-0.23862500	-0.94972900
H	1.07578400	0.62138100	1.46084800
H	2.48326800	1.43369400	0.79900200
C	1.92308000	-0.33599300	-0.27633700
C	1.25257000	-1.49772100	-0.27606900
H	-2.77500700	-0.23862500	-0.94972900
C	-1.92308000	-0.33599300	-0.27633700
H	0.00000000	-2.86758100	0.79944400
C	-1.56421500	0.90320200	0.52366800
H	-1.18107200	2.52290400	-0.94966100
H	-1.07578400	0.62138100	1.46084800
H	-2.48326800	1.43369400	0.79900200
C	-0.67067000	1.83372900	-0.27642900
H	1.59424800	-2.28431400	-0.94930100
H	0.00000000	-1.24246700	1.46121300
C	-1.25256900	-1.49772200	-0.27606900
H	-1.59424700	-2.28431400	-0.94930100

Transition state

H	1.18022000	2.08077800	-1.13609300
C	0.70874000	1.48496300	-0.36165500
C	0.00000000	-1.86055300	0.68716900
C	1.61128600	0.93027600	0.68716900
H	2.39211700	-0.01828800	-1.13609300
H	1.14240500	0.65956800	1.63318600
H	2.54429000	1.46894700	0.85584900
C	1.64038500	-0.12869400	-0.36165500
C	0.93164500	-1.35626800	-0.36165500

H	-2.39211700	-0.01828800	-1.13609300
C	-1.64038500	-0.12869400	-0.36165500
H	0.00000000	-2.93789300	0.85584900
C	-1.61128600	0.93027600	0.68716900
H	-1.18022000	2.08077800	-1.13609300
H	-1.14240500	0.65956800	1.63318600
H	-2.54429000	1.46894700	0.85584900
C	-0.70874000	1.48496300	-0.36165500
H	1.21189700	-2.06249000	-1.13609300
H	0.00000000	-1.31913600	1.63318600
C	-0.93164500	-1.35626800	-0.36165500
H	-1.21189700	-2.06249000	-1.13609300

System 11 (B3LYP/6-31+G(d,p))

Reactant

C	-1.03130500	1.73174100	-0.86019700
C	0.21336100	2.52637800	-0.37894400
H	1.04247300	2.63598700	-1.08519900
H	-0.05321600	3.51949300	-0.00295600
H	-0.78335600	1.03483700	-1.66546300
H	-1.91045000	2.30729500	-1.16857700
C	-1.08962900	1.05757100	0.54523600
C	0.39741800	1.49870700	0.77854200
H	0.57035600	1.94607100	1.76457800
C	1.46073000	0.41467100	0.54511900
H	-1.72785300	1.68889700	1.17543800
C	-1.49702800	-0.40549900	0.77786300
C	-2.29411100	-1.07843200	-0.38036200
C	-0.98316100	-1.75836700	-0.86111300
H	-2.80334100	-0.41499100	-1.08660000

H	-1.97163700	-0.47976800	1.76352700
H	-3.02090100	-1.80619800	-0.00507100
H	-0.50318600	-1.19407400	-1.66534000
H	-1.04144700	-2.80721800	-1.17056600
C	-0.37111700	-1.47264400	0.54490900
C	1.09950400	-1.09391600	0.77815000
H	-0.59897200	-2.34134700	1.17458500
H	1.40079500	-1.46774500	1.76394000
C	2.08114000	-1.44775900	-0.37982800
H	1.76176600	-2.22083800	-1.08594200
C	2.01419400	0.02741500	-0.86088700
H	2.95160900	0.50145900	-1.17038000
H	2.32702800	0.65169900	1.17472400
H	1.28555500	0.16076600	-1.66519500
H	3.07482300	-1.71274500	-0.00420800

Product

C	-1.09852100	1.75642200	-0.70634200
C	0.16293200	2.59884400	-0.36500600
H	0.68777200	2.81442200	-1.30489800
H	-0.17272000	3.57016400	0.01723900
H	-0.83651300	0.94573600	-1.39105600
H	-1.78389900	2.41295000	-1.26428700
C	-1.80330600	1.20305800	0.50272900
C	1.12701700	2.01198700	0.65173400
H	1.16308800	2.52752300	1.61070800
C	1.94286400	0.95918000	0.50281500
H	-1.90003200	1.89111200	1.34381600
C	-2.30753200	-0.02974300	0.65166400
C	-2.33263200	-1.15871700	-0.36442800
C	-0.97139800	-1.82757000	-0.70604100

H	-2.78280500	-0.81317400	-1.30426400
H	-2.77255400	-0.25582000	1.61048900
H	-3.00452200	-1.93599000	0.01853000
H	-0.40085400	-1.19297600	-1.38893700
H	-1.19555400	-2.74864300	-1.26592000
C	-0.13980200	-2.16217500	0.50283400
C	1.18011400	-1.98316400	0.65114900
H	-0.68723500	-2.58986400	1.34400400
H	1.60887800	-2.27349800	1.60957900
C	2.17010900	-1.44092900	-0.36549600
H	2.09491600	-2.00326300	-1.30542700
C	2.07003700	0.07266000	-0.70657400
H	2.98082900	0.33879300	-1.26487600
H	2.58690800	0.69875500	1.34398700
H	1.23644100	0.25066900	-1.39075200
H	3.17924500	-1.63513900	0.01680700

Transition state

C	-1.12472100	1.80375000	-0.76045700
C	0.18437500	2.52494300	-0.42135900
H	0.89556100	2.61957100	-1.24962100
H	0.00000000	3.53600300	-0.04054200
H	-0.96514000	1.07159800	-1.55901400
H	-1.96677700	2.43999000	-1.06777600
C	-1.31506500	1.09863300	0.58001400
C	0.66815400	1.62944400	0.73543900
H	0.67951800	2.09987100	1.71705000
C	1.60897700	0.58956300	0.58001400
H	-1.57429600	1.76825100	1.39808100
C	-1.74521700	-0.23608400	0.73543900
C	-2.27885200	-1.10279800	-0.42135900

C	-0.99973300	-1.87591200	-0.76045700
H	-2.71639500	-0.53420700	-1.24962100
H	-2.15830000	-0.46145600	1.71705000
H	-3.06226900	-1.76800200	-0.04054200
H	-0.44546100	-1.37163500	-1.55901400
H	-1.12970500	-2.92327400	-1.06777600
C	-0.29391100	-1.68819600	0.58001400
C	1.07706300	-1.39336000	0.73543900
H	-0.74420200	-2.24750600	1.39808100
H	1.47878200	-1.63841500	1.71705000
C	2.09447700	-1.42214500	-0.42135900
H	1.82083500	-2.08536400	-1.24962100
C	2.12445400	0.07216200	-0.76045700
H	3.09648200	0.48328400	-1.06777600
H	2.31849800	0.47925500	1.39808100
H	1.41060100	0.30003700	-1.55901400
H	3.06226900	-1.76800200	-0.04054200

System 12 (ωB97X-D/6-31+G(d,p))

Reactant

C	1.95980500	1.47461800	0.59611900
H	1.92210500	1.34540600	1.67569200
C	1.49852100	0.54002400	-0.23204000
H	1.53304800	0.69297100	-1.30922200
C	0.90189000	-0.76133800	0.22063200
H	0.86713400	-0.81123600	1.31857800
O	-0.39724700	-0.97101000	-0.32322200
C	-1.36972300	-0.15563900	0.16264600
C	-2.54589600	-0.01091600	-0.44238200
H	-2.76581800	-0.51499300	-1.37682300
H	1.49410600	-1.60622000	-0.14046200

H	2.39536300	2.39730300	0.22621800
H	-1.12879700	0.35358700	1.09598200
H	-3.30627600	0.61408100	0.00852900

Product

C	0.33768900	1.21241700	0.29190800
H	0.34114600	1.12280900	1.38530700
C	1.34787700	0.26887500	-0.29928000
H	1.44725800	0.29629400	-1.38472000
C	2.08986300	-0.58919700	0.39876800
H	2.01661500	-0.65319000	1.48218100
O	-2.27605800	-1.10599100	-0.58305200
C	-1.60657500	-0.40176000	0.13575800
C	-1.07827400	0.95856900	-0.24897300
H	-1.12481100	1.05706500	-1.33780800
H	2.79597600	-1.25456800	-0.08753100
H	0.61704200	2.24658500	0.05922600
H	-1.35535100	-0.73376800	1.16701700
H	-1.76989300	1.69892400	0.17676100

Transition state

C	0.56643700	1.43926200	0.32726800
H	0.36050200	1.36694300	1.39065800
C	1.33711400	0.47778300	-0.29988200
H	1.64296400	0.64159300	-1.32960900
C	1.31231400	-0.83747100	0.18189400
H	1.21084600	-1.01090300	1.24925500
O	-0.42855600	-1.37425600	-0.25163200
C	-1.25243700	-0.52808600	0.25763500
C	-1.47064000	0.71828500	-0.29375200
H	-1.24215900	0.89159700	-1.33885800

H	1.83659700	-1.61996900	-0.35452000
H	0.47221500	2.43658400	-0.09219900
H	-1.62686900	-0.72335300	1.27412900
H	-2.18238100	1.39291900	0.17521800

System 13 (ωB97X-D/6-31+G(d,p))

Reactant

C	0.07198300	2.42987900	0.62484800
H	0.04089700	2.31195300	1.70596500
C	0.41846700	1.42263500	-0.17292600
H	0.43372700	1.55324800	-1.25448400
C	0.80566400	0.05229800	0.31388100
H	0.69100800	0.00842600	1.40796400
O	-0.03829200	-0.94177300	-0.27764900
C	-1.33461200	-0.93387300	0.12624600
C	-2.29355700	-1.56948900	-0.54269300
H	-2.08340000	-2.09549900	-1.46726700
H	-0.18895600	3.40599600	0.22869600
H	-3.30430900	-1.57366400	-0.15473300
H	-1.53333500	-0.39029100	1.04992700
C	2.23120700	-0.31447500	-0.06584000
H	2.35553200	-0.27952400	-1.15214700
H	2.93303000	0.38911500	0.38943300
H	2.46431700	-1.32557600	0.27736500

Product

C	-0.93391100	1.13536500	0.21787100
H	-0.92205800	1.11680800	1.31497100
C	0.43661700	0.81581000	-0.31133500
H	0.55140800	0.84978800	-1.39633000

C	1.48511500	0.47466500	0.43905600
H	1.36159200	0.43509600	1.52272200
O	-1.92314100	-2.24225800	-0.51838500
C	-1.75353900	-1.25548200	0.15904000
C	-1.99874600	0.15846500	-0.30605400
H	-2.05559600	0.16275100	-1.39879900
H	-1.22228300	2.15159500	-0.07526000
H	-2.98667600	0.45215400	0.07592000
H	-1.40945600	-1.35374800	1.21227200
C	2.84807000	0.13474400	-0.08584400
H	2.88341300	0.19866800	-1.17707200
H	3.60557100	0.81319200	0.32227300
H	3.13659300	-0.88101600	0.20631800

Transition state

C	-0.90124200	1.54220800	0.28961400
H	-1.13412000	1.37547900	1.33636200
C	0.34771000	1.23340100	-0.20727100
H	0.59581700	1.52683600	-1.22516100
C	1.10268600	0.20479100	0.37909200
H	0.96448900	0.03666500	1.44527500
O	0.05496400	-1.30935600	-0.11955100
C	-1.16191100	-1.13265500	0.25255400
C	-2.03596800	-0.30575900	-0.42097700
H	-1.84427100	-0.04440600	-1.45514300
H	-1.53927000	2.25994100	-0.21696700
H	-3.05509700	-0.19383200	-0.06026200
H	-1.45201300	-1.49368400	1.25165100
C	2.43282900	-0.21448200	-0.16412300
H	2.45285700	-0.13107700	-1.25346200
H	3.22188300	0.42318400	0.25009900

H	2.64538800	-1.24928400	0.11067700

System 14 (ωB97X-D/6-31+G(d,p))

Reactant

C	1.49673900	0.82089600	1.62108500
H	0.98035000	0.64584700	2.56142100
C	1.23739600	0.08902400	0.53563100
C	0.22378000	-1.02884200	0.58366400
H	-0.23470900	-1.09742000	1.57948400
O	-0.78713500	-0.88458100	-0.41063100
C	-1.63412000	0.16110500	-0.22544600
C	-2.41485800	0.62487700	-1.19834600
H	-2.38378300	0.20249900	-2.19662500
H	0.69880400	-1.98777500	0.35647800
H	2.23817900	1.61469900	1.60711900
H	-3.10681900	1.43131500	-0.99110800
C	1.90767600	0.30617000	-0.79227400
H	1.16282500	0.53823800	-1.56055800
H	2.63007100	1.12430200	-0.74634300
H	2.42870800	-0.60249300	-1.11598400
H	-1.64450200	0.58165200	0.78021800

Product

C	0.10662100	1.03845500	0.78716300
H	-0.34932400	0.82512900	1.76058700
C	1.08309600	-0.06116900	0.43285600
C	1.26069900	-1.11585500	1.23249700
H	0.71102900	-1.22268600	2.16388000
O	-2.05735800	-0.50137000	-1.56269200
C	-1.79339900	-0.03073400	-0.48041700
C	-0.99789100	1.23169600	-0.26801600

H	-0.59828200	1.56180600	-1.23066300
H	1.96273200	-1.90597400	0.98186400
H	0.64686900	1.98763000	0.89197200
H	-1.69562400	2.00347700	0.08418700
C	1.82542000	0.09503200	-0.86841100
H	1.14309300	0.01142000	-1.72222000
H	2.30227600	1.08046800	-0.93033700
H	2.59738400	-0.66954100	-0.98086900
H	-2.14440100	-0.53202600	0.44760700

Transition state

C	0.40329900	1.09668000	0.94188000
H	-0.19023500	0.98222300	1.84286400
C	1.06504600	0.00747900	0.39959100
C	0.49185300	-1.25327200	0.62699600
H	-0.04223100	-1.43750900	1.55367400
O	-1.03474600	-1.17430200	-0.47192500
C	-1.72931800	-0.14420000	-0.13835400
C	-1.34774000	1.14111600	-0.46580500
H	-0.68401400	1.30780100	-1.30781800
H	0.92708600	-2.13628400	0.17092700
H	0.73630800	2.11017700	0.73452500
H	-1.96700300	1.97837800	-0.15488000
C	2.00127100	0.18455100	-0.76945300
H	1.46337200	0.02249300	-1.71301800
H	2.43162500	1.18929000	-0.79057300
H	2.82531200	-0.53389200	-0.73457700
H	-2.52872300	-0.28238500	0.60515900

System 15 (ωB97X-D/6-31+G(d,p))

Reactant

C	-1.20372000	-1.95540500	-0.53044600
C	-0.24615300	-1.36065500	0.17689100
O	1.01672900	-1.17864100	-0.30463300
C	1.68640700	-0.03293300	0.21752500
C	1.06326700	1.24596200	-0.25746200
C	0.50428800	2.14693600	0.55074400
H	-0.97872700	-2.25739900	-1.55081500
H	-0.40887200	-1.01622600	1.20068900
H	2.71628100	-0.12884100	-0.13548800
H	1.69496900	-0.07211200	1.31737200
H	1.05503700	1.40106400	-1.33608100
H	0.50954300	1.95806200	1.62578300
C	-2.57241100	-2.24356600	0.01215000
H	-2.78181800	-3.31930100	0.02018000
H	-2.68127600	-1.87472400	1.03711200
H	-3.34774100	-1.76918500	-0.59985700
C	-0.15027000	3.41931600	0.10493000
H	-0.11207900	3.52878500	-0.98234000
H	-1.20073100	3.44264700	0.41561100
H	0.33671200	4.29088900	0.55615000

Product

C	-0.87071100	-0.44382300	-0.36563200
C	-0.05880600	-1.68527400	-0.06373700
O	0.23156200	-2.53296000	-0.87525200
C	2.29588600	0.86545800	0.59543200
C	1.22253700	0.91319100	-0.19152500
C	-0.20450600	0.79407200	0.27983600
H	-0.88684200	-0.32595100	-1.45605500

H	0.23988500	-1.80448000	1.00196500
H	3.29960600	0.95573100	0.19259100
H	2.20528900	0.73248500	1.67131600
H	1.35487600	1.04359500	-1.26690900
H	-0.19438800	0.64398500	1.36954100
C	-2.30171200	-0.69151300	0.13834900
H	-2.71220300	-1.60544300	-0.29986000
H	-2.32337900	-0.79368900	1.22964900
H	-2.96151100	0.13467600	-0.13650900
C	-0.97227600	2.08764300	-0.02277100
H	-1.05926400	2.24414100	-1.10417700
H	-1.98012900	2.07098800	0.40057400
H	-0.44485900	2.94698600	0.40023100

Transition state

C	-0.83536500	-0.87660900	-0.39346400
C	0.28234200	-1.51046700	0.12757200
O	1.46058000	-1.37307600	-0.34653100
C	2.13296200	0.34247400	0.28790200
C	1.13696500	1.19271200	-0.17768000
C	-0.13143900	1.17946100	0.38898700
H	-0.76240900	-0.49465200	-1.40812000
H	0.17138100	-2.00631400	1.10839500
H	3.09231400	0.29758100	-0.21370000
H	2.14067300	0.03096700	1.32752700
H	1.25266700	1.62807600	-1.16831000
H	-0.22246700	0.86083100	1.42540700
C	-2.21065300	-1.16914900	0.13845300
H	-2.72618300	-1.89904500	-0.49631800
H	-2.16519400	-1.57925200	1.15266800
H	-2.84304100	-0.27612500	0.16540100

C	-1.22571500	2.08075200	-0.10995300
H	-1.14613500	2.24413400	-1.18843000
H	-2.22064400	1.68777500	0.11077400
H	-1.15019000	3.05558400	0.38605500

System 16 (ωB97X-D/6-31+G(d,p))

Reactant

C	1.78567000	-1.25492500	0.36760400
C	0.68811500	-0.93275800	-0.31220400
O	-0.54516200	-1.42134500	0.00264600
C	-1.61940800	-0.51902600	-0.26716300
C	-1.64404800	0.61882200	0.71363000
C	-1.25180000	1.87608300	0.48684000
H	1.68110000	-1.88834400	1.24545400
H	0.72149900	-0.28650000	-1.19276700
H	-2.52404000	-1.12438700	-0.17783100
H	-1.55092600	-0.16707200	-1.30481600
H	-1.96769600	0.35383900	1.71803200
C	3.16122500	-0.80418700	-0.02662000
H	3.81007500	-1.65600800	-0.26002900
H	3.13145800	-0.15625700	-0.90860900
H	3.64165000	-0.24644600	0.78500100
C	-0.72213800	2.46482800	-0.78794400
H	-0.75356500	1.77062800	-1.63008100
H	-1.29123400	3.35845100	-1.06538400
H	0.31895400	2.77852800	-0.64962600
H	-1.29950300	2.57028500	1.32517500

Product

C	1.02593600	-0.25737500	0.46569300

C	0.69615800	-1.37078900	-0.50409700
O	0.69271500	-2.54550700	-0.21451100
C	-2.50094900	0.39222900	0.02944600
C	-1.38950500	0.29435300	0.75754800
C	-0.03503400	0.87780200	0.42973700
H	1.00815600	-0.70780300	1.46465500
H	0.48135100	-1.05783900	-1.54818300
H	-3.42164200	-0.08169500	0.35405000
H	-2.53862300	0.94069700	-0.90733800
H	-1.42524100	-0.28006900	1.68378600
C	2.45154000	0.23711700	0.17747800
H	3.18002600	-0.54723900	0.39904100
H	2.57967100	0.52830800	-0.87020900
H	2.68433300	1.10762800	0.79914800
C	-0.01726200	1.71962600	-0.84784100
H	-0.25709500	1.13029800	-1.73876600
H	-0.75215800	2.52673800	-0.77834200
H	0.96151000	2.18056900	-1.00153900
H	0.23355900	1.54451900	1.26285800

Transition state

C	1.13149400	-0.64285900	0.45243600
C	0.33498400	-1.21469400	-0.52383500
O	-0.83653000	-1.68369000	-0.29205300
C	-2.07376800	-0.23065700	-0.08558100
C	-1.39504400	0.55868000	0.84273000
C	-0.22063600	1.22125400	0.51090000
H	0.87916800	-0.85937600	1.48620900
H	0.64543200	-1.09180800	-1.57530200
H	-2.91596200	-0.83057100	0.23836400
H	-2.08418000	0.02747700	-1.13851200

H	-1.56459000	0.34417600	1.89468800
C	2.53066100	-0.17096900	0.17358600
H	3.26841700	-0.88829900	0.55044300
H	2.70315800	-0.04730100	-0.90059300
H	2.73827200	0.78850800	0.66084800
C	0.06784600	1.85466000	-0.82415000
H	-0.40421800	1.32960500	-1.65618200
H	-0.30928000	2.88424000	-0.81951100
H	1.14295100	1.90232400	-1.01735900
H	0.33984600	1.65805300	1.33681200

System 17 (ωB97X-D/6-31+G(d,p))

Reactant

C	-1.93618800	-0.63021400	-0.76646700
C	-0.91589200	0.19719000	-0.98830700
O	-0.61215100	1.24114800	-0.16293300
C	0.78417400	1.38709300	0.10661300
C	1.25295700	0.36426100	1.10259000
C	1.92977900	-0.75681000	0.83618200
H	-0.28304000	0.10990200	-1.87324400
H	0.89211400	2.39603200	0.51076700
H	1.34815000	1.33767000	-0.83407400
H	0.94866700	0.54964100	2.13071200
C	-2.82642600	-0.59882700	0.43864000
H	-2.45332000	0.11089400	1.17994400
H	-3.84803000	-0.30590700	0.17029700
H	-2.88537100	-1.59000600	0.90129700
C	2.41269800	-1.24980200	-0.49597500
H	2.21887700	-0.54877100	-1.31012400
H	3.48958300	-1.44785300	-0.46643500

H	1.91848900	-2.19561800	-0.74460300
H	2.15527800	-1.41297100	1.67626600
H	-2.13401000	-1.37554800	-1.53252300

Product

C	-0.83023000	-0.81518800	-0.27246100
C	-1.03559100	0.35008600	-1.21878900
O	-2.04880700	1.00787100	-1.28745900
C	1.80144600	1.43862300	0.81211200
C	0.79760300	0.59333100	1.04369300
C	0.58020900	-0.75046600	0.38792900
H	-0.18300700	0.58020300	-1.88995700
H	1.85807600	2.38976500	1.33161800
H	2.59774100	1.22043800	0.10628200
H	0.03788700	0.88440200	1.76821000
C	-1.97481900	-0.94127700	0.72968400
H	-2.03889600	-0.06336900	1.37852300
H	-2.93327400	-1.02690600	0.21337500
H	-1.83446700	-1.82708000	1.35624400
C	1.69563600	-1.15833000	-0.57657200
H	1.78966900	-0.46765600	-1.42100000
H	2.66146100	-1.18634100	-0.06374500
H	1.50192500	-2.15629800	-0.98113600
H	0.55744200	-1.49735000	1.19422000
H	-0.83044300	-1.70830000	-0.91773900

Transition state

C	-1.15355100	-0.78180100	-0.48231400
C	-0.72131400	0.33728600	-1.17204800
O	-0.64777500	1.50541500	-0.64454100
C	0.94121000	1.57075100	0.44470300

C	0.82978100	0.38605500	1.17509600
C	0.93121500	-0.85601200	0.56233000
H	-0.23550100	0.18068800	-2.14706400
H	0.72755200	2.51692900	0.92801200
H	1.60723100	1.64208500	-0.40773800
H	0.30226400	0.43264600	2.12361100
C	-2.04847600	-0.71041200	0.72263400
H	-1.98566500	0.27392900	1.18998300
H	-3.08991500	-0.87382600	0.42129500
H	-1.80119200	-1.47514800	1.46630900
C	1.85877700	-1.18664100	-0.57706600
H	2.06157000	-0.33243200	-1.22510500
H	2.81635800	-1.52941600	-0.16668900
H	1.45742200	-1.99364500	-1.19531700
H	0.64549400	-1.71865400	1.16277500
H	-1.14927300	-1.72183100	-1.03375000

Optimized Cartesian coordinates for minima and transition state structures associated with reactions listed in Table 3 of the manuscript.

System 1 (ωB97X-D/6-31G)

Reactant

C	-2.33896500	-0.67088200	0.95298700
C	-2.34420900	0.66744100	0.95087500
C	0.66175600	1.50204300	1.73544900
C	1.21763700	0.73924900	0.79014100
C	1.23079500	-0.73638500	0.79770300
C	0.72388500	-1.49858700	1.77036700
C	-1.85520300	-1.14919600	-0.36975600

C	-1.86177500	1.14604400	-0.37250000
H	0.67879700	2.58245800	1.67179700
H	0.74638700	-2.57922900	1.71074700
O	-1.74217200	2.27077200	-0.80952400
O	-1.73213000	-2.27387900	-0.80552000
H	0.29747500	-1.06114600	2.66554800
H	0.19064700	1.06498300	2.60821600
H	-2.63804800	-1.35130300	1.73472700
H	-2.64925400	1.34784400	1.73030500
Cl	1.97000500	-1.57927100	-0.62363200
Cl	1.99296100	1.58132500	-0.61176500
O	-1.55319600	-0.00138800	-1.14126700

Product

C	-1.36591000	-0.77223600	1.09100400
C	-1.36637000	0.77119700	1.09099200
C	0.01048700	1.41264700	1.38394400
C	1.10625500	0.66621200	0.67138400
C	1.10666000	-0.66576800	0.67138100
C	0.01133500	-1.41287900	1.38391800
C	-1.84426800	-1.15662600	-0.30020000
C	-1.84488600	1.15528800	-0.30023900
H	-0.00837500	2.46200400	1.08146800
H	-0.00691300	-2.46223100	1.08139300
O	-1.97740500	2.26103200	-0.77951400
O	-1.97622300	-2.26246000	-0.77942500
H	0.19214500	-1.38741700	2.46530400
H	0.19130800	1.38724200	2.46532900
H	-2.09235700	-1.17122600	1.80549900
H	-2.09307300	1.16976900	1.80546000
Cl	2.38251800	-1.65098300	-0.11706600

Cl	2.38148000	1.65221000	-0.11709300
O	-2.13862300	-0.00076100	-1.03758300

Transition state

C	-1.76675100	-0.69444900	0.94732900
C	-1.76667600	0.69463700	0.94731100
C	0.30154500	1.42621900	1.56246400
C	1.11801100	0.70527800	0.72155600
C	1.11795000	-0.70538200	0.72154400
C	0.30143700	-1.42626000	1.56245700
C	-1.66854800	-1.15427000	-0.45777200
C	-1.66840800	1.15441000	-0.45780500
H	0.22940600	2.50272000	1.45751400
H	0.22918000	-2.50275200	1.45749000
O	-1.72267100	2.26760800	-0.94097800
O	-1.72295900	-2.26747200	-0.94092000
H	0.03081100	-1.02491300	2.53108400
H	0.03083900	1.02489200	2.53107700
H	-2.19551400	-1.33422400	1.70392400
H	-2.19538300	1.33447800	1.70388100
Cl	1.98738500	-1.60604200	-0.57391900
Cl	1.98754200	1.60587700	-0.57388300
O	-1.49367700	0.00005000	-1.26245600

System 2 (ωB97X-D/6-31G)

Reactant

C	1.36883300	0.89812700	1.45000000
C	2.11867700	-0.11482900	1.00008100
C	0.02307300	-2.62910900	0.50142900
C	-0.69361700	-1.75880000	-0.22404500

C	-1.56514600	-0.72480700	0.34244800
C	-1.64061700	-0.30730900	1.60736100
C	0.77168900	1.60625000	0.28657800
C	2.05874400	-0.13083000	-0.48526300
H	0.67387900	-3.34690800	0.01458200
H	-2.31970800	0.47558300	1.91989800
O	2.60930000	-0.85045900	-1.29225500
O	0.06464600	2.58955600	0.23597600
H	-1.01953300	-0.76616100	2.36963700
H	-0.02577900	-2.67240400	1.58569100
H	1.19186800	1.21450000	2.46588100
H	2.70246000	-0.82965700	1.55809800
Cl	-2.62926400	0.08741100	-0.89996700
O	1.20704900	0.92792200	-0.87905300
H	-0.62789500	-1.78296500	-1.30721200

Product

C	0.51247300	0.44586500	1.32424600
C	1.39015900	-0.72474700	0.82748700
C	0.61252800	-2.03081900	0.53268200
C	-0.69274200	-1.74177100	-0.16962200
C	-1.43066100	-0.72975900	0.28032800
C	-0.99884700	0.12033500	1.43940500
C	0.73527200	1.55193000	0.30567300
C	2.03880700	-0.20378000	-0.44377800
H	1.24070800	-2.69448100	-0.06653000
H	-1.56512100	1.05283900	1.49307000
O	2.78614800	-0.77751800	-1.20826800
O	0.24073300	2.65869700	0.26274800
H	-1.17140800	-0.42061800	2.37809400
H	0.42231300	-2.54098600	1.48565400

H	0.86017100	0.82194500	2.29118000
H	2.19589600	-0.94400800	1.53513100
Cl	-3.02955600	-0.32781000	-0.47538100
O	1.64752100	1.12422900	-0.67013000
H	-1.00062400	-2.35706500	-1.00628800

Transition state

C	0.83574100	0.69385600	1.32917800
C	1.68812700	-0.30338900	0.86600000
C	0.47949700	-2.21378200	0.54608600
C	-0.57391400	-1.73584500	-0.20766100
C	-1.42299900	-0.73804000	0.29684900
C	-1.25552800	-0.13410800	1.52250000
C	0.52732400	1.59494800	0.19445800
C	1.92915800	-0.07168300	-0.57325800
H	1.20124000	-2.88477700	0.09223200
H	-1.84545200	0.73218600	1.79936200
O	2.65909600	-0.63228500	-1.36825900
O	-0.08354200	2.64453800	0.14732400
H	-0.84330800	-0.71111500	2.34240300
H	0.44075000	-2.23367800	1.62950100
H	0.77271500	1.05517500	2.34462000
H	2.39492000	-0.86553900	1.45719800
Cl	-2.60105500	0.00458200	-0.86908600
O	1.11056900	1.02102300	-0.96344300
H	-0.63633500	-1.98808900	-1.26074500

System 3 (ωB97X-D/6-31G(d))

Reactant

C	-0.66578700	0.67237300	1.41402600
C	0.66569600	0.67248200	1.41402900

C	1.52996500	-2.14167400	0.16176700
C	0.73454900	-1.90150600	-0.88707400
C	-0.73427500	-1.90155100	-0.88707200
C	-1.52967700	-2.14198200	0.16171900
C	-1.12387500	1.14375700	0.07979600
C	1.12371600	1.14393000	0.07979800
H	2.61027300	-2.09320100	0.06419700
H	-2.60998700	-2.09353900	0.06415900
O	2.22819100	1.34059300	-0.33151900
O	-2.22837900	1.34025800	-0.33152200
H	-1.14294500	-2.41161200	1.14170300
H	1.14324600	-2.41109300	1.14181500
H	-1.35870600	0.40858200	2.20091000
H	1.35865400	0.40880300	2.20091800
O	-0.00009700	1.38471100	-0.68786400
H	-1.20034500	-1.64810700	-1.83723000
H	1.20060300	-1.64821100	-1.83727900

Product

C	-0.76817300	-0.11767800	0.95806300
C	0.76853000	-0.11765500	0.95793600
C	1.41116600	-1.41034900	0.41199700
C	0.66692100	-1.90762600	-0.79941600
C	-0.66674100	-1.90763200	-0.79934300
C	-1.41086100	-1.41037200	0.41215900
C	-1.13463100	1.06051100	0.07202500
C	1.13479300	1.06052000	0.07179800
H	2.46434100	-1.21822300	0.19183000
H	-2.46406000	-1.21824500	0.19210600
O	2.22117000	1.44380700	-0.24666000
O	-2.22107800	1.44379300	-0.24620000

H	-1.38370100	-2.16732800	1.20702600
H	1.38408400	-2.16728700	1.20689100
H	-1.17419100	0.09645000	1.95141800
H	1.17469200	0.09654700	1.95121800
O	0.00003300	1.69945200	-0.36955400
H	-1.23240200	-2.26172000	-1.65648000
H	1.23249200	-2.26171700	-1.65661100

Transition state

C	0.28887000	0.69175300	1.16644700
C	0.28879500	-0.69178600	1.16644500
C	-1.67758600	-1.43227300	0.31474600
C	-1.75301900	-0.70370400	-0.85201500
C	-1.75294100	0.70388600	-0.85202300
C	-1.67743300	1.43245900	0.31473000
C	1.09387400	1.13031100	0.00630300
C	1.09375100	-1.13042800	0.00629800
H	-1.53569100	-2.50838800	0.27514300
H	-1.53541600	2.50855700	0.27511700
O	1.45290000	-2.22159100	-0.33365900
O	1.45314600	2.22143500	-0.33365100
H	-2.09584000	1.05349500	1.24139000
H	-2.09594400	-1.05325200	1.24140500
H	0.15766700	1.34081700	2.02116200
H	0.15752800	-1.34083600	2.02116000
O	1.43128900	-0.00007600	-0.72092200
H	-1.58835300	1.21436200	-1.79755600
H	-1.58849000	-1.21420900	-1.79754300

System 4 (ωB97X-D/6-31G(d))

Reactant

C	-0.02791800	-0.91444500	1.40884100
C	-1.21151600	-0.30408900	1.41006200
C	-0.64372800	2.59669600	0.24633600
C	-0.09218500	2.04411100	-0.84171200
C	1.16897700	1.29894200	-0.90951800
C	2.03299300	1.10094800	0.09686300
C	0.16197900	-1.54330800	0.07523600
C	-1.83469900	-0.51189100	0.07583000
H	-1.59765700	3.11197100	0.18635900
H	-0.63851600	2.11381600	-1.78057500
O	-2.90595700	-0.17920600	-0.33588000
O	1.05141500	-2.22951100	-0.33460800
O	-0.94750300	-1.24309000	-0.69156500
H	1.83833000	1.55551800	1.06868800
H	-0.16378200	2.57644500	1.22185700
H	-1.70671600	0.24707900	2.19744900
H	0.70817600	-0.99898100	2.19671700
H	1.39422700	0.84583000	-1.87418400
C	3.28495400	0.28937400	-0.01006200
H	4.16533900	0.89289500	0.24430000
H	3.26572300	-0.55681100	0.68787800
H	3.41978700	-0.11271300	-1.01875600

Product

C	0.52597900	-0.24631600	0.90269700
C	-0.86061600	0.41895800	0.96814600
C	-0.89737700	1.88475300	0.48469500
C	-0.09042700	2.03027000	-0.77778600
C	1.11156600	1.45587700	-0.83879100

C	1.63547600	0.70279700	0.36106900
C	0.30191300	-1.46137000	0.01821600
C	-1.72272100	-0.43292100	0.05397500
H	-1.93810500	2.18594700	0.34288400
H	-0.50404500	2.58327700	-1.61612100
O	-2.86897900	-0.27636200	-0.24767900
O	1.06526700	-2.33221800	-0.27938100
O	-0.99724100	-1.48878900	-0.43839900
H	1.78713000	1.42999700	1.17279400
H	-0.48270000	2.52023700	1.27853400
H	-1.29411500	0.35304300	1.97088000
H	0.84377300	-0.62631900	1.87883300
H	1.73110300	1.51682900	-1.73060900
C	2.97401400	0.01442000	0.10339300
H	3.73473800	0.76771000	-0.12764200
H	3.30897800	-0.54741700	0.98130800
H	2.91722400	-0.68257300	-0.73651400

Transition state

C	0.14378000	-0.58132900	1.16592200
C	-1.05767400	0.10924300	1.15417000
C	-0.77708300	2.10369500	0.39522700
C	-0.15378900	1.87409300	-0.81896700
C	1.09476200	1.23855800	-0.91683500
C	1.81339500	0.82662400	0.18554000
C	0.14832100	-1.49350100	0.01820800
C	-1.83689700	-0.41117200	0.00036400
H	-1.78846300	2.50057800	0.40623700
H	-0.73885900	1.98246800	-1.72892700
O	-2.96836000	-0.19973100	-0.33316600
O	0.92522500	-2.34227300	-0.32236300

O	-1.01272500	-1.25101500	-0.71687700
H	1.65448200	1.33161300	1.13409500
H	-0.19423600	2.31789400	1.28597200
H	-1.57585500	0.49791000	2.02106400
H	0.80292100	-0.73542700	2.00819900
H	1.41659300	0.89578400	-1.89832100
C	3.06853000	0.01839500	0.07933800
H	3.94215100	0.68265300	0.11562300
H	3.16286700	-0.68654300	0.91074400
H	3.10520800	-0.55041600	-0.85323600

System 5 (ωB97X-D/6-31G)

Reactant

C	-0.64303000	-0.07902800	1.26560400
C	-1.13649900	2.26302300	-1.03696600
C	1.19396000	2.45559000	-0.73644400
C	0.68320900	-0.10856400	1.42745800
H	-1.24952600	0.65286200	1.78182600
H	1.16173600	0.60496600	2.09031400
C	0.16954900	1.73759600	-1.57413000
H	0.28833400	1.95856600	-2.64522300
H	0.26643100	0.64872300	-1.46795800
C	-0.88767500	3.15682400	-0.05183300
C	0.56577100	3.27598300	0.13658700
H	-2.10701900	1.95933200	-1.40667900
H	2.25992000	2.30675100	-0.84041100
C	-1.35066000	-1.01358300	0.37593800
O	-0.82086300	-1.86285700	-0.35137800
O	-2.69760600	-0.84214200	0.44274000
C	-3.52073600	-1.71765000	-0.38731000

H	-3.34776100	-2.76244100	-0.12296200
H	-4.54617100	-1.42825300	-0.17017500
H	-3.28953800	-1.56419300	-1.44321500
C	1.59416100	-1.12059900	0.82332200
O	1.97975400	-2.13041400	1.41143600
O	2.02274000	-0.76444700	-0.41306700
C	2.85547000	-1.72976300	-1.12919700
H	2.29770100	-2.65521100	-1.28077800
H	3.07987700	-1.25273100	-2.08029000
H	3.77048000	-1.93338100	-0.57027300
H	1.03768600	3.92244200	0.86589400
H	-1.62676500	3.70463600	0.51920800

Product

C	-0.91005500	0.65996800	0.41474400
C	-0.99840500	1.87163800	-0.59855500
C	1.21517900	1.75558000	-0.17687800
C	0.64581000	0.58358000	0.69379700
H	-1.45488400	0.87920400	1.33196800
H	0.81818600	0.76884000	1.75874500
C	0.29811800	1.66713800	-1.42094800
H	0.47223400	2.48072500	-2.12950000
H	0.34401700	0.70239000	-1.92892000
C	-0.62602800	3.10555300	0.21688000
C	0.69041700	3.03585400	0.46735800
H	-1.94121900	1.91288300	-1.14339500
H	2.28805300	1.69552000	-0.34151700
C	-1.49767500	-0.59042500	-0.18376400
O	-1.13307500	-1.13433900	-1.23108700
O	-2.54137500	-1.05487900	0.55068700
C	-3.18395100	-2.28311300	0.08842600

H	-2.45716300	-3.09688700	0.06273100
H	-3.96431100	-2.48397400	0.81872800
H	-3.61041000	-2.13851600	-0.90594800
C	1.22813500	-0.78369600	0.42368000
O	0.89866700	-1.79896700	1.04355600
O	2.17894100	-0.79626700	-0.54334500
C	2.74761900	-2.09461000	-0.89702900
H	1.95956300	-2.75959300	-1.25407900
H	3.46286100	-1.88152900	-1.68811000
H	3.24398100	-2.54042500	-0.03323600
H	1.28214100	3.70087000	1.08392000
H	-1.33548900	3.83550000	0.58558100

Transition state

C	-0.72073000	0.20044600	0.96322800
C	-1.13581300	1.91008600	-0.71859200
C	1.14051600	1.92025600	-0.27534000
C	0.66686000	0.34833200	1.07228700
H	-1.36738000	0.70125600	1.66820300
H	1.01943300	0.84430300	1.97085300
C	0.15619500	1.44292700	-1.32333200
H	0.34116800	2.01817400	-2.24595500
H	0.21415300	0.38534900	-1.57280100
C	-0.85413100	2.96537700	0.14685600
C	0.53157800	2.99789300	0.39132900
H	-2.11471300	1.65796800	-1.10527000
H	2.20988200	1.79968700	-0.38694100
C	-1.33532100	-0.86256900	0.18610700
O	-0.75728800	-1.64260200	-0.59088700
O	-2.68819000	-0.92978900	0.39473700
C	-3.41172500	-1.97174400	-0.32120600

H	-3.02968000	-2.95835400	-0.05132100
H	-4.44782000	-1.86263200	-0.00721800
H	-3.31947000	-1.83138300	-1.40034300
C	1.59561400	-0.76985500	0.69086200
O	1.89862800	-1.66019700	1.48922900
O	2.12036200	-0.71035700	-0.55891200
C	2.90213300	-1.86225400	-0.99691800
H	2.27892800	-2.75766100	-0.97866200
H	3.20606000	-1.62408600	-2.01376400
H	3.77258400	-2.00244200	-0.35353700
H	1.02874800	3.66538900	1.08337600
H	-1.59105500	3.59461300	0.62836500

System 6 (M06-2X/6-31+G(d)

Reactant

C	2.22020200	-0.77368700	0.56289500
C	2.27981200	0.52072800	0.17891600
C	1.53340800	0.68758700	-1.07145400
C	1.02284700	-0.50537200	-1.44443200
H	2.68859300	-1.21291800	1.43715700
H	2.79403500	1.32180400	0.70001100
H	1.40956800	1.63045900	-1.59317400
H	0.42147600	-0.70866700	-2.32378000
C	-0.48389800	-0.04325100	1.86281300
H	0.03132500	0.75747900	2.38145900
H	-0.42651700	-1.04727300	2.27068400
C	-1.28670600	1.53877000	0.20884700
C	-1.89810600	-0.83988100	0.05704900
N	-1.34442200	2.61396000	-0.21319900
N	-2.44873600	-1.69924400	-0.48740300
C	-1.20314500	0.20948800	0.75846500

C	1.43977200	-1.55452100	-0.45555400
H	2.07227400	-2.31720900	-0.93457100
H	0.58739100	-2.10096500	-0.02743300

Product

C	1.59437600	-0.65125500	0.90091600
C	2.19816200	0.57487100	0.24253600
C	1.54237000	0.78747600	-0.90470600
C	0.49551300	-0.30176800	-1.03297200
H	2.19855500	-1.14534500	1.66237700
H	2.94877500	1.21459000	0.69501000
H	1.63537100	1.63193200	-1.57848100
H	0.05280700	-0.46315800	-2.01575700
C	0.19118300	-0.21866700	1.41828500
H	0.21981300	0.68356500	2.03157200
H	-0.28772600	-1.01652900	1.99101600
C	-1.10027500	1.40588900	-0.04403500
C	-1.73460400	-0.89863900	-0.05159500
N	-1.46205500	2.49890900	-0.14157100
N	-2.59390900	-1.66323100	-0.16323100
C	-0.60085700	0.02940600	0.07631400
C	1.20216400	-1.47736700	-0.33839300
H	2.06613000	-1.82288700	-0.91039200
H	0.54024200	-2.32109600	-0.11454800

Transition state

C	1.66757500	-0.58288200	0.82638300
C	2.04496200	0.64861400	0.27737400
C	1.50743200	0.76952300	-1.02553000
C	0.87073600	-0.40631900	-1.34913900
H	2.13657600	-0.99933000	1.71295300

H	2.56529600	1.43631600	0.81272900
H	1.52132500	1.67082400	-1.62703000
H	0.32789000	-0.60874300	-2.26649100
C	-0.14439600	-0.12269400	1.56468600
H	0.13066300	0.71263300	2.19921700
H	-0.25597500	-1.06968200	2.08590200
C	-1.24670100	1.47045400	0.06697700
C	-1.84332900	-0.90234200	-0.04581700
N	-1.38055800	2.57831600	-0.25287600
N	-2.48662300	-1.77064800	-0.47085800
C	-1.02727000	0.13009100	0.50310700
C	1.19869200	-1.44147800	-0.32604500
H	2.07121500	-2.01002800	-0.68769700
H	0.40706400	-2.16346100	-0.11542500

System 7 (ωB97X-D/6-31G(d))

Reactant

C	0.49143400	-0.72660400	-1.31553700
C	-1.17173300	1.37907800	0.74027500
C	-2.66734300	-0.43229500	0.72153200
C	-0.35723800	-1.74691900	-1.21336300
H	0.44701500	-0.01673900	-2.13470200
H	-1.13489100	-1.91294700	-1.95145200
H	-0.29098300	-2.44778500	-0.38595900
C	-1.49918800	0.11894300	1.48438200
H	-1.75864800	0.32191000	2.53368900
H	-0.64843000	-0.57578200	1.50682000
C	-2.03576700	1.52980300	-0.28144300
C	-2.96964400	0.40128800	-0.29203200
H	-0.36152500	2.04680100	1.00952500
H	-3.17728900	-1.35331200	0.97921500

C	1.54534300	-0.51498200	-0.29735400
O	1.68525300	-1.15949500	0.72224800
O	2.35650400	0.49496100	-0.64564000
C	3.41796700	0.77299900	0.26689100
H	4.07238200	-0.09568700	0.37696800
H	3.96959400	1.60722500	-0.16714100
H	3.02290100	1.05081700	1.24778700
H	-3.76962600	0.27215600	-1.01342800
H	-2.05089200	2.34705700	-0.99473800

Product

C	-0.00512100	-0.01510900	-0.61008500
C	-0.79591800	0.97866000	0.33133100
C	-2.12447800	-0.83048100	0.27587200
C	-0.91894900	-1.26663100	-0.61382600
H	0.11527200	0.43040600	-1.59955300
H	-1.22838600	-1.54674200	-1.62385500
H	-0.40041200	-2.11620800	-0.16175000
C	-1.38795500	-0.01040000	1.35166600
H	-2.06672600	0.47527500	2.05838900
H	-0.63106000	-0.58615800	1.89365600
C	-2.04263100	1.35644500	-0.44599100
C	-2.83446900	0.28058100	-0.47675300
H	-0.19033800	1.80306600	0.71117300
H	-2.74657000	-1.65905100	0.61784700
C	1.37255500	-0.27347700	-0.04511100
O	1.68205000	-1.16708000	0.71237300
O	2.23932700	0.66543600	-0.45692800
C	3.56084900	0.56029000	0.07321500
H	4.01926000	-0.38998600	-0.21282000
H	4.11896100	1.39178500	-0.35812400

H	3.54936500	0.63890400	1.16354600
H	-3.76061600	0.16214700	-1.02935300
H	-2.18083600	2.29664400	-0.96902900

Transition state

C	0.17638800	-0.38767800	-0.96467700
C	-0.95501900	1.20035500	0.52716600
C	-2.26043100	-0.69920800	0.40234300
C	-0.74835900	-1.41636700	-0.84984000
H	0.15660800	0.28939100	-1.80917000
H	-1.37759900	-1.65857700	-1.69885100
H	-0.49648000	-2.25817300	-0.20995800
C	-1.29786800	-0.01068400	1.33597900
H	-1.86551500	0.31898100	2.22117500
H	-0.45084600	-0.60573600	1.67850000
C	-1.99845800	1.43822400	-0.35231400
C	-2.81642900	0.29869600	-0.40507000
H	-0.18761900	1.91505100	0.80159600
H	-2.78403700	-1.61084500	0.67263000
C	1.40023900	-0.39201000	-0.16427400
O	1.64452700	-1.12948100	0.77595300
O	2.27405000	0.54580500	-0.59031900
C	3.49731400	0.61344900	0.13476100
H	4.04343000	-0.33219900	0.07447500
H	4.07663400	1.40950300	-0.33527300
H	3.31785900	0.85222600	1.18709100
H	-3.65983100	0.16380000	-1.07367200
H	-2.10548000	2.31733000	-0.97805900

System 8 (ωB97X-D/6-31G)

Reactant

C	-3.80251600	-0.93031500	-0.54287700
C	-2.54630500	-1.40855300	-0.79059200
C	-1.37797300	-0.58307400	-0.65129600
C	-1.56398000	0.78675400	-0.23562400
C	-2.90390400	1.24278400	0.01328500
C	-3.98493500	0.41965400	-0.13360600
C	-0.07997300	-1.07584200	-0.91216400
C	-0.45222300	1.64435700	-0.08579700
C	0.82646400	1.18676100	-0.47481700
C	1.01247500	-0.18059200	-0.88643900
C	2.33378700	-0.60464100	-1.25543100
H	2.49348300	-1.62892900	-1.56596700
C	3.39571700	0.25521300	-1.23520900
C	3.21028700	1.60850400	-0.84000400
C	1.97123000	2.05416400	-0.47189600
H	-4.66569800	-1.57487500	-0.66953300
H	-2.43633500	-2.43111600	-1.12828900
H	-3.06762100	2.27499000	0.29664900
H	-4.98599500	0.79581300	0.04814800
H	4.38270900	-0.09112100	-1.52110600
H	4.05622400	2.28758000	-0.83782600
H	1.84851800	3.09434000	-0.19678100
C	0.11655100	0.18359500	2.69821400
C	0.24082800	-1.11453800	2.39535500
C	0.16122700	-2.53414200	-1.23099500
H	-0.65395100	-3.17327100	-0.89037000
H	0.28446100	-2.70077400	-2.30864800
H	1.06483600	-2.89877700	-0.73418000
C	-0.62466900	3.04202400	0.46616600
H	0.25306300	3.35877000	1.03428800
H	-0.78748400	3.78063100	-0.32918900

H	-1.47144200	3.10503600	1.15250400
H	0.96866200	0.85417000	2.71909800
H	-0.85505600	0.60217600	2.93304400
H	-0.62155300	-1.77253400	2.36789000
C	1.49392200	-1.71784500	2.06642800
N	2.50758200	-2.22834700	1.77925100

Product

C	-3.63039600	-0.67515000	-1.14230400
C	-2.40363700	-1.32197900	-0.95776500
C	-1.34867000	-0.64313600	-0.35329000
C	-1.51822800	0.68590300	0.07459200
C	-2.74155700	1.32510300	-0.10800300
C	-3.79828200	0.64208400	-0.71987500
C	0.03587700	-1.22436500	-0.06812800
C	-0.28875900	1.28043600	0.75727700
C	0.89027900	1.08305700	-0.19405400
C	1.06409000	-0.24387600	-0.62787500
C	2.13037800	-0.57388300	-1.45940500
H	2.27713200	-1.59566300	-1.79077100
C	3.02513700	0.42089900	-1.86726600
C	2.85279000	1.73587100	-1.43994500
C	1.78509800	2.06938000	-0.59970400
H	-4.45038300	-1.20241000	-1.61793900
H	-2.28381100	-2.34668100	-1.29123800
H	-2.88209500	2.34990100	0.21750500
H	-4.74963800	1.14241100	-0.86614800
H	3.85614700	0.16412800	-2.51527300
H	3.54860500	2.50540100	-1.75686800
H	1.66288800	3.09495200	-0.26929000
C	0.00117300	0.34614900	1.98286200

C	0.18098200	-1.13010700	1.51329100
C	0.21128000	-2.66159700	-0.54684900
H	-0.52289200	-3.32043500	-0.07132100
H	0.08172600	-2.73079200	-1.63155300
H	1.20732600	-3.04089000	-0.29927600
C	-0.47389500	2.71855600	1.23030500
H	0.42496200	3.07334000	1.74508100
H	-0.67740800	3.39351300	0.39227900
H	-1.30861000	2.78769100	1.93581300
H	0.90171400	0.70588700	2.48909700
H	-0.83234700	0.41462500	2.68810500
H	-0.60662300	-1.75831800	1.94447000
C	1.46883600	-1.67654800	1.94185600
N	2.50497900	-2.11001600	2.26479800

Transition state

C	-3.77067100	-0.88041200	-0.73873400
C	-2.50810900	-1.43105600	-0.79951200
C	-1.35899100	-0.65190100	-0.50451000
C	-1.52712200	0.70627600	-0.12118600
C	-2.83603500	1.24119200	-0.04802000
C	-3.93578700	0.46806800	-0.36106300
C	-0.02682900	-1.19450600	-0.53479000
C	-0.34791700	1.44940300	0.28259300
C	0.89088200	1.07743300	-0.37065600
C	1.05878700	-0.28233900	-0.75519200
C	2.31526400	-0.70379700	-1.26533400
H	2.45988800	-1.73932200	-1.54744500
C	3.34753100	0.19397600	-1.42856100
C	3.17306800	1.54521800	-1.06603400
C	1.97406100	1.97417000	-0.53447600

H	-4.63802800	-1.48126000	-0.98960900
H	-2.39254800	-2.46412000	-1.10584000
H	-2.97871900	2.27818800	0.23194600
H	-4.93009500	0.89993600	-0.32382000
H	4.29643400	-0.13843900	-1.83434100
H	3.98616600	2.24962300	-1.20493700
H	1.85746500	3.01608700	-0.26095600
C	-0.02448400	0.45268900	2.09974600
C	0.17240300	-0.92030300	1.90879200
C	0.18240600	-2.67280800	-0.73338600
H	-0.58501300	-3.25629100	-0.21933100
H	0.15174500	-2.94047500	-1.79784200
H	1.15064300	-2.98957600	-0.33734000
C	-0.51848800	2.87422900	0.76579300
H	0.37596400	3.22622800	1.28556100
H	-0.71500800	3.55757400	-0.06953700
H	-1.34980800	2.95674700	1.47075900
H	0.82646000	1.06724900	2.37827500
H	-0.97515200	0.77310300	2.51342600
H	-0.65557600	-1.61082800	2.02068900
C	1.46717300	-1.49790500	1.93827000
N	2.53604600	-1.98431200	1.91255700

System 9 (ωB97X-D/6-31G(d))

Reactant

C	1.12937500	-0.68478100	0.60033600
C	-0.76456200	-1.47727700	-1.69204100
C	-0.72001200	1.46477700	-1.67671600
C	1.10542000	0.67713900	0.63899200
C	-1.69937600	-0.73923400	-1.06744000
C	-1.69656300	0.74981000	-1.09055400

H	-0.78665800	-2.56220500	-1.63997900
C	0.24512000	-1.46384700	1.41326500
N	-0.46160200	-2.07958600	2.09302600
C	2.07519700	-1.38829100	-0.21313800
N	2.84590800	-1.95508100	-0.86488300
C	2.03649300	1.45719800	-0.11948900
N	2.79916900	2.08090200	-0.72727400
C	0.17974700	1.37850200	1.47689900
N	-0.56584400	1.93655400	2.16481500
H	0.10108700	1.01410300	-2.22594600
H	0.01492500	-1.04912900	-2.31492300
C	-2.81896500	1.46350200	-0.38137100
H	-2.85652500	1.20233600	0.68255700
H	-2.69999300	2.54727400	-0.45374800
H	-3.79187000	1.19909900	-0.81207100
C	-2.78296800	-1.42506900	-0.27475700
H	-2.76791800	-1.12293100	0.77878500
H	-3.77676100	-1.17745500	-0.66570800
H	-2.66609700	-2.51081500	-0.31150900
H	-0.74180600	2.55088200	-1.66555700

Product

C	0.70002000	-0.83007500	0.01144500
C	-0.45794900	-1.39831500	-0.88758500
C	-0.33243600	1.28829000	-1.02917300
C	0.59790600	0.76682100	0.11030100
C	-1.75949600	-0.65038700	-0.71960900
C	-1.70666200	0.68320100	-0.84266600
H	-0.56455600	-2.46146400	-0.65984600
C	0.62681100	-1.44575600	1.34811200
N	0.53911000	-1.96031000	2.37921300

C	1.97735400	-1.23329300	-0.60294700
N	2.94598800	-1.57535800	-1.13249000
C	1.92365800	1.40146400	0.01630000
N	2.94340300	1.93476200	-0.09017500
C	-0.00655600	1.18015800	1.39167000
N	-0.50763900	1.55176900	2.36455900
H	0.12943000	1.01647700	-1.98652500
H	-0.11376800	-1.32788900	-1.92613700
C	-2.84474400	1.65106100	-0.71704900
H	-2.70421500	2.28623000	0.16706000
H	-2.88230200	2.31528200	-1.58905400
H	-3.81495600	1.15951700	-0.62617900
C	-2.97180600	-1.48913400	-0.44673000
H	-2.85388100	-2.02230500	0.50504000
H	-3.89171200	-0.90459600	-0.39286400
H	-3.09949800	-2.24986200	-1.22679400
H	-0.35874500	2.37904600	-0.97586800

Transition state

C	0.97625900	-0.71251200	0.32059800
C	-0.46554800	-1.40207500	-1.32915000
C	-0.44785000	1.38934100	-1.31980000
C	0.94646200	0.71293600	0.34151500
C	-1.60266100	-0.71183000	-0.94589800
C	-1.59903400	0.70990300	-0.95430100
H	-0.42885200	-2.48222500	-1.21436300
C	0.28778400	-1.43637200	1.35242600
N	-0.29829900	-2.00961400	2.17150800
C	2.10106600	-1.37682700	-0.27518500
N	2.98881600	-1.91638900	-0.78795400
C	2.06405400	1.44165100	-0.19137500

N	2.94695100	2.03437800	-0.65068100
C	0.20976600	1.37055600	1.38608700
N	-0.41599800	1.89065300	2.21093500
H	0.26784300	0.97586100	-2.02134800
H	0.23955500	-0.99870200	-2.04687300
C	-2.73876400	1.46106000	-0.32505300
H	-2.86580000	1.17994200	0.72751300
H	-2.57721500	2.54002600	-0.36941400
H	-3.68108800	1.23422400	-0.83706700
C	-2.73208900	-1.44771800	-0.27975200
H	-2.79736600	-1.18585000	0.78378600
H	-3.69298100	-1.18690300	-0.73708300
H	-2.60077700	-2.52920200	-0.35268400
H	-0.41029100	2.47095600	-1.21978600

System 10 (B3LYP/6-31+G(d))

Reactant

C	-1.42538500	0.67338700	-1.75534700
C	-1.46219200	-0.66348000	-1.77805600
C	2.06894900	-1.45714400	-0.91183700
C	2.39360000	-0.72936500	0.17102900
C	2.37323100	0.76258000	0.14518600
H	2.10413600	-2.54374900	-0.89580300
C	2.80534700	1.45380500	-0.92411100
H	2.76812000	2.54041400	-0.94686300
C	-1.68666300	1.13678100	-0.35057700
C	-1.75218600	-1.15814800	-0.38926700
O	-1.87725300	-2.30640500	-0.00862200
O	-1.73747000	2.27936200	0.06397400
H	-1.23987600	1.37353500	-2.56009900
H	-1.31818700	-1.34413100	-2.60763400

N	-1.86898400	-0.02053300	0.41387100
C	-2.17994900	-0.04536400	1.83312100
H	-3.16147000	-0.49894100	2.00238500
H	-1.42689800	-0.62327500	2.37670700
H	-2.18543600	0.98645800	2.18923300
H	1.75087800	-0.98988300	-1.83947100
H	3.22468200	0.95805300	-1.79527200
C	1.87475100	1.47628900	1.38432000
H	1.82107700	2.55642100	1.22022200
H	0.87504600	1.12920500	1.67519800
H	2.53655500	1.29744600	2.24187200
C	2.78053300	-1.39983100	1.47217800
H	3.76519600	-1.05760700	1.81812300
H	2.06533700	-1.17165900	2.27292400

Product

C	-0.24704900	0.76525900	-1.24992300
C	-0.28642100	-0.77952500	-1.22219800
C	1.07847400	-1.42511300	-0.89311900
C	1.80089300	-0.70863900	0.23696400
C	1.83528700	0.63966900	0.21287200
H	0.91631000	-2.48023700	-0.64781900
C	1.14958200	1.35119000	-0.94297200
H	1.04249300	2.42148200	-0.73645000
C	-1.26947300	1.20167500	-0.19965300
C	-1.32860500	-1.12083900	-0.15696600
O	-1.66731600	-2.23050000	0.21307500
O	-1.54519300	2.34302500	0.12175400
H	-0.59446700	1.16167600	-2.21174500
H	-0.65480500	-1.19153300	-2.16956100
N	-1.85691100	0.06281600	0.34695700

C	-2.87999000	0.09430700	1.38254100
H	-3.74265500	-0.49840600	1.06705900
H	-2.48799900	-0.32585000	2.31374200
H	-3.16768700	1.13546200	1.53512200
H	1.69524100	-1.40753200	-1.80500100
H	1.76358100	1.26845300	-1.85314300
C	2.52144900	1.53553700	1.21305100
H	1.80098400	2.22792900	1.67038100
H	3.01986500	0.98892800	2.01696200
H	3.27825400	2.15964100	0.71583300
C	2.44204300	-1.60187500	1.26884800
H	2.96635400	-1.05274300	2.05435400
H	1.68855100	-2.24210600	1.74835900
H	3.16757900	-2.27906000	0.79498500

Transition state

C	-0.63920700	0.70861100	-1.57803900
C	-0.64215500	-0.68675800	-1.58466700
C	1.46530300	-1.40419800	-1.12410000
C	1.78593400	-0.72120000	0.04281700
C	1.79388400	0.70639900	0.05276200
H	1.34776700	-2.48431600	-1.09964500
C	1.48210400	1.40868800	-1.10443200
H	1.37402900	2.48934800	-1.06572400
C	-1.27457200	1.16577200	-0.31004800
C	-1.28332200	-1.14875400	-0.32039100
O	-1.56627600	-2.28129400	0.03543300
O	-1.54397800	2.29947300	0.05149800
H	-0.64966300	1.35336900	-2.44740900
H	-0.66073500	-1.32151800	-2.46130200
N	-1.53266500	0.00405000	0.43640100

C	-2.17628700	-0.00922300	1.73791400
H	-3.13682200	-0.53096900	1.68258900
H	-1.54629700	-0.52072500	2.47283100
H	-2.33437700	1.02787500	2.03955000
H	1.69566200	-0.99268700	-2.09949400
H	1.70431700	1.00708500	-2.08574000
C	1.92625100	1.45239900	1.36364400
H	1.83375000	2.53129700	1.21376300
H	1.16598400	1.14973500	2.09479900
H	2.90407600	1.26037500	1.82483700
C	1.90778000	-1.48606600	1.34352600
H	2.88257500	-1.30296300	1.81447800
H	1.14332400	-1.19123500	2.07393500
H	1.81281700	-2.56246900	1.17834900

System 11 (M06-2X/6-31+G(d))

Reactant

C	-0.65931000	0.66661600	-1.42049200
C	-0.65949900	-0.66677800	-1.42032200
C	2.03808500	-1.17655800	0.13929200
C	1.39099200	-0.73283400	1.23899100
C	1.39121700	0.73278900	1.23877300
H	2.20556900	-2.21164700	-0.13796100
H	0.92864300	-1.34770300	2.00424900
H	0.92905500	1.34802600	2.00384900
C	2.03844300	1.17598800	0.13894200
C	2.54886500	-0.00047900	-0.64319300
H	2.20624200	2.21094400	-0.13861800
H	3.64899800	-0.00064800	-0.67375000
H	2.21582900	-0.00058600	-1.68970200
C	-1.32058200	1.12355600	-0.16720800

C	-1.32090000	-1.12321700	-0.16692200
O	-1.56840500	-2.22806600	0.21436400
O	-1.67952500	0.00031200	0.55416100
O	-1.56777300	2.22857200	0.21379700
H	-0.28272000	1.36578000	-2.15594300
H	-0.28310300	-1.36622400	-2.15560300

Product

C	0.05686000	0.76877500	-0.90858300
C	0.05663000	-0.76903900	-0.90836600
C	1.42186200	-1.13019600	-0.21694300
C	1.31335300	-0.66988300	1.22688300
C	1.31354500	0.66981100	1.22670600
H	1.73429800	-2.16066800	-0.38242200
H	1.15330600	-1.32793500	2.07470700
H	1.15369000	1.32813400	2.07435700
C	1.42219100	1.12971400	-0.21724000
C	2.29297400	-0.00044500	-0.80591400
H	1.73493000	2.16005200	-0.38298500
H	3.30807700	-0.00054000	-0.40053400
H	2.32420000	-0.00059000	-1.90120900
C	-1.15840700	1.14182500	-0.09306600
C	-1.15873800	-1.14149000	-0.09272700
O	-1.57175600	-2.22532000	0.19545100
O	-1.79937500	0.00032500	0.34273600
O	-1.57111400	2.22586100	0.19478200
H	-0.01530300	1.22313000	-1.89968300
H	-0.01569400	-1.22365300	-1.89933500

Transition state

C	-0.26181600	0.69456100	-1.12987300

C	-0.26181500	-0.69456000	-1.12987300
C	1.60271700	-1.15439900	-0.00558400
C	1.22835300	-0.70188600	1.26197100
C	1.22835200	0.70188500	1.26197200
H	1.76806600	-2.19588400	-0.26100900
H	0.87261200	-1.32918500	2.07228400
H	0.87261100	1.32918300	2.07228600
C	1.60271600	1.15440100	-0.00558300
C	2.25961500	0.00000100	-0.71377200
H	1.76806400	2.19588600	-0.26100700
H	3.32553200	0.00000200	-0.43516100
H	2.19350500	0.00000200	-1.80259300
C	-1.25339700	1.13072900	-0.12661800
C	-1.25339600	-1.13072900	-0.12661800
O	-1.64886700	-2.22476100	0.16237700
O	-1.72491500	-0.00000100	0.52295600
O	-1.64887000	2.22475900	0.16237700
H	0.01643000	1.35393000	-1.94130100
H	0.01643100	-1.35392900	-1.94130100

System 12 (B3LYP/6-31+G(d))

Reactant

C	0.47376400	-1.13959900	0.30657100
C	0.99872800	2.34620600	1.04026000
C	-0.99045900	2.56906700	-0.21065600
C	-0.62341100	-1.04745700	-0.45635400
C	-0.49751400	2.41920800	1.20500700
H	-0.79801200	3.27090100	1.83587000
H	-0.90878400	1.52200300	1.69275900
C	1.30658800	2.44787700	-0.27384200
C	0.06986700	2.58452300	-1.05184900

H	1.69491300	2.23551900	1.86463400
H	-2.03671200	2.65637900	-0.48329000
H	0.03238700	2.67846700	-2.13261600
H	2.30214300	2.42789200	-0.70583200
H	0.40191000	-1.20091700	1.38812800
H	-0.55075100	-0.99692600	-1.53820400
C	1.82811500	-1.16913700	-0.30058700
O	2.07889300	-1.05693800	-1.48580000
C	-1.97667300	-1.02113200	0.15219400
O	-2.21855800	-0.95365200	1.34420000
O	2.77147900	-1.35046300	0.65135100
O	-2.93159100	-1.08665000	-0.80134600
C	4.13179200	-1.40353500	0.18551600
H	4.73648400	-1.56640100	1.07791400
H	4.25849000	-2.22519600	-0.52459800
H	4.40306700	-0.46217200	-0.30012300
C	-4.29232400	-1.08466800	-0.33215900
H	-4.90688200	-1.14840100	-1.23028400
H	-4.46949800	-1.94320800	0.32120400
H	-4.50285000	-0.16331500	0.21764200

Product

C	0.56142900	-0.05630400	0.52080800
C	0.94262300	1.42361200	0.93349700
C	-0.94293500	1.70257400	-0.27509200
C	-0.70511900	0.13165900	-0.35563100
C	-0.47697100	1.98898900	1.17224600
H	-0.46833600	3.05854200	1.40530100
H	-1.04295200	1.44410600	1.93570400
C	1.32220700	2.16229000	-0.34304700
C	0.20019700	2.32503000	-1.06236100

H	1.65451300	1.47061700	1.75870400
H	-1.95188200	2.00806500	-0.56004500
H	0.11381900	2.71569300	-2.07165500
H	2.33720200	2.40156700	-0.64500700
H	0.30468200	-0.60657600	1.43305300
H	-0.53100400	-0.17259800	-1.38936100
C	1.67504000	-0.81899400	-0.16666500
O	1.62991600	-1.31514500	-1.27478700
C	-1.90869600	-0.63041400	0.16223000
O	-2.06308500	-1.05001300	1.29412300
O	2.76585800	-0.89762800	0.63138800
O	-2.84423300	-0.76319800	-0.80438000
C	3.88950800	-1.62265800	0.09708300
H	4.65566900	-1.57899000	0.87179100
H	3.60914300	-2.65869600	-0.11117900
H	4.24346800	-1.15278700	-0.82448700
C	-4.05884200	-1.43682900	-0.42382100
H	-4.67413200	-1.45114300	-1.32385900
H	-3.83966500	-2.45415600	-0.08908700
H	-4.56136700	-0.89243200	0.38037400

Transition state

C	0.52461900	-0.44777100	0.41910200
C	0.97684800	1.67461400	0.90925900
C	-0.97716600	1.87439100	-0.30758500
C	-0.63385800	-0.32575800	-0.36888200
C	-0.49765600	1.91551600	1.12409100
H	-0.62817300	2.94405000	1.50197900
H	-1.00305900	1.23652900	1.81243200
C	1.28814000	2.15605000	-0.37508000
C	0.10424300	2.27005300	-1.11425100

H	1.69184200	1.58792300	1.72116200
H	-2.01900600	1.98067900	-0.59338900
H	0.04653400	2.49682500	-2.17370800
H	2.28798400	2.27723500	-0.77710700
H	0.42141600	-0.73945100	1.45891300
H	-0.53953600	-0.42356800	-1.44369800
C	1.79645900	-0.81207200	-0.23487500
O	2.02854700	-0.75462800	-1.43118800
C	-1.94201600	-0.71101800	0.19942100
O	-2.20852700	-0.81668700	1.38687800
O	2.71813600	-1.22366200	0.67576500
O	-2.85571700	-0.93390000	-0.77969600
C	3.99467500	-1.61343300	0.14284800
H	4.58540800	-1.92412600	1.00548700
H	3.87870300	-2.44067600	-0.56287900
H	4.47151200	-0.77175400	-0.36776300
C	-4.16510600	-1.33120100	-0.33821500
H	-4.74571000	-1.47388500	-1.25032400
H	-4.10983200	-2.26190300	0.23311500
H	-4.61269700	-0.55308500	0.28670100

System 13 (MPW1PW91/6-31+G(d))

Reactant

C	-1.81077700	0.02875700	-0.21926600
O	-2.20213500	-0.78870400	-1.32936200
O	-0.79742100	-0.82889500	-0.75317800
C	-2.38606700	-0.37910600	1.14939300
C	-1.64933900	1.53043300	-0.51851200
H	-2.44625000	-1.50030300	1.22267100
H	-1.21174100	1.67360600	-1.54518100
H	-1.72831500	0.01478800	1.97636700

H	-3.41656500	0.06049400	1.28082800
H	-2.65270100	2.04322600	-0.46467000
H	-0.97139600	2.00578400	0.24701900
C	2.29054600	0.09950800	0.54589700
C	1.75539100	-0.32638200	1.73332400
H	1.66087200	-1.41637000	1.97521100
H	1.38987300	0.39962200	2.50489400
C	2.79904600	-0.88415200	-0.52874900
C	2.42547000	1.59611900	0.19373000
H	2.67376500	-1.95775800	-0.20804900
H	2.23996900	-0.73521400	-1.50054000
H	3.89363600	-0.70247800	-0.75089500
H	3.50814100	1.86720100	0.00742900
H	1.86425000	1.83381800	-0.75939300
H	2.02939900	2.25910500	1.01542200

Product

C	-2.88886200	-0.02271000	-0.64956700
O	-3.38244200	-0.75386500	-1.53066800
O	0.88179100	0.07675100	0.95683900
C	-2.86957800	-0.44178400	0.83857300
C	-2.25745500	1.34736600	-0.99034000
H	-3.37438400	-1.43767200	0.97551900
H	-2.28544300	1.53098300	-2.09974700
H	-1.80024900	-0.49889600	1.19862900
H	-3.38868000	0.33915900	1.46852500
H	-2.81776800	2.17049900	-0.45619100
H	-1.19144100	1.38057400	-0.61922700
C	2.28770600	0.11795200	0.50555200
C	1.92493000	-0.48498100	1.83214300
H	1.88921900	-1.59990700	1.94556500

H	2.10574000	0.09447800	2.77488200
C	2.59810000	-0.80415900	-0.69675500
C	2.89752100	1.53821000	0.45005600
H	2.08667900	-1.80208200	-0.58082400
H	2.24477100	-0.32876000	-1.65883800
H	3.71053300	-0.97816800	-0.78278200
H	4.02493900	1.48188000	0.41959600
H	2.55098300	2.07912200	-0.47935300
H	2.59270800	2.14235900	1.35169800

Transition state

C	-1.59709300	0.00142200	-0.18304400
O	-1.89347700	-0.79776400	-1.26355600
O	-0.28766900	-0.68494700	-0.32658300
C	-2.33842800	-0.36350900	1.13642900
C	-1.52808200	1.52640900	-0.47839300
H	-2.26544800	-1.47267100	1.32015200
H	-0.92924900	1.70653300	-1.41522600
H	-1.92228100	0.19261000	2.02525900
H	-3.42744000	-0.08320000	1.03441900
H	-2.57513100	1.91950700	-0.63510100
H	-1.06873900	2.09919300	0.37777000
C	1.87265000	-0.02479500	0.28889800
C	1.03753100	-0.60431100	1.25700400
H	1.04304000	-1.70615100	1.43621600
H	0.52014700	0.03320800	2.01571100
C	2.68144200	-0.89216400	-0.68209400
C	2.04321900	1.49324200	0.16387200
H	2.45313300	-1.98763700	-0.56234400
H	2.47354700	-0.58736200	-1.74978000
H	3.78733200	-0.73007800	-0.50527400

H	3.12930900	1.75947700	0.33673100
H	1.78770900	1.84095800	-0.88007000
H	1.41581100	2.05953200	0.90661900

System 14 (ωb97X-D/6-311+G(d,p))

Reactant

C	-2.41042000	0.92311900	-0.28843100
O	-3.00254000	1.11963100	0.96138700
O	-1.55906800	1.31223800	0.74411300
C	-2.71261800	1.96272800	-1.32679300
C	-2.29358300	-0.50107100	-0.74405400
H	-2.74912300	2.95148800	-0.86993500
H	-2.05145700	-1.14740900	0.09929300
H	-1.94079600	1.94571100	-2.09875200
H	-3.67349500	1.74311000	-1.79789300
H	-3.23629500	-0.82211800	-1.19324900
H	-1.50861600	-0.58131000	-1.49857500
C	1.12200100	0.44558000	-1.51645200
C	0.93448200	1.76306200	-1.45510400
H	0.93817600	-0.06043100	-2.46232600
H	1.07017400	2.33097300	-0.54062100
H	0.62486400	2.31908800	-2.33252100
C	1.54399200	-0.43559100	-0.41117100
C	1.39783400	-1.81893700	-0.55262700
C	1.77869900	-2.68767000	0.46408000
C	2.32100400	-2.18546100	1.64140500
C	2.47939100	-0.80970900	1.79253900
C	2.09724000	0.05573200	0.77718900
H	0.97763900	-2.21763900	-1.47085100
H	1.65416100	-3.75691200	0.33428200
H	2.62394300	-2.85948100	2.43467400

H	2.90994800	-0.41057900	2.70420200
H	2.24370600	1.12222700	0.90688800

Product

C	-3.15527400	1.03655400	-0.32728400
O	-3.33477600	1.21566900	0.86046000
O	-0.14161900	1.42184500	-0.26841200
C	-3.20838100	2.16241100	-1.32339300
C	-2.91025300	-0.34583900	-0.88048000
H	-3.51706600	3.09107700	-0.84505400
H	-2.36538200	-0.95343300	-0.15749800
H	-2.21238000	2.28419200	-1.75824200
H	-3.89217700	1.91058500	-2.13909800
H	-3.88497800	-0.81282000	-1.05793700
H	-2.38042500	-0.31722500	-1.83330800
C	0.54436800	0.34477900	-0.90777500
C	0.90814600	1.73986600	-1.17696200
H	-0.04829100	-0.16547900	-1.66327400
H	1.80497500	2.14884400	-0.71917500
H	0.59205400	2.20478300	-2.10675700
C	1.36162600	-0.55462900	-0.04785100
C	1.49266600	-1.89709800	-0.39791000
C	2.26254300	-2.75718300	0.37889200
C	2.90222600	-2.28113100	1.51751100
C	2.76608900	-0.94254800	1.87764600
C	1.99886500	-0.08409600	1.10125500
H	0.98833100	-2.27298900	-1.28259100
H	2.35700100	-3.79963600	0.09652300
H	3.50030600	-2.94981100	2.12616400
H	3.25679900	-0.56805100	2.76899300
H	1.88506600	0.95420400	1.39387300

Transition state

C	-2.58393000	0.33599500	-0.38586000
O	-2.59107000	0.17476900	-1.72308100
O	-1.43505600	-0.51830500	-0.51043500
C	-3.73730000	-0.30833200	0.35935900
C	-2.24003700	1.73277300	0.09876400
H	-3.88110500	-1.33158200	0.00923600
H	-1.34237200	2.08891300	-0.40890900
H	-3.56498100	-0.31139300	1.43850300
H	-4.64811000	0.26463000	0.16783300
H	-3.07108400	2.40430600	-0.13229600
H	-2.08135200	1.75527200	1.17939100
C	0.06310600	-0.47462300	1.19244900
C	-0.73109900	-1.57236400	1.03610000
H	-0.29668400	0.31377200	1.84722400
H	-0.41694700	-2.43886600	0.46946600
H	-1.61914000	-1.68894700	1.64245800
C	1.35406500	-0.22575400	0.56460700
C	1.97998200	1.00566700	0.79548400
C	3.20500200	1.29997600	0.21222800
C	3.82132800	0.36598300	-0.61327300
C	3.20913200	-0.86352700	-0.85073100
C	1.98734200	-1.15938000	-0.26770900
H	1.49692000	1.73583800	1.43653700
H	3.67686900	2.25743600	0.39956000
H	4.77712800	0.59269100	-1.07166300
H	3.68856700	-1.59234800	-1.49384200
H	1.52576200	-2.11991600	-0.46387400

System 15 (ωB97X-D/6-31G(d))

Reactant

C	-0.37836200	0.77399700	-1.02010300
C	0.92278900	0.50564700	-0.82186100
H	1.60605200	0.83238600	-1.60668100
C	1.59143100	-0.04805400	0.36413300
C	-1.51790500	0.59330700	-0.10960100
H	-0.62644000	1.29281700	-1.94682200
H	-2.12125600	1.49153900	0.03269000
H	2.42689300	0.55362100	0.72616900
C	-1.91337000	-0.52622800	0.49674100
C	1.33185000	-1.19596600	0.99047300
H	-1.41595000	-1.47591100	0.33973000
H	-2.78377300	-0.53123500	1.14637400
H	0.57359400	-1.88678900	0.64141400
H	1.90707000	-1.49930200	1.86040900

Product

C	-0.39909200	0.86855900	-1.05250600
C	1.00016000	0.80382900	-0.61344700
H	1.71262900	1.50665700	-1.03701900
C	1.39233600	-0.11782700	0.27435600
C	-1.35464500	0.21974000	-0.37622500
H	-0.64458800	1.46763500	-1.92534400
H	-2.39624000	0.29092400	-0.67873400
H	2.43353200	-0.19014500	0.57798100
C	-1.01261300	-0.55731400	0.87141000
C	0.40856500	-1.12998300	0.80846200
H	-1.73436800	-1.36385100	1.03786200
H	-1.09913300	0.11930800	1.73668700
H	0.42234800	-2.01068100	0.14649500

H	0.71348300	-1.48433400	1.79871700

Transition state

C	0.69919400	1.23279800	0.16225900
C	-0.69968300	1.23264200	0.16189100
H	-1.17233800	2.21220200	0.11517800
C	-1.47374500	0.12345300	-0.19348200
C	1.47367200	0.12396500	-0.19332700
H	1.17166100	2.21248100	0.11633900
H	2.31242200	0.32639800	-0.86072600
H	-2.31222900	0.32543000	-0.86134900
C	1.13686600	-1.20083600	0.06166800
C	-1.13645200	-1.20110000	0.06218500
H	0.92986300	-1.49101700	1.07869700
H	1.63166800	-1.97970000	-0.51762700
H	-0.92948100	-1.49089200	1.07931600
H	-1.63067700	-1.98042800	-0.51698900

System 16 (ωB97X-D/6-311+G(2df,p))

Reactant

C	-0.01541300	-0.19656100	-0.11229900
H	0.90710200	-0.40030600	-0.64404000
H	-0.84363400	-0.07152400	-0.80040000
H	-0.22602700	-0.97194000	0.61548000
Br	0.21216100	1.47901700	0.85396600
Cl	-0.46883500	-3.22880800	-1.86481700

Product

C	-0.19133300	-1.33253300	-0.77018700
H	0.76908100	-0.91020300	-1.04804600

H	-1.00059900	-0.66623200	-1.05146000
H	-0.22332800	-1.54943800	0.29278200
Br	0.28631100	2.01179300	1.16411600
Cl	-0.40232300	-2.87667500	-1.66253300

Transition state

C	-0.75780300	-0.00003100	0.00090100
H	-0.76194900	-0.92747300	-0.53965900
H	-0.76194700	0.93191900	-0.53184900
H	-0.76195800	-0.00454100	1.07438900
Br	1.70218600	0.00000400	-0.00011500
Cl	-3.10257800	0.00000900	-0.00025000

System 17 (ωB97X-D/TZVP)

Reactant

N	-1.36926100	-0.81437300	-0.51830800
N	-2.46668000	-0.68143500	-0.61542800
Ti	1.18275100	0.75772300	0.46968200
O	-0.18727700	-0.96189200	-0.41541200

Product

N	-1.33912900	-0.02596100	-0.22304800
N	-2.39067800	-0.32047900	-0.43277000
Ti	0.59083600	0.40572900	0.27580500
O	1.44920800	-0.88569600	-0.17636000

Transition state

N	-1.17969800	-0.81658100	0.00000000
N	-2.28587300	-0.70615100	0.00000000
Ti	1.10268200	0.87621400	0.00000000
O	0.00000000	-1.07719900	0.00000000

System 18 (B3LYP/6-31G(d))

Reactant

C	-0.67450700	0.74846600	0.23886400
C	0.66371600	0.77671600	0.16852800
H	1.40733700	1.55281000	0.33186500
C	0.79013500	-0.68459600	-0.22529700
C	-0.78022500	-0.71612200	-0.14884900
H	-1.42888200	1.49274600	0.48163300
H	-1.19204700	-1.38834900	0.61411000
H	-1.28238800	-0.92427700	-1.10179500
H	1.29836200	-1.33354100	0.49870600
H	1.20810300	-0.88136100	-1.22037400

Product

C	-0.72037800	0.47510800	0.29567800
C	0.71303900	0.56867900	-0.01688200
H	1.11353200	1.57908200	-0.10739200
C	1.54703700	-0.46793900	-0.16807700
C	-1.54016000	-0.50969900	-0.09305200
H	-1.13379500	1.30046800	0.87651200
H	-2.58768700	-0.52297300	0.19389900
H	-1.19412000	-1.32752500	-0.72031900
H	1.21394200	-1.49405700	-0.03329300
H	2.59363400	-0.32262800	-0.41976600

Transition state

C	-0.68438900	0.73294100	0.08313500
C	0.68283500	0.73384800	-0.08307200
H	1.33835700	1.54203700	-0.40460300
C	1.06551200	-0.62491000	0.11923000

C	-1.06412200	-0.62656300	-0.11914700
H	-1.34147700	1.54019600	0.40390200
H	-1.88065900	-1.10106100	0.43636900
H	-0.87055300	-1.08763700	-1.08058100
H	0.87341400	-1.08608600	1.08078300
H	1.88189800	-1.09934200	-0.43675100

System 19 (MPW1PW91/6-31+G(d,p))

Reactant

C	0.83799400	-0.16470400	2.75798100
C	1.20055200	0.18860200	1.23850600
C	-1.10823000	0.18547800	1.22558500
C	-0.75849100	-0.16900500	2.74882700
H	1.27781200	-1.15313800	3.07479200
H	1.24093500	0.62983700	3.45231200
H	-1.19625600	-1.16010400	3.05993300
H	-1.17339000	0.62237400	3.43959100
C	0.04633800	1.21535200	0.90188900
H	0.05045600	1.54677700	-0.17611200
H	0.04142200	2.11831800	1.58228400
C	0.73825300	-1.03610300	0.39369800
H	1.41272000	-1.83661900	-0.00105500
C	-0.63460800	-1.03647700	0.38522800
H	-1.30642300	-1.82832200	-0.02903000
H	2.26086700	0.53287400	1.08129800
H	-2.16719300	0.52575000	1.05586200
C	1.14079700	0.24887400	-3.21929300
H	1.69402400	-0.07761800	-2.31260800
H	1.60532100	0.58180800	-4.17173000
N	-1.34036500	0.21759500	-3.08296000
N	-0.18221600	0.23301400	-3.15304700

Product

C	0.85201900	-0.32051200	2.17489300
C	1.18378000	0.37211300	0.79358400
C	-1.13666500	0.33826600	0.81915200
C	-0.74774700	-0.36205200	2.18371500
H	1.31608900	-1.34658100	2.25748100
H	1.24716900	0.29672800	3.03359400
H	-1.15776300	-1.41173300	2.25404400
H	-1.16598200	0.21912400	3.05605000
C	0.00544900	1.41830100	0.67910200
H	-0.02176800	1.97903500	-0.30029700
H	0.00356600	2.16895800	1.52272300
C	0.83064800	-0.65385100	-0.35949700
H	1.28195600	-1.66913900	-0.16886300
C	-0.76179700	-0.66100500	-0.34319400
H	-1.25438100	-1.66873500	-0.21743800
H	2.23053900	0.78668200	0.72595900
H	-2.19845200	0.70831300	0.76400200
C	1.12498800	-0.15585400	-1.81856100
H	1.73558400	0.79379100	-1.86661400
H	1.63944100	-0.91780500	-2.47342400
N	-1.19471700	-0.11966000	-1.69774000
N	-0.22587900	0.14515100	-2.45882900

Transition state

C	2.28239400	0.85213300	-0.24139800
C	0.80677100	1.14662400	0.29526500
C	0.89455000	-1.16322000	0.26433300
C	2.34944900	-0.74560500	-0.25012900
H	2.45403500	1.30363500	-1.26086200

H	3.05356700	1.28920900	0.45959500
H	2.56981000	-1.16918700	-1.27180600
H	3.14587000	-1.12398400	0.45746400
C	0.64176600	-0.03020600	1.33401600
H	-0.38058700	-0.08078600	1.80777700
H	1.42623000	-0.01032300	2.14720300
C	-0.16688000	0.67789300	-0.83478600
H	-0.37109200	1.30877000	-1.73620400
C	-0.09381200	-0.73425600	-0.86005600
H	-0.31871900	-1.37451600	-1.74816600
H	0.65450500	2.19500400	0.67950500
H	0.81158300	-2.22862800	0.61867200
C	-2.30050300	1.14240500	0.00281200
H	-2.19296100	1.68738800	0.97651700
H	-2.90403600	1.66146000	-0.78598400
N	-2.28022900	-1.29370100	0.04195500
N	-2.63843000	-0.18239200	0.15746600

System 20 (ωB97X-D/6-31+G(d,p))

Reactant

C	2.06793300	0.72765300	1.42212900
H	1.72582100	0.29457900	2.36001800
C	1.73249200	0.19591000	0.24881200
H	2.07321300	0.65123600	-0.67940500
C	0.88538700	-1.03438300	0.09308000
H	0.51630700	-1.37929100	1.06825800
O	-0.18357500	-0.83337500	-0.82485800
C	-1.13957900	0.09561500	-0.48608100
C	-1.57473000	0.92853800	-1.43233000
H	-1.13396600	0.91640100	-2.42248800
H	1.46947000	-1.84656200	-0.34856600

H	2.69972500	1.60757100	1.48861600
H	-2.39107100	1.61229900	-1.23289400
C	-1.68325800	0.03602500	0.91348400
H	-0.94130900	0.36675400	1.64799800
H	-2.55513200	0.68611300	1.00300800
H	-1.98168100	-0.98668200	1.16814600

Product

C	0.84126600	1.07611700	0.43373200
H	0.45760100	1.00670100	1.45808800
C	1.60755100	-0.16976900	0.08891300
H	2.00914200	-0.21714500	-0.92354400
C	1.80563600	-1.19628700	0.91447600
H	1.41838500	-1.18990500	1.93140100
O	-1.71647400	-0.18166800	-1.71022100
C	-1.34565600	0.25235600	-0.63803600
C	-0.30371700	1.35618400	-0.55608000
H	0.08404500	1.51613600	-1.56613700
H	2.36581800	-2.07324000	0.60640700
H	1.52006600	1.93740600	0.41140500
H	-0.82260000	2.27491200	-0.25136000
C	-1.90597500	-0.27507500	0.66396700
H	-1.16016200	-0.93064300	1.12780900
H	-2.11455100	0.53703000	1.36789500
H	-2.81115700	-0.85083500	0.46920000

Transition state

C	1.20743600	1.13053400	0.61519000
H	0.60634000	1.06216500	1.51806600
C	1.80745800	-0.00126400	0.09337000
H	2.52139000	0.11143700	-0.71808200

C	1.16146200	-1.23847500	0.24327500
H	0.64213000	-1.45118900	1.17458400
O	-0.34718200	-1.03907600	-0.78854200
C	-0.99301000	0.00661400	-0.38232800
C	-0.55112400	1.27036100	-0.73551800
H	0.07704700	1.38216500	-1.61066700
H	1.56263900	-2.11564900	-0.25159100
H	1.61413800	2.11656100	0.41054700
H	-1.09944200	2.15089700	-0.41069600
C	-2.01965700	-0.19333900	0.70470800
H	-1.52793900	-0.56832900	1.61313800
H	-2.54955800	0.72945400	0.95311900
H	-2.74467500	-0.95148300	0.39773500

System 21 (MN15-L/6-31G(d))

Reactant

C	3.06783500	-0.21127700	1.19487800
C	1.67843100	-0.41146400	1.21940800
C	0.99765100	-0.53495700	0.00343900
C	1.65530200	-0.46530000	-1.22942400
C	3.04478900	-0.26425900	-1.23955000
C	3.75090500	-0.13774000	-0.03111000
H	3.61767500	-0.11061600	2.14042200
H	1.11899200	-0.46761500	2.16257500
H	1.07794600	-0.56214900	-2.15836300
H	3.57675900	-0.20472700	-2.19869700
H	4.83776600	0.01947200	-0.04486200
C	-1.28064900	0.18182900	0.01973800
N	-2.54086200	-0.29839300	0.07684000
C	-2.88170000	-1.72510400	0.03182100
C	-3.67522200	0.62839500	0.03476500

H	-3.57756100	-1.95351600	0.86152100
H	-3.38702400	-1.95763300	-0.92741700
H	-1.98326500	-2.34759400	0.13091400
H	-3.58627600	1.38587500	0.83346100
H	-3.72456700	1.14977200	-0.94096200
H	-4.59578600	0.03767300	0.18420400
S	-0.87888100	1.80786000	-0.04811300
O	-0.37082900	-0.83112700	0.02323200

Product

C	3.34587600	0.26970600	1.13751800
C	1.98960100	0.62219100	1.23838500
C	1.13242900	0.42033800	0.13986100
C	1.62897700	-0.13623800	-1.05639600
C	2.97929100	-0.50333500	-1.14097700
C	3.84027900	-0.29656100	-0.04809200
H	4.01396400	0.43034900	1.99474200
H	1.59138200	1.05314300	2.16719500
H	0.94971700	-0.28849600	-1.90534800
H	3.36445900	-0.94543300	-2.07012000
H	4.89977500	-0.57736400	-0.12325900
C	-1.44566900	-0.60098200	-0.03075900
N	-2.80325500	-0.48006300	0.07851800
C	-3.63449400	-1.61640600	-0.32243600
C	-3.49105500	0.80140300	0.23078900
H	-4.45700100	-1.73935800	0.40768400
H	-4.07314400	-1.44778600	-1.32856900
H	-3.01757300	-2.52708300	-0.34092800
H	-3.04492900	1.39879900	1.04657300
H	-3.48067000	1.39626100	-0.70676300
H	-4.54055900	0.59066700	0.50302900

S	-0.55714400	0.97571400	0.25954200
O	-0.85072400	-1.63778000	-0.28784600

Transition state

C	3.12136700	-0.20614600	1.21017100
C	1.72770200	-0.03355100	1.22826000
C	1.06103700	0.07820500	-0.00166300
C	1.72721100	-0.04311300	-1.23088400
C	3.12092800	-0.21506200	-1.21196600
C	3.82983000	-0.29613100	-0.00069800
H	3.65325100	-0.27285700	2.17047700
H	1.17151200	0.04283100	2.17078600
H	1.17044500	0.02551700	-2.17361200
H	3.65251000	-0.28862000	-2.17193600
H	4.91898100	-0.43085000	-0.00039600
C	-1.32672300	-0.03438500	0.01957100
N	-2.63758500	-0.31721900	0.07120900
C	-3.10872900	-1.70184000	-0.01640500
C	-3.67219200	0.71129100	-0.02001000
H	-3.86081300	-1.87511500	0.77680000
H	-3.58387300	-1.87787100	-1.00293800
H	-2.26380200	-2.39326500	0.11540000
H	-3.28189700	1.67883400	0.33609700
H	-4.02763200	0.81816800	-1.06541500
H	-4.52447700	0.40966300	0.61744400
S	-0.62080100	1.53405600	-0.00880300
O	-0.43886000	-0.96455100	0.00142600

System 22 (M06-2X/6-31+G(d))

Reactant

C	2.38284400	0.62291000	-2.15636100

C	1.76892100	-0.06720000	-1.05842200
C	2.19211900	0.26894300	0.27788900
C	3.22745600	1.25151900	0.42804800
C	3.79212800	1.87259500	-0.64743300
C	3.35676000	1.55838800	-1.96429000
H	2.08521300	0.37643000	-3.16923600
H	3.59456100	1.48846400	1.42030400
H	4.58117700	2.60481200	-0.50071400
H	3.80852700	2.05775400	-2.81612000
C	0.79004300	-1.05765700	-1.27059700
C	0.32279400	-1.80254400	-0.16881600
C	0.70399200	-1.43087100	1.16710300
C	1.59314700	-0.35836400	1.38806400
C	-0.99314200	-3.65674100	0.73261200
C	-0.64407500	-3.26905300	2.05526700
C	0.17133000	-2.19128900	2.26034400
C	-0.53393500	-2.93993000	-0.33512900
H	-1.63260900	-4.52014000	0.57273800
H	-1.01545100	-3.83933400	2.90202400
H	0.44845600	-1.92554400	3.27470700
H	-0.81550200	-3.25126000	-1.33489100
C	1.90222000	0.06755200	2.80390400
C	0.26058000	-1.32974700	-2.65882700
H	-0.75878600	-1.71904000	-2.62565300
H	0.21933300	-0.41237600	-3.25076600
H	0.88308400	-2.05072900	-3.20451800
H	0.98389600	0.13179700	3.39515600
H	2.57350900	-0.64199800	3.30418700
H	2.35739600	1.05585600	2.84676100
C	-1.43252400	1.14556000	-0.54796400
C	-0.90531000	1.54549200	0.61724200

C	0.11712300	2.61262700	0.61970100
O	0.52940900	3.20390600	-0.35303300
O	0.53875700	2.88124100	1.87393400
C	1.47645200	3.95065400	1.98000800
H	1.75847400	3.99311100	3.03191400
H	2.34613700	3.75782200	1.34739300
H	1.01237600	4.89074900	1.67012500
C	-4.53568800	-1.72791600	-1.16319000
C	-3.89759800	-1.65732300	0.07644600
C	-2.87669600	-0.73872700	0.28929600
C	-2.48019100	0.13524600	-0.73320900
C	-3.11628000	0.04296900	-1.97938600
C	-4.13806400	-0.87822800	-2.19457600
H	-5.33226700	-2.44810600	-1.32609900
H	-4.18424700	-2.33430200	0.87629900
H	-2.36020200	-0.72382700	1.24645200
H	-2.80663600	0.70922500	-2.78160700
H	-4.62424300	-0.93112100	-3.16435700
H	-1.19850400	1.13946300	1.58074900
H	-1.06845800	1.64190600	-1.4486640

Product

C	2.51297300	0.27861200	-2.19170100
C	1.67209200	0.00937600	-1.11744900
C	2.06121600	0.37671300	0.17902600
C	3.28678200	0.99539100	0.39524000
C	4.13190100	1.25698600	-0.68632100
C	3.74338700	0.90464200	-1.97424000
H	2.22184000	0.00849800	-3.20237600
H	3.59265000	1.28030100	1.39793400
H	5.09018600	1.73989600	-0.51863800

H	4.39676500	1.11405900	-2.81620600
C	0.29343600	-0.63001900	-1.20717000
C	0.24042600	-1.74512600	-0.17997500
C	0.57408900	-1.33560300	1.11972800
C	0.99816000	0.12353900	1.23572400
C	-0.33865500	-3.93166200	0.65753700
C	-0.02231800	-3.52314000	1.94933600
C	0.43808500	-2.22350400	2.18251800
C	-0.20875800	-3.04009800	-0.41018600
H	-0.69614200	-4.94134800	0.47757500
H	-0.12939900	-4.21352900	2.78098200
H	0.68126800	-1.91727000	3.19552500
H	-0.48161000	-3.35735000	-1.41230900
C	1.42772600	0.49570400	2.64897300
C	-0.07230000	-1.06958000	-2.61687900
H	-1.06297000	-1.53085600	-2.64241000
H	-0.09047500	-0.20887500	-3.29450500
H	0.65582400	-1.79310000	-2.99981200
H	0.58962600	0.39971200	3.34669400
H	2.23680000	-0.16363400	2.98158300
H	1.77966600	1.52682700	2.70764700
C	-0.71961800	0.46784900	-0.66566600
C	-0.26316700	0.95263500	0.73480800
C	0.08175000	2.43357500	0.69474100
O	0.40278800	3.05616400	-0.28885200
O	0.02404800	2.99136100	1.91782400
C	0.45633200	4.35213200	1.98350400
H	0.36740200	4.63896100	3.03028400
H	1.49215600	4.43381300	1.64429600
H	-0.17576900	4.98218500	1.35415400
C	-4.76284600	-1.05809100	-0.97472700

C	-3.98346700	-1.38699300	0.13292400
C	-2.69280900	-0.87804000	0.26266200
C	-2.15242400	-0.02939100	-0.71269700
C	-2.95444200	0.30573700	-1.80954500
C	-4.24452400	-0.20381700	-1.94596500
H	-5.76710800	-1.45897900	-1.07673600
H	-4.37660800	-2.04866100	0.89960000
H	-2.09983900	-1.16581200	1.12773600
H	-2.55476000	0.96987900	-2.57328900
H	-4.84368700	0.06898900	-2.81007000
H	-1.05347300	0.81727400	1.48030100
H	-0.62916500	1.31158500	-1.35709500

Transition state

C	1.89988400	0.46205300	2.69052000
C	1.17961600	0.71081900	1.49860500
C	1.90036000	0.95963500	0.30304500
C	3.31424000	0.96686900	0.33820900
C	3.99135700	0.75648700	1.51938600
C	3.27735900	0.49649300	2.70433300
H	1.36340700	0.27067700	3.61416000
H	3.87468000	1.16475500	-0.57029300
H	5.07674900	0.78793500	1.53607400
H	3.81363400	0.32687100	3.63330900
C	-0.26070600	0.67258800	1.43389800
C	-0.87584300	1.48879000	0.41847700
C	-0.16748600	1.68098500	-0.79540900
C	1.14503200	1.09282500	-0.91737300
C	-2.75331900	2.73647100	-0.48974000
C	-2.05483700	2.91705900	-1.69794800
C	-0.79034200	2.38498700	-1.85192500

C	-2.18112500	2.01959400	0.54043000
H	-3.74852100	3.15454500	-0.37042600
H	-2.50773900	3.48083200	-2.50829700
H	-0.25850400	2.53788400	-2.78559600
H	-2.73696400	1.87444000	1.46115100
C	1.86742000	1.22035000	-2.23572700
C	-1.03660200	0.33633100	2.68112700
H	-2.07673100	0.09702000	2.45049000
H	-0.60773000	-0.53390300	3.18656700
H	-1.02709800	1.17585700	3.38876800
H	1.22253100	0.92209500	-3.06673900
H	2.18144600	2.25916500	-2.40311700
H	2.75140600	0.58392800	-2.27695500
C	-0.41945300	-1.22280400	0.24059900
C	0.38772200	-1.03741800	-0.89255200
C	1.71273700	-1.68262900	-0.86458300
O	2.29891800	-2.04523000	0.13256700
O	2.23236000	-1.82536800	-2.10508600
C	3.52792500	-2.42077700	-2.14780800
H	3.80106800	-2.45787600	-3.20179500
H	4.24309000	-1.81711400	-1.58213600
H	3.49966600	-3.42623900	-1.72136100
C	-4.67217500	-1.73208700	0.00919400
C	-4.01722900	-0.94204500	-0.93534000
C	-2.63852500	-0.76392000	-0.87196600
C	-1.88220900	-1.37422000	0.13987600
C	-2.55499600	-2.16338800	1.08557300
C	-3.93392100	-2.34326700	1.02232300
H	-5.74805200	-1.87044000	-0.04404000
H	-4.58291400	-0.45357400	-1.72388100
H	-2.14999300	-0.12743500	-1.60701700

H	-1.98126200	-2.64722500	1.87322300
H	-4.43123200	-2.96420200	1.76202400
H	-0.06207400	-0.92809000	-1.87470500
H	0.05160000	-1.76380300	1.05939100

Values of the external parameter μ for the testing reaction set presented in Table 3 of the manuscript.

Table S1. External parameter μ in E_h

No.	$\mu[\mathrm{E}_h]$
1	0.01172099
2	0.00964619
3	0.01534064
4	0.01460426
5	0.01841486
6	0.00952677
7	0.02154924
8	0.01953110
9	0.00671141
10	0.01044064
11	0.01102385
12	0.01230222
13	0.01557511
14	0.02372702
15	0.02278763
16	0.02092953
17	0.00069965
18	0.06113551
19	0.02342654
20	0.04144491
21	0.01550286
22	0.06592490