

Theoretical mechanistic insights on the electrophilic addition of hydrogen halides to alkynes

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Electronic Supporting Information

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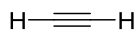
1. Details of Calculations

The calculations were performed with the Gaussian 09,¹ ORCA,² and uESE³ programs. Density functional theory (DFT) calculations using the B3LYP-D3(BJ) theoretical method were used to locate all the stationary points involved.⁴⁻⁷ Structural optimization were obtained at the B3LYP-D3(BJ)/def2-tzvp level under the SMD solution model which computed by a self-consistent reaction field (SCRF) in Gaussian 09, while frequency calculations are under the same level and the substrates, intermediates and products characterized by no imaginary vibrational mode but transition states characterized by only one.^{8,9} Intrinsic reaction coordinate (IRC) calculations for typical transition states were performed, helping to confirm the transition states.^{10,11} The Gibbs energies of correction (ΔG_{corr}) are given by frequency calculations. The energies in gas (E_{gas}) can be obtained at a high level DLPNO-CCSD(T)/aug-cc-pVTZ by using the ORCA program.^{12,13} The wavefunctions were obtained at the same level in order to get CM5 charges by Multiwfn program,¹⁴⁻²³ and the CM5 charges of molecules can be used to calculate the solvation free energies (G_{uESE}) by the usage of uESE program.

References

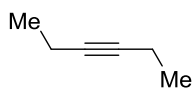
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2. Coordinates of All Stationary Points



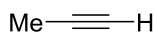
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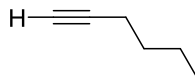
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C	2.61399500	0.87735800	0.00009700
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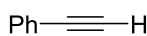
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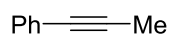
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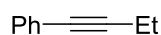
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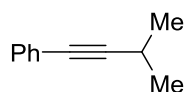
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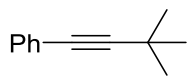
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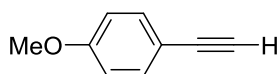
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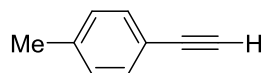
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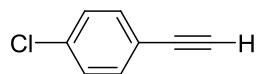
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C	-0.80389700	1.20787400	-0.08447700

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C	0.57399400	1.20718400	-0.22877600
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H	-1.34321800	-2.14434000	-0.03283900
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C	3.39221500	0.00000300	0.71966300
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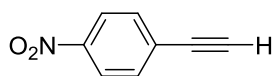
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H	-4.79550200	0.00024900	0.00953300
C	-1.10163500	-0.00004800	0.00124300
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H	1.53313000	2.13953100	-0.01591400
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C	3.21683900	0.00002400	0.01325000
H	3.62241000	0.88510700	-0.47885000
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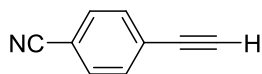
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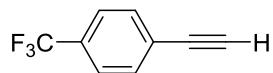
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C	1.05765700	1.21211000	-0.00000600
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C	-0.32414600	1.21576000	-0.00001000
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C	-0.99573400	0.00000000	-0.00001700
H	-0.87738700	2.14262600	-0.00001000
H	-0.87751400	-2.14263400	-0.00001400
N	-2.45683600	0.00004300	-0.00002900
O	-3.03714700	-1.07812800	0.00003900
O	-3.03708300	1.07824900	0.00005000



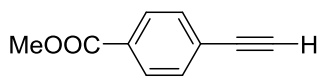
7e

C	-3.99970000	-0.00002400	0.00000200
C	-2.79697500	0.00001200	-0.00000400
H	-5.06554500	-0.00001300	0.00001700
C	-1.37364700	0.00000700	-0.00000400
C	-0.66714500	-1.21094300	-0.00000200
C	-0.66713800	1.21095300	-0.00000200
C	0.71443100	-1.21349100	0.00000000
H	-1.21077800	-2.14556800	-0.00000200
C	0.71443700	1.21349400	0.00000000
H	-1.21076700	2.14558100	-0.00000200
C	1.41022800	0.00000000	0.00000000
H	1.26042500	-2.14683900	0.00000100
H	1.26043700	2.14683900	0.00000100
C	2.83505600	-0.00000400	0.00000300
N	3.98789100	-0.00000700	0.00000500



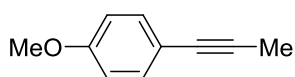
7f

C	-4.87170600	-0.27834800	-0.04123900
C	-3.67374900	-0.17201500	-0.03008700
H	-5.93318300	-0.37245600	-0.05044300
C	-2.25473300	-0.04626300	-0.01461200
C	-1.44289700	-1.18725600	-0.04357400
C	-1.65700700	1.21952300	0.03328500
C	-0.06438500	-1.06420300	-0.02086100
H	-1.89958100	-2.16666500	-0.08077300
C	-0.27829400	1.34030300	0.05592600
H	-2.27945100	2.10340600	0.05559300
C	0.51726400	0.19877500	0.03419400
H	0.55464000	-1.95034900	-0.04109100
H	0.17463900	2.32119900	0.09531900
C	2.01044700	0.33203000	0.02197300
F	2.43531600	1.43819300	0.66808000
F	2.50278800	0.41641200	-1.24039300
F	2.62742100	-0.72071900	0.59869700



7g

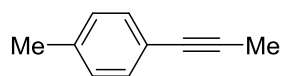
C	-4.87349000	-0.27773800	-0.00003400
C	-3.67480400	-0.17588700	-0.00001100
H	-5.93513200	-0.36857300	-0.00007100
C	-2.25597300	-0.05476900	0.00000500
C	-1.44793300	-1.19976700	0.00002000
C	-1.65263200	1.21073600	0.00000500
C	-0.06968100	-1.08153900	0.00003600
H	-1.91033600	-2.17731100	0.00002000
C	-0.27504100	1.32313100	0.00002100
H	-2.27260500	2.09686200	-0.00000600
C	0.52725300	0.18085500	0.00003700
H	0.54481000	-1.97012200	0.00004800
H	0.19211600	2.29810900	0.00002200
C	2.00029000	0.35635900	0.00005400
O	2.55726600	1.43597000	0.00000700
O	2.66459800	-0.80537100	0.00001300
C	4.10190000	-0.72046200	-0.00003100
H	4.44901700	-0.19854800	0.89112000
H	4.45177100	-1.74899900	-0.00006200
H	4.44896100	-0.19851300	-0.89118400



10a

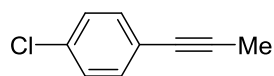
C	-2.35762100	-0.03620100	0.00113300
C	-3.56064100	-0.12342300	-0.00022000
C	-0.93601900	0.06515600	0.00232700
C	-0.13332800	-1.07992200	-0.00718200
C	-0.30099100	1.31846700	0.01278500
C	1.25247500	-0.99192700	-0.00656200
H	-0.60204900	-2.05525200	-0.01524000
C	1.07601100	1.41536100	0.01347400
H	-0.90219000	2.21824900	0.02034100
C	1.86376700	0.26124600	0.00373800
H	1.83824200	-1.89923800	-0.01413400

H	1.56472500	2.38118200	0.02148500
O	3.21061300	0.45794800	0.00511900
C	4.06055500	-0.68580400	-0.00464000
H	3.90326800	-1.28656300	-0.90368700
H	5.07758300	-0.30000500	-0.00180000
H	3.90387000	-1.30136000	0.88444600
C	-5.01000000	-0.23176500	-0.00220600
H	-5.35743800	-0.84709900	-0.83608400
H	-5.37283500	-0.68792500	0.92253400
H	-5.47621000	0.75191300	-0.09563400



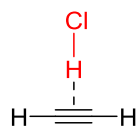
10b

C	1.91547900	0.00001000	0.00180500
C	3.12140000	0.00000600	0.00376600
C	0.48980200	0.00000900	-0.00039800
C	-0.22869700	-1.20322500	-0.00390900
C	-0.22870100	1.20324000	-0.00391900
C	-1.61455800	-1.19636600	-0.00940200
H	0.30955800	-2.14226000	-0.00587900
C	-1.61456200	1.19637600	-0.00941300
H	0.30955000	2.14227700	-0.00589800
C	-2.33403800	0.00000400	-0.01029100
H	-2.14915900	-2.13909700	-0.01544600
H	-2.14916700	2.13910500	-0.01546600
C	-3.83544500	0.00000200	0.01569400
H	-4.24171200	-0.88478800	-0.47665500
H	-4.24171600	0.88477000	-0.47669000
H	-4.20663000	0.00002100	1.04528300
C	4.57458600	-0.00000600	0.00547800
H	4.96573500	-0.88331500	0.51595300
H	4.96905700	-0.00044600	-1.01391400
H	4.96575300	0.88372100	0.51521200



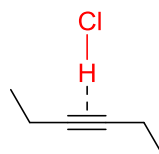
10c

C	-2.33335500	0.00045800	0.00077000	H	5.65581800	-0.00267600	1.02178900
C	-3.53888400	0.00033900	0.00025900	H	5.65998700	-0.88385700	-0.51008700
C	-0.90870300	0.00032800	0.00080400				
C	-0.19350100	1.20571300	0.00097700				
C	-0.19385800	-1.20527500	0.00020700				
C	1.19223600	1.20967600	0.00030900				
H	-0.73105400	2.14446500	0.00163400				
C	1.19187500	-1.20966500	-0.00048500				
H	-0.73170400	-2.14386000	0.00023900				
C	1.87292000	-0.00009600	-0.00049200				
H	1.73627400	2.14403100	0.00041600				
H	1.73562600	-2.14418600	-0.00101400				
Cl	3.62219600	-0.00036000	-0.00145700				
C	-4.99132700	-0.00019100	-0.00016600				
H	-5.38185300	-0.87327400	-0.52822200				
H	-5.38311900	-0.02249200	1.01993600				
H	-5.38269800	0.89415700	-0.49057500				

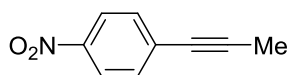


Int1a

C	1.96631800	-0.59955400	0.00039700
C	1.96633300	0.59956100	0.00003700
H	1.96895000	1.66640600	-0.00002500
H	-0.27928700	0.00003300	-0.00004600
H	1.96891000	-1.66639900	0.00037900
Cl	-1.57796700	-0.00004200	-0.00013400



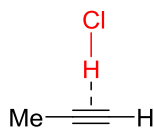
Int1b



10d

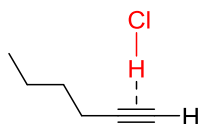
C	2.61346000	-0.00000300	0.00073200
C	3.81910800	-0.00000700	-0.00048700
C	1.19299500	0.00000300	0.00091100
C	0.48198700	1.21118900	0.00087100
C	0.48198900	-1.21118400	0.00068500
C	-0.89909800	1.21529700	0.00029700
H	1.02439000	2.14632800	0.00124300
C	-0.89909600	-1.21529500	0.00010400
H	1.02439400	-2.14632100	0.00090900
C	-1.57341500	0.00000000	-0.00014400
H	-1.45182300	2.14257900	0.00016600
H	-1.45181900	-2.14257800	-0.00017800
N	-3.03077000	-0.00000200	-0.00086600
O	-3.61328600	-1.07834100	-0.00120600
O	-3.61329000	1.07833500	-0.00101600
C	5.26957100	0.00000700	-0.00069800
H	5.66002100	0.88643800	-0.50556400

C	0.60321400	-0.98513300	-0.49716900
C	-0.60335000	-0.98507700	-0.49716600
H	-0.00006900	1.07274900	-0.51420100
C	2.06231700	-0.98283600	-0.45545400
H	2.43967800	-0.23031500	-1.15420900
H	2.42887000	-1.94828600	-0.81586400
C	2.61175500	-0.70865600	0.94833100
H	2.27398900	-1.46929500	1.65392600
H	3.70310300	-0.71535800	0.93216900
H	2.28130200	0.26511600	1.31288600
C	-2.06245700	-0.98267900	-0.45547500
H	-2.43976400	-0.23021200	-1.15431600
H	-2.42906800	-1.94814600	-0.81578300
C	-2.61189500	-0.70831800	0.94827400
H	-3.70324300	-0.71497100	0.93210500
H	-2.27417300	-1.46889800	1.65395500
H	-2.28139500	0.26547600	1.31273100
Cl	0.00036000	2.38517800	-0.55085000



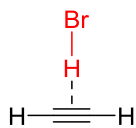
Int1c

C	-1.49626700	0.24429000	0.00060400
C	-1.17906000	1.40478900	0.00076800
H	-0.92502300	2.43980800	0.00086300
H	0.78782200	0.45390300	-0.00146400
C	-1.86513800	-1.15971200	0.00009800
H	-0.97515000	-1.79305600	0.00080200
H	-2.45646400	-1.40404100	0.88482600
H	-2.45489000	-1.40386000	-0.88573400
Cl	2.04961800	0.12217300	-0.00080500



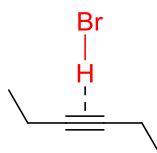
Int1d

C	-0.47028600	1.65905300	0.12207700
C	-1.32453700	1.84218700	-0.70544400
H	-1.26229000	-0.34903300	-0.85888700
C	0.56645200	1.42793900	1.12147800
H	0.11438000	1.49380000	2.11435200
H	1.29681800	2.24013000	1.05650100
C	1.28416100	0.07622500	0.96799800
H	1.97277400	-0.03053900	1.81012200
H	0.55301300	-0.73102400	1.05722700
H	-2.07730600	2.03592400	-1.43178200
C	2.05263800	-0.06695200	-0.34181000
H	1.37157100	0.08672700	-1.18287500
H	2.80363900	0.72708300	-0.40520500
C	2.72574700	-1.42907200	-0.47689700
H	1.98467300	-2.23128700	-0.45828000
H	3.27866600	-1.50674500	-1.41458800
H	3.42833700	-1.60459400	0.34147200
Cl	-1.41772500	-1.60312700	-1.17328000



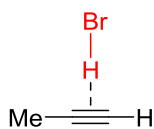
Int2a

C	-0.59945200	2.67244800	0.00000000
C	0.59970500	2.67233200	0.00000000
H	-1.66634700	2.67576100	0.00000000
H	1.66660100	2.67544700	0.00000000
Br	0.00002800	-1.03484300	0.00000000
H	-0.00005700	0.40503000	0.00000000



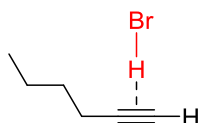
Int2b

C	-0.56715000	1.50017400	-0.20727600
C	0.56565600	1.50262000	0.20833200
Br	0.01068000	-2.03005500	-0.00402700
H	0.00527000	-0.57330200	-0.00342600
C	-1.95060700	1.50045500	-0.67247700
C	-2.96193800	1.30491700	0.46116400
H	-2.07599400	0.71286900	-1.42166500
H	-2.14942800	2.44483300	-1.18753700
H	-3.97777600	1.31145600	0.06226000
H	-2.80235400	0.35358100	0.97105000
H	-2.87895800	2.10360000	1.19992000
C	1.94909500	1.50958000	0.67364700
C	2.96194500	1.32506400	-0.46050700
H	2.07934800	0.71960800	1.41948800
H	2.14190300	2.45297000	1.19274800
H	3.97761300	1.33706500	-0.06132300
H	2.80929200	0.37439700	-0.97380200
H	2.87358100	2.12562400	-1.19657300



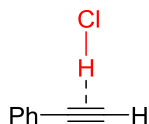
Int2c

C	-2.20812100	0.20981600	-0.00006300
C	-1.91929700	1.37766900	0.00004800
Br	1.52822700	0.26664400	0.00017900
H	0.11036800	0.55653800	-0.00032800
C	-2.54480600	-1.20177900	-0.00002600
H	-3.13001400	-1.45922500	-0.88515200
H	-1.64213700	-1.81714200	-0.00035300
H	-3.12943400	-1.45930700	0.88545900
H	-1.69706900	2.42001100	0.00024000



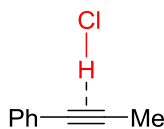
Int2d

C	-0.07437600	2.00590800	0.02848300
C	0.79841700	2.60480700	-0.54460400
Br	2.61840400	-0.49823800	0.04738800
H	1.77810700	0.66774500	-0.12768500
C	-1.12508700	1.24836100	0.69160700
H	-0.68323300	0.67043700	1.50941400
H	-1.82583000	1.94963100	1.15477200
H	1.55893800	3.15642200	-1.04777100
C	-1.87976400	0.31041700	-0.26156400
H	-1.16796300	-0.37931300	-0.72332800
H	-2.31457600	0.90177300	-1.07202400
C	-2.97331300	-0.47766000	0.45090000
H	-2.52669400	-1.06064400	1.26298600
H	-3.67439700	0.22003700	0.92060100
C	-3.73111700	-1.40849600	-0.48831500
H	-3.05815500	-2.13462000	-0.95201900
H	-4.50504700	-1.96636900	0.04376900
H	-4.21850600	-0.84886900	-1.29109800



Int3a

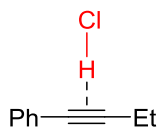
C	0.59373300	1.40562200	0.47318000
C	1.58444500	2.07238600	0.63468200
H	2.44952400	2.67406300	0.79534600
H	2.36792900	0.31059500	-0.47215400
Cl	3.06782400	-0.62195200	-1.05102800
C	-0.56206600	0.59626200	0.27545200
C	-0.63186800	-0.67916300	0.85099600
C	-1.63086900	1.06336300	-0.50034700
C	-1.75350400	-1.46931000	0.65224000
H	0.19608400	-1.04064100	1.44605000
C	-2.74870000	0.26567600	-0.69167200
H	-1.57480700	2.04735800	-0.94651100
C	-2.81300400	-0.99986800	-0.11736200
H	-1.80058900	-2.45429800	1.09866000
H	-3.57172600	0.63193200	-1.29183000
H	-3.68732700	-1.61967900	-0.27016700



Int3b

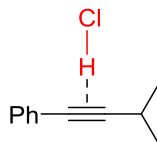
C	1.78863700	1.39415800	0.22323500
C	0.64678600	1.00524800	0.17214700
H	1.89526400	-0.78533000	-0.09551700
C	3.16050800	1.87090500	0.29254400
H	3.79509300	1.15272200	0.81503900
H	3.21308000	2.82057200	0.82880400
Cl	2.33887500	-2.00679100	-0.21721400
H	3.57168700	2.02283500	-0.70709000
C	-0.70173000	0.54441900	0.10868900
C	-1.60152000	1.10508500	-0.80806700
C	-1.14252800	-0.47964300	0.95808500
C	-2.91069200	0.65129800	-0.86874800
H	-1.26394500	1.89396200	-1.46638600
C	-2.45273600	-0.92932700	0.88894200
H	-0.45088200	-0.91740300	1.66482800
C	-3.34029600	-0.36616500	-0.02241400

H	-3.59742000	1.09170400	-1.57969800
H	-2.78192500	-1.72158600	1.54839900
H	-4.36196600	-0.71890200	-0.07342700



Int3c

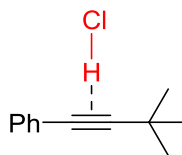
C	-1.48913800	-0.95093500	0.57490300
C	-0.31813600	-0.70214900	0.41164200
H	-1.43494500	1.07249800	-0.27193600
C	-2.90241800	-1.26262000	0.74505200
H	-3.38627400	-0.43605000	1.27325400
H	-2.99331200	-2.13883400	1.39406700
Cl	-1.79896100	2.24706000	-0.71351300
C	1.06584200	-0.41502300	0.22067800
C	1.88300000	-1.30764500	-0.48642400
C	1.62475500	0.76440800	0.73152200
C	3.22719800	-1.02367900	-0.67472700
H	1.45454800	-2.21853400	-0.88324900
C	2.96939100	1.04144800	0.53548400
H	0.99862300	1.45709200	1.27798400
C	3.77420800	0.15016300	-0.16649500
H	3.85006600	-1.72019400	-1.22162400
H	3.39050300	1.95653600	0.93217300
H	4.82345400	0.36971100	-0.31779500
C	-3.62021400	-1.52408800	-0.58402400
H	-3.16798900	-2.36511800	-1.11151900
H	-4.67021400	-1.75719300	-0.40027100
H	-3.57208800	-0.64841600	-1.23257100



Int3d

C	1.36735800	-0.56773900	-0.18724000
C	0.16208200	-0.49759500	-0.13713500

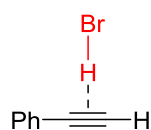
H	0.92499300	1.52764200	0.21524600
C	2.82291000	-0.69486200	-0.23507900
Cl	1.05286900	2.81341400	0.41364700
C	-1.25980800	-0.40941700	-0.07494400
C	-1.97668600	-1.17212000	0.85708100
C	-1.95691500	0.44584000	-0.93909300
C	-3.35895000	-1.08020500	0.91817700
H	-1.44108000	-1.83177300	1.52689700
C	-3.33921600	0.53304800	-0.86895700
H	-1.40753900	1.03745300	-1.65933100
C	-4.04404200	-0.22839600	0.05758300
H	-3.90332000	-1.67392500	1.64154800
H	-3.86806500	1.19783100	-1.54007800
H	-5.12313700	-0.15832200	0.10895300
C	3.40490000	-0.81758800	1.17976100
H	3.03702000	-1.72090200	1.67047400
H	4.49403100	-0.87192000	1.13058800
H	3.13258600	0.04115700	1.79481100
C	3.23612600	-1.87868800	-1.12067200
H	4.32484700	-1.93570300	-1.17695300
H	2.86308200	-2.81817000	-0.70839500
H	2.84495000	-1.76987600	-2.13303800
H	3.21796300	0.22066200	-0.68844200



Int3e

C	1.42644600	-0.50690500	-0.24150300
C	0.21961700	-0.48222700	-0.19257100
H	0.81278800	1.47564000	0.55969900
C	2.89062900	-0.56915400	-0.31750900
Cl	0.82355500	2.70142600	1.00918800
C	-1.20502600	-0.45105500	-0.13163500
C	-1.90122500	-1.35616900	0.68095400
C	-1.92670600	0.49072400	-0.87765800
C	-3.28640100	-1.31896200	0.74057100

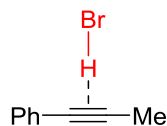
H	-1.34680600	-2.08207700	1.26004900
C	-3.31165700	0.52246400	-0.81074900
H	-1.39269100	1.19320100	1.50289800
C	-3.99547100	-0.38099800	-0.00342900
H	-3.81420200	-2.02272500	1.37078200
H	-3.85879800	1.25465400	-1.38995000
H	-5.07602600	-0.35373700	0.04656100
C	3.48574700	-0.37469700	1.09006700
H	3.12976200	-1.14768500	1.77169300
H	4.57428400	-0.43369600	1.03773800
H	3.21340500	0.59832400	1.49927100
C	3.29893000	-1.94944200	-0.86724900
H	4.38699100	-2.01069900	-0.92829400
H	2.94330100	-2.74773300	-0.21522400
H	2.88658200	-2.10797100	-1.86406300
C	3.40156100	0.53747100	-1.25866000
H	2.98659000	0.41708400	-2.25974800
H	3.12666500	1.52496800	-0.88757700
H	4.48956200	0.48609900	-1.32628400



Int4a

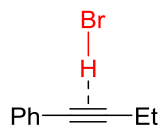
C	-0.20729800	1.65599700	0.53712500
C	0.70288200	2.42681300	0.70815800
H	1.49178000	3.12299800	0.86508800
H	1.66175000	0.66448900	-0.40138600
C	-1.26668200	0.72768900	0.32193400
C	-1.97196000	0.19320900	1.40810800
C	-1.60432800	0.33393800	-0.97963700
C	-2.99659800	-0.71554200	1.19137200
H	-1.70916100	0.49547000	2.41254600
C	-2.62898600	-0.57708000	-1.18604700
H	-1.05733800	0.74324300	-1.81766000
C	-3.32711900	-1.10288100	-0.10356000
H	-3.53743300	-1.12397000	2.03475200

H	-2.88288100	-0.87798000	-2.19378300
H	-4.12622000	-1.81353000	-0.26848000
Br	2.41845600	-0.31701200	-1.14003900



Int4b

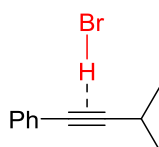
C	0.76857200	2.06362300	0.36302600
C	-0.23145000	1.38993900	0.29431100
H	1.39592100	0.14777500	-0.51686800
C	1.97155300	2.87246800	0.44558600
H	2.68074400	2.44595800	1.15837300
H	1.73402600	3.88822200	0.77042200
H	2.46550600	2.93840700	-0.52699100
C	-1.40600500	0.58684900	0.20133400
C	-2.45061900	0.95452500	-0.65754400
C	-1.52355200	-0.58775100	0.95692500
C	-3.58620500	0.16454000	-0.75291200
H	-2.36112200	1.85839000	-1.24539300
C	-2.66246700	-1.37233600	0.85409200
H	-0.71766300	-0.87712700	1.61831700
C	-3.69619600	-0.99942100	0.00117500
H	-4.38774600	0.45777000	-1.41888700
H	-2.74330700	-2.27824900	1.44125200
H	-4.58414700	-1.61375000	-0.07660000
Br	2.18931800	-0.91474400	-1.10191300



Int4c

C	0.99602600	1.79193400	0.39155300
C	-0.11876200	1.34858100	0.25014800
H	1.21217100	-0.38972000	0.47818900
C	2.34724600	2.31976800	0.53260400
H	2.82257900	1.84750400	1.39684500

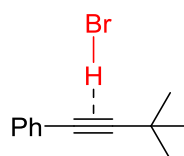
H	2.28652200	3.38759700	0.76139900
C	-1.43118800	0.81589100	0.08675900
C	-2.18450400	1.11946000	-1.05550500
C	-1.98047700	-0.02745400	1.06231900
C	-3.45757200	0.59227300	-1.21310400
H	-1.76215000	1.76761500	-1.81127100
C	-3.25349400	-0.55208200	0.89575000
H	-1.40111400	-0.26650500	1.94362200
C	-3.99564600	-0.24430200	-0.24006500
H	-4.03101800	0.83339100	-2.09855800
H	-3.66734000	-1.20331100	1.65440400
H	-4.98863200	-0.65507700	-0.36687100
C	3.20717100	2.10205000	-0.71983800
H	2.76014800	2.59089700	-1.58564800
H	4.20355500	2.51659800	-0.56444000
H	3.30685700	1.03929600	-0.94092600
Br	1.77760700	-1.71711200	0.62859200



Int4d

C	0.96287400	-1.24785300	-0.20987300
C	-0.21247200	-0.97076300	-0.16497500
H	0.83708700	0.81182800	0.57233200
C	2.37447100	-1.62357400	-0.26418800
C	-1.59299900	-0.61912700	-0.11234700
C	-2.35117400	-0.88780100	1.03516400
C	-2.20350100	0.01591000	-1.20235600
C	-3.68988100	-0.52944500	1.08602900
H	-1.88139000	-1.37464500	1.87957300
C	-3.54281200	0.37012000	-1.14277600
H	-1.61882500	0.22833900	-2.08760600
C	-4.28942500	0.09936700	-0.00056200
H	-4.26730200	-0.73996200	1.97729200
H	-4.00476000	0.86139800	-1.98973600
H	-5.33428600	0.37936700	0.04311300

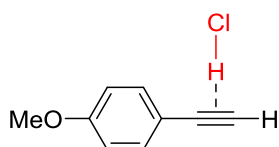
C	2.90816500	-1.95546700	1.13568100
H	2.38804800	-2.82092400	1.55103800
H	3.97329400	-2.18767400	1.08189100
H	2.77607800	-1.11701000	1.82060000
C	2.58782000	-2.78899200	-1.24088600
H	3.64982600	-3.03485000	-1.29838500
H	2.04737100	-3.67646200	-0.90595600
H	2.23909300	-2.53411800	-2.24248800
Br	1.14318800	2.13688800	1.07481800
H	2.92957200	-0.75911900	-0.64501700



Int4e

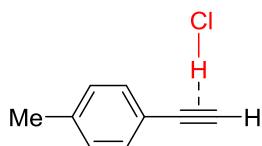
C	-1.17513800	1.18190700	-0.20998200
C	0.01996400	1.01496100	-0.15019900
H	-0.79659900	-0.90598300	0.49113400
C	-2.62082900	1.41939900	-0.29054300
C	1.42890300	0.80801100	-0.07806800
C	2.03991800	0.51201000	1.14806600
C	2.21914800	0.88638600	-1.23286300
C	3.40910200	0.30103000	1.21363200
H	1.43258900	0.44684200	2.04047000
C	3.58802300	0.67615900	-1.15819500
H	1.74986900	1.11134600	-2.18093800
C	4.18694400	0.38275000	0.06301900
H	3.87026200	0.07144300	2.16524600
H	4.18913400	0.73942500	-2.05579600
H	5.25492300	0.21752600	0.11744500
C	-3.24805100	1.23366800	1.10355200
H	-2.81231100	1.92995500	1.82062900
H	-4.32199400	1.41970900	1.04884700
H	-3.09362100	0.21885500	1.47056100
C	-2.85897700	2.86072200	-0.78056700
H	-3.93169500	3.05147400	-0.84611500
H	-2.42021300	3.58271500	-0.09136300

H	-2.41950100	3.01323700	-1.76670400
Br	-0.93678500	-2.26278600	0.98313700
C	-3.24921800	0.42352600	-1.28381900
H	-3.09812800	-0.60499500	-0.95572200
H	-4.32256200	0.60758900	-1.35564700
H	-2.81140700	0.53700400	-2.27594500



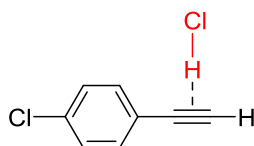
Int5a

C	1.81627700	1.44146400	0.14437300
C	2.94005500	1.87858000	0.12154200
H	3.92009200	2.29181500	0.10955900
C	0.50199800	0.89865400	0.17212100
C	0.09923000	0.05663400	1.22200200
C	-0.41182900	1.18182400	-0.84697800
C	-1.17130500	-0.47779400	1.24580200
H	0.79688100	-0.17569300	2.01482600
C	-1.69247700	0.64960500	-0.82844600
H	-0.11459400	1.82631700	-1.66296900
C	-2.07927400	-0.18590600	0.22147300
H	-1.48560900	-1.12830400	2.05060500
H	-2.37435800	0.88835400	-1.63005800
O	-3.30123700	-0.75591800	0.33245300
C	-4.26686300	-0.50184300	-0.68468800
H	-3.91741200	-0.85937400	-1.65575900
H	-5.15691500	-1.05216700	-0.39312400
H	-4.49986200	0.56334000	-0.74807900
Cl	3.60291300	-1.57844100	-0.05202300
H	3.22973700	-0.33156900	-0.01039200



Int5b

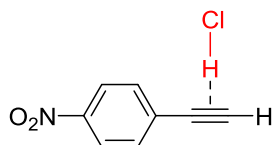
C	1.28037500	1.43020800	0.43246600
C	2.37111600	1.93101100	0.54590300
H	3.32487200	2.39165100	0.66489000
C	0.00332900	0.81800100	0.28705400
C	-0.26270200	-0.41889300	0.88802600
C	-1.00092200	1.43355900	-0.47011200
C	-1.50181700	-1.01674700	0.73198400
H	0.50891800	-0.90670100	1.46885900
C	-2.23610100	0.82406900	-0.61551500
H	-0.80335400	2.38614200	-0.94380400
C	-2.51028500	-0.40814900	-0.01845800
H	-1.69032000	-1.97612100	1.19872400
H	-3.00129700	1.31143400	-1.20766400
Cl	3.36826200	-1.05189900	-0.99845700
H	2.84762400	0.01097900	-0.45436100
C	-3.85930200	-1.05058200	-0.15760700
H	-3.78475600	-2.13888500	-0.14108200
H	-4.34916800	-0.75179000	-1.08518600
H	-4.51454200	-0.75648900	0.66825700



Int5c

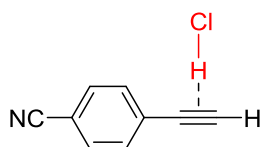
C	1.75765800	1.42893200	0.41899400
C	2.87916500	1.85613000	0.52477400
H	3.86433100	2.24835200	0.63441300
C	0.44089200	0.90428300	0.28299100
C	0.09907200	-0.31108300	0.88898500
C	-0.52248700	1.59079500	-0.46616200
C	-1.17685500	-0.83138800	0.75000500
H	0.83855700	-0.84881700	1.46656000
C	-1.80052100	1.07618100	-0.60673500
H	-0.26524200	2.52889600	-0.93884300
C	-2.11483700	-0.13130300	0.00284700
H	-1.43840000	-1.77062000	1.21667700
H	-2.54347100	1.60660100	-1.18550800

Cl	3.65615600	-1.21635500	-1.02814000
H	3.21859600	-0.11722900	-0.48725900
Cl	-3.72476500	-0.78364500	-0.17588000



Int5d

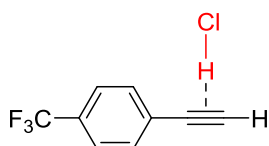
C	2.04339200	1.43358900	0.38116600
C	3.16991200	1.84827900	0.47225300
H	4.16233000	2.22787400	0.56372000
C	0.71297000	0.94121500	0.26680400
C	0.39249700	-0.33952100	0.73817400
C	-0.28083800	1.73703600	-0.32019600
C	-0.89871800	-0.81935600	0.62538800
H	1.15979300	-0.95259900	1.18926200
C	-1.57377900	1.26297300	-0.43514200
H	-0.03100400	2.72415100	-0.68270000
C	-1.86276100	-0.00913800	0.04061900
H	-1.15862600	-1.80431400	0.98217500
H	-2.34862500	1.86566900	-0.88386100
Cl	4.06876500	-1.32330000	-0.82648400
H	3.57348100	-0.21327600	-0.37076300
N	-3.23128100	-0.51312100	-0.07856100
O	-4.06070500	0.19205200	-0.63777700
O	-3.48402300	-1.61681900	0.38596700



Int5e

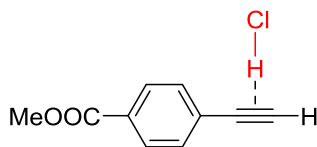
C	2.72991600	1.86916100	0.50765600
C	1.61302300	1.43078000	0.40647200
H	3.71335200	2.26852000	0.60945500
C	0.30026700	0.89456700	0.27810200
C	-0.01454200	-0.33818500	0.86556100

C	-0.67858000	1.59062500	-0.44338300
C	-1.28385600	-0.86755700	0.73367800
H	0.74167500	-0.87546400	1.42066900
C	-1.94979500	1.06557900	-0.57584800
H	-0.43370400	2.54070700	-0.89745800
C	-2.25529900	-0.16615100	0.01229400
H	-1.52960300	-1.81913400	1.18419400
H	-2.70715500	1.60003500	-1.13226600
Cl	3.52792000	-1.23353600	-1.04527700
H	3.08653200	-0.13618000	-0.50902000
C	-3.56572300	-0.71044700	-0.12426900
N	-4.62602000	-1.14907400	-0.23344500



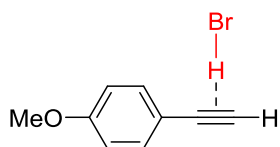
Int5f

C	-3.63016800	1.76265600	-0.54647900
C	-2.48633300	1.40235400	-0.43943000
H	-4.63560500	2.09525000	-0.65054700
C	-1.13709300	0.96398200	-0.30577700
C	-0.73933100	-0.26702400	-0.84080800
C	-0.20047100	1.75657900	0.36968100
C	0.57002800	-0.69604800	-0.70322300
H	-1.46064500	-0.88398400	-1.35717700
C	1.10774300	1.32562300	0.50385100
H	-0.50616400	2.70522500	0.78737900
C	1.49232400	0.09888700	-0.03047300
H	0.86996300	-1.64922300	-1.11403500
H	1.82553700	1.93947000	1.02925100
Cl	-4.04630600	-1.48946000	0.91505400
H	-3.77941900	-0.31823200	0.42477600
C	2.92433200	-0.34008800	0.08050400
F	3.68488600	0.17559900	-0.91688200
F	3.49260600	0.05838600	1.23753100
F	3.05956100	-1.67915100	0.01251800



Int5g

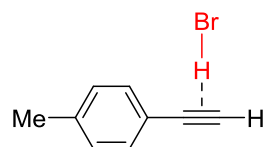
C	3.68769300	1.76572100	0.46881200
C	2.54692900	1.38387800	0.41114600
H	4.69005200	2.11853500	0.52411600
C	1.20171500	0.92124000	0.33843700
C	0.86185700	-0.34438700	0.83557100
C	0.20843800	1.72552300	-0.23542400
C	-0.44440000	-0.79054900	0.75848200
H	1.62687000	-0.96844900	1.27533000
C	-1.09735300	1.27354200	-0.30793200
H	0.47028000	2.70091600	-0.62072700
C	-1.43292000	0.01256500	0.18850300
H	-0.71450300	-1.76538800	1.13839400
H	-1.85975200	1.89678700	-0.75052100
Cl	4.13756500	-1.40023500	-1.14121800
H	3.84490500	-0.26428600	-0.58619500
C	-2.82260500	-0.51575600	0.13267300
O	-3.15521900	-1.59920400	0.55980300
O	-3.67536800	0.34153400	-0.44497100
C	-5.04421500	-0.08978300	-0.54159500
H	-5.45239700	-0.27625100	0.45030200
H	-5.57211100	0.72629700	-1.02498800
H	-5.11275000	-0.99747900	-1.13888700



Int6a

C	0.88803400	1.89373900	0.37026900
C	1.92617100	2.50732000	0.39936500
H	2.82698000	3.07463100	0.44738500
C	-0.31806700	1.14291400	0.32572000
C	-0.51575600	0.05837500	1.19629900

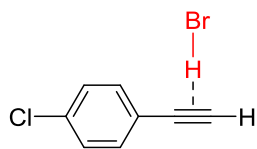
C	-1.32612300	1.46166800	-0.58909800
C	-1.68185000	-0.67559200	1.14906100
H	0.25598500	-0.20137300	1.90852500
C	-2.50279900	0.72995500	-0.63953100
H	-1.18542400	2.29201900	-1.26823200
C	-2.68506700	-0.34454500	0.23234300
H	-1.83995200	-1.51176800	1.81755100
H	-3.26362600	1.00094900	-1.35565900
O	-3.79744600	-1.11957500	0.26341500
C	-4.87667000	-0.79894400	-0.61330400
H	-4.57385800	-0.88694500	-1.65926800
H	-5.65607900	-1.52715800	-0.40127800
H	-5.25652500	0.20669800	-0.41911500
Br	3.25730800	-0.67550000	-0.79551100
H	2.59464700	0.52740400	-0.34224300



Int6b

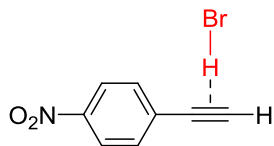
C	0.39137500	1.79523600	0.56072000
C	1.39193900	2.45391600	0.69730300
H	2.26302500	3.05128100	0.83962700
C	-0.77348900	0.99816600	0.37829100
C	-1.01738600	-0.10487700	1.20612200
C	-1.68379300	1.29239100	-0.64446500
C	-2.14503700	-0.88475500	1.01265300
H	-0.31556100	-0.34552200	1.99374700
C	-2.80766900	0.50390400	-0.82503600
H	-1.49971600	2.13783800	-1.29410500
C	-3.06049200	-0.59536200	-0.00160000
H	-2.31811200	-1.73715400	1.65856100
H	-3.50136200	0.74315200	-1.62210500
Br	2.77929600	-0.27432600	-1.32604900
H	2.10465300	0.73809600	-0.54637300
C	-4.29683200	-1.42620400	-0.18299800
H	-4.13155800	-2.45805200	0.12973300

H	-4.62593900	-1.42828700	-1.22301600
H	-5.11977200	-1.02993300	0.41982500



Int6c

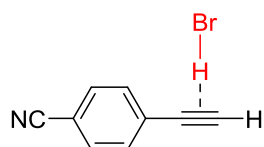
C	0.86174200	1.92315000	0.40256600
C	1.90850500	2.51178200	0.49966600
H	2.82029100	3.05500700	0.59893700
C	-0.35934200	1.20262800	0.27701700
C	-0.58120500	0.05002600	1.04085600
C	-1.34642400	1.63125100	-0.61901200
C	-1.76296000	-0.66083700	0.91309900
H	0.17632300	-0.28768400	1.73484800
C	-2.53101400	0.92590900	-0.74876800
H	-1.18083200	2.51948000	-1.21329200
C	-2.72735400	-0.21424700	0.01945000
H	-1.93177600	-1.55177000	1.50141500
H	-3.29260100	1.25738700	-1.44047900
Br	3.24120100	-0.68584200	-0.73537700
H	2.57849200	0.51084900	-0.27560100
Cl	-4.22038200	-1.10512100	-0.14259200



Int6d

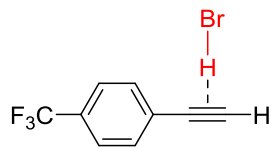
C	1.18028700	1.94809900	0.53931100
C	2.24292400	2.49961900	0.66552900
H	3.17381200	3.00516400	0.78818300
C	-0.06111700	1.27107100	0.38037600
C	-0.31964200	0.10293900	1.11094200
C	-1.02166400	1.76084700	-0.51518100
C	-1.51837600	-0.56621800	0.95149600
H	0.42359400	-0.27338800	1.79961500

C	-2.22280500	1.09694900	-0.67780200
H	-0.81834200	2.65992700	-1.07953500
C	-2.45244100	-0.05729800	0.05922500
H	-1.72992700	-1.46695300	1.50715200
H	-2.97127800	1.46320100	-1.36386500
Br	3.30085100	-0.64107200	-1.08301600
H	2.78720400	0.53104800	-0.42469700
N	-3.72420700	-0.76177400	-0.11012000
O	-4.53675000	-0.30590300	-0.90379100
O	-3.91786300	-1.77354100	0.55077500



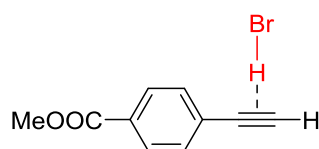
Int6e

C	1.74668300	2.53118100	0.47777600
C	0.71074700	1.92397300	0.38750300
H	2.65224300	3.08690400	0.56741000
C	-0.50056300	1.18568600	0.27027800
C	-0.69136200	0.02338400	1.02951800
C	-1.50224600	1.61197500	-0.61206800
C	-1.86122100	-0.70185900	0.90877500
H	0.08087100	-0.30408100	1.71145300
C	-2.67460000	0.89119000	-0.73355100
H	-1.35229800	2.50826100	-1.19762900
C	-2.85656400	-0.26856800	0.02705000
H	-2.01133400	-1.60039600	1.49095200
H	-3.44986300	1.21638900	-1.41328900
H	2.45618700	0.50166800	-0.28376400
C	-4.06607700	-1.01298400	-0.09653600
N	-5.04498800	-1.61326900	-0.19603400
Br	3.13498400	-0.68374200	-0.74130800



Int6f

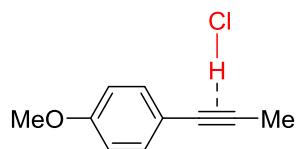
C	-2.73568600	2.54027100	-0.38416500
C	-1.65323700	2.01852700	-0.30912800
H	-3.68496100	3.01554400	-0.45604400
C	-0.38190400	1.38244300	-0.21624200
C	-0.06053400	0.32167000	-1.07236300
C	0.55154200	1.80362000	0.73857200
C	1.17037000	-0.30369100	-0.97437600
H	-0.78062800	-0.00985200	-1.80661700
C	1.78275900	1.17752100	0.83240500
H	0.30420900	2.61873900	1.40359700
C	2.09094000	0.12310000	-0.02182300
H	1.41083200	-1.12528900	-1.63390400
H	2.49812500	1.50455200	1.57323700
H	-3.19561800	0.28583300	0.02783000
C	3.44347900	-0.52578600	0.04808900
F	4.32733100	0.06731100	-0.79246600
F	3.98359100	-0.45693400	1.28148500
F	3.40500400	-1.82908400	-0.29642700
Br	-3.62984000	-1.07382200	0.21733200



Int6g

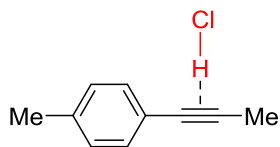
C	2.81492700	2.45075300	0.48546100
C	1.72126100	1.94811600	0.44003800
H	3.77570200	2.90946400	0.53972700
C	0.44088400	1.32884100	0.37687700
C	0.17988100	0.17713600	1.13150100
C	-0.56133800	1.85727600	-0.44690100
C	-1.05977000	-0.42976600	1.06040300
H	0.95316000	-0.23231600	1.76677900
C	-1.80128100	1.24745800	-0.51091700
H	-0.35836800	2.74411000	-1.03137900
C	-2.05832500	0.09993800	0.24196800
H	-1.26536500	-1.31975100	1.63876400
H	-2.57040300	1.66036600	-1.14730000

H	3.22463500	0.37919000	-0.39608100
C	-3.37342200	-0.58774400	0.20536800
O	-3.63074200	-1.59636100	0.83062800
O	-4.25797400	0.02188000	-0.59136400
C	-5.56118900	-0.58353600	-0.68054500
H	-6.03459100	-0.61011100	0.30035900
H	-6.12851600	0.04816800	-1.35842300
H	-5.48296200	-1.59471600	-1.07862600
Br	3.69988200	-0.86747100	-0.94050800



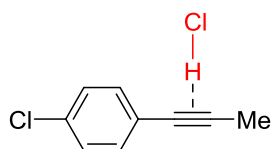
Int7a

C	1.60567000	0.98050400	0.29047700
C	2.79216100	1.18799200	0.38697200
C	0.20861500	0.73100100	0.16766000
C	-0.36826400	-0.40720300	0.73896000
C	-0.62096300	1.61775500	-0.53845900
C	-1.72648800	-0.66385900	0.61648800
H	0.25604700	-1.10260000	1.28432200
C	-1.97264300	1.37111600	-0.66231400
H	-0.19181200	2.50289200	-0.98903700
C	-2.53573300	0.22803100	-0.08699200
H	-2.13867200	-1.55327200	1.06901500
H	-2.61480100	2.05264800	-1.20511700
O	-3.87327000	0.07069100	-0.26558900
C	-4.50455100	-1.08232500	0.28703300
H	-4.41681600	-1.09617500	1.37617500
H	-5.55354800	-1.00680400	0.01009600
H	-4.08407900	-2.00036000	-0.13031300
C	4.21750400	1.44248900	0.50867400
H	4.40223100	2.36738900	1.06019500
H	4.71313000	0.62733700	1.04058600
H	4.68410800	1.53697000	-0.47492400
H	2.65548100	-0.71254800	-0.61422700
Cl	2.98067900	-1.84253700	-1.18920600



Int7b

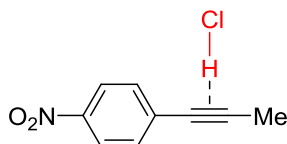
C	-1.12249500	-0.99913600	0.29409900
C	-2.28346000	-1.32730000	0.35492600
C	0.24557200	-0.60649800	0.21296800
C	0.68778300	0.57353600	0.82334500
C	1.17229300	-1.38470600	-0.49371000
C	2.01631000	0.95704600	0.72775300
H	-0.01789100	1.18882300	1.36612700
C	2.49700300	-0.99063300	-0.57950400
H	0.84261600	-2.29554800	-0.97621400
C	2.94476000	0.18468500	0.02854600
H	2.33795600	1.87585500	1.20330800
H	3.19786300	-1.60432400	-1.13314400
C	4.38821500	0.58942900	-0.05037800
H	4.51244300	1.65770200	0.13039000
H	4.81406100	0.35348900	-1.02725000
H	4.98254800	0.05678300	0.69844800
C	-3.67768100	-1.72875500	0.42758700
H	-3.76456700	-2.76997700	0.74657400
H	-4.22615800	-1.10896200	1.14007200
H	-4.16266000	-1.63407300	-0.54715800
Cl	-2.65146300	1.66240100	-1.32268700
H	-2.26378500	0.58377800	-0.69380600



Int7c

C	-1.54394000	-1.01026800	0.27612000
C	-2.71449700	-1.30048700	0.33612400
C	-0.16420400	-0.66168600	0.20028500
C	0.31164600	0.49573200	0.83010200
C	0.73536600	-1.46395000	-0.51343000

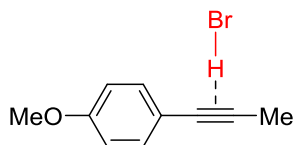
C	1.65008300	0.84413100	0.75070600
H	-0.37399800	1.12473900	1.38167600
C	2.07554500	-1.12263500	-0.59510300
H	0.37855900	-2.35834500	-1.00604900
C	2.52013600	0.03024100	0.03809900
H	2.01235300	1.73886400	1.23734800
H	2.76601400	-1.74510300	-1.14688600
Cl	4.20949500	0.46668700	-0.06492600
C	-4.12236200	-1.64822100	0.40858500
H	-4.57239300	-1.66059000	-0.58703600
H	-4.25464900	-2.63784700	0.85203500
H	-4.66977100	-0.92676700	1.01889600
H	-2.64701400	0.63859300	-0.68386400
Cl	-3.01187100	1.73908900	-1.28400800



Int7d

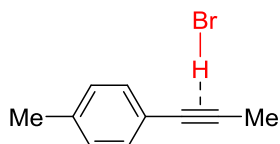
C	-1.82372200	1.03281700	-0.25902900
C	-2.99252100	1.33188600	-0.30547500
C	-0.44362900	0.69279200	-0.19958100
C	0.01262600	-0.51956800	-0.73902600
C	0.47273700	1.56562100	0.40681200
C	1.35079100	-0.85672700	-0.67092200
H	-0.68891000	-1.19392800	-1.20932100
C	1.81270600	1.23713600	0.47433600
H	0.12382200	2.50002900	0.82333800
C	2.23361400	0.02763000	-0.06447600
H	1.70859700	-1.78911900	-1.08008900
H	2.52437400	1.90249600	0.93890800
N	3.64871900	-0.32433300	0.01137900
O	4.41832700	0.47593500	0.52878600
O	4.00533900	-1.40358000	-0.44483300
C	-4.39490200	1.69562200	-0.36647100
H	-4.60812800	2.24592700	-1.28628700
H	-5.02963900	0.80689100	-0.35145500

H	-4.66985400	2.32851400	0.47981200
Cl	-3.19980400	-1.90893000	1.08338900
H	-2.88440600	-0.74604700	0.59153300



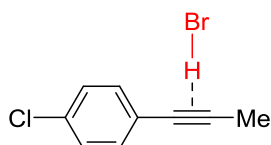
Int8a

C	0.89577100	1.52141200	0.34458100
C	2.02960000	1.92190400	0.46473900
C	-0.43408600	1.03735800	0.19029300
C	-0.90020900	-0.03312300	0.95939500
C	-1.30548900	1.61673600	-0.74684100
C	-2.19166300	-0.51800500	0.80925700
H	-0.24083800	-0.49259000	1.68403200
C	-2.59110200	1.14135300	-0.90141700
H	-0.96074500	2.44446400	-1.35243400
C	-3.04388200	0.07015200	-0.12531900
H	-2.51979900	-1.34596100	1.41968400
H	-3.26589500	1.58563300	-1.62165100
O	-4.32366500	-0.32618800	-0.34971600
C	-4.84664100	-1.40637900	0.42010500
H	-4.84866700	-1.16574100	1.48590400
H	-5.86977800	-1.54508900	0.07834800
H	-4.27952400	-2.32458100	0.24939600
C	3.38624300	2.41799000	0.61960700
H	4.02754100	1.66432100	1.08229600
H	3.81873300	2.68222400	-0.34830300
H	3.40523400	3.30931800	1.25158900
Br	2.77482300	-1.02456700	-1.39844700
H	2.22863600	0.10750200	-0.66899600



Int8b

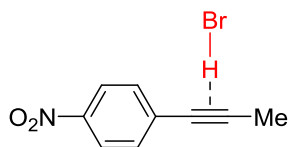
C	0.37090000	1.49806100	0.29532200
C	1.45768900	2.02208600	0.35546400
C	-0.90387100	0.86619600	0.21779700
C	-1.17535000	-0.28461800	0.96635600
C	-1.90679600	1.37565400	-0.61928300
C	-2.41387300	-0.90262200	0.87854000
H	-0.40961500	-0.69095500	1.61411500
C	-3.13864600	0.74996600	-0.69590400
H	-1.70837700	2.26301500	-1.20617000
C	-3.41641900	-0.39932800	0.04998200
H	-2.60426700	-1.79354800	1.46490100
H	-3.90181700	1.15784600	-1.34859800
C	-4.75945700	-1.06362600	-0.04440900
H	-4.80636000	-1.95755100	0.57755800
H	-4.98282900	-1.35513500	-1.07384400
H	-5.55541200	-0.38644000	0.27639900
C	2.76293200	2.65431000	0.43513400
H	2.70523000	3.59784200	0.98333500
H	3.47719300	2.00825400	0.95047100
H	3.15619800	2.86743700	-0.56174300
H	1.81039700	0.08859600	-0.58322500
Br	2.44534700	-1.06882600	-1.18557200



Int8c

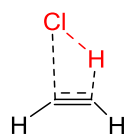
C	0.81238200	1.54144400	0.26768900
C	1.92407700	2.00925300	0.32560100
C	-0.49620700	0.98334000	0.19595300
C	-0.83099800	-0.14301000	0.95878700
C	-1.46603100	1.54671000	-0.64344500
C	-2.10045600	-0.69317800	0.88741200
H	-0.09116300	-0.58677800	1.61109500
C	-2.73814000	1.00349200	-0.71747500
H	-1.21765000	2.41484600	-1.23885300
C	-3.04314900	-0.11286500	0.04963700

H	-2.35362200	-1.56316500	1.47712700
H	-3.48389300	1.44194300	-1.36572000
Cl	-4.64771800	-0.79952400	-0.04054500
C	3.25839300	2.57575800	0.40327900
H	3.69024600	2.69820000	-0.59289500
H	3.23384100	3.55741500	0.88265900
H	3.92158200	1.93249100	0.98557800
Br	2.81966700	-1.21381100	-1.02122100
H	2.21309800	-0.00442400	-0.50375600



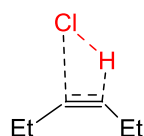
Int8d

C	1.10221300	1.58617400	0.32289600
C	2.21986400	2.03716600	0.39358600
C	-0.21414100	1.05376100	0.24023900
C	-0.57281300	-0.06288400	1.01039800
C	-1.15945300	1.63030900	-0.62151100
C	-1.84462600	-0.59520200	0.92130800
H	0.15286900	-0.50812600	1.67643200
C	-2.43372200	1.10484100	-0.71404300
H	-0.88412700	2.48924000	-1.21721300
C	-2.75808200	-0.00343200	0.05840800
H	-2.12848800	-1.45537700	1.50823500
H	-3.16753900	1.54029500	-1.37518000
N	-4.10199500	-0.56543200	-0.04380800
O	-4.90199100	-0.02050900	-0.79431500
O	-4.37066900	-1.55684900	0.62352200
C	3.55855400	2.58558200	0.48873500
H	3.75800900	2.93723700	1.50371300
H	4.30923200	1.82986500	0.24401800
H	3.68569500	3.42496900	-0.19767700
H	2.31650300	-0.07910100	-0.54226000
Br	2.74870800	-1.33215300	-1.11174300



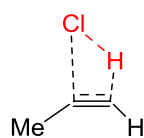
TS1a

C	-1.60470900	-0.48510900	-0.00002000
C	-1.28951600	0.71379700	0.00004700
H	-0.95708900	1.73278500	0.00010000
H	-0.45422900	-0.81439400	-0.00004300
H	-2.42872600	-1.17973000	-0.00005400
Cl	1.35190500	-0.08315800	-0.00001100



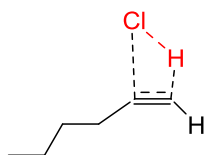
TS1b

C	-0.68941400	0.03068300	-0.34809500
C	0.49693300	0.38584200	-0.12530800
H	-0.57377100	-1.10165500	-0.32741700
C	-2.02363000	0.68503300	-0.56801300
H	-1.88252400	1.76147700	-0.65515400
H	-2.41009300	0.31769500	-1.52056400
C	-2.99782900	0.34908400	0.55846000
H	-3.96433400	0.81391000	0.35653800
H	-3.14726900	-0.72832200	0.64314100
H	-2.63333400	0.72000100	1.51750500
C	1.81770400	0.84649900	0.12579100
H	2.17370300	0.48572500	1.09169200
H	2.49714900	0.52659000	-0.66536400
C	1.72489900	2.40353200	0.14700600
H	1.06262800	2.74909000	0.93915000
H	2.73058600	2.77572900	0.33922200
H	1.38078100	2.79170300	-0.81013400
Cl	0.91676100	-2.61749600	-0.05729500



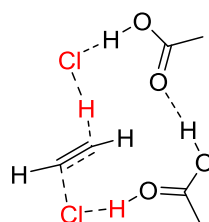
TS1c

C	0.69812900	1.44276900	-0.00000100
C	1.14643700	0.26857800	-0.00000100
H	-0.43390700	1.34333600	0.00000000
C	1.66189200	-1.04645600	-0.00000100
H	1.39498800	-1.59288500	0.90592500
H	1.39498600	-1.59288500	-0.90592700
Cl	-1.86005500	-0.21569300	0.00000100
H	1.21176800	2.39565100	-0.00000100
H	2.75931900	-0.91057900	-0.00000200



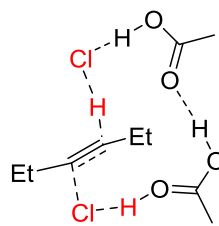
TS1d

C	-1.50504900	1.69353400	0.04005100
C	-0.69380000	0.73428700	-0.03069300
H	-2.53488700	1.21978300	-0.06101400
H	-1.34520000	2.75451600	0.16716500
Cl	-3.37288600	-0.68280100	-0.31444500
C	0.25598800	-0.31105100	-0.10474900
H	0.10962700	-1.02260400	0.70917000
H	0.19169500	-0.82225000	-1.06638000
C	1.67136500	0.36101300	0.03650800
H	1.80385600	1.08998000	-0.76339700
H	1.72294000	0.89245900	0.98713900
C	2.75835700	-0.71060300	-0.03416200
H	2.59317000	-1.44324000	0.75960400
H	2.67369700	-1.24666200	-0.98262600
C	4.15079400	-0.10188400	0.09888000
H	4.91537800	-0.87828800	0.04661700
H	4.34585200	0.61538000	-0.70095900
H	4.26480400	0.41753000	1.05254100



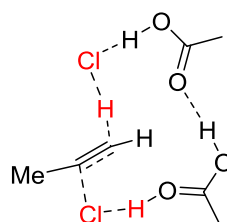
TS2a

H	1.73776300	1.90557800	-0.51900500
H	-2.01688700	0.35913200	0.59748600
C	-1.96558300	-1.20051700	-0.62636800
O	-1.45966400	-0.48854200	0.29543100
O	-1.21083700	-2.03603400	-1.22801300
H	-0.20446200	-1.89335500	-0.97720000
C	-3.37996900	-1.08815900	-1.04035600
H	-4.02176200	-0.96714000	-0.16910600
H	-3.47922000	-0.18801100	-1.65476900
H	-3.67162200	-1.95426300	-1.62832300
C	1.60703400	-1.59332900	0.45432200
O	1.17308700	-1.43564900	-0.68644300
O	2.63087200	-0.90348300	0.90710400
H	2.91141100	-0.20004900	0.26388400
C	1.02997000	-2.54268600	1.44717700
H	0.50123500	-1.96535200	2.20939100
H	0.33808000	-3.23011500	0.96747700
H	1.82729300	-3.09354500	1.94599700
C	-0.03753800	2.35994700	0.49613400
H	-0.02253700	2.85465500	1.44210400
C	0.38494500	1.86271800	-0.55159200
H	0.08547600	1.35800900	-1.45127300
Cl	-2.60048700	2.00646500	0.96911700
Cl	3.30385700	1.67462000	-0.67927600



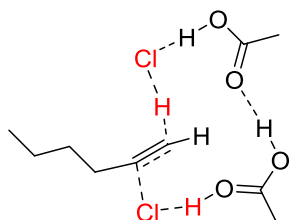
TS2b

H	-1.92503200	0.37867400	0.83111700
H	1.98772100	0.71020800	-0.55509500
C	2.56239400	-0.98221000	0.36296600
O	1.79968100	-0.35437900	-0.42816200
O	2.20022500	-2.13660100	0.77897600
H	1.21809500	-2.35293200	0.50175500
C	3.85878100	-0.43770200	0.82362300
H	4.46176300	-0.15923000	-0.04190900
H	3.67485200	0.47457400	1.39587200
H	4.38121700	-1.16383000	1.43947100
C	-0.63809600	-2.33179800	-0.93424300
O	-0.24141300	-2.43239500	0.22665100
O	-1.86011400	-1.94337300	-1.21797200
H	-2.36505200	-1.67245900	-0.39309400
C	0.19394500	-2.62852900	-2.13566400
H	0.28581100	-1.72659600	-2.74269900
H	1.17970200	-2.98236700	-1.84656600
H	-0.30902500	-3.38330300	-2.74272600
C	-0.83337900	1.38275400	-0.33944300
C	-0.83182200	0.93355000	0.81964700
C	-0.06709700	0.78417900	2.08479400
H	0.01814100	-0.28389300	2.29709900
H	0.93288900	1.18337100	1.91366200
C	-0.74080300	1.49628200	3.25598100
H	-0.15473500	1.34679000	4.16431100
H	-0.81494900	2.56873300	3.06974200
H	-1.74433900	1.10618000	3.43001900
C	-1.48017100	3.19013700	-1.94408700
H	-1.81961700	3.32633900	-2.97121300
H	-2.25117700	3.56601000	-1.27089800
H	-0.57193700	3.77322700	-1.79739500
C	-1.20760600	1.70804600	-1.68733100
H	-2.11847500	1.11129200	-1.85593500
H	-0.45791900	1.30983100	-2.37477700
Cl	-3.36464600	-0.68717200	1.07968600
Cl	1.94151100	2.42050600	-0.64767900



TS2c

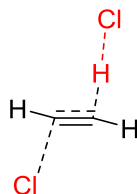
H	1.64543800	1.42203800	-1.27954800
H	-2.08012500	0.41969500	0.33257000
C	-2.08033500	-1.38672400	-0.55103900
O	-1.54852100	-0.52452000	0.20622300
O	-1.38084200	-2.39062400	-0.92984500
H	-0.38304500	-2.28122800	-0.67152700
C	-3.47438700	-1.27977800	-1.03468900
H	-4.13659400	-1.00191900	-0.21554900
H	-3.51545200	-0.47760200	-1.77726000
H	-3.79005300	-2.21194700	-1.49489200
C	1.42437900	-1.54618700	0.68625600
O	1.04739700	-1.86103600	-0.44072400
O	2.43035600	-0.71892800	0.87507600
H	2.76903500	-0.34868200	0.00935800
C	0.80438400	-2.03962900	1.95008300
H	0.35298000	-1.19955100	2.48106300
H	0.04715000	-2.78998600	1.74022100
H	1.57741700	-2.45763500	2.59646400
C	0.30547300	2.00611000	0.06866900
C	0.44391200	1.68583700	-1.12274100
H	-0.14930800	1.54621400	-2.00896400
C	0.56500800	2.29720100	1.44371900
H	0.09571700	1.57357400	2.10882900
H	1.65667600	2.22919500	1.56393600
H	0.25717200	3.30949100	1.70710500
Cl	-2.61296900	2.03967100	0.46470800
Cl	3.27525400	0.86435400	-1.59365700



TS2d

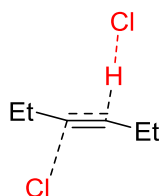
H	-0.01729000	1.70268400	-1.82513100
H	0.54541100	-2.06814900	-0.09477200
C	2.54525900	-1.87877700	0.02954800
O	1.37744700	-1.46676900	0.28687700
O	3.53475300	-1.09057700	0.21589300
H	3.21471000	-0.12474600	0.44163400
C	2.81811200	-3.25512300	-0.45265200
H	2.81281700	-3.92223500	0.41313700
H	2.02247800	-3.57824600	-1.12175900
H	3.78947600	-3.30604200	-0.93483500
C	1.82910300	1.57331100	1.36008500
O	2.64647300	1.24499600	0.50215300
O	0.94640000	2.52183900	1.15388500
H	0.96669400	2.84717900	0.20654100
C	1.72371200	0.92020300	2.70112900
H	1.04603200	0.06861900	2.60628300
H	2.69594600	0.55107000	3.01825700
H	1.31339000	1.60542400	3.43843000
C	-1.00352600	0.19024000	-0.97125700
C	-0.23758100	0.47987500	-1.90502300
H	0.30776400	-0.00785700	-2.69133500
C	-1.88504200	0.26864800	0.15592800
H	-1.47187100	-0.30853100	0.98540700
H	-1.83010400	1.32811600	0.45648600
C	-0.84176000	-2.75640700	-0.79463400
Cl	0.50936200	3.35821700	-1.72820600
C	-3.34082400	-0.12626600	-0.13052800
H	-3.35229200	-1.16072700	-0.47654000
H	-3.72511600	0.49411000	-0.94333700
C	-4.21765200	0.02458900	1.10828000
H	-3.80760600	-0.59088500	1.91494200

H	-4.17756300	1.06086000	1.45815300
C	-5.66611800	-0.37425400	0.84462500
H	-5.73251400	-1.41567400	0.52189700
H	-6.27571200	-0.26222200	1.74264800
H	-6.10711600	0.24590100	0.06090700



TS'2a

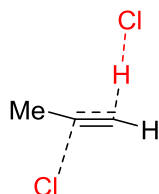
H	1.95361100	1.70528300	-0.61217600
C	0.03294700	2.21681000	0.36234000
H	0.12898800	2.72673900	1.29149800
C	0.42880400	1.65954300	-0.66364800
H	0.13115400	1.16278300	-1.56454300
Cl	-2.46952500	2.45413900	0.84836900
Cl	3.41035900	1.65757500	-0.72992800



TS'2b

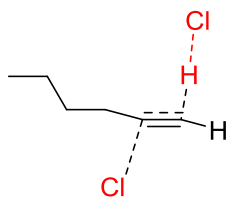
H	-2.00163400	0.37130600	0.70253400
C	-0.68092900	1.34602900	-0.41675800
C	-0.72654500	0.90549400	0.73327000
C	-0.07964700	0.72745600	2.04909300
H	-0.16350300	-0.31938300	2.35020300
H	0.97956600	0.95891400	1.91656000
C	-0.69406800	1.62502200	3.12653300
H	-0.19152600	1.46203900	4.08115000
H	-0.58615800	2.67565200	2.85582400
H	-1.75547300	1.41056500	3.25519400
C	-1.36912600	3.18090400	-1.97010900
H	-1.67878300	3.36146900	-3.00028500

H	-2.17067300	3.50491200	-1.30541800
H	-0.47675800	3.76722200	-1.75877400
C	-1.06553500	1.69377600	-1.76979300
H	-1.95394800	1.08797900	-1.99248400
H	-0.28048100	1.36696600	-2.45341000
Cl	-3.39499900	-0.32607400	0.93946700
Cl	1.93237900	2.51644500	-0.58804800



TS'2c

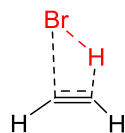
H	1.91694900	1.26817900	-1.08419000
C	0.30909800	1.88394900	0.08735000
C	0.51995700	1.52205100	-1.07315700
H	0.07666900	1.33473700	-2.02907400
C	0.61954900	2.21193500	1.46158200
H	0.07436800	1.57048900	2.15126500
H	1.69604400	2.05735800	1.60028800
H	0.37583900	3.24931200	1.68247800
Cl	-2.38099700	2.47089200	0.45968000
Cl	3.41246000	0.95628900	-1.23968400



TS'2d

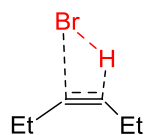
H	-0.23894400	1.78922400	-1.79484500
C	-0.89783700	0.03762000	-0.91405700
C	-0.17915500	0.38817900	-1.85475800
H	0.44739700	0.04792200	-2.65308300
C	-1.80152700	0.17761100	0.20865000
H	-1.45353600	-0.45469600	1.02570700
H	-1.69825600	1.22145700	0.53767000

Cl	-0.91456800	-2.77441600	-0.73048200
Cl	-0.20817800	3.33772000	-1.84734700
C	-3.26709000	-0.12618200	-0.12144100
H	-3.32349400	-1.14299100	-0.51196700
H	-3.60021500	0.54832300	-0.91521500
C	-4.17000000	0.01978600	1.09899500
H	-3.82470700	-0.66288400	1.88180800
H	-4.07358500	1.03129100	1.50739500
C	-5.63455900	-0.26609300	0.78041600
H	-5.75909200	-1.28056300	0.39461100
H	-6.26229900	-0.16594200	1.66798200
H	-6.01291700	0.42505200	0.02324100



TS3a

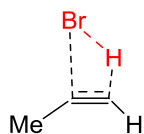
C	-2.10515200	-0.53308100	-0.00001800
C	-1.94476300	0.70068000	0.00005300
H	-1.73257800	1.75135900	0.00010600
H	-0.96615000	-0.85913700	-0.00004500
Br	0.95504500	-0.04761800	-0.00000600
H	-2.90581200	-1.25912700	-0.00005100



TS3b

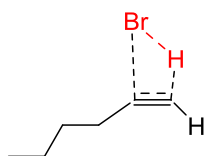
C	-0.92673000	-0.51641900	-0.32786100
C	-0.74210300	0.71158200	-0.11670300
H	0.12684100	-0.94389700	-0.30293900
Br	2.28621900	-0.33606100	-0.01169600
C	-2.11733200	-1.40989500	-0.55081900
H	-3.01876000	-0.80075800	-0.59979500
H	-1.98112400	-1.88661900	-1.52375800
C	-2.22846300	-2.46935600	0.54220100
H	-3.08250900	-3.11725200	0.33783500

H	-1.33137700	-3.08876600	0.58565000	H	2.62255200	0.92809000	-0.94864500
H	-2.37397600	-2.01121900	1.52168400	H	2.67858700	1.04990500	0.81096300
C	-0.61438800	2.10832300	0.11616000	C	3.54637800	-0.77220400	0.02455900
H	-0.13909300	2.29718500	1.07975300	H	3.41232500	-1.33984200	0.94843700
H	-0.04061500	2.58448100	-0.68011500	H	3.35657000	-1.46103600	-0.80201100
C	-2.06899600	2.67394400	0.13070200	C	4.97288600	-0.23755700	-0.05789400
H	-2.65725400	2.22531000	0.92942200	H	5.69081700	-1.05824900	-0.02393800
H	-1.98989500	3.74602500	0.30755200	H	5.13538400	0.31222600	-0.98709200
H	-2.56621800	2.50866500	-0.82360300	H	5.19149600	0.43420100	0.77458800
				Br	-2.85186100	-0.36590000	0.20010700



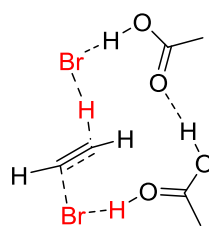
TS3c

C	1.38909700	1.43826800	0.00020400
C	1.78472600	0.24411200	0.00019900
H	0.25362600	1.43577700	0.00008700
Br	-1.40810500	-0.06525200	-0.00015800
C	2.25497000	-1.08915100	0.00020200
H	1.96785700	-1.62704300	0.90507800
H	1.96805100	-1.62698300	-0.90477100
H	1.96523200	2.35628200	0.00029900
H	3.35700200	-0.99952200	0.00032700



TS3d

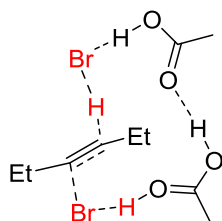
C	-0.54822800	1.88597600	-0.02903800
C	0.19058400	0.86619400	0.01801600
H	-1.62612200	1.55872300	0.02791100
H	-0.26786400	2.92818300	-0.11007800
C	1.06753800	-0.23777300	0.06649500
H	0.95980300	-0.78138100	1.00630800
H	0.90288700	-0.90506900	-0.78083500
C	2.52459300	0.36314700	-0.02150300



TS4a

H	-1.75065300	-1.45583300	-0.45746600
H	2.15715400	0.23624800	0.36423300
C	1.89115000	1.73185600	-0.90462200
O	1.52942900	1.04418300	0.10166300
O	1.04779000	2.53849300	-1.41998800
H	0.09606900	2.41753300	-1.01167600
C	3.24256600	1.63174000	-1.49353700
H	3.98766300	1.85564800	-0.72801100
H	3.41153300	0.60165600	-1.81592500
H	3.34446600	2.31035300	-2.33507400
C	-1.47282200	2.00624200	0.70119700
O	-1.24009400	1.98983200	-0.50551100
O	-2.43906500	1.27827100	1.22654000
H	-2.84535500	0.68030200	0.55148900
C	-0.70985200	2.80309400	1.70168200
H	-0.06049700	2.12403300	2.25924300
H	-0.10391100	3.55877600	1.20878900
H	-1.39381800	3.26636400	2.41241100
C	0.12615900	-1.85781300	0.43336300
H	0.20893600	-2.35122700	1.37591700

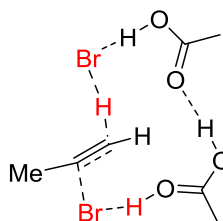
C	-0.36191200	-1.36225800	-0.58043700
H	-0.17323300	-0.85474900	-1.50707300
Br	-3.43730800	-1.29729900	-0.54423900
Br	2.95492300	-1.47345800	0.78512800



TS4b

H	1.68452000	-0.97407300	0.56929000
H	-2.29116500	0.54294400	-0.18401500
C	-1.81952600	2.29051600	0.65348700
O	-1.60062300	1.36820600	-0.18921600
O	-0.89575800	3.14368500	0.88058700
H	0.00158000	2.88140200	0.41693500
C	-3.11041500	2.43771600	1.35979400
H	-3.79694800	2.96682300	0.69152500
H	-3.54199000	1.45904500	1.56583600
H	-2.98393200	3.01760000	2.27009500
C	1.39137300	1.99929800	-1.27145700
O	1.27273800	2.30082200	-0.08595200
O	2.29378000	1.12890400	-1.67540100
H	2.77128500	0.71546100	-0.90432300
C	0.55345500	2.54974400	-2.37420300
H	-0.07559600	1.75034700	-2.77146400
H	-0.07310400	3.36158400	-2.01539300
H	1.19498000	2.89836500	-3.18417900
C	0.07139100	-1.33152400	-0.36764800
C	0.41143100	-0.95275900	0.75712600
Br	3.51220500	-0.76146600	0.61476200
Br	-3.20838200	-1.10414900	-0.11065700
C	0.05358200	-0.50281200	2.12238800
H	0.55634200	0.44749700	2.31453100
H	-1.02390400	-0.33031100	2.13527600
C	0.43924200	-1.52769800	3.18758300

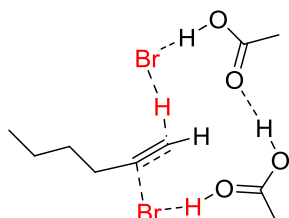
H	0.17675800	-1.14883600	4.17668900
H	-0.09178000	-2.46741000	3.02885500
H	1.51066000	-1.73060000	3.17441700
C	-0.33435300	-3.27389500	-1.88186800
H	-0.32463400	-3.54537800	-2.93800900
H	0.38217900	-3.90477000	-1.35505600
H	-1.33006400	-3.46432000	-1.48308100
C	0.02689600	-1.79575600	-1.72926500
H	1.02676600	-1.59343800	-2.14095800
H	-0.66148100	-1.15983300	-2.29207400



TS4c

H	-1.74647400	-1.29462100	-1.03445200
H	2.25987100	0.13734400	-0.02937600
C	1.90377500	1.96579600	-0.76200000
O	1.57720200	0.96887800	-0.04992100
O	1.02775000	2.86970400	-0.98597000
H	0.09089000	2.59652300	-0.62654300
C	3.26209600	2.13861200	-1.31997800
H	3.93296700	2.41697200	-0.50241300
H	3.61964400	1.19149700	-1.72456000
H	3.26845900	2.91732800	-2.07718500
C	-1.41322600	1.67601000	0.94491800
O	-1.21872400	1.99145800	-0.22580500
O	-2.34961200	0.80996500	1.28031900
H	-2.79622300	0.43437400	0.47468600
C	-0.63245900	2.20058800	2.10181600
H	0.04333000	1.41837800	2.45561100
H	-0.05029700	3.06959600	1.80666100
H	-1.30327300	2.45460300	2.92212800
C	-0.11359100	-1.64467800	0.08171100
C	-0.47278900	-1.41193200	-1.07783700

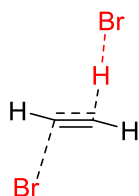
H	-0.10224100	-1.25973500	-2.07505600
Br	-3.53848000	-0.96975100	-1.14880800
Br	3.14769700	-1.52162800	-0.01018400
C	-0.07700700	-1.89047700	1.49132700
H	0.46319500	-1.10744500	2.02235000
H	-1.11881700	-1.89151800	1.84258500
H	0.36105100	-2.86312600	1.71697300



TS4d

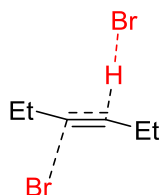
H	1.55542000	1.16327100	-1.38698900
H	-1.37625400	-1.87495000	-0.04015200
C	0.03805200	-3.29229700	0.02419100
O	-0.37730900	-2.12388300	0.28715700
O	1.27357800	-3.55986100	0.21473000
H	1.81840500	-2.71221000	0.47502800
C	-0.84928300	-4.36134500	-0.48280200
H	-1.59638200	-4.59078900	0.28040900
H	-1.38742900	-3.99962200	-1.36053700
H	-0.27474700	-5.25104400	-0.72317900
C	2.20860600	-0.66411900	1.59146200
O	2.51414300	-1.40152100	0.65839100
O	2.49042100	0.62408200	1.57594800
H	2.89451000	0.89554500	0.70767100
C	1.48420300	-1.10244300	2.81803900
H	0.46032100	-0.72508500	2.77471100
H	1.46648400	-2.18679100	2.88706600
H	1.95744300	-0.67415700	3.70161300
C	-0.28723500	0.93611000	-0.60147800
C	0.44800100	0.53725500	-1.51125100
H	0.48676900	-0.14944400	-2.33741300
Br	3.24588100	1.85181500	-1.30365700
Br	-2.98480100	-1.15198300	-0.67982500

C	-0.88039700	1.58835000	0.52654400
H	-1.20290000	0.83054700	1.24564100
H	-0.05124000	2.13170600	1.00829700
C	-2.02460000	2.55060400	0.18052200
H	-2.80256800	1.98623200	-0.33659300
H	-1.65337200	3.30872800	-0.51344400
C	-2.59957700	3.21233000	1.42755600
H	-2.94602700	2.43621800	2.11759900
H	-1.80725100	3.75999500	1.94849100
C	-3.75028700	4.15769000	1.10462600
H	-4.56779500	3.62753200	0.60943000
H	-4.15207700	4.61559800	2.01116100
H	-3.42632500	4.96354100	0.44074800



TS'4a

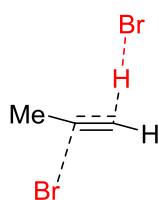
H	-1.89225500	-1.30983400	-0.47265900
C	0.09535900	-1.76905600	0.27074800
H	0.20168000	-2.31647000	1.17690600
C	-0.42149800	-1.19200500	-0.68091600
H	-0.29563700	-0.64328300	-1.59131000
Br	-3.52208100	-1.29671700	-0.47997900
Br	2.93328300	-1.91869300	0.49358500



TS'4b

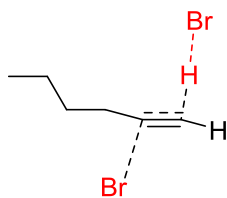
H	1.82071300	-0.81426100	0.39492800
C	0.15013500	-1.24048900	-0.51373000
C	0.44520900	-0.88814700	0.62368800
Br	3.52044100	-0.59984100	0.49188500

Br	-3.05657700	-1.48272900	-0.17628700
C	0.12600200	-0.55459400	2.02438300
H	0.63219000	0.37487100	2.29366800
H	-0.95122400	-0.38008200	2.06771500
C	0.52968300	-1.66786000	2.99470800
H	0.27934200	-1.37894500	4.01630000
H	0.00155200	-2.59178500	2.75831600
H	1.60183300	-1.85965800	2.94371900
C	-0.08299300	-3.14982400	-2.10288900
H	-0.05024400	-3.38983000	-3.16603500
H	0.68153900	-3.73450500	-1.59074800
H	-1.05978800	-3.42479600	-1.70849900
C	0.15397400	-1.65003000	-1.90067300
H	1.13019100	-1.35495000	-2.30718700
H	-0.59738900	-1.06526700	-2.43545600



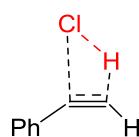
TS'4c

H	-1.89921200	-1.20761300	-0.62866800
C	-0.11603600	-1.53001300	0.33352600
C	-0.51879000	-1.36671100	-0.81532700
H	-0.29254100	-1.28089900	-1.85732900
Br	-3.57809800	-0.97324700	-0.63726300
Br	3.03825400	-1.67323200	0.25722700
C	-0.06961400	-1.68875000	1.76543700
H	0.57122200	-0.93499100	2.21870900
H	-1.09124100	-1.57101200	2.14646200
H	0.29838300	-2.67661100	2.03917100



TS'4d

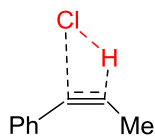
H	-1.76566800	-0.97183300	-1.22806500
C	0.16130000	-0.84495700	-0.58362400
C	-0.55112900	-0.35350000	-1.45717800
H	-0.64069800	0.32418100	-2.28042600
Br	-3.35247900	-1.60599200	-1.12121400
Br	3.07111400	0.54481500	-0.78026200
C	0.64539600	-1.64111200	0.51698600
H	1.19431000	-0.99129500	1.20109000
H	-0.25133300	-1.98618200	1.05190300
C	1.50827100	-2.83768100	0.09730100
H	2.36267900	-2.46011000	-0.46664600
H	0.92897500	-3.47795000	-0.57328100
C	1.98768600	-3.64053000	1.30199000
H	2.56782800	-2.98558800	1.95934200
H	1.12333700	-3.97619600	1.88449200
C	2.83447200	-4.84465700	0.90118800
H	3.71831500	-4.53115800	0.34097900
H	3.17295400	-5.40129900	1.77705900
H	2.26586000	-5.53016400	0.26805900



TS5a

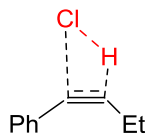
C	-2.04123500	1.65939100	0.00006300
C	-0.88208200	1.13679400	0.00004200
H	-2.87035400	0.92841800	0.00003600
H	-2.21837900	2.73085200	0.00009900
C	0.36510800	0.58402200	0.00002300
C	1.01073900	0.29632900	-1.23216900
C	1.01074800	0.29626700	1.23219600
C	2.26769500	-0.26062400	-1.21985000
H	0.49592500	0.51300500	-2.15772300
C	2.26770400	-0.26068400	1.21983900
H	0.49594100	0.51289900	2.15776400
C	2.88983500	-0.53881000	-0.00001400
H	2.77238200	-0.48923000	-2.14839000

H	2.77239800	-0.48933500	2.14836500
H	3.87720400	-0.98280600	-0.00002900
Cl	-2.90978300	-1.38291900	-0.00010900



TS5b

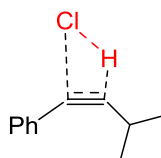
C	-2.10760200	-0.81489700	0.00000100
C	-0.85112300	-0.60183300	0.00000000
H	-2.65863100	0.14657800	0.00000100
C	0.49948200	-0.38861900	0.00000000
C	1.20072200	-0.28475000	1.23028800
C	1.20072300	-0.28475100	-1.23028800
C	2.56214700	-0.08805600	1.21906100
H	0.64803500	-0.35481600	2.15666800
C	2.56214800	-0.08805700	-1.21906100
H	0.64803600	-0.35481800	-2.15666800
C	3.23726600	0.00953100	0.00000000
H	3.10875300	-0.00363900	2.14825300
H	3.10875400	-0.00364100	-2.14825200
H	4.30825600	0.16866000	0.00000100
C	-2.83660500	-2.12567100	0.00000300
H	-2.15301900	-2.97191400	-0.00000100
H	-3.47796800	-2.17697200	0.88147200
H	-3.47797600	-2.17697000	-0.88146000
Cl	-2.08720300	2.39070900	-0.00000900



TS5c

C	1.80752800	-0.22176900	-0.32636400
C	0.54071400	-0.26390300	-0.20198900
H	2.18462600	0.81252800	-0.21230800
C	-0.82063500	-0.33031400	-0.08762700
C	-1.63326900	-0.19680800	-1.24405400

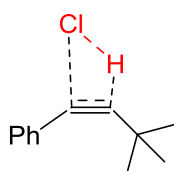
C	-1.41820900	-0.53679300	1.18324800
C	-3.00149700	-0.27187800	-1.12251700
H	-1.15916600	-0.02848700	-2.20089600
C	-2.78842800	-0.60865500	1.28276900
H	-0.78301800	-0.62399300	2.05355900
C	-3.57391000	-0.47549000	0.13518000
H	-3.63307700	-0.16776500	-1.99397800
H	-3.25846600	-0.76163500	2.24448100
H	-4.65165900	-0.52810400	0.22360000
C	2.76097500	-1.36382700	-0.58070300
C	3.83179100	-1.44243700	0.50337200
H	4.39526700	-0.51012500	0.56888500
H	3.38989300	-1.64092500	1.48138100
H	4.53017300	-2.24973500	0.27510400
H	2.20885900	-2.30054700	-0.65301600
H	3.22613700	-1.17672600	-1.55197200
Cl	1.21088500	2.88253200	0.21273200



TS5d

C	1.51752500	-0.11513800	-0.00002000
C	0.24863500	-0.20930500	-0.00001200
H	1.84356600	0.94286900	-0.00003500
C	-1.11443100	-0.33753900	-0.00000500
C	-1.81991700	-0.40702900	-1.22967900
C	-1.81991100	-0.40696700	1.22967600
C	-3.18918100	-0.54428300	-1.21909800
H	-1.26661200	-0.34206300	-2.15540400
C	-3.18917600	-0.54422000	1.21910700
H	-1.26660300	-0.34195300	2.15539400
C	-3.86830800	-0.61150200	0.00000800
H	-3.73932000	-0.59493400	-2.14788100
H	-3.73931000	-0.59482200	2.14789500
H	-4.94545900	-0.71495900	0.00001300
C	2.54001500	-1.23810700	0.00000000

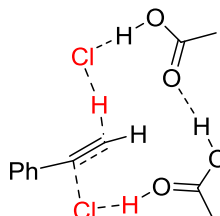
C	3.38911800	-1.14249700	-1.26939500
H	3.92460800	-0.19222800	-1.30680600
H	4.12257200	-1.95033400	-1.27954300
H	2.77421800	-1.22493100	-2.16572900
C	3.38907900	-1.14248300	1.26942000
H	4.12253100	-1.95032200	1.27960000
H	3.92457000	-0.19221500	1.30683500
H	2.77415200	-1.22490400	2.16573500
H	2.00556000	-2.18948100	-0.00000300
Cl	0.76263600	2.98615400	0.00004100



TS5e

C	1.50391300	-0.15288600	-0.00000700
C	0.23392000	-0.22695500	-0.00000700
H	1.83618800	0.90313200	-0.00001600
C	-1.13081600	-0.33215200	-0.00000800
C	-1.83690900	-0.39280500	-1.22950300
C	-1.83691200	-0.39279200	1.22948600
C	-3.20773000	-0.51423700	-1.21907300
H	-1.28253400	-0.33491900	-2.15499900
C	-3.20773400	-0.51422500	1.21905300
H	-1.28254000	-0.33489700	2.15498300
C	-3.88759800	-0.57364800	-0.00001000
H	-3.75851000	-0.55889300	-2.14779700
H	-3.75851600	-0.55887100	2.14777600
H	-4.96585500	-0.66490400	-0.00001100
C	2.52724400	-1.28304800	0.00000100
C	3.38948600	-1.11719400	-1.25926600
H	3.87738200	-0.14220100	-1.27674700
H	4.16110400	-1.88907200	-1.27243500
H	2.78763400	-1.21778700	-2.16314000
C	3.38948600	-1.11717700	1.25926600
H	4.16110400	-1.88905400	1.27244600

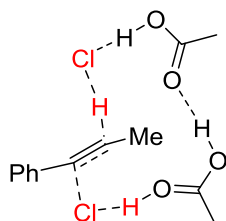
H	3.87738100	-0.14218300	1.27673600
H	2.78763300	-1.21775900	2.16314200
Cl	0.77784900	2.94914500	-0.00005300
C	1.83554100	-2.64781100	0.00001000
H	1.21023000	-2.77234300	0.88584400
H	1.21023100	-2.77235500	-0.88582200
H	2.58325600	-3.44169600	0.00001600



TS6a

H	-0.08419600	1.17475700	-2.19578100
H	0.90097900	-2.12013900	-0.05413100
C	2.82178900	-1.60961800	0.18547800
O	1.57989500	-1.36089700	0.28086700
O	3.64793100	-0.64930900	0.32953800
H	3.15869500	0.28903500	0.35069900
C	3.33972400	-2.96632300	-0.09880000
H	4.41426000	-3.00417800	0.05644600
H	2.82833200	-3.70093500	0.52250400
H	3.11436100	-3.20441500	-1.14223000
C	1.54841400	1.85793700	0.96856000
O	2.38788900	1.49204900	0.13867100
O	0.55421200	2.63919600	0.65091900
H	0.53519900	2.87389000	-0.34690400
C	1.60058300	1.44270800	2.40306900
H	0.78216100	1.87198100	2.97450000
H	1.56581900	0.35349000	2.46310000
H	2.55422100	1.76456100	2.82535900
C	-1.07698600	-0.24758700	-1.16290000
C	-0.16764000	0.07192400	-1.98844200
H	0.52960300	-0.59242400	-2.47805700
C	-2.10986200	-0.24841500	-0.25194700
C	-1.82924200	-0.08584800	1.12495800

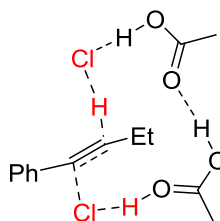
C	-3.44643700	-0.36574900	-0.69804500
C	-2.86867700	-0.02880000	2.02581100
H	-0.80177300	-0.00913800	1.44786600
C	-4.47377800	-0.30622000	0.21885200
H	-3.64092200	-0.49508200	-1.75351400
C	-4.18501500	-0.13943900	1.57350900
H	-2.66763400	0.10099800	3.08043200
H	-5.50078300	-0.38753300	-0.10997300
H	-4.99700400	-0.09440600	2.28818900
Cl	-0.38454300	-3.05958900	-0.77970300
Cl	0.22927100	3.29570900	-2.20332200



TS6b

H	-0.13527000	1.07969600	-2.01092500
H	0.86732300	-2.06218000	0.39343200
C	2.76172200	-1.46692000	0.51447500
O	1.51871300	-1.27225800	0.69506100
O	3.55176000	-0.46956500	0.58451100
H	3.02781600	0.44974700	0.59201600
C	3.32037700	-2.80237400	0.20969100
H	4.39748900	-2.80283500	0.35359300
H	2.84054000	-3.56379000	0.82256100
H	3.09975600	-3.03056200	-0.83699200
C	1.36883400	2.02356500	1.10236200
O	2.22740600	1.61603600	0.31314700
O	0.37029400	2.76720300	0.71321400
H	0.36345300	2.91452900	-0.29752500
C	1.40339200	1.71108000	2.56231400
H	0.52653500	2.09427500	3.07690600
H	1.47890900	0.63127100	2.69735700
H	2.30289800	2.15830800	2.99067800
C	-0.99404700	-0.35954700	-1.02846700

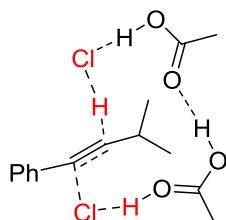
C	-0.06915100	-0.04600200	-1.83658700
C	-2.08129700	-0.28878100	-0.17042800
C	-1.87915300	-0.03485200	1.20310500
C	-3.38972900	-0.43221400	-0.67775700
C	-2.96718600	0.08700100	2.04068000
H	-0.87093700	0.05654500	1.57886500
C	-4.46877800	-0.30749700	0.17354700
H	-3.52697200	-0.63341900	-1.73112000
C	-4.25740000	-0.04855200	1.52688600
H	-2.82248700	0.28842400	3.09354000
H	-5.47569100	-0.40861600	-0.20833500
H	-5.10766200	0.04838400	2.19007600
C	1.04290000	-0.73826200	-2.53973400
H	0.97160400	-0.54581800	-3.61150700
H	1.99414700	-0.32183700	-2.20143800
H	1.00743400	-1.80845700	-2.35211200
Cl	0.08044500	3.13064000	-2.21355000
Cl	-0.36206000	-3.09140800	-0.34054100



TS6c

H	0.00800600	1.13798900	1.80565700
H	-0.76264000	-2.06573500	-0.59416500
C	-2.63031600	-1.46986000	-0.94430700
O	-1.37335100	-1.28490600	-0.98040500
O	-3.39687900	-0.46992400	-1.13123200
H	-2.86452100	0.44674000	-1.10214500
C	-3.23307000	-2.79545600	-0.68258000
H	-4.28436900	-2.79252100	-0.95739200
H	-2.68846900	-3.57347400	-1.21519600
H	-3.14413100	-3.00070100	0.38832200
C	-1.17065200	2.01581300	-1.48163700
O	-2.10148900	1.61559300	-0.77437300

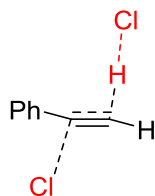
O	-0.21758600	2.76891300	-1.00782700	C	-2.44172400	-0.72808200	-1.79712300
H	-0.31494800	2.94067500	-0.00478200	O	-1.18858800	-0.67598200	-1.57921900
C	-1.06385500	1.70597800	-2.93830200	O	-3.11139700	0.35132500	-1.76666500
H	-0.04388800	1.82356800	-3.29553900	H	-2.54197800	1.16315300	-1.35870900
H	-1.43182700	0.70126300	-3.13981900	C	-3.13282100	-2.00458200	-2.10136700
H	-1.70317000	2.41163000	-3.47627800	H	-4.20491600	-1.89905400	-1.96985900
C	0.95408100	-0.32429200	0.93993000	H	-2.91823700	-2.27037900	-3.13935700
C	-0.03734200	0.01085600	1.65566900	H	-2.73076900	-2.79826500	-1.47251300
C	2.10387100	-0.25379800	0.16522000	C	-0.77426700	2.61781100	-0.95653600
C	1.99991200	-0.05781100	-1.22820200	O	-1.81344100	2.07048300	-0.56963900
C	3.37289600	-0.32363500	0.77598400	O	0.11026700	3.09188900	-0.13167600
C	3.14357300	0.08348100	-1.98471400	H	-0.09998800	2.88909600	0.84880000
H	1.02085800	-0.02835500	-1.68253600	C	-0.44760100	2.79626900	-2.40744600
C	4.50907500	-0.17717200	0.00552200	H	0.57448400	3.13615700	-2.54442900
H	3.43708200	-0.48165600	1.84363400	H	-0.60759600	1.85826300	-2.93852100
C	4.39425900	0.02644700	-1.36857200	H	-1.13393600	3.53313000	-2.82845600
H	3.07268100	0.24126300	-3.05254500	C	0.91847900	-0.71338600	0.81099800
H	5.48624000	-0.21825800	0.46761400	C	-0.05649800	-0.55380000	1.60621600
H	5.28915000	0.14070800	-1.96712500	C	2.11709500	-0.51521900	0.13447300
C	-1.20338400	-0.67096500	2.29628000	C	2.13070800	0.09161900	-1.13880000
H	-2.10708400	-0.22760000	1.86851400	C	3.33116300	-0.88428500	0.75002800
H	-1.17312500	-1.72648900	2.03206100	C	3.33285900	0.33621800	-1.76787200
C	-1.20563400	-0.48383500	3.81189100	H	1.19375800	0.35221000	-1.60616900
H	-1.23069400	0.57295800	4.08145600	C	4.52824500	-0.63588100	0.10743400
H	-2.08488200	-0.96587400	4.24316900	H	3.30596000	-1.35242900	1.72366700
H	-0.31781600	-0.93154600	4.26203900	C	4.52845300	-0.02787600	-1.14657300
Cl	-0.23005300	3.21323800	1.91435600	H	3.35041700	0.80778200	-2.74057200
Cl	0.40912800	-3.05642100	0.28913200	H	5.46245300	-0.91073500	0.57692200



TS6d

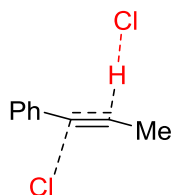
H	0.03056000	0.47498100	2.08001400	H	-3.37634800	-1.16267900	2.26006600
H	-0.70960400	-1.60437200	-1.36209700	H	-2.47352100	0.30238300	2.68206100
				H	-2.69737500	-0.13114300	0.99441700

H	-1.31335500	-2.21078700	1.35393400
Cl	-0.13825300	2.46202400	2.73847600
Cl	0.17565000	-2.97326400	-0.69719100



TS'6a

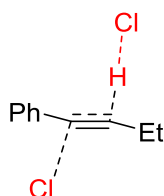
H	-0.16910300	1.59892500	-1.89619300
C	-0.92283500	-0.22739800	-1.13796300
C	-0.03361900	0.22349900	-1.86819100
H	0.79342700	-0.08416700	-2.47720200
C	-2.02778400	-0.34804900	-0.27271900
C	-1.84214400	-0.29412700	1.11741700
C	-3.32212400	-0.48250700	-0.79853300
C	-2.93562900	-0.36849700	1.96228800
H	-0.84076600	-0.19861900	1.51257600
C	-4.40875800	-0.55608200	0.05516800
H	-3.45371200	-0.53132800	-1.87013400
C	-4.21728800	-0.50049400	1.43354800
H	-2.79260700	-0.32618300	3.03368600
H	-5.40639000	-0.65908000	-0.35012300
H	-5.06958800	-0.56069900	2.09781700
Cl	-0.48337400	-3.19389700	-1.19220500
Cl	-0.17913500	3.14861100	-2.03769100



TS'6b

H	0.21597100	1.37000000	1.89170900
C	0.88300600	-0.33205700	1.04056000
C	-0.03693700	0.05207100	1.77244100
C	2.03397400	-0.41946700	0.23263600

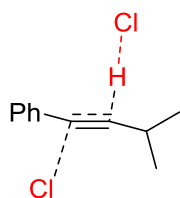
C	1.92457900	-0.36227000	-1.16586400
C	3.30036400	-0.54906100	0.82414800
C	3.06169100	-0.42580500	-1.95161400
H	0.94456100	-0.27925200	-1.61372600
C	4.43295400	-0.60779900	0.02958300
H	3.37618600	-0.59959500	1.90124600
C	4.31534400	-0.54678900	-1.35626400
H	2.97513100	-0.38368200	-3.02913000
H	5.40838200	-0.70315800	0.48756700
H	5.20217400	-0.59636900	-1.97469000
C	-1.24397100	-0.33774900	2.52519000
H	-1.10569500	-0.14650500	3.59044400
H	-2.10398500	0.24655700	2.19512700
H	-1.42941900	-1.39933100	2.35784000
Cl	0.26695600	2.93848100	2.20564800
Cl	0.08169500	-3.23003300	0.68435000



TS'6c

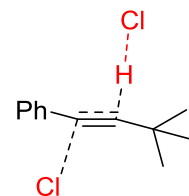
H	0.03765700	1.35770300	1.67843700
C	0.80255400	-0.35275300	0.90392200
C	-0.18763500	0.03379200	1.53468600
C	2.01993700	-0.46276100	0.20358200
C	2.05130700	-0.30094100	-1.19053000
C	3.21229400	-0.72225600	0.89820600
C	3.25385200	-0.38930600	-1.87059600
H	1.12812600	-0.11008700	-1.71934500
C	4.40973800	-0.80908200	0.20946800
H	3.17838900	-0.85550500	1.97025200
C	4.43213200	-0.64282600	-1.17305400
H	3.27624600	-0.26254700	-2.94469400
H	5.32730200	-1.00825500	0.74677200
H	5.37018700	-0.71255600	-1.70835400
C	-1.45163700	-0.36564500	2.19612900

H	-2.24623100	0.31648800	1.88615100
H	-1.68618200	-1.36909400	1.83435400
C	-1.32958900	-0.36104700	3.72155200
H	-1.05887900	0.62832400	4.09175300
H	-2.28131400	-0.64817000	4.17123100
H	-0.56898800	-1.07203600	4.04542400
Cl	0.03493600	2.92169500	1.99354800
Cl	0.07902100	-3.32423600	0.79406000



TS'6d

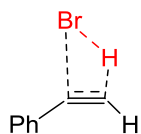
H	1.45876800	-1.32693100	-0.00115700
C	-0.00663800	0.06951600	-0.00055600
C	1.22725100	0.01401000	-0.00091000
C	-1.38917200	-0.19907400	-0.00020300
C	-2.08193700	-0.33925500	-1.21326000
C	-2.08126300	-0.33953400	1.21320500
C	-3.43784100	-0.61793800	-1.20781800
H	-1.54394400	-0.22146600	-2.14328800
C	-3.43717100	-0.61821500	1.20845100
H	-1.54275500	-0.22195800	2.14296200
C	-4.11620000	-0.75679800	0.00048900
H	-3.96978500	-0.72484700	-2.14373800
H	-3.96859500	-0.72533800	2.14464100
H	-5.17694200	-0.97170000	0.00075800
C	2.49262400	0.79871100	-0.00115400
C	3.30656400	0.52514500	1.26610800
H	3.61284200	-0.52098200	1.31479400
H	4.20309200	1.14780400	1.26872100
H	2.72628900	0.75663800	2.15989000
C	3.30585100	0.52550700	-1.26895100
H	4.20238400	1.14815800	-1.27188600
H	3.61209200	-0.52061000	-1.31811400
H	2.72507700	0.75726500	-2.16234000



TS'6e

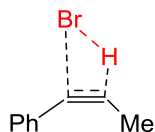
H	2.16147600	1.84161900	-0.00091100
Cl	1.97988300	-2.82736300	-0.00150600
Cl	-0.28569100	3.13371200	-0.00006700
H	2.00577100	-0.04533000	0.09123700
C	0.07338900	0.10290400	0.00171000
C	0.92197600	-0.80195800	0.01098300
C	-0.53222000	1.37483000	-0.00333200
C	-0.78839200	2.02594700	-1.21967800
C	-0.84878200	2.01212500	1.20607400
C	-1.35130200	3.29027100	-1.22175100
H	-0.54701000	1.52486000	-2.14633300
C	-1.40988900	3.27723400	1.19415100
H	-0.65358600	1.50044100	2.13781400
C	-1.66327300	3.91597200	-0.01722400
H	-1.55032700	3.79038000	-2.16017400
H	-1.65355300	3.76777600	2.12705800
H	-2.10605100	4.90355600	-0.02265600
C	1.14149400	-2.28960300	-0.01260500
C	0.45320200	-2.85055700	-1.26830300
H	0.90081700	-2.43374500	-2.17227500
H	0.57781900	-3.93572900	-1.29321900
H	-0.60926200	-2.61033700	-1.25448500
C	0.48755800	-2.87769000	1.24905800
H	0.61330800	-3.96295300	1.25029300
H	0.95542900	-2.47742600	2.15016400
H	-0.57535500	-2.63993300	1.26435900
C	2.63393100	-2.63508000	-0.03914900
H	3.14762600	-2.25032700	0.84164400
H	2.75080800	-3.72001300	-0.06270800
H	3.12153200	-2.21597600	-0.91980900
Cl	-2.65334100	-1.17175000	-0.06328300

Cl	3.42051500	0.78243300	0.20743800
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TS7a

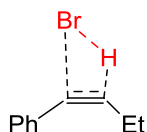
C	1.30034600	-0.72076700	-0.00000100
C	0.02941900	-0.67824700	0.00000100
H	1.80064300	0.26791000	-0.00000200
Br	1.00753900	2.54069100	-0.00000300
C	-1.33637100	-0.65851800	0.00000200
C	-2.04466200	-0.65288700	-1.23104000
C	-2.04465900	-0.65288500	1.23104500
C	-3.41977300	-0.64399000	-1.21878800
H	-1.48772300	-0.64748300	-2.15752200
C	-3.41977100	-0.64398700	1.21879600
H	-1.48771900	-0.64747900	2.15752700
C	-4.10287300	-0.63916700	0.00000500
H	-3.97243900	-0.63562200	-2.14818000
H	-3.97243500	-0.63561700	2.14818900
H	-5.18547900	-0.62790500	0.00000600
H	1.86895400	-1.64650900	0.00000000



TS7b

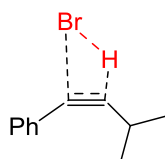
C	1.32865600	-0.73593300	-0.04973500
C	0.05524700	-0.69096700	-0.02498700
H	1.75205800	0.28903000	-0.10978400
Br	0.91438800	2.54845600	-0.20485200
C	-1.31326700	-0.66838200	0.00297500
C	-2.04867100	-0.72301400	-1.20971500
C	-1.99645300	-0.60056200	1.24518400
C	-3.42394000	-0.70551800	-1.17034100
H	-1.51167100	-0.76641900	-2.14703500
C	-3.37218700	-0.58414400	1.26264000

H	-1.42008300	-0.55165200	2.15854400
C	-4.08123700	-0.63316200	0.06010000
H	-3.99609200	-0.74159000	-2.08730900
H	-3.90484700	-0.52759800	2.20208900
H	-5.16346400	-0.61341800	0.08213600
C	2.23364900	-1.93191300	-0.00928700
H	2.85711200	-1.93873400	-0.90512100
H	2.89564500	-1.85003700	0.85462000
H	1.67584000	-2.86403500	0.04991400



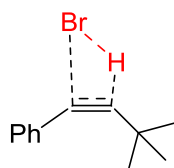
TS7c

C	1.38353700	-0.55591400	-0.47754900
C	0.12210400	-0.56187600	-0.30417500
H	1.76985300	0.47590000	-0.61248000
Br	0.85003000	2.70491700	-0.68542800
C	-1.23372100	-0.60986400	-0.11797300
C	-2.09892300	-0.73689500	-1.23554800
C	-1.77247400	-0.54849600	1.19340800
C	-3.45904000	-0.80008600	-1.03681700
H	-1.67162500	-0.77292800	-2.22786500
C	-3.13548400	-0.61445800	1.37062600
H	-1.09943400	-0.44276000	2.03293300
C	-3.97362100	-0.73683200	0.26013600
H	-4.12906600	-0.89328400	-1.88056000
H	-3.55865400	-0.56560600	2.36454000
H	-5.04526500	-0.78195900	0.40763300
C	2.33387300	-1.72903800	-0.49113900
H	2.82480400	-1.73148900	-1.46750500
H	1.77746400	-2.66106900	-0.39581900
C	3.37602900	-1.60141600	0.61649700
H	4.08004500	-2.43387300	0.56195900
H	3.93905100	-0.67114700	0.52377300
H	2.90589900	-1.61753400	1.60139100



TS7d

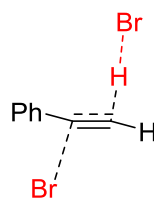
C	1.23890100	-0.87252600	0.00559300
C	-0.02768100	-0.74540600	-0.00355300
H	1.76520000	0.09756000	0.01554000
Br	1.09561000	2.51580100	0.02483500
C	-1.38939600	-0.62860500	-0.01351200
C	-2.08647000	-0.55941600	-1.24940100
C	-2.10574600	-0.57422000	1.21205100
C	-3.45698000	-0.44156800	-1.24839800
H	-1.52324500	-0.59163500	-2.17082400
C	-3.47608300	-0.45624100	1.19100200
H	-1.55701800	-0.61757300	2.14172800
C	-4.14587600	-0.38899600	-0.03365800
H	-4.00019300	-0.38353600	-2.18075700
H	-4.03383700	-0.40937800	2.11537000
H	-5.22347800	-0.29073600	-0.04150600
C	2.04038600	-2.16419800	0.00409400
C	2.90198400	-2.21560000	-1.25921500
H	3.60054400	-1.37752600	-1.28616300
H	3.47756100	-3.14249900	-1.27020100
H	2.28914900	-2.18058600	-2.15998500
C	2.88223700	-2.23080400	1.27994300
H	3.45765300	-3.15782600	1.28878400
H	3.58022200	-1.39318300	1.32778000
H	2.25546500	-2.20651200	2.17142900
H	1.34117800	-3.00163300	-0.00635900



TS7e

C	-1.26808600	-0.46909700	0.00024100
C	0.00362200	-0.52804200	0.00016400

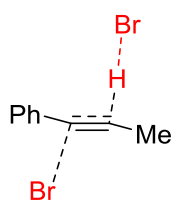
H	-1.64506000	0.56706000	0.00029000
Br	-0.62087200	2.85651700	0.00039400
C	1.36694500	-0.62634900	0.00009300
C	2.07406700	-0.68261000	1.23057900
C	2.07394600	-0.68257000	-1.23046300
C	3.44517100	-0.79371700	1.21966600
H	1.51922500	-0.62909400	2.15609200
C	3.44505100	-0.79367700	-1.21968800
H	1.51901400	-0.62902500	-2.15592000
C	4.12509400	-0.84756400	-0.00004500
H	3.99664200	-0.83428000	2.14810100
H	3.99643200	-0.83421000	-2.14817800
H	5.20402200	-0.93031400	-0.00009900
C	-2.26157400	-1.62901400	0.00028500
C	-3.12682600	-1.48608300	1.26012400
H	-3.64371400	-0.52611500	1.27695300
H	-3.87511200	-2.28058100	1.27470400
H	-2.52157500	-1.56833100	2.16355500
C	-3.12697400	-1.48606100	-1.25945000
H	-3.87526700	-2.28055500	-1.27395100
H	-3.64385800	-0.52609000	-1.27620600
H	-2.52183000	-1.56830300	-2.16295300
C	-1.53285600	-2.97373600	0.00023000
H	-0.90475000	-3.08124200	-0.88573100
H	-0.90464100	-3.08125500	0.88611200
H	-2.25925900	-3.78695900	0.00026800



TS'8a

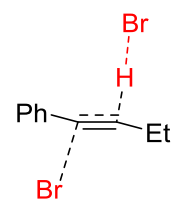
H	-2.62175500	-0.69840200	-0.02084800
C	-0.52255600	-0.56161100	-0.03290200
C	-1.41608900	-1.40743400	-0.04238100
C	0.30400500	0.57073900	-0.01764300
C	0.72819100	1.11609600	1.20623100

C	0.71128300	1.16121600	-1.22622600
C	1.54207400	2.23401200	1.21447100
H	0.41784300	0.64778300	2.12939800
C	1.52526100	2.27887900	-1.20431200
H	0.38801600	0.72738100	-2.16172300
C	1.94164800	2.81374800	0.01258100
H	1.87275100	2.65300900	2.15507800
H	1.84294300	2.73255500	-2.13323900
H	-1.64948900	-2.45311000	-0.06015200
Br	2.62020600	-2.49448500	-0.09060300
Br	-4.17415500	-0.04326500	0.00209500
H	2.58336500	3.68502600	0.02428200



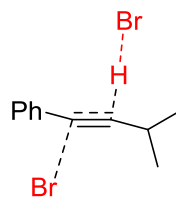
TS'8b

H	2.03756400	-0.59950300	0.02613400
C	0.07879000	-0.15651100	-0.01531400
C	0.75346800	-1.18399900	-0.01591100
C	-0.45169200	1.14785500	-0.00640400
C	-0.68732600	1.82224100	-1.21500200
C	-0.74803900	1.78097700	1.21112000
C	-1.20428400	3.10623300	-1.20056000
H	-0.46598400	1.32436400	-2.14848100
C	-1.26472000	3.06515700	1.21449000
H	-0.57322600	1.25147700	2.13703900
C	-1.49325300	3.72813800	0.01141700
H	-1.38678200	3.62383200	-2.13276600
H	-1.49404400	3.55093100	2.15345600
Br	-2.95466000	-1.68464700	-0.11712300
Br	3.69205500	-0.24786700	0.07348000
H	-1.90044800	4.73082700	0.01828100
C	0.87625200	-2.64888900	-0.03774600
H	1.40172700	-3.00140400	0.85070200
H	-0.12414400	-3.08265700	-0.07012300



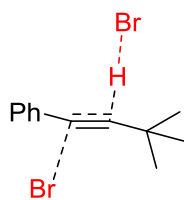
TS'8c

H	1.90012300	-0.27780000	-0.16963300
C	-0.02687900	0.22851700	0.04751000
C	0.63088800	-0.81065200	0.02346900
C	-0.55679800	1.53160500	0.03914400
C	-1.00050400	2.10399900	-1.16493800
C	-0.64242600	2.26976100	1.23136500
C	-1.51289400	3.38948300	-1.17146800
H	-0.93974900	1.52639500	-2.07640000
C	-1.15495600	3.55541700	1.21287700
H	-0.30661800	1.82022200	2.15524300
C	-1.58977300	4.11569900	0.01442600
H	-1.85537900	3.82789400	-2.09913800
H	-1.21971400	4.12264200	2.13164500
Br	-3.03440800	-1.66124400	0.23857200
Br	3.56566200	0.01517000	-0.39347000
H	-1.99236700	5.12018800	0.00499000
C	0.71482700	-2.28583800	0.05437300
H	1.55723300	-2.58353500	0.68162200
C	0.86688200	-2.87697300	-1.34910600
H	1.76754100	-2.50467200	-1.83835700
H	0.93226700	-3.96402200	-1.28769500
H	0.00336900	-2.61728500	-1.96155500
H	-0.20988000	-2.64169900	0.51373000



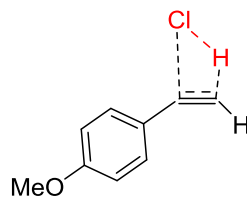
TS'8d

H	-2.09307700	-0.78184000	0.00157000	C	-1.48667300	1.71559700	0.66855500
C	-0.14734400	-0.40096800	0.00010500	C	-0.67607400	3.61350100	-1.22265900
C	-0.86160500	-1.40394900	0.00072400	H	0.81016400	2.17830000	-1.81418000
C	0.40622800	0.89307300	-0.00042300	C	-2.14429300	2.92995000	0.57697100
C	0.67686900	1.54498600	1.21341900	H	-1.79920500	0.95209200	1.37129900
C	0.67510300	1.54475200	-1.21478200	C	-1.73903500	3.87755000	-0.36005100
C	1.19805400	2.82702800	1.20725100	H	-0.36902600	4.35489400	-1.94795400
H	0.47618400	1.03203900	2.14336600	H	-2.97531000	3.14049700	1.23657500
C	1.19629600	2.82679600	-1.20961900	Br	-2.78619800	-1.55721900	2.20664200
H	0.47306500	1.03162700	-2.14433800	Br	3.39969000	0.21165100	1.69265500
C	1.45781100	3.46814100	-0.00143500	H	-2.25554500	4.82666800	-0.42223900
H	1.40587400	3.32870000	2.14281400	C	1.11673000	-2.26569400	-0.05565500
H	1.40275500	3.32828700	-2.14558000	C	-0.07040500	-2.79201500	-0.87684000
Br	3.03422600	-1.81775200	-0.00209700	H	-0.09216500	-2.33082800	-1.86548600
Br	-3.75401000	-0.35944400	0.00275000	H	0.02409200	-3.87273900	-1.00126300
H	1.86702700	4.47003000	-0.00182900	H	-1.01027900	-2.57981700	-0.36675900
C	-1.03607400	-2.88095000	0.00099000	C	1.11052300	-2.90734300	1.34077400
H	-2.10882200	-3.08713300	0.00179500	H	1.21094200	-3.98957600	1.23812500
C	-0.41579100	-3.47796400	1.26992600	H	1.93962400	-2.53791700	1.94385900
H	-0.87025600	-3.05451200	2.16639300	H	0.17408200	-2.69022100	1.85547500
H	-0.57366300	-4.55821800	1.28053200	C	2.43915900	-2.56203700	-0.77573700
H	0.65501700	-3.27485500	1.28690600	H	3.28894300	-2.18167900	-0.20972600
C	-0.41765000	-3.47820200	-1.26874200	H	2.55350000	-3.64154800	-0.88897700
H	-0.57552600	-4.55845900	-1.27890800	H	2.45321900	-2.10927200	-1.76853100
H	-0.87343900	-3.05492700	-2.16462100				
H	0.65312900	-3.27508300	-1.28733700				



TS'8e

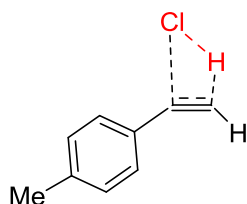
H	1.95309800	-0.24348000	0.80029100
C	0.25474200	0.21537300	-0.10621700
C	0.95147400	-0.78219800	0.10284000
C	-0.41148400	1.44378700	-0.19905600
C	-0.01566300	2.40079800	-1.15271100



TS9a

C	-3.02539100	-1.56550200	0.52977500
C	-1.81612900	-1.20060700	0.33818100
H	-3.79500200	-0.80020000	0.37464800
H	-3.28366800	-2.57694000	0.83085900
C	-0.53554800	-0.82639700	0.13859600
C	0.22902100	-0.28014400	1.21254400
C	0.06897400	-0.95348600	-1.15185700

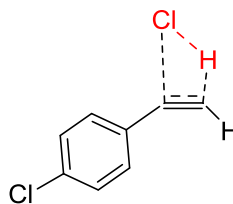
C	1.52245200	0.10974700	1.01937400
H	-0.23912300	-0.17153300	2.18098700
C	1.35825100	-0.56704900	-1.34161000
H	-0.51818200	-1.35356500	-1.96649400
C	2.10196300	-0.03346600	-0.26149100
H	2.08831300	0.52838900	1.83693300
H	1.84124500	-0.65010200	-2.30537100
O	3.34388900	0.30846800	-0.54656800
C	4.20428600	0.85806700	0.46966800
H	5.15700200	1.02296200	-0.02448400
H	3.80262500	1.80366300	0.83307100
H	4.32579300	0.14863300	1.28804500
Cl	-3.57548700	1.54887200	-0.25900800



TS9b

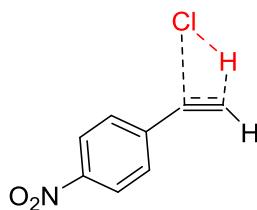
C	-2.54045600	-1.71025500	0.00003700
C	-1.35279900	-1.24890000	0.00001100
H	-3.34021000	-0.95319700	-0.00006100
H	-2.75866100	-2.77448400	0.00015700
C	-0.08390700	-0.76566800	0.00001800
C	0.58333400	-0.50642100	1.22981400
C	0.58353800	-0.50685900	-1.22975600
C	1.86161400	-0.01463900	1.21597000
H	0.06353000	-0.69659000	2.15852200
C	1.86182400	-0.01508600	-1.21587100
H	0.06389900	-0.69737000	-2.15848600
C	2.52109000	0.24072000	0.00005800
H	2.37538300	0.18517500	2.14711300
H	2.37575900	0.18439000	-2.14699600
C	3.89716700	0.80877400	0.00007500
H	4.45169200	0.51556400	-0.89127100
H	3.83473000	1.90320100	0.00022700
H	4.45174900	0.51535000	0.89132000

Cl	-3.26507600	1.41929200	-0.00015600
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TS9c

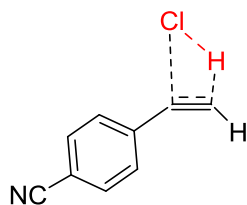
C	3.00531600	-1.62190800	-0.00093500
C	1.79880200	-1.22022000	-0.00063800
H	3.75773300	-0.81144500	-0.00036600
H	3.28850700	-2.67052400	-0.00160200
C	0.50350700	-0.79570100	-0.00040700
C	-0.17214200	-0.57275700	-1.22986200
C	-0.17219800	-0.57409200	1.22926000
C	-1.47745200	-0.15090100	-1.22653100
H	0.35601500	-0.73084300	-2.15953900
C	-1.47750000	-0.15220400	1.22632900
H	0.35591600	-0.73317800	2.15879200
C	-2.11831100	0.05125700	-0.00000600
H	-2.00638900	0.02731500	-2.15152700
H	-2.00645900	0.02504500	2.15149700
Cl	-3.75958700	0.57369500	0.00023200
Cl	3.57823300	1.49184400	0.00193800



TS9d

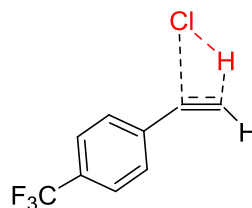
C	3.33877500	-1.54094900	-0.00053700
C	2.12462200	-1.18143300	-0.00041800
H	4.04090400	-0.67285100	-0.00023900
H	3.68958900	-2.56837800	-0.00087900
C	0.80487000	-0.79072300	-0.00028200
C	0.13049400	-0.59760100	-1.22938100
C	0.13049300	-0.59849600	1.22895400

C	-1.19512000	-0.22406300	-1.22613500
H	0.66476700	-0.73768400	-2.15788900
C	-1.19513200	-0.22499900	1.22597800
H	0.66477300	-0.73922600	2.15735900
C	-1.82581500	-0.05068400	-0.00001500
H	-1.73617700	-0.06555000	-2.14616500
H	-1.73620100	-0.06720800	2.14612500
N	-3.25339900	0.34222400	0.00011900
O	-3.79968700	0.49139900	-1.07923100
O	-3.79978700	0.49035000	1.07956200
Cl	3.77075400	1.52088400	0.00054200



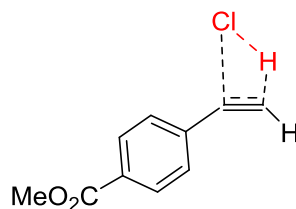
TS9e

C	2.98795700	-1.42746800	0.00001000
C	1.76580700	-1.09010800	0.00000700
H	3.68060000	-0.55596100	0.00000500
C	0.44312100	-0.72301300	0.00000500
C	-0.23507100	-0.53652400	-1.22954300
C	-0.23507300	-0.53651600	1.22955000
C	-1.56012800	-0.17135300	-1.22583900
H	0.30118700	-0.67386000	-2.15753600
C	-1.56013000	-0.17134500	1.22584200
H	0.30118400	-0.67384600	2.15754500
C	-2.21745500	0.01029800	0.00000000
H	-2.09512400	-0.02006300	-2.15225000
H	-2.09512700	-0.02004900	2.15225100
H	3.34881500	-2.45153600	0.00001700
Cl	3.37240000	1.66210800	-0.00003000
C	-3.59285900	0.39169800	-0.00000200
N	-4.70326200	0.69607300	-0.00000400



TS9f

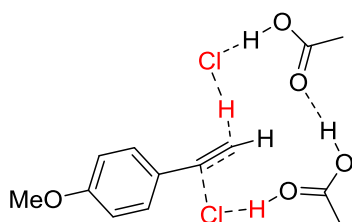
C	-3.92194600	0.74708600	1.08059700
C	-2.68329600	0.63752500	0.83078400
H	-4.56242400	0.13138700	0.41246400
C	-1.34225600	0.52329600	0.56503200
C	-0.72793500	1.40445600	-0.35948700
C	-0.57842700	-0.47177500	1.21976500
C	0.61721500	1.28417100	-0.61498200
H	-1.32693300	2.15291200	-0.85797700
C	0.76890100	-0.58086900	0.95203400
H	-1.06372300	-1.14133800	1.91532600
C	1.35518400	0.29363500	0.03914500
H	1.09936400	1.94625100	-1.32097700
H	1.35980700	-1.34024200	1.44208900
H	-4.33742100	1.37367000	1.86421500
Cl	-4.11940300	-1.26696100	-1.29095600
C	2.82880000	0.18882100	-0.27951300
F	3.02478500	-0.05409800	-1.59068100
F	3.44007800	-0.78913700	0.40480700
F	3.46988900	1.34084800	0.00819300



TS9g

C	-3.92423600	0.74456800	1.07661400
C	-2.68463600	0.63719000	0.82673400
H	-4.56626900	0.12279400	0.41768700
C	-1.34506000	0.52391500	0.56351000
C	-0.73195100	1.39330300	-0.37344800
C	-0.57605900	-0.45909800	1.23497800

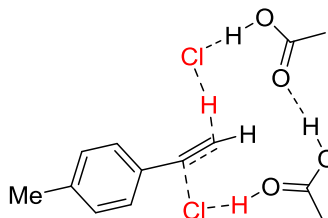
C	0.61514500	1.27683000	-0.62081600
H	-1.33485600	2.12929200	-0.88602400
C	0.76986100	-0.56330500	0.97167700
H	-1.06144900	-1.11973700	1.93926900
C	1.36487400	0.30187600	0.04609800
H	1.10519700	1.92581500	-1.33219200
H	1.36569400	-1.31018000	1.47388900
H	-4.33838800	1.38028400	1.85371700
Cl	-4.12773100	-1.29749500	-1.28559500
C	2.82711700	0.22049300	-0.26613700
O	3.39777100	1.01379800	-0.98097500
O	3.41686800	-0.81271500	0.32575200
C	4.82833800	-0.97854800	0.07436000
H	5.11317700	-1.87415200	0.61820700
H	5.00512500	-1.10378300	-0.99298200
H	5.37686500	-0.11316700	0.44390700



TS10a

H	0.88469700	1.14288700	-2.18199300
H	1.74742000	-2.01801900	0.00305000
C	3.51146500	-1.28512300	0.50678800
O	2.23526000	-1.25637800	0.52242800
O	4.13948900	-0.24436000	0.86965500
H	3.48891300	0.61322900	0.93117000
C	4.26190500	-2.48157200	0.06860300
H	5.31898600	-2.37109300	0.29303000
H	3.85170500	-3.37510900	0.53876500
H	4.12934700	-2.58787400	-1.01203400
C	1.59923700	1.86472600	1.38007600
O	2.62325500	1.68555000	0.70485900
O	0.59561800	2.55755000	0.93556900
H	0.72307500	2.88350500	-0.04077600

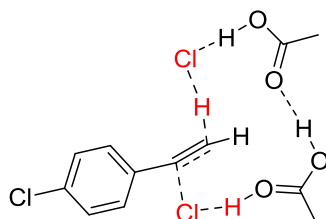
C	1.44323300	1.31307600	2.76039200
H	0.44733400	1.49779200	3.15340700
H	1.65369900	0.24319700	2.75132100
H	2.18441500	1.78739600	3.40737800
C	-0.10345400	-0.44811200	-1.43199100
C	0.89512800	0.04335400	-2.06952000
H	1.72283800	-0.51813300	-2.47487600
C	-1.30040500	-0.46364100	-0.75543800
C	-1.33170200	-0.38254100	0.66083700
C	-2.51963100	-0.51327600	-1.46902400
C	-2.52542700	-0.31572200	1.31947500
H	-0.40045500	-0.37168000	1.20675400
C	-3.72259600	-0.44437900	-0.80940600
H	-2.49364700	-0.59169200	-2.54718700
C	-3.73309100	-0.33937800	0.59197800
H	-2.57393400	-0.23614300	2.39698900
H	-4.64410300	-0.46543700	-1.37023100
O	-4.84368700	-0.25542400	1.32336800
C	-6.12372300	-0.24579000	0.67410200
H	-6.28605300	-1.17761800	0.13088200
H	-6.85207400	-0.15487700	1.47512700
H	-6.20498100	0.60877800	0.00102900
Cl	0.70720600	3.45502100	-1.83190200
Cl	0.66731700	-2.95377400	-1.13639000



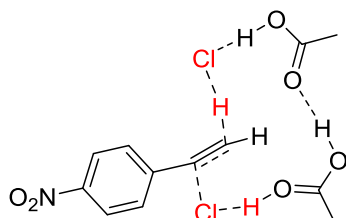
TS10b

H	0.56082100	1.15728200	-2.19536700
H	1.37346900	-2.04644400	0.01249000
C	3.16554300	-1.34523700	0.51549000
O	1.89566200	-1.26341400	0.50219200
O	3.83539600	-0.31766100	0.85373500
H	3.22801000	0.55458400	0.89132100

C	3.88119100	-2.58431000	0.14055200	H	-0.91368700	1.42826800	2.20913500
H	4.94131100	-2.49194700	0.35871500	H	-1.56463300	-2.00649000	0.16614200
H	3.44721700	-3.43775500	0.66158900	C	-3.31991000	-1.46687600	-0.61008000
H	3.74066300	-2.74929000	-0.93124900	O	-2.08246000	-1.26335600	-0.39748600
C	1.36911300	1.90701300	1.30107300	O	-4.03157800	-0.49745700	-1.02801100
O	2.38416400	1.67773900	0.63283800	H	-3.50864300	0.42762800	-0.97620600
O	0.37851800	2.61026100	0.83311400	C	-3.95384400	-2.78412500	-0.38287300
H	0.52036500	2.89713000	-0.14616200	H	-4.98565300	-2.77474800	-0.72184100
C	1.20347300	1.42468500	2.70546000	H	-3.38339500	-3.56048700	-0.89389000
H	0.17261300	1.50877400	3.03925100	H	-3.91715800	-3.00464700	0.68721700
H	1.55280200	0.39609100	2.79015500	C	-1.75018500	1.88492400	-1.30058500
H	1.83496700	2.04245100	3.34946100	O	-2.77033900	1.60987100	-0.65871600
C	-0.48347200	-0.36988200	-1.40089600	O	-0.81790200	2.65903200	-0.82181000
C	0.52374100	0.05078900	-2.05864200	H	-1.01154400	2.97606300	0.13380400
H	1.32112700	-0.55369600	-2.46486600	C	-1.50537900	1.37555800	-2.68322900
C	-1.65537300	-0.42608000	-0.68618800	H	-0.47844200	1.54430300	-2.99608800
C	-1.63269800	-0.34338000	0.72634400	H	-1.75428200	0.31595900	-2.73861000
C	-2.89594300	-0.51137600	-1.36102100	H	-2.17645400	1.90681300	-3.36300500
C	-2.81337000	-0.31725800	1.42600700	C	0.17128000	-0.14054500	1.54052100
H	-0.68136900	-0.30512700	1.23535100	C	-0.85440400	0.30647100	2.13971800
C	-4.06611200	-0.48267000	-0.64084900	H	-1.66411700	-0.27249100	2.55998800
H	-2.90533600	-0.58686100	-2.43954500	C	1.35680200	-0.27842000	0.85269500
H	-2.79871400	-0.24717000	2.50592500	C	1.35401200	-0.29178200	-0.56104300
H	-5.01642600	-0.53714900	-1.15588200	C	2.57769500	-0.38099300	1.55655500
C	-4.04765300	-0.37896400	0.75826600	C	2.53856200	-0.39282500	-1.24993200
C	-5.32605500	-0.30208000	1.52456100	H	0.41442400	-0.23056500	-1.08931600
H	-5.20661000	-0.67006700	2.54347000	C	3.76318100	-0.48172400	0.86527800
H	-5.65304300	0.74150000	1.58807000	H	2.56899100	-0.37631100	2.63739700
H	-6.12145900	-0.86049800	1.03025000	H	2.55364100	-0.40107100	-2.33019500
Cl	0.31140900	-3.04707300	-1.00470300	H	4.70504400	-0.55564000	1.38938500
Cl	0.53596600	3.37679600	-1.99229300	C	3.73144400	-0.48785700	-0.52942600
				Cl	5.22023200	-0.62008300	-1.39799200
				Cl	-0.58003100	-2.91953000	1.30560500
				Cl	-1.09198600	3.54353400	1.97632600



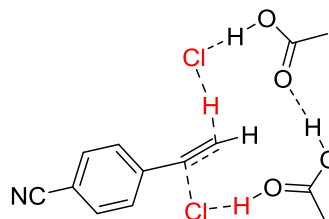
TS10c



TS10d

H	-1.14074700	1.35474900	2.37381400
H	-1.68209700	-2.09671500	0.00819000
C	-3.50303400	-1.53623400	-0.68564400
O	-2.29602500	-1.27642300	-0.41453200
O	-4.29705700	-0.57044000	-0.96585500
H	-3.84691300	0.35500100	-0.81674800
C	-4.04467500	-2.91409200	-0.68837800
H	-5.07703200	-2.91813300	-1.02571200
H	-3.42740400	-3.54964400	-1.32422600
H	-3.98303200	-3.31420400	0.32649300
C	-2.14301500	1.97653000	-1.03175800
O	-3.13388600	1.60556600	-0.40329000
O	-1.23301100	2.75668900	-0.49696800
H	-1.42610800	2.94649100	0.47043400
C	-1.86586300	1.56577600	-2.44019800
H	-1.02891200	2.11617100	-2.86146200
H	-1.64021700	0.49666100	-2.45134100
H	-2.76093900	1.71988100	-3.04320700
C	-0.01973700	-0.15157500	1.60048200
C	-1.07035700	0.17200800	2.19395900
H	-1.92628300	-0.38171800	2.54877600
C	1.18702400	-0.22460800	0.91035300
C	1.19519200	-0.02612500	-0.48401100
C	2.38618600	-0.46883700	1.60574500
C	2.38904300	-0.05745200	-1.17232700
H	0.26555800	0.14998100	-1.00239800
C	3.58046600	-0.50812900	0.91516000
H	2.36122400	-0.62455300	2.67460400
H	2.42529000	0.09892300	-2.23916900
H	4.51448900	-0.69434100	1.42231100
C	3.55529000	-0.29725300	-0.45683700

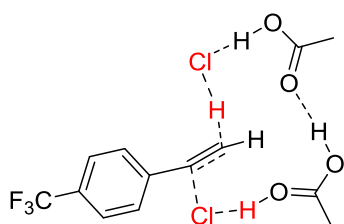
N	4.83410300	-0.32440000	-1.19462500
O	5.85324100	-0.54931400	-0.56266900
O	4.80167100	-0.11785000	-2.39711200
Cl	-0.65222600	-3.14891400	0.81453000
Cl	-1.44576300	3.15252300	2.50801900



TS10e

H	-0.71064600	1.34970400	2.27860700
H	-1.29377800	-2.07570200	-0.27284400
C	-3.23295800	-1.52911300	-0.63243600
O	-2.01134500	-1.23217500	-0.54325000
O	-4.10491700	-0.59275300	-0.72076600
H	-3.67090800	0.34554100	-0.60790400
C	-3.71704500	-2.93334100	-0.66994400
H	-4.76824300	-2.98273500	-0.40267500
H	-3.58999100	-3.30670700	-1.68917700
H	-3.10836300	-3.55429200	-0.01549700
C	-2.11089900	2.09616000	-0.96012600
O	-2.99698600	1.62241200	-0.25123100
O	-1.21262300	2.92774200	-0.49163100
H	-1.29966900	3.03875500	0.50185600
C	-1.94843800	1.75575500	-2.40835600
H	-1.28260600	2.45243300	-2.90911800
H	-1.52782000	0.74976000	-2.47395600
H	-2.92213000	1.74113800	-2.89477900
C	0.47539100	-0.11040100	1.46020000
C	-0.57970200	0.16773500	2.06686400
C	1.68381900	-0.20929800	0.78489400
C	1.71061200	-0.10546400	-0.62118900
C	2.87788700	-0.41425400	1.50554200
C	2.90900800	-0.19739200	-1.29180200
H	0.78717100	0.03906600	-1.16021500

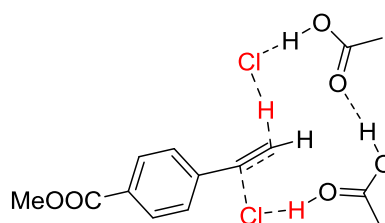
C	4.07631700	-0.50857800	0.83183500
H	2.84190700	-0.49632100	2.58186400
H	2.94581300	-0.11895100	-2.36824800
H	4.99956900	-0.66523400	1.36982500
C	4.09045400	-0.39996700	-0.56476300
Cl	-0.20188200	-3.16967700	0.24126900
Cl	-1.08550000	3.08988000	2.53050700
H	-1.40750700	-0.42963600	2.41456900
C	5.33302100	-0.49789500	-1.26279300
N	6.33431300	-0.57535200	-1.82658100



TS10f

H	-1.57340300	1.20617700	2.40621600
H	-1.93758400	-2.08289700	-0.10343200
C	-3.74221500	-1.53845300	-0.81640700
O	-2.53671700	-1.27475500	-0.52977900
O	-4.53543800	-0.57309800	-1.08656600
H	-4.09284900	0.35887400	-0.89832600
C	-4.27034400	-2.92079000	-0.84605600
H	-5.29921800	-2.92895800	-1.19381300
H	-3.64046000	-3.54068200	-1.48514100
H	-4.21502600	-3.33544500	0.16345800
C	-2.40838200	1.98447000	-0.99487400
O	-3.42249000	1.57717900	-0.42382200
O	-1.53766800	2.75579600	-0.39586600
H	-1.77541700	2.92295000	0.57604300
C	-2.07295900	1.62807900	-2.40645200
H	-1.20413800	2.17490600	-2.76271100
H	-1.87687300	0.55489600	-2.45973100
H	-2.93388000	1.83679300	-3.04264600
C	-0.35531000	-0.20136000	1.61059700
C	-1.44794200	0.08560200	2.16681300

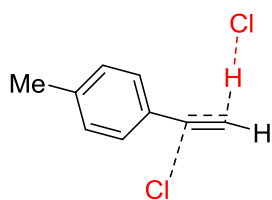
C	0.88252000	-0.22974100	0.99418400
C	0.97421700	0.02760500	-0.38949300
C	2.04458500	-0.48870700	1.74980900
C	2.20911100	0.02953900	-1.00083100
H	0.07482900	0.22081500	-0.95442700
C	3.27415100	-0.48924000	1.12715800
H	1.95642200	-0.68833300	2.80808600
H	2.29188700	0.22933500	-2.05918100
H	4.17066600	-0.68896100	1.69669000
C	3.34888300	-0.23346700	-0.24184600
C	4.70478100	-0.19783300	-0.90323800
F	5.28613000	1.01329200	-0.74986600
F	5.54733100	-1.10623600	-0.37867400
F	4.63454700	-0.43483200	-2.22493300
Cl	-0.90640400	-3.12746300	0.76528400
Cl	-1.92556500	3.15563500	2.54326800
H	-2.27760300	-0.55790100	2.42297000



TS10g

H	-1.83809300	0.88756700	2.54432200
H	-1.84466600	-2.05380200	-0.32493000
C	-3.53283800	-1.44656400	-1.22084700
O	-2.36894300	-1.21825500	-0.77234100
O	-4.27747400	-0.45407500	-1.52570900
H	-3.86969100	0.45244400	-1.19119400
C	-4.06535800	-2.81628900	-1.39268300
H	-5.00762300	-2.79557100	-1.93263300
H	-3.33377500	-3.43948100	-1.90646200
H	-4.22322400	-3.24697600	-0.40008200
C	-2.23556800	2.11257800	-0.81425700
O	-3.29586300	1.59237600	-0.45885500
O	-1.49089800	2.80552600	0.00702900

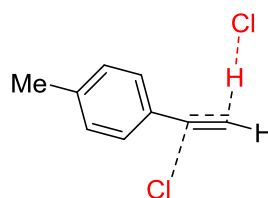
H	-1.87375500	2.83608600	0.94970100
C	-1.71634400	2.03124500	-2.21180100
H	-0.64870400	2.23192800	-2.25404200
H	-1.94488300	1.05822900	-2.64390000
H	-2.23509500	2.78927500	-2.80525500
C	-0.50974700	-0.39849200	1.70734100
C	-1.64361000	-0.19024600	2.22243500
C	0.76795700	-0.33116100	1.18325500
C	0.94993700	-0.02189600	-0.18212300
C	1.88454800	-0.55476600	2.01693900
C	2.22345200	0.05953100	-0.69801000
H	0.08569200	0.13613500	-0.80927600
C	3.15329700	-0.46871400	1.48745000
H	1.72955700	-0.79286700	3.05964400
H	2.37332700	0.29345600	-1.74123200
H	4.02240500	-0.63618300	2.10722300
C	3.32544600	-0.16881400	0.13377400
Cl	-0.94351700	-3.16844400	0.63591700
Cl	-2.33051000	2.83683900	2.85631200
H	-2.44709600	-0.89680000	2.37581600
C	4.72357800	-0.10993200	-0.39170800
O	5.70370200	-0.28871300	0.29717600
O	4.76950800	0.15362800	-1.69562600
C	6.08200800	0.21694700	-2.29016400
H	6.59002900	-0.74004800	-2.17834900
H	5.91307400	0.44083500	-3.33937000
H	6.66887000	1.00511600	-1.82045100



TS'10a

H	-3.35875000	-0.40472800	-0.04363000
C	-1.36701100	0.21940200	0.03250700
C	-2.61084700	0.44315400	-0.05020600
H	-2.94398200	1.48091900	-0.13480800

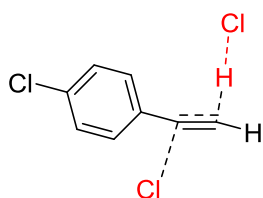
C	-0.03831000	-0.07001800	0.11682400
C	0.61047300	-0.15736700	1.38180100
C	0.72562100	-0.27127000	-1.06275500
C	1.94469300	-0.43254900	1.45268900
H	0.02957600	0.00168100	2.27882000
C	2.06630000	-0.54554200	-0.99242100
H	0.23191100	-0.19734700	-2.02114900
C	2.68851400	-0.62786300	0.26890100
H	2.45899700	-0.50191400	2.40065500
H	2.63275100	-0.69199700	-1.89833700
O	3.97936000	-0.88522000	0.44162600
C	4.82781000	-1.09034500	-0.69860400
H	4.84247200	-0.20104700	-1.32855000
H	5.81698700	-1.27284800	-0.29179400
H	4.49534500	-1.95604800	-1.27153100
Cl	-4.69528200	-1.98813700	-0.02481600
Cl	-1.56547600	3.65218700	-0.28239300



TS'10b

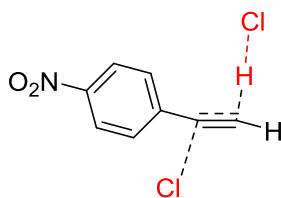
H	2.96371000	-0.67414300	0.00877200
C	1.19855800	0.48785400	-0.06786700
C	2.42964600	0.59260300	-0.08306000
H	3.20937900	1.32610300	-0.14477000
C	-0.12737700	0.03198500	-0.04017300
C	-0.75747200	-0.38386000	-1.22403000
C	-0.83000400	-0.04343700	1.17362100
C	-2.04983700	-0.87160000	-1.18532200
H	-0.21872700	-0.32243500	-2.15917300
C	-2.12095900	-0.53141800	1.19505300
H	-0.34923700	0.28811100	2.08293300
H	-2.52528800	-1.19746400	-2.10176400
H	-2.65417200	-0.59016700	2.13552200
C	-2.75339700	-0.95238100	0.01988900

C	-4.16681700	-1.45515800	0.05166600
H	-4.38221800	-1.97196700	0.98718000
H	-4.86865500	-0.62017600	-0.02938400
H	-4.36606300	-2.13365600	-0.77760600
Cl	0.29158100	3.48375200	-0.04231300
Cl	3.72354900	-2.03385400	0.09876200



TS'10c

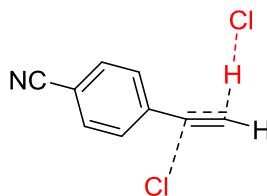
H	0.96740200	1.74593600	-1.90675000
C	-0.08504700	-0.04501100	-1.49069200
C	0.96457000	0.36580500	-1.99854900
H	1.85823100	0.01752300	-2.47813800
C	-1.34017100	-0.10485800	-0.85426500
C	-1.42041600	-0.19133200	0.54388000
C	-2.52012000	-0.04559600	-1.61119100
C	-2.65081700	-0.21446100	1.17312800
H	-0.51139000	-0.24465000	1.12547100
C	-3.75290400	-0.06840600	-0.98661300
H	-2.45747500	0.01326000	-2.68823800
H	-2.71980900	-0.28056800	2.24916800
H	-4.66524800	-0.02274500	-1.56327300
C	-3.80589500	-0.15391100	0.40064400
Cl	-5.35758400	-0.18331600	1.19046200
Cl	0.02171000	-2.99920200	-1.74475800
Cl	1.12446400	3.29255000	-1.88240900



TS'10d

H	-3.21651400	-1.23079900	-0.00020200
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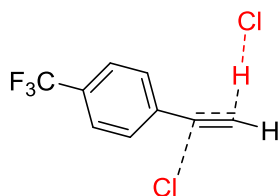
C	-1.96448300	0.54592200	0.00055500
C	-3.16025800	0.23583700	0.00062100
C	-0.55846900	0.31882400	0.00039000
C	0.12889400	0.17911800	-1.21278900
C	0.12865200	0.17628900	1.21337000
C	1.48148000	-0.09732600	-1.21733600
H	-0.40688900	0.29439200	-2.14399800
C	1.48124500	-0.10021800	1.21753400
H	-0.40732900	0.28929900	2.14473500
C	2.13920900	-0.23133300	0.00001500
H	2.02404900	-0.20866900	-2.14359100
H	2.02361500	-0.21378700	2.14363600
N	3.56812100	-0.52687700	-0.00018900
O	4.13846700	-0.64732700	1.07801000
O	4.13891000	-0.64368100	-1.07856400
Cl	-1.57789700	3.19465100	0.00059800
Cl	-3.42878400	-2.70702200	-0.00117600
H	-4.15683900	0.63340100	0.00083600



TS'10e

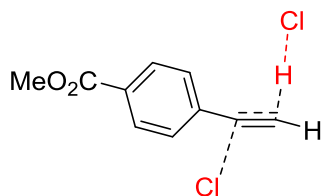
H	-0.63635900	1.98035500	1.58496100
C	0.33120300	0.07385600	1.39323800
C	-0.71155700	0.56931700	1.83534600
C	1.60603500	0.03702600	0.76677200
C	1.70140400	-0.12035900	-0.62199000
C	2.76852600	0.20436900	1.53041000
C	2.93665100	-0.11376300	-1.23857800
H	0.80109700	-0.25346500	-1.20373200
C	4.00625500	0.21171100	0.91884000
H	2.68751900	0.32055200	2.60121900
H	3.01537300	-0.23568800	-2.30944700
H	4.90588800	0.33957100	1.50376400
C	4.09460900	0.04937500	-0.46888100

Cl	0.41842100	-2.63044000	1.75874600
Cl	-0.70094600	3.48180100	1.39031100
H	-1.63194800	0.32800600	2.32817900
C	5.37262700	0.05347100	-1.10311500
N	6.40546900	0.05789800	-1.61584500



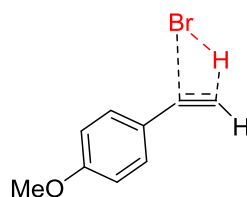
TS'10f

H	3.54635200	-1.29642900	-0.15932400
C	2.31193100	0.46605000	-0.18202400
C	3.50398800	0.14226900	-0.20378800
C	0.90128900	0.30394900	-0.14176700
C	0.18040900	0.13579800	-1.32834500
C	0.23329100	0.25944600	1.08945400
C	-1.18780100	-0.07405100	-1.28748100
H	0.69876300	0.17548200	-2.27592000
C	-1.13102700	0.04977600	1.12822100
H	0.79337200	0.39623300	2.00358800
H	-1.74034800	-0.20404300	-2.20678000
H	-1.64560600	0.01558900	2.07934700
C	-1.84069700	-0.11590100	-0.06079800
C	-3.32222000	-0.33432200	0.01622500
F	-3.63822400	-1.39988400	0.79255900
F	-3.96510700	0.72735100	0.56157400
F	-3.88748700	-0.55146900	-1.18659200
Cl	2.07722900	3.22523500	-0.24576900
Cl	3.75338400	-2.79360100	-0.11729900
H	4.50184100	0.53514600	-0.24208500



TS'10g

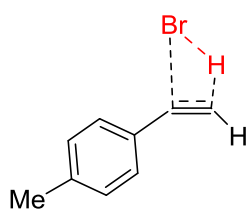
H	-1.69017300	1.97002200	1.65501900
C	-0.66252600	0.09407900	1.62254200
C	-1.76208700	0.57058200	1.92377800
C	0.68240400	0.03925300	1.17592200
C	0.96844300	-0.21590800	-0.17197500
C	1.73037200	0.28601100	2.07321100
C	2.27770800	-0.22426400	-0.61300300
H	0.15635200	-0.41430200	-0.85620200
C	3.03779700	0.27751400	1.62639600
H	1.50412800	0.47887500	3.11202000
H	2.49773900	-0.42207100	-1.65119100
H	3.85450300	0.46752200	2.30790200
C	3.32132600	0.02057300	0.28386300
Cl	-0.70973400	-2.66669500	2.00643000
Cl	-1.76793800	3.47007800	1.41062300
H	-2.73184700	0.31144000	2.29893700
C	4.74483800	0.02067700	-0.14585100
O	5.68060300	0.24129900	0.59159300
O	4.88768700	-0.25137900	-1.45132700
C	6.23407400	-0.27294000	-1.95336400
H	6.81819900	-1.03314300	-1.43725600
H	6.14667700	-0.51036400	-3.00911900
H	6.70420100	0.69977500	-1.81732700



TS11a

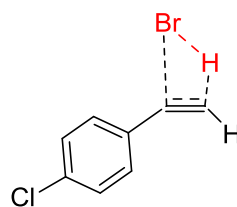
C	-2.11717900	2.19742400	-0.46627400
C	-0.97068300	1.66240500	-0.28972300
H	-2.98611500	1.53128800	-0.36966300
Br	-3.17350000	-0.94719600	0.09311300
C	0.25132100	1.11655600	-0.10582700
C	0.95508500	0.54371500	-1.20567600
C	0.84821100	1.08472300	1.19295800
C	2.18175000	-0.02912700	-1.02703000

H	0.49390000	0.55975300	-2.18334500
C	2.07239800	0.51878700	1.36807800
H	0.30761300	1.50910800	2.02742100
C	2.75352500	-0.04696000	0.26440400
H	2.69967500	-0.46889000	-1.86511400
H	2.54569200	0.47776000	2.33933400
O	3.93181100	-0.57816700	0.53828900
C	4.70443700	-1.21064700	-0.49929100
H	5.61352700	-1.54763100	-0.01043200
H	4.16087000	-2.06304100	-0.90680800
H	4.94579600	-0.49386700	-1.28426500
H	-2.23614800	3.25146200	-0.70210200



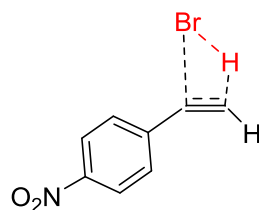
TS11b

C	1.58231500	2.23574100	-0.00000700
C	0.48481100	1.58920400	-0.00000600
H	2.50026100	1.62130700	-0.00000200
Br	2.91646300	-0.79022600	0.00000800
C	-0.70394300	0.92888100	-0.00000500
C	-1.33379000	0.58712800	1.22839400
C	-1.33378300	0.58711200	-1.22840300
C	-2.54112500	-0.06106200	1.21473700
H	-0.84397700	0.84289600	2.15775300
C	-2.54111900	-0.06107800	-1.21474400
H	-0.84396500	0.84286800	-2.15776300
C	-3.16507800	-0.39692200	-0.00000300
H	-3.02505500	-0.32177700	2.14690200
H	-3.02504300	-0.32180600	-2.14690800
C	-4.46338900	-1.12813800	-0.00000200
H	-5.05024600	-0.90251600	-0.89040600
H	-4.27262800	-2.20728600	0.00000000
H	-5.05024700	-0.90251200	0.89039900
H	1.62530800	3.32153600	-0.00001300



TS11c

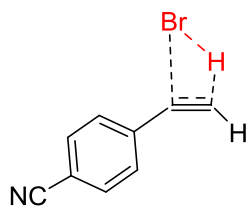
C	-2.11341800	2.19314100	0.00000200
C	-0.96791100	1.64114400	0.00000200
H	-2.96920900	1.48819900	0.00000000
Br	-3.16129300	-0.90414800	-0.00000300
C	0.26836400	1.06303500	0.00000200
C	0.91273500	0.76003000	-1.22840900
C	0.91273400	0.76002700	1.22841200
C	2.15297900	0.17292800	-1.22553700
H	0.41087400	0.98748100	-2.15841000
C	2.15297700	0.17292400	1.22554000
H	0.41087100	0.98747500	2.15841300
C	2.75912700	-0.11985900	0.00000200
H	2.65498800	-0.06860000	-2.15127000
H	2.65498500	-0.06860600	2.15127300
Cl	4.31075100	-0.87116200	0.00000100
H	-2.26551300	3.26878100	0.00000300



TS11d

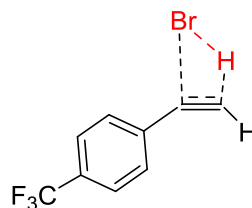
C	2.45023200	2.16534200	-0.01628400
C	1.28827800	1.65776600	-0.01250400
H	3.26680300	1.40946400	-0.01070000
Br	3.37583000	-0.96105200	0.00796800
C	0.03134000	1.10273100	-0.00848100
C	-0.61507500	0.83439300	1.22344700
C	-0.61553700	0.81756200	-1.23637200
C	-1.88162100	0.29425700	1.22338000
H	-0.10338700	1.04995300	2.14953300

C	-1.88160200	0.27631800	-1.22838500
H	-0.10446900	1.02104500	-2.16553600
C	-2.48483500	0.02781800	-0.00063000
H	-2.40235100	0.07551200	2.14198900
H	-2.40214700	0.04375500	-2.14369900
N	-3.85032100	-0.55407200	0.00360700
O	-4.37655900	-0.74225900	1.08626900
O	-4.35702800	-0.80396600	-1.07586600
H	2.66537800	3.22827100	-0.02396200



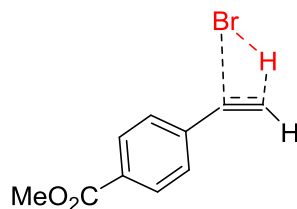
TS11e

C	-2.10166100	2.06748700	0.00001200
C	-0.94657400	1.54405300	0.00000900
H	-2.93295800	1.32404800	0.00000500
C	0.30950000	0.98901600	0.00000700
C	0.95733800	0.71144100	-1.22889500
C	0.95733300	0.71142200	1.22890700
C	2.22081100	0.17094800	-1.22524600
H	0.44531700	0.92179900	-2.15707200
C	2.22080600	0.17092900	1.22525500
H	0.44530900	0.92176400	2.15708600
C	2.84870900	-0.09881900	0.00000300
H	2.73125900	-0.05047300	-2.15160900
H	2.73125000	-0.05050800	2.15161600
H	-2.29963400	3.13544500	0.00001900
Br	-3.06212100	-1.01460600	-0.00000700
C	4.16021600	-0.65922000	0.00000100
N	5.21985800	-1.11021100	0.00000000



TS11f

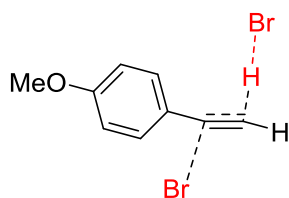
C	-3.08044600	1.88757700	-0.59701700
C	-1.88706400	1.49373800	-0.42304500
H	-3.84928200	1.10321100	-0.41278400
C	-0.58803400	1.09030800	-0.23825600
C	0.14575600	0.55666100	-1.32399500
C	0.02001000	1.22757300	1.03435700
C	1.45585600	0.17219500	-1.13756400
H	-0.33366800	0.44975100	-2.28659200
C	1.32742500	0.83912200	1.20499400
H	-0.55510500	1.62896300	1.85651300
C	2.03687500	0.31403400	0.12125900
H	2.02320700	-0.23809300	-1.95973800
H	1.80208200	0.93607600	2.17178600
H	-3.35721000	2.89365300	-0.89932400
Br	-3.78539400	-1.15807600	0.23512100
C	3.47351900	-0.09027000	0.35045400
F	4.03982800	-0.63879400	-0.73519500
F	3.57693600	-0.98549100	1.35277500
F	4.22528700	0.97651200	0.69802300



TS11g

C	-3.08346800	1.88877700	-0.59311200
C	-1.88795000	1.49780900	-0.42280300
H	-3.85303400	1.10596300	-0.41004200
C	-0.59029400	1.09534900	-0.24030200
C	0.14022400	0.54916400	-1.32506100
C	0.02428200	1.24257700	1.02871700

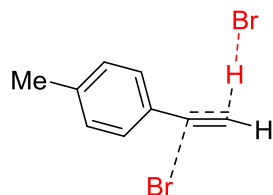
C	1.44684600	0.16243200	-1.13839100
H	-0.34409400	0.43592800	-2.28453100
C	1.33221800	0.85439900	1.19557700
H	-0.54735900	1.65309400	1.84893700
C	2.04390100	0.31344700	0.11894100
H	2.01044000	-0.25769300	-1.95754500
H	1.82067000	0.95623700	2.15381800
H	-3.35994200	2.89557800	-0.89315900
Br	-3.79381100	-1.17093700	0.22205400
C	3.46309700	-0.09162300	0.36245600
O	4.03134300	0.08223700	1.41787900
O	4.02440300	-0.65732300	-0.70230100
C	5.39640900	-1.07882700	-0.55355000
H	5.67224900	-1.50543700	-1.51330000
H	6.02699000	-0.22249500	-0.31776600
H	5.47261500	-1.82584800	0.23540200



TS'12a

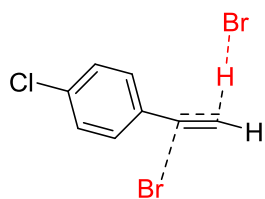
H	-2.65357000	-0.73293500	0.09001000
C	-0.51907300	-0.55358400	0.09156900
C	-1.36161200	-1.44476000	0.14231000
C	0.27609500	0.59486200	0.03034800
C	0.58697800	1.31427100	1.20278500
C	0.78906600	1.04348300	-1.19734700
C	1.37081700	2.44099000	1.14081900
H	0.20263900	0.96915900	2.15242400
C	1.57763700	2.17501200	-1.26431800
H	0.57251000	0.48213300	-2.09470700
C	1.87328300	2.88181900	-0.09271200
H	1.61801200	3.00092600	2.03213800
H	1.96451900	2.49534800	-2.21895900
H	-1.58854300	-2.48828900	0.21366000
Br	2.71437100	-2.60281200	-1.11029700

Br	-4.16872100	-0.12346500	0.06809000
C	3.18983100	4.49334000	-1.26756000
H	3.76036800	5.37427400	-0.98838000
H	3.85172500	3.75651300	-1.72581100
H	2.40293900	4.77273200	-1.97070900
O	2.63258700	3.99233900	-0.05179900



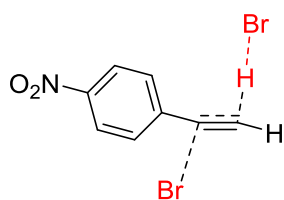
TS'12b

H	3.17289400	-0.19422300	0.03257100
C	1.23107700	0.67217400	-0.02000600
C	2.40533100	1.03219500	-0.01759200
C	-0.01324900	0.02570400	-0.01386600
C	-0.65753900	-0.26062500	1.20041300
C	-0.62764000	-0.34630300	-1.22126400
C	-1.87802200	-0.90746600	1.19897200
H	-0.19046800	0.03448300	2.12940100
C	-1.84775700	-0.99236000	-1.20464100
H	-0.13606100	-0.11962300	-2.15687700
C	-2.49511000	-1.28105000	0.00132200
H	-2.36743800	-1.12532200	2.13967400
H	-2.31323100	-1.27768700	-2.13958900
H	3.10547800	1.84180800	-0.03439200
Br	-0.60165600	3.81043100	-0.00164500
Br	4.22614300	-1.46489100	0.08946800
C	-3.83876800	-1.94870500	0.00569500
H	-3.92899400	-2.66342100	-0.81278800
H	-4.63079700	-1.20521300	-0.12159700
H	-4.02228500	-2.46736700	0.94632900



TS'12c

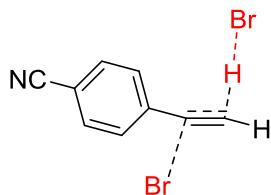
H	3.10351200	-0.22643700	0.00002200
C	1.19072700	0.66826700	-0.00001300
C	2.37827700	0.98740800	-0.00001700
C	-0.06360400	0.03974400	-0.00000900
C	-0.69393000	-0.27948800	1.21356200
C	-0.69388300	-0.27959100	-1.21357700
C	-1.92509800	-0.90587800	1.21527500
H	-0.21194200	-0.02385200	2.14610000
C	-1.92505100	-0.90598100	-1.21528500
H	-0.21185800	-0.02403500	-2.14611800
C	-2.52920500	-1.21239100	-0.00000400
H	-2.41819500	-1.15240400	2.14412400
H	-2.41811200	-1.15258600	-2.14413200
H	3.08679800	1.79074200	-0.00003600
Br	-0.50680600	3.74094800	-0.00005600
Br	4.14507600	-1.53649500	0.00006200
Cl	-4.08041500	-1.99929200	0.00000000



TS'12d

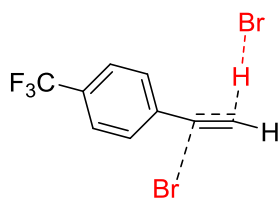
H	2.80398300	-0.75222600	-1.52515300
C	1.57636300	0.54845800	-0.26503000
C	2.74640800	0.49910800	-0.62956100
C	0.20530000	0.21237700	-0.11460600
C	-0.19530500	-0.66354200	0.90507300
C	-0.74091100	0.69622000	-1.03005400
C	-1.51700500	-1.04223200	1.01663000
H	0.53809200	-1.03115200	1.60813200

C	-2.06440400	0.32199700	-0.92486000
H	-0.42619900	1.37206900	-1.81202700
C	-2.43659800	-0.54126800	0.10070300
H	-1.83911000	-1.71366500	1.79781200
H	-2.80306000	0.68869600	-1.62109200
H	3.73628700	0.90692300	-0.62199400
Br	1.02516600	2.87896900	1.52819200
Br	3.05631000	-2.00552300	-2.47702700
N	-3.83198700	-0.94089300	0.21332500
O	-4.63472800	-0.49787800	-0.60192000
O	-4.14980100	-1.70645500	1.11786200



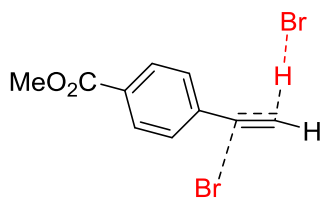
TS'12e

H	3.02684900	-0.22460300	0.00254600
C	1.15959600	0.74908600	0.00082600
C	2.36247000	1.01036700	0.00161100
C	-0.08947200	0.09463100	0.00014000
C	-0.70231200	-0.24793700	1.21488100
C	-0.70050900	-0.24882500	-1.21525900
C	-1.90624100	-0.92205000	1.21560500
H	-0.22787500	0.02718700	2.14527900
C	-1.90443600	-0.92294000	-1.21727800
H	-0.22469100	0.02561800	-2.14515300
C	-2.51110600	-1.25953700	-0.00116200
H	-2.38531500	-1.18766200	2.14686400
H	-2.38212700	-1.18923300	-2.14905200
H	3.10243900	1.78501800	0.00187400
Br	-0.45396300	3.56308700	-0.00136000
Br	4.01572300	-1.58285300	0.00376300
C	-3.75665900	-1.95674100	-0.00183200
N	-4.76087900	-2.52275000	-0.00237000



TS'12f

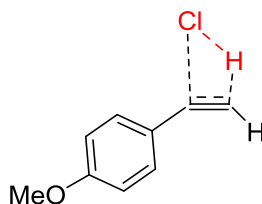
H	-3.20311200	-0.66279800	-0.03256500
C	-1.50106700	0.58474200	-0.08748000
C	-2.72816300	0.66434400	-0.11336600
C	-0.16226100	0.14338600	-0.05984700
C	0.46848000	-0.24232700	-1.25093400
C	0.53284200	0.06276700	1.15559600
C	1.77243500	-0.70233600	-1.22538200
H	-0.06963500	-0.17085700	-2.18486700
C	1.83542200	-0.39678400	1.17608800
H	0.04629900	0.37648000	2.06721200
C	2.45378500	-0.77567200	-0.01388800
H	2.26074200	-0.99505200	-2.14349500
H	2.37470900	-0.45180400	2.11070200
H	-3.57760000	1.31483200	-0.16321800
Br	-0.41635200	3.66636500	-0.01367600
Br	-3.97986100	-2.14345700	0.05591600
C	3.85528300	-1.31745700	0.02037600
F	3.86516500	-2.65704800	0.23391200
F	4.51602100	-1.10924500	-1.13555200
F	4.59385800	-0.76807300	1.00500400



TS'12g

H	3.05504300	-0.19890600	0.00391300
C	1.16539700	0.75669400	0.00189400
C	2.35829700	1.05212000	0.00105700
C	-0.07569500	0.08695400	0.00413900
C	-0.67450400	-0.27770200	1.21893500

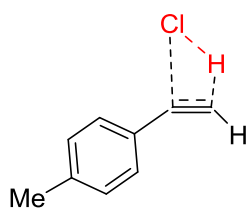
C	-0.70082700	-0.24358500	-1.20798700
C	-1.87297000	-0.96525100	1.22002700
H	-0.19231500	-0.01113700	2.14827800
C	-1.89756300	-0.93136200	-1.19889300
H	-0.24027600	0.05101100	-2.13970500
C	-2.49046100	-1.29675200	0.01165700
H	-2.33486000	-1.24628400	2.15424300
H	-2.39010300	-1.19307600	-2.12419500
H	3.09163000	1.83207000	-0.00109700
Br	-0.41266900	3.59858700	-0.04662300
Br	4.05372600	-1.52578200	0.00845800
C	-3.77901500	-2.04068000	-0.03652100
O	-4.34101200	-2.35981900	-1.06074900
O	-4.25422600	-2.32492000	1.18354900
C	-5.49905500	-3.04301200	1.23023500
H	-5.71637100	-3.17859100	2.28512900
H	-6.28619900	-2.46562100	0.74813800
H	-5.39857900	-4.00630600	0.73262800



TS13a

C	3.00327800	-0.73426800	-0.12570900
C	1.73163100	-0.60607700	-0.03971500
H	3.52529100	0.23107100	-0.09842200
C	0.38895000	-0.48401800	0.05789100
C	-0.40493100	-0.29928500	-1.11229600
C	-0.25465800	-0.50414100	1.33472500
C	-1.75803900	-0.13934900	-1.02176400
H	0.08820300	-0.27189800	-2.07402300
C	-1.60342700	-0.35307000	1.42404300
H	0.35025000	-0.63235900	2.22154400
C	-2.37064600	-0.16333200	0.25065700
H	-2.34657400	0.01120600	-1.91351200
H	-2.11563200	-0.36067300	2.37622800

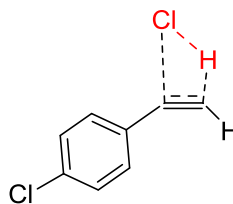
O	-3.66918500	-0.01230700	0.44201300
C	-4.54569100	0.23061000	-0.67402100
H	-5.53900200	0.31287300	-0.24305100
H	-4.27556900	1.16319300	-1.16930500
H	-4.51090700	-0.60310000	-1.37526400
C	3.77658200	-2.01360000	-0.25631100
H	4.47844100	-2.09731500	0.57567700
H	3.12526100	-2.88550800	-0.26495300
H	4.35942500	-1.99076000	-1.17921500
Cl	2.68433500	2.55712200	-0.01570400



TS13b

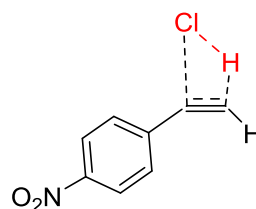
C	-2.57977300	-0.77702300	-0.00155000
C	-1.31335700	-0.61354600	-0.00113900
H	-3.10405100	0.19465700	-0.00528200
C	0.03716600	-0.44557400	-0.00087700
C	0.74809300	-0.35026700	1.22689400
C	0.74953900	-0.35860600	-1.22845200
C	2.10745800	-0.17566000	1.21442500
H	0.19829700	-0.40944900	2.15594900
C	2.10885800	-0.18389400	-1.21557600
H	0.20081900	-0.42411300	-2.15771900
C	2.80956400	-0.08314100	-0.00048500
H	2.65170900	-0.10044100	2.14659300
H	2.65420400	-0.11500000	-2.14760000
C	4.28051500	0.15555200	-0.00056900
H	4.75466500	-0.26270500	-0.88840300
H	4.47035200	1.23485400	-0.00740100
H	4.75304300	-0.25129200	0.89337300
C	-3.34798500	-2.06588300	0.00217900
H	-3.99319400	-2.09553300	0.88206200
H	-3.98886600	-2.10310000	-0.88059700
H	-2.69074200	-2.93292100	0.00744100

Cl	-2.42637400	2.45648900	-0.01172800
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TS13c

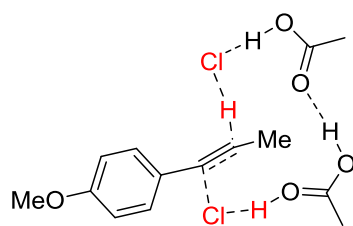
C	2.97299700	-0.75711900	0.00001900
C	1.70733000	-0.60643700	0.00003100
H	3.47214600	0.23254500	0.00003500
C	0.35029800	-0.44871800	0.00002400
C	-0.35748400	-0.36733900	-1.22769900
C	-0.35750300	-0.36732100	1.22773400
C	-1.72127800	-0.21232600	-1.22584200
H	0.19142600	-0.41983100	-2.15733800
C	-1.72129600	-0.21230100	1.22585300
H	0.19139300	-0.41980100	2.15738300
C	-2.38923300	-0.13402400	0.00000000
H	-2.27388600	-0.14535900	-2.15167700
H	-2.27391800	-0.14531700	2.15167800
Cl	-4.10174100	0.06711400	-0.00001500
C	3.77590700	-2.02340600	-0.00002700
H	4.41961100	-2.03718400	-0.88128600
H	4.41956000	-2.03727600	0.88126900
H	3.14256800	-2.90790200	-0.00008800
Cl	2.77737000	2.44042300	-0.00006000



TS13d

C	3.24975000	-0.74190700	0.00030100
C	1.98974000	-0.59137800	0.00381600
H	3.70937400	0.27903500	-0.00394800
C	0.61961000	-0.42764400	0.00292400

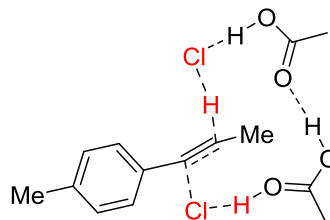
C	-0.07898600	-0.37332900	-1.22542300
C	-0.07850200	-0.33810600	1.22944400
C	-1.44935500	-0.23101000	-1.22556400
H	0.47159400	-0.43649100	-2.15284700
C	-1.44919000	-0.20012200	1.22575600
H	0.47292100	-0.37003300	2.15798100
C	-2.10035400	-0.14768000	-0.00078300
H	-2.00954600	-0.18415100	-2.14662700
H	-2.01001700	-0.12548400	2.14458900
N	-3.57167300	0.00262900	-0.00142000
O	-4.11916400	0.22447700	-1.06792800
O	-4.15190300	-0.10535800	1.06566600
C	4.10266500	-1.97230300	-0.00088700
H	3.50385100	-2.88012300	0.00795900
H	4.73863400	-1.96160300	-0.88750800
H	4.75354300	-1.95390000	0.87466300
Cl	3.00661400	2.37901100	-0.00012400



TS14a

H	-0.28210000	1.23901600	1.96731700
H	-1.20438000	-1.92523700	-0.33243900
C	-3.04123400	-1.38975300	-0.80858300
O	-1.77670400	-1.18668300	-0.79672900
O	-3.80624200	-0.41405300	-1.04943200
H	-3.26982900	0.55615200	-1.01143800
C	-3.61064700	-2.74055100	-0.57713400
H	-4.66551300	-2.67237600	-0.33090400
H	-3.48971600	-3.32101100	-1.49531800
H	-3.05239000	-3.25106200	0.20683300
C	-1.65528200	2.03641600	-1.45633500
O	-2.59330900	1.67365800	-0.72657600
O	-0.73785800	2.84852700	-1.04583100

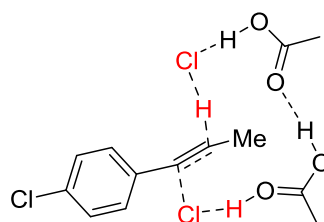
H	-0.79987900	3.07265300	-0.03552700
C	-1.49892800	1.54541100	-2.86187700
H	-0.77519800	2.14321400	-3.40765600
H	-1.15268000	0.51019300	-2.82548300
H	-2.46218400	1.55533500	-3.36912300
C	0.57066600	-0.37282100	1.23984500
C	-0.41666700	0.13618200	1.88114600
C	1.78848800	-0.38306800	0.58299500
C	1.85060000	-0.18389600	-0.81246300
C	2.99429800	-0.57954500	1.29920400
C	3.05660300	-0.15556700	-1.47091000
H	0.93094900	-0.04983400	-1.36251400
C	4.19867900	-0.55477300	0.64888200
H	2.94994700	-0.74358000	2.36651600
H	3.08149500	0.00996100	-2.53640700
H	5.12959700	-0.69310100	1.18047800
C	4.24405900	-0.34281700	-0.74196500
C	-1.67575300	-0.39949200	2.46719700
H	-1.72958900	-0.12488400	3.52171900
H	-2.52782100	0.07143400	1.97350300
H	-1.72707900	-1.47935500	2.36473700
Cl	-0.11111200	-2.87164400	0.77526200
Cl	-0.60213600	3.47290200	1.78960600
C	5.60488700	-0.12434000	-2.69630800
H	6.67235900	-0.16098500	-2.88868900
H	5.10033700	-0.91249300	-3.25633900
H	5.21047700	0.85173300	-2.98101500
O	5.46209100	-0.33524700	-1.28613700



TS14b

H	0.40301700	1.18524700	-2.03590800
H	1.06964500	-2.07276600	0.24667100

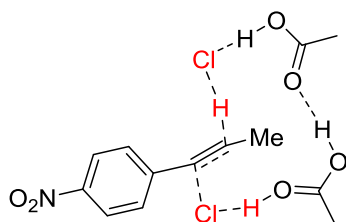
C	2.91880900	-1.54045500	0.72289700
O	1.66449500	-1.32388800	0.69519600
O	3.69424100	-0.56651600	0.98454300
H	3.18223900	0.36879500	0.95671200
C	3.49835800	-2.87377200	0.45063000
H	4.54166200	-2.90170600	0.75217700
H	2.92179100	-3.64741600	0.95596900
H	3.43050200	-3.05999700	-0.62508700
C	1.48991500	1.91140600	1.33498100
O	2.45095800	1.54945000	0.64465900
O	0.56344700	2.69871400	0.87029500
H	0.69552200	2.93091100	-0.12206700
C	1.32069500	1.49645000	2.76042200
H	0.35468200	1.80044500	3.15394700
H	1.44345200	0.41664700	2.84638700
H	2.11348000	1.96464400	3.34862100
C	-0.57278400	-0.32553500	-1.28603100
C	0.45240100	0.06360600	-1.93495000
C	-1.76331400	-0.27704500	-0.58144700
C	-1.74926000	-0.09400500	0.81735400
C	-3.00091900	-0.37051200	-1.25556000
C	-2.93489800	0.01616200	1.50790800
H	-0.80104700	-0.04376700	1.33203800
C	-4.17538100	-0.26080000	-0.54840700
H	-3.00745400	-0.52096600	-2.32640100
H	-2.92123900	0.16873600	2.57941000
H	-5.12368400	-0.32389400	-1.06731400
C	-4.16460100	-0.06516100	0.84112500
C	-5.45344100	0.04678300	1.58983600
H	-5.29064800	0.26831000	2.64366300
H	-6.08172000	0.83129200	1.16072000
H	-6.01887100	-0.88663500	1.51673600
C	1.65979500	-0.58148400	-2.51532200
H	1.76549100	-0.28392000	-3.55990000
H	2.54512700	-0.21827200	-1.98824600
H	1.59485500	-1.66394200	-2.44169100
Cl	-0.06590000	-3.01169400	-0.76905500
Cl	0.66674800	3.33159800	-1.99558300



TS14c

H	-0.77104100	1.13133200	2.15841400
H	-1.35037600	-2.04305200	-0.39486700
C	-3.16864300	-1.44603000	-0.95834700
O	-1.92420800	-1.23905700	-0.80275800
O	-3.93216600	-0.44582400	-1.15743200
H	-3.42948200	0.47622000	-0.99660700
C	-3.75847600	-2.80226000	-0.91120700
H	-4.79034600	-2.78092000	-1.24981000
H	-3.16253500	-3.48902900	-1.51192100
H	-3.72299100	-3.15632600	0.12274200
C	-1.71652900	2.01596900	-1.19169100
O	-2.69822200	1.62337100	-0.55117400
O	-0.78257200	2.74547100	-0.64866400
H	-0.94073700	2.91634600	0.34662000
C	-1.52136900	1.71132100	-2.64041800
H	-0.51776500	1.96534700	-2.97067900
H	-1.73268600	0.65916800	-2.82999600
H	-2.24416900	2.30076700	-3.21014000
C	0.23363700	-0.32400700	1.35602800
C	-0.82219400	0.00566300	1.97394700
C	1.45741100	-0.28691700	0.70993700
C	1.51648000	-0.03039100	-0.67679400
C	2.65008100	-0.47296200	1.43964700
C	2.73416800	0.05080000	-1.31247000
H	0.59906600	0.09782600	-1.23160300
C	3.86941000	-0.39223000	0.80422800
H	2.59549400	-0.67490100	2.50010900
H	2.79430500	0.25253900	-2.37222300
H	4.79012700	-0.52648900	1.35339600
C	3.89817000	-0.13135300	-0.56490200
Cl	5.43084900	-0.02828000	-1.36555200

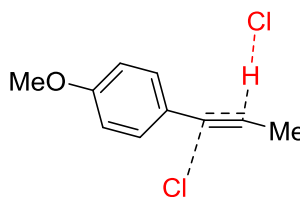
C	-2.05961500	-0.66794200	2.44810400
H	-2.92103600	-0.22481000	1.94469300
H	-2.01425700	-1.73676900	2.25443700
H	-2.18378500	-0.48776000	3.51723700
Cl	-0.29787300	-3.08582100	0.55310200
Cl	-0.95676100	3.19407900	2.26740300



TS14d

H	0.97658000	0.93016200	-2.27014400
H	1.56237300	-1.98643200	0.58787000
C	3.34772200	-1.27537100	1.14276400
O	2.10628500	-1.12155600	0.93801000
O	4.07742000	-0.23667900	1.29012100
H	3.55791700	0.64091200	1.05792700
C	3.99050100	-2.60630900	1.20497900
H	4.96173800	-2.53419100	1.68730800
H	3.34670100	-3.31800700	1.71843500
H	4.12975500	-2.96137700	0.17951700
C	1.75354000	2.17589000	1.01191500
O	2.78390200	1.75800300	0.48079600
O	0.83350200	2.81380600	0.33066300
H	1.05135600	2.85397500	-0.65095400
C	1.45888500	2.02216100	2.46721800
H	0.41762400	2.23974300	2.68962000
H	1.71963700	1.01606200	2.79335200
H	2.09278000	2.72341600	3.01614500
C	0.04507100	-0.51665000	-1.38391700
C	1.10959000	-0.22944800	-1.97473500
C	-1.21549900	-0.42693000	-0.77442400
C	-1.30410700	-0.05670300	0.57914500
C	-2.37949000	-0.66918400	-1.52229700
C	-2.54042000	0.08320900	1.17395100

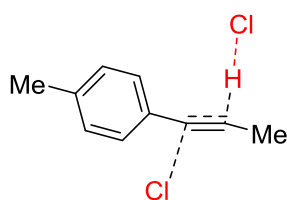
H	-0.40076100	0.10912900	1.14585600
C	-3.61964200	-0.52928600	-0.92964500
H	-2.29551200	-0.95952900	-2.55959300
H	-2.63585400	0.37159600	2.20932200
H	-4.52885400	-0.70443700	-1.48394600
C	-3.67306900	-0.15450200	0.40546600
N	-4.99329600	-0.00010500	1.03910600
O	-5.98433800	-0.20198300	0.35503600
O	-5.02834300	0.32299500	2.21653400
C	2.42394200	-0.79104400	-2.35962400
H	2.46962500	-1.84688400	-2.09896500
H	2.58115500	-0.66623700	-3.43170200
H	3.21409700	-0.23917500	-1.84684900
Cl	0.58779800	-3.15258300	-0.24357600
Cl	1.14059900	2.71470500	-2.67696000



TS'14a

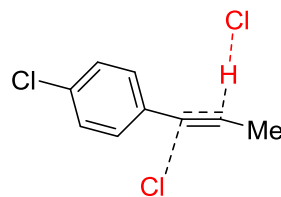
H	2.13586500	-1.31620400	-0.04705300
C	0.53602100	-0.11803400	0.28896700
C	1.76917600	-0.04473500	0.24836200
C	-0.82574700	-0.43012100	0.27887800
C	-1.46948600	-0.89602700	1.44423500
C	-1.58716400	-0.25690900	-0.88827700
C	-2.81367700	-1.18160300	1.43316700
H	-0.89195300	-1.02450600	2.34896200
C	-2.93957000	-0.53684200	-0.90465900
H	-1.10243600	0.11271700	-1.78077000
C	-3.56182000	-1.00110700	0.26025800
H	-3.31786900	-1.54027500	2.31994800
H	-3.50165500	-0.38878000	-1.81357600
C	2.94823500	0.83492600	0.37938700
H	3.56276000	0.51985600	1.22432600
H	3.56728400	0.77536100	-0.51691500

H	2.59833500	1.85809200	0.52841600
C	-5.69930900	-1.11508700	-0.80065800
H	-5.36815800	-1.74892700	-1.62542300
H	-6.69932200	-1.40730700	-0.49381400
H	-5.70189400	-0.06989300	-1.11532300
O	-4.87222000	-1.29873000	0.34862600
Cl	0.19316500	3.21682100	0.67563500
Cl	2.83955700	-2.70264500	-0.38922200



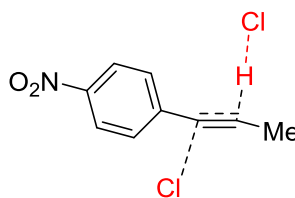
TS'14b

H	-2.43536500	-1.13896500	0.00038100
C	-0.97325600	0.25370900	0.00000900
C	-2.20783700	0.20555300	0.00007800
C	0.40279900	-0.03484100	0.00000200
C	1.09848100	-0.18529400	-1.20947100
C	1.09859900	-0.18480800	1.20947400
C	2.44865500	-0.48058300	-1.20177900
H	0.56616000	-0.06469700	-2.14255400
C	2.44876600	-0.48009800	1.20177300
H	0.56636400	-0.06383400	2.14255800
C	3.14764000	-0.62847900	-0.00000900
H	2.97504800	-0.59771400	-2.14082000
H	2.97524800	-0.59685200	2.14081200
C	4.62207100	-0.91095700	-0.00000100
H	5.18869800	0.02469900	0.00053000
H	4.91886700	-1.47229200	-0.88613100
H	4.91868300	-1.47315000	0.88565200
C	-3.47678900	0.95566900	-0.00003100
H	-4.06957500	0.70022700	-0.87962900
H	-4.06947500	0.70065100	0.87975900
H	-3.25678400	2.02339700	-0.00029900
Cl	-0.52143500	3.27486900	-0.00066500
Cl	-2.99307200	-2.62286300	0.00072900



TS'14c

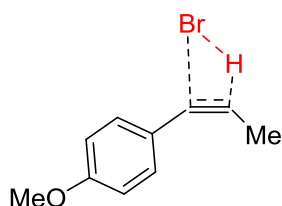
H	2.99453500	-0.19426000	-0.23832100
C	1.20141300	0.71388600	-0.00440000
C	2.40339500	1.00346800	-0.04902900
C	-0.03681000	0.04239600	-0.00530500
C	-0.57821700	-0.44880100	1.19257300
C	-0.73885700	-0.14929800	-1.20518100
C	-1.78780300	-1.11845100	1.19336400
H	-0.04341600	-0.29334400	2.11856300
C	-1.94888900	-0.81813000	-1.21105600
H	-0.32781700	0.23689800	-2.12688500
C	-2.46191900	-1.29569600	-0.00997600
H	-2.20904300	-1.49776300	2.11304400
H	-2.49342800	-0.96756200	-2.13207600
C	3.39179700	2.09619000	0.02108200
H	4.09099500	1.92502400	0.84085400
H	3.97219800	2.14415500	-0.90144500
H	2.85764500	3.03414600	0.17542600
Cl	-0.01004900	3.42559800	0.41829300
Cl	3.94267200	-1.46094000	-0.45999400
Cl	-3.98781800	-2.13624300	-0.01273200



TS'14d

H	-2.67224200	-1.28168000	-0.55145300
C	-1.65435700	0.43300800	0.03897600
C	-2.82644600	0.07551500	-0.14495600
C	-0.23975400	0.26508600	0.03298500
C	0.36389200	-0.30381800	-1.09887700

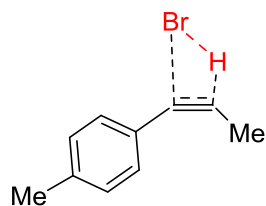
C	0.54851200	0.60552800	1.14131200
C	1.72680600	-0.53848700	-1.12147700
H	-0.24571300	-0.56602900	-1.95103900
C	1.90979800	0.37769600	1.12309200
H	0.07891000	1.07110600	1.99336300
C	2.48204000	-0.19240600	-0.00959700
H	2.20350100	-0.97557100	-1.98476800
H	2.52966800	0.63426400	1.96778100
N	3.92559700	-0.43343000	-0.03061900
O	4.57742200	-0.12291900	0.95868900
O	4.41399700	-0.93540400	-1.03557600
C	-4.24252000	0.46603800	-0.11841800
H	-4.69558500	0.33730600	-1.10284000
H	-4.80094800	-0.15803900	0.58171000
H	-4.31611300	1.51098800	0.18727200
Cl	-1.73795100	3.00571900	0.80894700
Cl	-2.75955400	-2.73359900	-1.02479000



TS15a

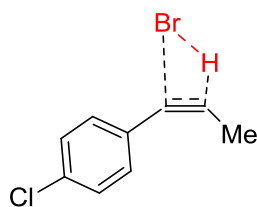
C	-2.32996000	1.55477500	-0.14040100
C	-1.10169200	1.20573600	-0.04682000
H	-3.01323200	0.69102600	-0.11397200
Br	-2.72697600	-1.81334200	0.09998300
C	0.20143100	0.85410200	0.05378100
C	0.95974300	0.55688400	-1.11538200
C	0.83301400	0.75020300	1.33145300
C	2.26767200	0.17211300	-1.02314100
H	0.47612700	0.62813400	-2.07993200
C	2.13676700	0.37126700	1.42319000
H	0.25372600	0.96582100	2.21848100
C	2.86800400	0.07212800	0.25042400
H	2.82790500	-0.05837700	-1.91589300
H	2.63629400	0.27858800	2.37777700

O	4.12227000	-0.30086000	0.44373100
C	4.95285200	-0.65949500	-0.67543800
H	5.90803300	-0.94042200	-0.24188100
H	4.52316900	-1.50550300	-1.21167600
H	5.08319400	0.19370000	-1.34146400
C	-2.87395700	2.94726400	-0.27053800
H	-3.55017600	3.14924600	0.56254300
H	-2.08512400	3.69705900	-0.28142200
H	-3.45514300	3.02293300	-1.19167900



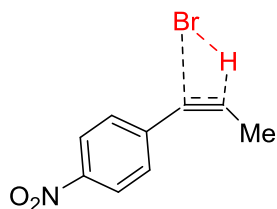
TS15b

C	1.88363400	1.60888600	-0.04477400
C	0.68472200	1.16998900	-0.02800100
H	2.61741700	0.78231700	-0.09637300
Br	2.53983600	-1.66972000	-0.18660400
C	-0.60625000	0.73401800	-0.00841100
C	-1.25354500	0.46216600	1.22749100
C	-1.32202800	0.55461500	-1.22324100
C	-2.55574700	0.03321500	1.23516500
H	-0.70086600	0.59280800	2.14764200
C	-2.62353800	0.12472600	-1.19055100
H	-0.82125500	0.75531800	-2.16033500
C	-3.26077600	-0.14731400	0.03252500
H	-3.05168300	-0.17573300	2.17416700
H	-3.17150300	-0.01398100	-2.11349700
C	-4.66127800	-0.65586600	0.05251100
H	-5.22768600	-0.30460400	-0.81001300
H	-4.64928800	-1.75094800	0.01134400
H	-5.17815600	-0.37097600	0.96893900
C	2.34633400	3.03612900	-0.00363800
H	2.99057400	3.17904700	0.86594800
H	2.94210200	3.24555400	-0.89405100
H	1.51416600	3.73548300	0.04572900



TS15c

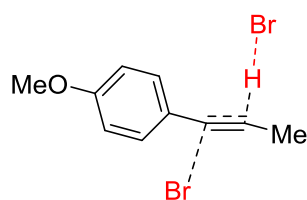
C	-2.29410800	1.56009100	-0.00000500
C	-1.07698800	1.18229400	-0.00000400
H	-2.97423600	0.68097000	0.00000400
Br	-2.77265200	-1.71775100	0.00004200
C	0.23559700	0.79779000	-0.00000300
C	0.92201400	0.60311000	-1.22677600
C	0.92201800	0.60313000	1.22677000
C	2.24432600	0.23346100	-1.22492100
H	0.38919000	0.74068800	-2.15718100
C	2.24433100	0.23348100	1.22491500
H	0.38919900	0.74072100	2.15717500
C	2.89329900	0.05555400	-0.00000300
H	2.77932600	0.07823300	-2.15068400
H	2.77933500	0.07826800	2.15067900
Cl	4.55721000	-0.40053400	-0.00000200
C	-2.85335800	2.95216800	-0.00001400
H	-3.48393400	3.08361800	-0.88107800
H	-3.48393500	3.08362900	0.88104700
H	-2.07009200	3.70728800	-0.00001800



TS15d

C	-2.58549900	1.52395700	0.00000900
C	-1.36928800	1.16069700	0.00000500
H	-3.23392900	0.60939200	-0.00000300
Br	-2.99256500	-1.70363200	-0.00005300
C	-0.04150600	0.78522600	0.00000400
C	0.64188000	0.61290100	-1.22687100

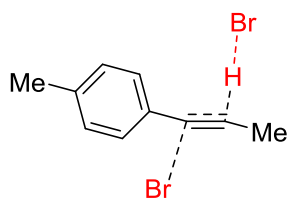
C	0.64187700	0.61288300	1.22687800
C	1.97898200	0.28256800	-1.22504400
H	0.10474700	0.73701700	-2.15611600
C	1.97897900	0.28255100	1.22505000
H	0.10474100	0.73698500	2.15612300
C	2.61808600	0.12972000	0.00000300
H	2.52415600	0.14326100	-2.14582600
H	2.52415000	0.14323200	2.14583200
N	4.05523100	-0.20876600	0.00000200
O	4.60946000	-0.33684000	-1.07936300
O	4.60945900	-0.33685000	1.07936700
C	-3.20516200	2.88869500	0.00002400
H	-2.45314700	3.67435500	0.00003000
H	-3.84041900	2.99013000	-0.88131000
H	-3.84041600	2.99011200	0.88136200



TS'16a

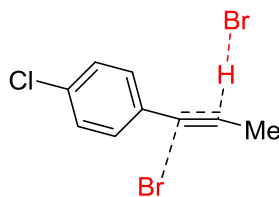
H	2.11251500	-1.28969500	-0.00194100
C	0.58761000	-0.01492000	0.32798100
C	1.81196200	0.08141200	0.29605900
C	-0.77848800	-0.32756100	0.31151100
C	-1.41149400	-0.86988900	1.44812200
C	-1.54644500	-0.09137200	-0.83904200
C	-2.75297600	-1.17164900	1.42378500
H	-0.82948600	-1.04898100	2.34145200
C	-2.89641000	-0.38677200	-0.86744000
H	-1.07058400	0.33948900	-1.70841700
C	-3.50786200	-0.93192500	0.26668600
H	-3.24797900	-1.59065000	2.28906600
H	-3.46330100	-0.18888100	-1.76379000
Br	0.43266200	3.75790800	0.04252200
Br	2.79838200	-2.78150200	-0.33966800
C	3.06520400	0.84431900	0.39652900

H	3.62703200	0.53860700	1.28055400
H	3.69441900	0.66245800	-0.47554200
H	2.82533000	1.90699400	0.45883500
C	-5.64459000	-1.02573100	-0.79825800
H	-5.30215600	-1.60797300	-1.65603300
H	-6.63920600	-1.35249900	-0.50896800
H	-5.66724500	0.03450900	-1.05725200
O	-4.81458800	-1.25579700	0.33987300



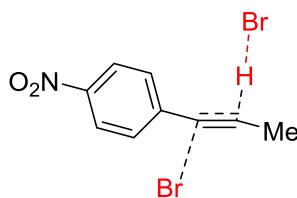
TS'16b

H	3.00551700	-0.19850200	-0.26511600
C	1.22374800	0.67105900	-0.01098400
C	2.39474900	1.04482900	-0.05081800
C	-0.02068900	0.01986800	-0.01088700
C	-0.59748800	-0.41725000	1.19390500
C	-0.71038000	-0.19799600	-1.21472900
C	-1.82098300	-1.05780300	1.18440100
H	-0.07641800	-0.23711800	2.12367300
C	-1.93295300	-0.84339400	-1.20744200
H	-0.27535300	0.14696400	-2.14235700
C	-2.50766000	-1.28585300	-0.01292600
H	-2.25884500	-1.38549800	2.11894600
H	-2.45661500	-1.00475800	-2.14120300
Br	0.21513500	4.04803100	0.87861300
Br	4.05828900	-1.50917000	-0.51807700
C	-3.82244700	-2.00968200	-0.01258800
H	-4.42623000	-1.73146800	0.85189300
H	-3.66255500	-3.09062400	0.03693500
H	-4.39152900	-1.80060100	-0.91787400
C	3.42166100	2.09586500	0.01648700
H	4.15682600	1.86082800	0.78718500
H	3.95054200	2.17178900	-0.93459300
H	2.93300400	3.04401400	0.24748100



TS'16c

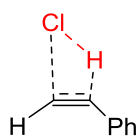
H	-2.52094100	-0.52375800	0.00098300
C	-0.74737900	0.40380100	0.00211200
C	-1.93074200	0.74108100	0.00242500
C	0.49317700	-0.25957400	0.00143800
C	1.11686100	-0.59377000	-1.21070600
C	1.11673600	-0.59646900	1.21289800
C	2.33223900	-1.25241600	-1.21399800
H	0.64175800	-0.32523600	-2.14328000
C	2.33211400	-1.25512100	1.21484800
H	0.64153700	-0.33001400	2.14601900
C	2.92809000	-1.57668000	0.00009600
H	2.81833000	-1.51043900	-2.14354900
H	2.81810900	-1.51521400	2.14387200
Br	0.73733200	3.43996400	0.00557500
Br	-3.55298700	-1.87835800	-0.00058300
Cl	4.46031200	-2.40454300	-0.00074700
C	-2.97726000	1.77476800	0.00352200
H	-3.61234700	1.67311600	-0.87733200
H	-3.61245200	1.67114300	0.88407000
H	-2.50749400	2.75855000	0.00465200



TS'16d

H	2.55001100	-0.88692800	0.00359900
C	1.00703200	0.43727100	0.00191200
C	2.23675400	0.48913500	0.00118800
C	-0.33934100	0.00518300	0.00177800
C	-1.01179200	-0.20424500	1.21533100

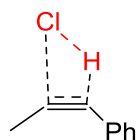
C	-1.00006900	-0.23545200	-1.21232400
C	-2.31863800	-0.65103700	1.21814900
H	-0.50015700	-0.00716000	2.14573700
C	-2.30649200	-0.68377000	-1.21629500
H	-0.47954800	-0.06224500	-2.14256600
C	-2.94612700	-0.88459300	0.00063100
H	-2.85187500	-0.81776800	2.14070100
H	-2.83045800	-0.87517600	-2.13936500
Br	0.18090800	3.42368100	-0.00639300
Br	3.25782300	-2.41706400	0.00489400
N	-4.33309900	-1.36341300	0.00006100
O	-4.86629300	-1.58115300	-1.07960700
O	-4.88723300	-1.52319900	1.07931200
C	3.47269900	1.28406500	-0.00154000
H	4.07519200	1.05933700	0.87937800
H	4.07337600	1.05589000	-0.88280700
H	3.20359500	2.34182000	-0.00328600



TS17a

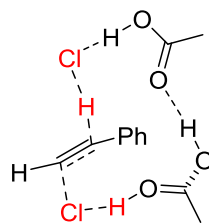
C	0.50789600	0.75526800	0.12764600
C	1.53078800	0.20650400	-0.33027600
H	1.02445300	0.43736500	-1.38709800
H	-0.38346100	1.23171100	0.47167600
C	2.80367600	-0.45346000	-0.17887200
C	3.51317500	-0.85999700	-1.31219800
C	3.32579600	-0.68552000	1.10001100
C	4.73739200	-1.49472900	-1.16664100
H	3.10279400	-0.67691400	-2.29574700
C	4.54922700	-1.32022400	1.23348600
H	2.77250700	-0.36881400	1.97356100
C	5.25533500	-1.72489700	0.10310000
H	5.28643700	-1.80932500	-2.04359400
H	4.95456800	-1.50058300	2.21993100
H	6.21068000	-2.22030100	0.21425100

Cl	-0.56722100	1.23993100	-2.29105800
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TS17b

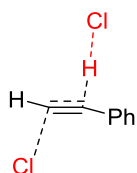
C	1.80490000	1.32245400	0.02909800
C	0.96852800	0.37439400	0.05324200
H	1.71641500	-0.48704600	0.13441600
C	-0.46898200	0.15092100	0.01020500
C	-0.95383300	-1.15746900	0.06982400
C	-1.36368100	1.22271100	-0.08938600
C	-2.32122100	-1.39131000	0.03016100
H	-0.25930300	-1.98305500	0.14674800
C	-2.72664700	0.98022200	-0.12835400
H	-0.99079600	2.23735500	-0.13573800
C	-3.20797700	-0.32560600	-0.06875300
H	-2.69293000	-2.40598600	0.07656400
H	-3.41655800	1.80990500	-0.20534400
H	-4.27366200	-0.50958700	-0.09956100
Cl	3.77826500	-0.83315000	0.23623100
C	2.71083200	2.41534200	-0.00103200
H	3.35688700	2.39587800	-0.87822200
H	2.05858200	3.30274200	-0.08001700
H	3.28625100	2.50400900	0.91997700



TS18a

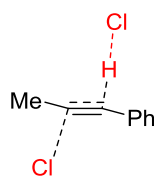
H	1.02186300	0.27579900	2.19438200
H	-2.25764800	-0.94186100	0.17677500
C	-2.93424400	0.68230900	-0.72754800
O	-1.98541500	-0.06699900	-0.33871600
O	-2.64803200	1.84959100	-1.14734500

H	-1.63516800	2.08143200	-0.97853400	C	-1.85679600	0.68605400	-0.01178000
C	-4.34762400	0.23488700	-0.73672800	C	0.54740600	-0.23727000	-0.00356200
H	-5.01771100	1.08655200	-0.79877100	C	0.38159600	-1.62564900	0.11414600
H	-4.49427800	-0.40422200	-1.61116900	C	1.83864900	0.28912200	-0.11623700
H	-4.55161000	-0.36717800	0.14753100	C	1.48859100	-2.46043100	0.11853100
C	0.76003700	2.12732000	-1.03848800	H	-0.62273400	-2.02052500	0.19462100
O	-0.30488200	2.40662100	-0.49114000	C	2.94154900	-0.55507600	-0.11327100
O	1.90439300	2.22208000	-0.40299200	H	1.97101100	1.35837600	-0.20497500
H	1.76498400	2.31980500	0.57631700	C	2.77138300	-1.92999500	0.00474500
C	0.88656400	1.62360500	-2.43829700	H	1.35122400	-3.53050900	0.21011300
H	1.76465600	2.05057500	-2.91872400	H	3.93605500	-0.13704200	-0.20263700
H	1.02988600	0.54110400	-2.38865200	H	-2.79329800	1.19076900	-0.00637600
H	-0.00894600	1.84208700	-3.01308500	H	3.63280600	-2.58564800	0.00801100
C	0.53076700	-0.80468500	1.58205600	Cl	-3.23865000	-1.44520700	-0.04697500
C	-0.50515500	-0.91450600	2.25987500	Cl	0.17287300	3.50042500	0.05090500
H	-1.18733200	-0.69529400	3.04816100				
C	1.29383900	-1.23341900	0.42858100				
C	2.61133900	-0.80538000	0.24500400				
C	0.70561700	-2.08231100	-0.51915700				
C	3.32547100	-1.20858800	-0.87426100				
H	3.06557000	-0.15012000	0.97349200				
C	1.42518700	-2.47703900	-1.63584700				
H	-0.30526800	-2.42946000	-0.36367300				
C	2.73434500	-2.03902200	-1.81918900				
H	4.34355200	-0.86884300	-1.00978700				
H	0.96465500	-3.13099100	-2.36473600				
H	3.29148400	-2.34795700	-2.69397600				
Cl	-2.43655100	-2.34253600	1.29158100				
Cl	1.73554800	1.69672500	2.62110600				



TS'18a

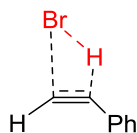
H	-0.31403000	2.09929800	0.01990400
C	-0.61951700	0.61434000	-0.00681600



TS'18b

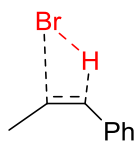
H	0.75760300	1.73814600	0.01552700
C	0.52413100	0.35748500	-0.00052400
C	1.72107800	0.03267000	0.00011500
C	-0.87167300	-0.01875800	-0.00084200
C	-1.22426400	-1.37156600	0.10274500
C	-1.87853800	0.94723700	-0.10192500
C	-2.56117000	-1.74010000	0.10653000
H	-0.43438100	-2.10884300	0.17032600
C	-3.21417500	0.56716000	-0.09896400
H	-1.60778700	1.99078500	-0.18148700
C	-3.56049100	-0.77535500	0.00648900
H	-2.82570200	-2.78691000	0.18772600
H	-3.98551400	1.32246000	-0.17900900
H	-4.60244400	-1.06918600	0.01022500
C	3.15033100	0.25502600	0.00977800
H	3.62007900	-0.15387800	-0.88340900

H	3.31054800	1.33917300	0.03727300
H	3.61469700	-0.19857000	0.88378000
Cl	0.84210200	3.30699500	0.03725600
Cl	2.07798900	-2.69499300	-0.04910100



TS19a

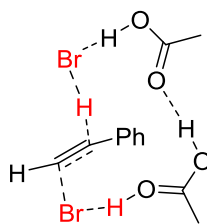
C	0.51799500	0.75330900	0.17072200
C	1.53205800	0.20767800	-0.31408900
H	1.05043700	0.42642400	-1.37482400
H	-0.37685900	1.23187000	0.50493700
C	2.80601500	-0.45415200	-0.16766100
C	3.51095400	-0.85848300	-1.30450600
C	3.33128800	-0.68896700	1.10928300
C	4.73507800	-1.49441700	-1.16356200
H	3.09801800	-0.67320700	-2.28666100
C	4.55437400	-1.32475100	1.23769700
H	2.78129100	-0.37385500	1.98514200
C	5.25657700	-1.72754600	0.10416600
H	5.28135300	-1.80768400	-2.04265600
H	4.96233800	-1.50733900	2.22263100
H	6.21185400	-2.22390300	0.21131800
Br	-0.62872700	1.27104000	-2.45375800



TS19b

C	0.92394900	1.56346900	-0.02655600
C	0.18289200	0.53637600	-0.05137200
H	0.96298600	-0.28389300	-0.12920800
C	-1.23831800	0.21367600	-0.00891400
C	-1.62837700	-1.12584800	-0.06565500
C	-2.20584300	1.22008500	0.08702400
C	-2.97592500	-1.45555700	-0.02669500

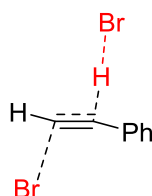
H	-0.87664000	-1.89986400	-0.13976300
C	-3.54812300	0.88204200	0.12530600
H	-1.90518700	2.25839700	0.13107800
C	-3.93568300	-0.45482400	0.06860500
H	-3.27493600	-2.49405300	-0.07082800
H	-4.29506600	1.66099200	0.19948000
H	-4.98574700	-0.71342800	0.09887200
Br	3.22566700	-0.58750300	-0.24149200
C	1.72335400	2.73325900	0.00359400
H	2.36314200	2.78141500	0.88467400
H	2.28692100	2.87995800	-0.91772100
H	0.98643100	3.55402200	0.07963100



TS20a

H	1.25540500	0.10831900	2.39643000
H	-2.60874100	-0.41576200	1.01880700
C	-2.29302800	0.14980300	-0.82306300
O	-2.20741700	0.33900700	0.43418200
O	-1.61007700	0.89265700	-1.59500200
H	-0.91483700	1.49309700	-1.07768700
C	-3.18775400	-0.87092000	-1.41707600
H	-2.83094100	-1.15719100	-2.40174100
H	-3.27310500	-1.73053300	-0.75535100
H	-4.18160900	-0.42532300	-1.51459000
C	1.19394100	2.51454300	-0.87866400
O	0.15595300	2.12841800	-0.34459300
O	2.27480900	2.76342900	-0.17559600
H	2.15154500	2.49253600	0.77058100
C	1.36091300	2.70401900	-2.35020100
H	2.11626200	3.45621600	-2.56259300
H	1.69620700	1.75281300	-2.77142800
H	0.41210900	2.96951200	-2.80942800

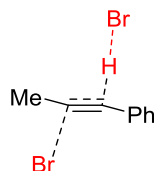
C	0.43872200	-0.84760100	1.84575100
C	-0.36717300	-0.88811800	2.78355300
H	-0.80634800	-0.70250200	3.73605400
C	0.79067300	-1.24232600	0.49956000
C	1.92434100	-0.73965400	-0.14250400
C	-0.04615300	-2.13833400	-0.17990600
C	2.19729200	-1.09949500	-1.45500000
H	2.58622400	-0.06935800	0.38504600
C	0.23350700	-2.49103100	-1.49063400
H	-0.90772800	-2.54504200	0.33167600
C	1.35035400	-1.96686500	-2.13544100
H	3.07692300	-0.70330400	-1.94492600
H	-0.42010400	-3.17986200	-2.00949600
H	1.56462500	-2.24287900	-3.15945100
Br	-2.95591900	-1.97460400	2.22942300
Br	2.37102100	1.39642100	2.79735500



TS'20a

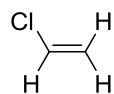
H	-1.48673800	-1.00368800	0.00417000
C	-0.15375100	-0.31595000	-0.01959900
C	0.52791200	-1.34445000	-0.02072000
H	0.76183300	-2.38200200	-0.01348300
C	-0.23891600	1.12552200	-0.01041600
C	-1.45091100	1.79608300	-0.20074400
C	0.93444200	1.86715300	0.19121800
C	-1.48852800	3.18410900	-0.19136400
H	-2.35741400	1.22829600	-0.35426900
C	0.88583000	3.25247900	0.20167200
H	1.86859400	1.33814100	0.32744000
C	-0.32366900	3.91569500	0.01077100
H	-2.43114300	3.69433000	-0.34164800
H	1.79571600	3.81774900	0.35786600
H	-0.35681100	4.99762200	0.01917200

Br	3.33337900	-1.11010300	-0.03460000
Br	-3.04619300	-1.53487600	0.04133800



TS'20b

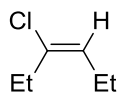
H	-1.52226400	-0.79273300	0.00040300
C	-0.27726400	-0.17968500	-0.00113200
C	0.32665900	-1.25754600	-0.00234700
C	-0.31300300	1.26485600	-0.00062400
C	-1.52368700	1.96391200	0.00145700
C	0.89582600	1.97342900	-0.00226100
C	-1.52439300	3.35229100	0.00189400
H	-2.45604100	1.41750900	0.00272000
C	0.88293500	3.35977300	-0.00181200
H	1.82614400	1.41944400	-0.00384000
C	-0.32412000	4.05399600	0.00026200
H	-2.46599200	3.88602100	0.00351000
H	1.82020700	3.90137500	-0.00308400
H	-0.32819400	5.13646500	0.00060600
Br	3.42346100	-0.83757400	-0.00659200
Br	-3.16517800	-1.35718900	0.00249300
C	0.55658200	-2.68051400	-0.00313600
H	1.10695800	-2.99172800	-0.88958700
H	1.10912900	-2.99237500	0.88173700
H	-0.42832500	-3.16461600	-0.00210100



syn-2a/anti-2a

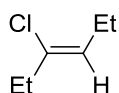
C	-1.63272100	-0.28492900	0.00002300
C	-0.57409500	0.50235600	0.00001500
H	-1.56008700	-1.36488100	0.00000800
H	-2.61995400	0.16076100	0.00004600
H	-0.61729300	1.58256200	0.00003000

Cl	1.06500600	-0.09929300	-0.00001800
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syn-2b

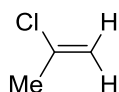
C	0.84405400	-0.52013400	-0.41605200
C	-0.34498100	-0.18267200	0.06897600
H	0.98192000	-1.53573900	-0.77135800
Cl	-1.62673300	-1.41162800	0.06702400
C	2.04881100	0.36811800	-0.50299400
C	3.18689300	-0.11454000	0.40331400
H	1.79476400	1.39967200	-0.25989600
H	2.39830100	0.37213700	-1.54047000
H	4.07275000	0.51076400	0.27969300
H	2.88725200	-0.08041100	1.45223200
H	3.46471400	-1.14400200	0.16816300
C	-0.79615500	1.13203500	0.62267000
C	-1.75471100	1.88575700	-0.30443400
H	0.08319800	1.74567800	0.81922300
H	-1.28027100	0.95795300	1.58684500
H	-2.06145200	2.82801700	0.15153500
H	-1.27380300	2.10670000	-1.25868400
H	-2.65085800	1.29766600	-0.50380300



anti-2b

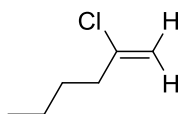
C	0.74592600	-0.84957400	0.23253700
C	-0.37694900	-0.23516200	-0.11972000
H	0.72225700	-1.93361600	0.15466000
Cl	-0.47637000	1.53487400	-0.07673100
C	-1.63916000	-0.89627200	-0.57733600
H	-1.89703900	-0.52570200	-1.57418200
H	-1.42711500	-1.96319500	-0.67739400
C	-2.82704200	-0.69340000	0.36392500
H	-3.09261200	0.36087800	0.45149400
H	-3.70151600	-1.22844500	-0.01130200

H	-2.60033700	-1.07063900	1.36349500
C	2.03855400	-0.24606700	0.67754900
H	1.88791100	0.78836300	0.98714700
H	2.39504000	-0.79371300	1.55534300
C	3.11025400	-0.30619000	-0.41657800
H	4.05860100	0.09428900	-0.05143900
H	3.28376900	-1.33361800	-0.74542700
H	2.80822100	0.27796600	-1.28841600



syn-2c/anti-2c

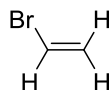
C	0.94516500	1.36262100	0.00000000
C	0.44729300	0.13655900	0.00000000
H	0.32120000	2.24537300	-0.00000100
Cl	-1.30776500	-0.08373100	0.00000000
C	1.20808200	-1.14277200	0.00000000
H	2.27913700	-0.93847500	0.00000000
H	0.96386600	-1.74164600	-0.88063700
H	2.01964800	1.49927400	-0.00000100
H	0.96386700	-1.74164500	0.88063900



syn-2d/anti-2d

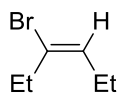
C	-2.19629500	1.44096300	-0.46562000
C	-1.42226500	0.50215400	0.05559300
H	-3.17667700	1.23223000	-0.87053800
Cl	-2.00923600	-1.16715800	0.09985900
C	-0.05331200	0.68485100	0.62463300
H	0.12438700	1.75944700	0.71250100
H	-1.84223300	2.46430600	-0.49217300
H	-0.02771900	0.26902700	1.63649300
C	1.05931300	0.04851900	-0.21499700
H	0.85738400	-1.01821600	-0.34357000
H	1.04741500	0.49339300	-1.21492100

C	2.43738000	0.23037000	0.41364200
H	2.63001300	1.29799900	0.56320900
H	2.43969800	-0.22508600	1.40939300
C	3.55516900	-0.37605700	-0.42709300
H	3.60168500	0.08727600	-1.41639200
H	4.52934900	-0.23960600	0.04830000
H	3.40347000	-1.44916600	-0.57109400



syn-3a/anti-3a

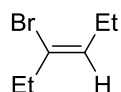
C	-2.10800500	-0.31259600	0.00003200
C	-1.08853900	0.52382600	0.00002400
H	-1.98735400	-1.38824700	0.00001800
H	-3.11672300	0.08424400	0.00005500
H	-1.18151200	1.60051300	0.00003900
Br	0.73293400	-0.04525000	-0.00001200



syn-3b

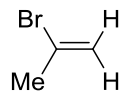
C	1.15466700	-0.49323000	-0.42819700
C	0.09942100	0.14280000	0.06394400
H	1.02765700	-1.50146800	-0.80753500
C	2.55275600	0.04665300	-0.49822200
C	3.51578200	-0.73589000	0.39792900
H	2.58125100	1.10456700	-0.23745100
H	2.89379400	-0.02706600	-1.53633700
H	4.53566300	-0.35932900	0.29241200
H	3.22852800	-0.64921500	1.44811700
H	3.52114700	-1.79763500	0.14008300
C	0.01266700	1.51911200	0.64226800
C	-0.63704200	2.53639000	-0.29723600
H	1.02285700	1.84744200	0.89317800
H	-0.54401700	1.48023400	1.58179600
H	-0.66699800	3.52152000	0.17217700
H	-0.07364900	2.61874500	-1.22893400

H	-1.66091200	2.25190000	-0.54508800
Br	-1.61208600	-0.78177800	0.02521600



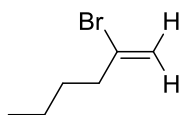
anti-3b

C	-0.95455700	1.12090300	0.18271000
C	0.22948500	0.61527600	-0.13522900
H	-1.03971600	2.19799600	0.04905600
C	1.41888200	1.38607300	-0.61563100
H	1.77439300	0.96011700	-1.55813100
H	1.07583600	2.40066900	-0.83443900
C	2.57226700	1.44262900	0.38621400
H	2.96440800	0.44766500	0.60156700
H	3.38998100	2.04534700	-0.01377400
H	2.24737500	1.89012900	1.32781800
C	-2.18879100	0.42669600	0.65708100
H	-1.95972600	-0.59829900	0.94817300
H	-2.55524400	0.93923100	1.55234800
C	-3.29237900	0.42939400	-0.40559400
H	-4.19762800	-0.04754100	-0.02387600
H	-3.55038300	1.44748400	-0.70663900
H	-2.97339100	-0.11301100	-1.29813500
Br	0.55077000	-1.29408300	0.01007900



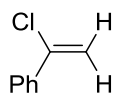
syn-3c/anti-3c

C	1.50308600	1.33678400	-0.00000100
C	0.95635100	0.13313000	0.00000000
H	0.92434000	2.24954700	-0.00000200
C	1.66286900	-1.17661500	0.00000100
H	2.74158600	-1.01175300	-0.00000100
H	1.39922300	-1.76762400	-0.88013600
H	2.58401300	1.42449900	-0.00000200
H	1.39922600	-1.76762100	0.88014200
Br	-0.97239000	-0.02291200	0.00000100



syn-3d/anti-3d

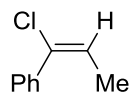
C	-1.43573000	2.03156600	-0.42975600
C	-0.81915800	0.95784100	0.03513500
H	-2.43140800	2.00776900	-0.84932700
C	0.55177700	0.89570100	0.62356100
H	0.89581900	1.92687100	0.74401900
H	-0.92679700	2.98838400	-0.39162500
H	0.49712200	0.45650200	1.62426000
C	1.56671500	0.11611200	-0.21758100
H	1.22774200	-0.91633700	-0.33582500
H	1.60573700	0.55060500	-1.22133100
C	2.96092200	0.12391100	0.40228000
H	3.30314400	1.15832300	0.51184400
H	2.90632400	-0.29064500	1.41436900
C	3.97630800	-0.66440800	-0.41699100
H	4.07021800	-0.25819700	-1.42777000
H	4.96657700	-0.63641900	0.04348000
H	3.68163500	-1.71331100	-0.50778600
Br	-1.74327600	-0.74350500	-0.03092900



syn-5a/anti-5a

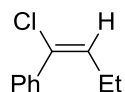
C	0.12387400	0.21032300	-0.03809800
C	1.05055700	1.23717000	-0.25464200
C	0.59884300	-1.08495300	0.18510500
C	2.41283800	0.97743500	-0.22610700
H	0.70029400	2.23802300	-0.46631900
C	1.96288900	-1.34149300	0.21572000
H	-0.10297200	-1.89142900	0.34260900
C	2.87529700	-0.31268100	0.01227800
H	3.11435100	1.78227500	-0.40299500
H	2.31271200	-2.34930300	0.39756500
H	3.93805900	-0.51557100	0.02926500

C	-1.31658200	0.52208300	-0.02490000
C	-1.86377800	1.66857600	0.36435800
H	-1.23897300	2.46459600	0.74467200
H	-2.92974900	1.83458700	0.32575500
Cl	-2.38387700	-0.76947500	-0.57674400



syn-5b

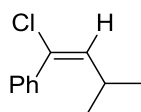
C	0.24905400	-0.05361000	0.02138200
C	0.96543300	0.89085500	0.76105600
C	0.95383600	-1.01049100	-0.71473000
C	2.35481200	0.88977000	0.74957300
H	0.43108100	1.61827300	1.35748400
C	2.34089400	-1.00706300	-0.72808100
H	0.41133300	-1.75582200	-1.28142100
C	3.04654500	-0.05596900	0.00272400
H	2.89575000	1.62531900	1.33160600
H	2.87289600	-1.74943700	-1.30963600
H	4.12925100	-0.05794800	-0.00489900
C	-1.22482800	-0.02539000	0.02091500
C	-2.02026600	1.01489700	-0.21426100
Cl	-1.98238200	-1.59038500	0.38390000
C	-1.57985400	2.38813500	-0.60368100
H	-1.77709800	3.10270600	0.20166400
H	-0.52093700	2.43768100	-0.85028300
H	-2.15407200	2.72748500	-1.47022600
H	-3.09094800	0.85996800	-0.14322700



syn-5c

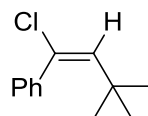
C	0.56720400	0.16056700	-0.10356800
C	1.05596100	-0.78171400	-1.01151800
C	1.40321000	0.60667500	0.92395900
C	2.34637700	-1.28092100	-0.88385800
H	0.42550900	-1.11286200	-1.82598700

C	2.68953800	0.10334300	1.05241500	H	-2.48025500	1.19558300	-0.14774900
H	1.04041800	1.34527800	1.62690200	C	-2.77578000	-1.55724300	-0.93247100
C	3.16521000	-0.84308400	0.14976800	H	-2.11936500	-1.59525500	-1.80366600
H	2.71309100	-2.00766900	-1.59785900	H	-3.08856100	-2.57771900	-0.69892400
H	3.32306700	0.45046700	1.85900600	H	-3.66707700	-0.98789200	-1.20941900
H	4.17131300	-1.23078000	0.24849800	C	-2.97841500	-0.94139400	1.50687300
C	-0.81275400	0.66297600	-0.23507600	H	-3.27473500	-1.96442600	1.74975500
C	-1.93423200	-0.04677400	-0.31841500	H	-2.47026700	-0.52053700	2.37684800
Cl	-0.93532600	2.43498700	-0.29121100	H	-3.88784700	-0.35987600	1.33327400
C	-2.05158000	-1.53532700	-0.20444600				
H	-2.39843500	-1.93714800	-1.16313300				
H	-1.07989300	-1.98728700	-0.00766000				
H	-2.86899000	0.49111100	-0.43817700				
C	-3.04327600	-1.93635700	0.89058200				
H	-4.03221700	-1.51010100	0.70575700				
H	-3.14878100	-3.02229600	0.93549900				
H	-2.70551800	-1.58783600	1.86905300				



syn-5d

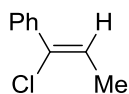
C	0.83373200	0.16946900	-0.06566400
C	1.02425900	-0.94021200	-0.89224700
C	1.84281600	0.52453300	0.83364400
C	2.19090100	-1.69027700	-0.80770000
H	0.26067300	-1.20570000	-1.61075600
C	3.00515300	-0.22791800	0.91919500
H	1.71138000	1.38944900	1.47069800
C	3.18271100	-1.33882800	0.09982900
H	2.32664800	-2.54568400	-1.45752200
H	3.77523400	0.05334400	1.62640700
H	4.09295900	-1.92148600	0.16455800
C	-0.42006200	0.94178700	-0.14548900
C	-1.66438600	0.48822900	-0.03560400
Cl	-0.17949400	2.68123100	-0.42548100
C	-2.07063300	-0.92474100	0.27217700
H	-1.17979500	-1.51401900	0.49593400



syn-5e

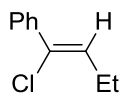
C	0.91119800	0.14654100	-0.17107500
C	1.24451600	-0.66476600	-1.25544000
C	1.80955000	0.27289100	0.88878200
C	2.44707800	-1.36105600	-1.26809500
H	0.55465400	-0.75276600	-2.08413500
C	3.00863100	-0.42592200	0.87754500
H	1.55761000	0.90978400	1.72663100
C	3.32904200	-1.24688900	-0.19975800
H	2.69336800	-1.99313800	-2.11133800
H	3.69317000	-0.33249800	1.71058000
H	4.26411000	-1.79163900	-0.20709400
C	-0.37593800	0.86983700	-0.16159600
C	-1.60421100	0.42029600	0.06221200
Cl	-0.18276800	2.59841900	-0.55875000
C	-2.08175000	-0.97134300	0.43569100
H	-2.40748100	1.14126400	-0.04843700
C	-2.54666500	-1.68231700	-0.84926200
H	-1.70687500	-1.85098200	-1.52425900
H	-2.99011200	-2.65003200	-0.60363200
H	-3.29577900	-1.09005900	-1.37822800
C	-3.29038500	-0.79291400	1.37295600
H	-3.70927100	-1.76547500	1.63709200
H	-2.99753200	-0.28632900	2.29467800
H	-4.07513200	-0.20292400	0.89526900

C	-1.03938500	-1.83684900	1.15370900
H	-0.20506900	-2.10197900	0.50887600
H	-0.64063600	-1.32597000	2.03110300
H	-1.51308300	-2.76260800	1.48613200



anti-5b

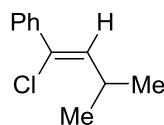
C	0.45917800	0.07142200	0.07659200
C	1.16525300	1.22711300	0.43067300
C	1.18302200	-1.05705600	-0.32003100
C	2.55118200	1.25975700	0.36419500
H	0.62493400	2.09691100	0.77869800
C	2.56921100	-1.02223700	-0.38563400
H	0.65569800	-1.96275300	-0.58451600
C	3.25990600	0.13606300	-0.04683300
H	3.07870600	2.16113600	0.64831400
H	3.11097200	-1.90394600	-0.70267700
H	4.34081000	0.15967400	-0.09237000
C	-1.01552400	0.07543000	0.10586900
C	-1.78353900	1.11988000	-0.20166000
H	-1.25257700	2.00842500	-0.52645700
Cl	-1.75827400	-1.45477300	0.58499900
C	-3.26961900	1.21612700	-0.17066300
H	-3.58127800	2.04940300	0.46523100
H	-3.65943400	1.42407900	-1.17115900
H	-3.73451000	0.30490800	0.19808700



anti-5c

C	0.81987300	-0.00044900	-0.04696200
C	1.27010700	-1.27794100	0.30542800
C	1.76728400	0.98399800	-0.34315300
C	2.62732000	-1.56656600	0.33730300
H	0.55276300	-2.04207800	0.57362100
C	3.12390000	0.69209400	-0.31185900

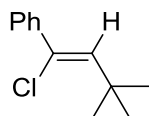
H	1.44084200	1.98029900	-0.60830600
C	3.56056800	-0.58388000	0.02639500
H	2.95609000	-2.55889800	0.61989900
H	3.84197900	1.46589200	-0.55272800
H	4.61937600	-0.80787800	0.05686800
C	-0.62827800	0.26918800	-0.12064000
C	-1.54660300	-0.59378700	-0.55109700
Cl	-1.11400400	1.88303600	0.42001200
C	-3.02773900	-0.42744600	-0.61005300
H	-3.30734100	0.60440100	-0.39998500
H	-3.36301400	-0.65071300	-1.62812800
C	-3.74373800	-1.36909300	0.36456800
H	-3.46630100	-1.14512500	1.39675500
H	-4.82694500	-1.26421800	0.27424500
H	-3.48969000	-2.41291700	0.16600700
H	-1.16355100	-1.55243300	-0.88829500



anti-5d

C	-1.12365500	-0.04197300	0.00605600
C	-1.72597700	-1.26278700	-0.31788300
C	-1.94256700	1.03198900	0.36714600
C	-3.10497300	-1.40994300	-0.25949600
H	-1.11052600	-2.09378800	-0.63576600
C	-3.32115500	0.88200700	0.42544900
H	-1.49774900	1.98670900	0.61208600
C	-3.90895900	-0.33913300	0.11421900
H	-3.55248500	-2.36067400	-0.52101700
H	-3.93804600	1.72355800	0.71483900
H	-4.98492500	-0.45247300	0.15294500
C	0.34767300	0.07886600	-0.02135000
C	1.19009700	-0.87667100	0.36773600
Cl	0.93970000	1.63238000	-0.62637300
C	2.69968500	-0.92356200	0.36453500
H	2.96069600	-1.91836300	0.73383600

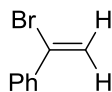
C	3.30210900	-0.80500500	-1.04085000
H	3.14739900	0.18555000	-1.46758200
H	4.37854300	-0.98817500	-0.99929800
H	2.86296100	-1.53794600	-1.72077100
H	0.69986300	-1.76207900	0.75909300
C	3.32582700	0.08556500	1.33606100
H	4.40514600	-0.07397000	1.39356800
H	3.15419100	1.11302000	1.01554100
H	2.91430300	-0.02811500	2.34110600



anti-5e

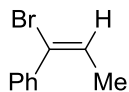
C	-1.11497700	-0.03758500	0.00194800
C	-1.72085500	-1.25514200	-0.32735900
C	-1.93100600	1.03626500	0.36984700
C	-3.10008300	-1.40048000	-0.26573000
H	-1.10736000	-2.08470100	-0.65153600
C	-3.30979200	0.88870800	0.43186300
H	-1.48128100	1.98809100	0.61542600
C	-3.90088600	-0.33009400	0.11677600
H	-3.55004300	-2.34844500	-0.53104600
H	-3.92409500	1.72928200	0.72768200
H	-4.97642300	-0.44158500	0.15913000
C	0.35756500	0.08175200	-0.02293700
C	1.19091600	-0.88433100	0.36132800
Cl	0.94674700	1.64105400	-0.60679800
C	2.70642800	-0.96360200	0.37674400
C	3.28578900	-0.79118400	-1.03845000
H	3.06996600	0.19376700	-1.44699000
H	4.37026700	-0.91781100	-1.00886300
H	2.87499700	-1.54091200	-1.71700000
H	0.68418800	-1.76705400	0.73766800
C	3.30287100	0.09150700	1.32568000
H	4.38789200	-0.02603700	1.37035600
H	3.08342500	1.10362900	0.99187000
H	2.90628900	-0.02969500	2.33528300

C	3.09465800	-2.35786100	0.89413600
H	4.18019400	-2.46358600	0.92453200
H	2.70902600	-2.52201200	1.90259900
H	2.69537500	-3.14083100	0.24581300



syn-6a/anti-6a

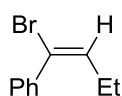
C	0.71136500	0.33044900	0.07229700
C	1.77766600	1.21099100	0.29063500
C	0.99284000	-1.01556900	-0.17765400
C	3.08884100	0.75934000	0.23799800
H	1.57447600	2.24798000	0.52060800
C	2.30511500	-1.46359200	-0.23322600
H	0.18023000	-1.71064700	-0.33589000
C	3.35814100	-0.57892200	-0.02695800
H	3.90062700	1.45237500	0.41658400
H	2.50499300	-2.50756500	-0.43627300
H	4.38045900	-0.93179600	-0.06241800
C	-0.66490300	0.85313300	0.08075000
C	-1.05218300	2.03945900	-0.37073000
H	-0.32842200	2.69891500	-0.83222100
H	-2.07524000	2.37808800	-0.30864600
Br	-2.00866200	-0.31465800	0.83419500



syn-6b

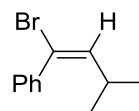
C	0.69253500	0.09151700	-0.01977100
C	1.58304100	0.67551200	0.88460100
C	1.15873900	-0.90761700	-0.87852600
C	2.91446000	0.27919200	0.91905100
H	1.22538900	1.43633200	1.56606400
C	2.48926700	-1.29851500	-0.84585700
H	0.47667000	-1.37455100	-1.57713300
C	3.37176700	-0.70634000	0.05291800
H	3.59253200	0.73849500	1.62737500

H	2.83910600	-2.06732700	-1.52325500
H	4.40876900	-1.01626600	0.08005400
C	-0.70769500	0.54716100	-0.06116800
C	-1.15317000	1.78278900	-0.26105500
C	-0.29961400	2.97158200	-0.56726600
H	-0.32234000	3.68884800	0.25916900
H	0.73840800	2.70659200	-0.75974700
H	-0.69393800	3.49185200	-1.44462200
H	-2.22142300	1.96257900	-0.22506200
Br	-2.01476700	-0.85946700	0.24083500



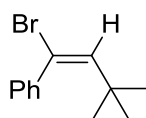
syn-6c

C	-0.79128100	-0.03489800	-0.06336900
C	-1.59255000	0.50721000	-1.07121100
C	-1.40430400	-0.67198600	1.01900000
C	-2.97742400	0.42684400	-0.99119900
H	-1.12489200	0.98452800	-1.92230100
C	-2.78709500	-0.74692900	1.09956900
H	-0.79396100	-1.10526500	1.80079700
C	-3.57836800	-0.19786600	0.09463300
H	-3.58546900	0.84852100	-1.78171500
H	-3.24938200	-1.23592600	1.94782100
H	-4.65738300	-0.26240900	0.15623100
C	0.67414900	0.08343600	-0.15375000
C	1.39619200	1.19262600	-0.26671700
C	0.86043000	2.59245100	-0.23356500
H	1.00213600	3.04675400	-1.22067300
H	-0.21199300	2.59004000	-0.03968200
H	2.47379900	1.10551800	-0.35630100
C	1.57961600	3.44458700	0.81412400
H	2.65506300	3.48086200	0.62456000
H	1.20200700	4.46908100	0.80248500
H	1.42960100	3.04008500	1.81755200
Br	1.61123600	-1.62104400	-0.12897700



syn-6d

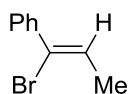
C	0.88701900	-0.18445600	-0.01400700
C	1.25091900	-1.12726000	-0.97830600
C	1.81211800	0.16509900	0.97338900
C	2.50666700	-1.72167000	-0.94531100
H	0.54842700	-1.38600700	-1.75880100
C	3.06400500	-0.43172000	1.00727800
H	1.54375400	0.90485700	1.71595800
C	3.41525700	-1.37771400	0.04828100
H	2.77547300	-2.44907100	-1.70023900
H	3.76780500	-0.15834000	1.78263400
H	4.39404300	-1.83861700	0.07325100
C	-0.45876400	0.41482800	-0.04419800
C	-1.62935200	-0.20794900	0.01869700
C	-1.82782700	-1.68581300	0.21296800
H	-0.85427500	-2.16078700	0.34207100
H	-2.53877800	0.38042400	-0.04592800
C	-2.50854500	-2.30121400	-1.01575200
H	-1.90453200	-2.16457300	-1.91376200
H	-2.66569200	-3.37142600	-0.86791100
H	-3.48283300	-1.83863100	-1.19174700
C	-2.65546100	-1.93360800	1.48048500
H	-2.80658700	-3.00397800	1.63289500
H	-2.15574800	-1.52893400	2.36171000
H	-3.63810800	-1.46202400	1.40106300
Br	-0.45840800	2.35280600	-0.20976800



syn-6e

C	0.98064500	-0.19099500	-0.11413900
C	1.42646400	-0.80783800	-1.28372000
C	1.84855100	-0.08111900	0.97306400
C	2.71139500	-1.33139100	-1.35542000

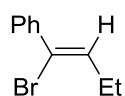
H	0.75881200	-0.88183000	-2.13185500
C	3.13061200	-0.60766100	0.90178100
H	1.50885500	0.40716900	1.87705900
C	3.56447300	-1.23623700	-0.26177900
H	3.04478400	-1.81464900	-2.26456800
H	3.79192300	-0.52952400	1.75489000
H	4.56452200	-1.64620200	-0.31610200
C	-0.39076100	0.34305200	-0.04395000
C	-1.54989500	-0.27497300	0.13418900
C	-1.84367500	-1.74573500	0.37495800
H	-2.44411000	0.33731000	0.08812600
C	-2.30191400	-2.35924800	-0.96165600
H	-1.48969400	-2.35151000	-1.68961500
H	-2.61870100	-3.39362900	-0.81014800
H	-3.14276800	-1.80484900	-1.38276800
C	-3.00724800	-1.80964800	1.38158500
H	-3.30080900	-2.84706600	1.55110600
H	-2.71738500	-1.37624600	2.34071600
H	-3.87856300	-1.26560600	1.01171800
Br	-0.44044200	2.28077400	-0.31581700
C	-0.67199000	-2.55770800	0.93718600
H	0.14852400	-2.64543300	0.22900500
H	-0.28335500	-2.10925600	1.85217600
H	-1.01939500	-3.56518500	1.17423300



anti-6b

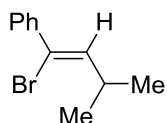
C	-1.15800200	1.62532100	0.40391100
C	-0.58246400	0.48500200	0.03169200
H	-0.47226800	2.39342700	0.75158500
C	0.87045000	0.23810200	0.01267600
C	1.73300000	1.24864600	-0.42761000
C	1.42390700	-0.96952500	0.44871200
C	3.10897700	1.06349300	-0.40936600
H	1.31961500	2.17604600	-0.80139600
C	2.79925900	-1.15173200	0.46687300

H	0.77468500	-1.76742100	0.78268600
C	3.64829500	-0.13621700	0.03972000
H	3.75970300	1.85492100	-0.75981400
H	3.20910300	-2.09121200	0.81596800
H	4.72083500	-0.28343200	0.04755700
C	-2.59919000	1.99148800	0.42495600
H	-2.91973400	2.21717600	1.44683900
H	-2.76547500	2.90079000	-0.16073300
H	-3.23890700	1.20453300	0.03101700
Br	-1.67388000	-1.00442600	-0.55742700



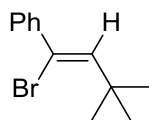
anti-6c

C	-1.06939600	0.24064200	-0.10510200
C	-1.66517700	1.39913500	0.40702300
C	-1.89508300	-0.81396300	-0.50562900
C	-3.04680000	1.50708400	0.49145400
H	-1.03964400	2.21073800	0.75428800
C	-3.27547600	-0.70351500	-0.42035400
H	-1.45442800	-1.72219400	-0.89358900
C	-3.85819600	0.45771700	0.07603700
H	-3.48866600	2.40947800	0.89526500
H	-3.89830100	-1.52833600	-0.74321200
H	-4.93535200	0.53941500	0.14760000
C	0.39726800	0.17894600	-0.23661500
C	1.17344300	1.18343000	-0.63432500
C	2.66130700	1.24105500	-0.73421200
H	3.08266900	0.23619800	-0.74217600
H	2.92965200	1.71142600	-1.68465500
C	3.27581400	2.05031400	0.41421200
H	3.06027600	1.58371900	1.37757900
H	4.36019000	2.11266500	0.30169400
H	2.88052500	3.06841600	0.43727200
H	0.64650800	2.09636100	-0.90013300
Br	1.19246100	-1.52236900	0.24655400



anti-6d

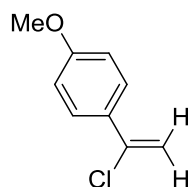
C	1.30654400	0.25939600	0.05702500
C	1.96944400	1.33071200	-0.55150200
C	2.07057200	-0.74167800	0.66391000
C	3.35592700	1.40848800	-0.53333900
H	1.39339800	2.09632700	-1.05420400
C	3.45553200	-0.66109900	0.68230300
H	1.57798700	-1.58338400	1.13170100
C	4.10483700	0.41431800	0.08483300
H	3.85111300	2.24212100	-1.01545200
H	4.02946900	-1.44178700	1.16558400
H	5.18595700	0.47141000	0.09362000
C	-0.16923800	0.23117100	0.06794300
C	-0.93610800	1.28903900	0.31832100
C	-2.43624100	1.47102700	0.33135300
H	-2.59513300	2.52802900	0.55849700
C	-3.08637600	1.21498100	-1.03372500
H	-3.03828500	0.16418900	-1.31733800
H	-4.13909800	1.50588500	-1.00273800
H	-2.59912500	1.79861200	-1.81742900
H	-0.36754500	2.18113300	0.56681500
C	-3.12353300	0.67514500	1.44843000
H	-4.17933800	0.95016300	1.50541800
H	-3.06591100	-0.39883800	1.27322600
H	-2.66745000	0.88371500	2.41835200
Br	-0.92726300	-1.50704500	-0.33483900



anti-6e

C	-1.13355100	-0.08221200	-0.01228600
C	-1.66345400	-1.27565000	-0.51445500
C	-2.01346900	0.88168100	0.48884300

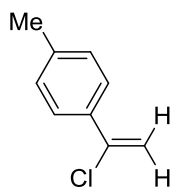
C	-3.03279500	-1.50722300	-0.49447100
H	-0.99716900	-2.01597200	-0.93615700
C	-3.38102700	0.64773100	0.51000800
H	-1.62176500	1.81488400	0.86942800
C	-3.89705300	-0.54778300	0.01975900
H	-3.42427200	-2.43413700	-0.89329900
H	-4.04600900	1.40172100	0.91086100
H	-4.96447900	-0.72530400	0.03037300
C	0.33035100	0.11368900	0.00270800
C	1.19983400	-0.82784400	0.36121700
C	2.71717600	-0.86959900	0.41078800
C	3.32619100	-0.63237500	-0.98209000
H	3.09959600	0.36206000	-1.36044400
H	4.41206500	-0.73729200	-0.92942000
H	2.94853100	-1.36502800	-1.69750300
H	0.71558300	-1.74376800	0.68912100
C	3.26541200	0.15983600	1.41473700
H	4.35110800	0.06252000	1.48345900
H	3.03371100	1.17973700	1.11497200
H	2.84541400	-0.00884100	2.40787400
C	3.12565100	-2.27390600	0.88459100
H	4.21231500	-2.35563500	0.93753800
H	2.72019700	-2.48529300	1.87631100
H	2.76057200	-3.04006800	0.19722200
Br	0.88824000	1.87898300	-0.56552300



syn-8a/anti-8a

C	-2.96495500	1.40241500	-0.50507100
C	-2.24296500	0.35321700	-0.12581400
H	-4.04511800	1.38293800	-0.51702100
H	-2.47158100	2.31054200	-0.82526500
Cl	-3.10188600	-1.12847800	0.31906500
C	-0.77770300	0.29123500	-0.03110200

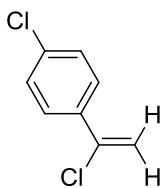
C	-0.04896300	1.45665800	0.25229500
C	-0.06551500	-0.88862400	-0.24178800
C	1.32980600	1.44120500	0.30184900
H	-0.57328900	2.38115700	0.45349400
C	1.32268000	-0.91734200	-0.19937100
H	-0.59662300	-1.80583200	-0.45490500
C	2.02882900	0.25277600	0.07224900
H	1.88686000	2.34064200	0.53030200
H	1.83542400	-1.85090000	-0.37585500
C	4.14677400	-0.84184300	-0.12114800
H	5.18921400	-0.54759700	-0.02239900
H	3.92335800	-1.63253900	0.59918800
H	3.96685600	-1.20603400	-1.13559000
O	3.38391700	0.33256200	0.14606500



syn-8b/anti-8b

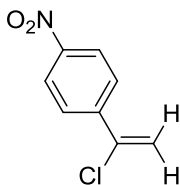
C	2.42464100	1.57734100	0.45077000
C	1.81106900	0.44684200	0.11607000
H	3.50050800	1.66531600	0.44891900
H	1.84488000	2.44041500	0.74670100
Cl	2.80822000	-0.95136800	-0.29343900
C	0.35595000	0.23282900	0.05244800
C	-0.49225200	1.30410000	-0.25274000
C	-0.22352700	-1.00986300	0.31691800
C	-1.86705400	1.13695000	-0.27176200
H	-0.07021400	2.27019000	-0.49389900
C	-1.60190200	-1.16808300	0.29871800
H	0.40765900	-1.85583900	0.54927200
C	-2.45016800	-0.10174700	0.00368000
H	-2.49996200	1.98169400	-0.51579700
H	-2.02553700	-2.14046600	0.51855600
C	-3.94090500	-0.28402000	-0.05336400
H	-4.46246200	0.59768700	0.32125300

H	-4.25723000	-1.14727800	0.53209900
H	-4.27250000	-0.44455000	-1.08306700



syn-8c/anti-8c

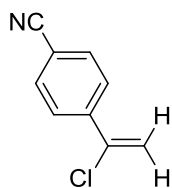
C	2.83017000	1.54363200	0.46876600
C	2.20178100	0.42781800	0.11804300
H	3.90801100	1.61939000	0.47265000
H	2.26147600	2.41146500	0.77521000
Cl	3.17086400	-0.98213000	-0.31587300
C	0.74195400	0.24333500	0.05479300
C	-0.07829300	1.33224200	-0.26113700
C	0.13996100	-0.98773300	0.32501200
C	-1.45772700	1.20411000	-0.28596200
H	0.36438200	2.28696200	-0.51006000
C	-1.23955400	-1.12820300	0.30603500
H	0.74906300	-1.84779800	0.56437400
C	-2.02761500	-0.02817300	0.00223400
H	-2.08101100	2.05045900	-0.53907600
H	-1.69400900	-2.08434300	0.52519400
Cl	-3.76716100	-0.19856200	-0.03309400



syn-8d/anti-8d

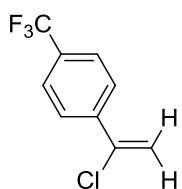
C	-3.09993800	1.52027200	-0.51751500
C	-2.46874800	0.41709800	-0.13231500
H	-4.17837100	1.58490400	-0.53662400
H	-2.53697800	2.38508200	-0.84191800
Cl	-3.42440600	-0.98573200	0.33605800
C	-1.00678200	0.24854900	-0.06960400
C	-0.19604300	1.36307300	0.18600600

C	-0.40121200	-0.99519600	-0.27680200
C	1.18016700	1.24608200	0.21446900
H	-0.64733700	2.32439900	0.38570100
C	0.97569200	-1.12525500	-0.25543800
H	-1.00828300	-1.86793400	-0.46669800
C	1.75015200	-0.00042000	-0.01003500
H	1.80517400	2.10217100	0.41821300
H	1.44280700	-2.08337900	-0.42486900
N	3.20449400	-0.13230900	0.02693500
O	3.87029500	0.85995300	0.29603000
O	3.69482900	-1.22862000	-0.21292900



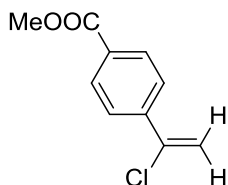
syn-8e/anti-8e

C	2.07037000	0.42297800	0.11248200
C	2.69322900	1.54182600	0.46343300
H	3.77101000	1.61804000	0.47740300
H	2.12204200	2.41018400	0.76318600
Cl	3.03804300	-0.98609000	-0.31457700
C	0.60950100	0.23975400	0.05324300
C	0.01300300	-0.99609300	0.32041200
C	-0.20904400	1.33275400	-0.25917200
C	-1.36276500	-1.13669900	0.30280900
H	0.62700100	-1.85344400	0.55493500
C	-1.58443700	1.20275100	-0.28347400
H	0.23599400	2.28653000	-0.50550000
C	-2.16842600	-0.03547100	0.00150600
H	-1.81741800	-2.09346900	0.51983800
H	-2.20985600	2.04870800	-0.53354900
C	-3.58570000	-0.17566400	-0.02496000
N	-4.73289500	-0.28903100	-0.04529900



syn-8f/anti-8f

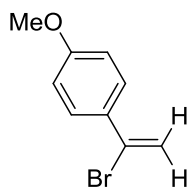
C	2.95372500	0.30412300	0.13869100
C	3.67702100	1.33118000	0.56782400
H	4.75703500	1.30475600	0.58616600
H	3.18706800	2.22567600	0.92866300
Cl	3.78906200	-1.15664100	-0.38758700
C	1.48236300	0.26241600	0.06363600
C	0.76909600	-0.92241300	0.24934300
C	0.77173900	1.44494400	-0.17927300
C	-0.61774900	-0.92790400	0.21869500
H	1.29594300	-1.84819500	0.43001600
C	-0.61039000	1.44305800	-0.21357500
H	1.30620100	2.36671900	-0.36192200
C	-1.30854600	0.25450600	-0.01014800
H	-1.15264700	-1.85394800	0.37390700
H	-1.14420600	2.36371600	-0.41006200
C	-2.80618000	0.27736500	-0.06972400
F	-3.26108800	0.59813700	-1.30657400
F	-3.33406900	1.19832800	0.77205400
F	-3.36313100	-0.90590400	0.25090300



syn-8g/anti-8g

C	2.95451800	0.30363500	0.13986500
C	3.67728100	1.33287700	0.56604200
H	4.75734900	1.30670100	0.58550300
H	3.18677600	2.22893700	0.92232300
Cl	3.79164000	-1.15879400	-0.38107700
C	1.48406800	0.26056800	0.06296200
C	0.77039000	-0.92526100	0.25679100

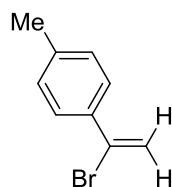
C	0.77270900	1.44053100	-0.18904700
C	-0.61397300	-0.93048700	0.22544000
H	1.29992500	-1.84833400	0.44456000
C	-0.60900200	1.43559800	-0.22367900
H	1.30826300	2.36052400	-0.37810100
C	-1.31634600	0.25104800	-0.01314200
H	-1.14869200	-1.85525800	0.38685200
H	-1.15195800	2.34827300	-0.42715200
C	-2.79767300	0.29506800	-0.06272500
O	-3.44290800	1.30276600	-0.27367300
O	-3.36261100	-0.89919800	0.15142500
C	-4.80039700	-0.94613700	0.10152800
H	-5.15443500	-0.65053900	-0.88561000
H	-5.06300100	-1.98061700	0.30524300
H	-5.22879700	-0.28909000	0.85753500



syn-9a/anti-9a

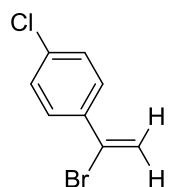
C	-2.18806000	1.90019100	-0.60595400
C	-1.60308900	0.77287100	-0.21975700
H	-3.26090500	2.02209300	-0.63584700
H	-1.57920700	2.74046700	-0.91737700
C	-0.15904600	0.54010600	-0.09281300
C	0.67374900	1.59061100	0.32308600
C	0.43669200	-0.68244500	-0.40071600
C	2.04164400	1.42630400	0.40506200
H	0.23729800	2.54030500	0.60215100
C	1.81191800	-0.86046700	-0.32668500
H	-0.17762100	-1.51484900	-0.71528900
C	2.62300700	0.19874700	0.07725500
H	2.67951400	2.23545300	0.73677200
H	2.23456500	-1.82094000	-0.58125200
C	4.62356500	-1.10123600	-0.11751500
H	5.68362000	-0.92755500	0.05301100

H	4.27763600	-1.90605600	0.53560100
H	4.46348300	-1.37740400	-1.16257000
O	3.97486500	0.12933500	0.19457500
Br	-2.74630600	-0.72123700	0.24888600



syn-9b/anti-9b

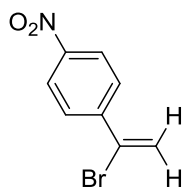
C	1.63949200	1.98765300	0.58425000
C	1.16907200	0.79423600	0.24261400
H	2.69566400	2.20812000	0.61523700
H	0.95000600	2.77688100	0.85524300
C	-0.24785400	0.41834000	0.12799700
C	-1.17584500	1.36344000	-0.32332000
C	-0.71837000	-0.84697000	0.48868800
C	-2.52608200	1.05563200	-0.39021500
H	-0.83381100	2.34013700	-0.63790000
C	-2.07040700	-1.14534400	0.42224300
H	-0.02157700	-1.59811800	0.83374900
C	-3.00031400	-0.20303800	-0.01955800
H	-3.22292300	1.80435800	-0.74710800
H	-2.41036000	-2.13009100	0.71931200
C	-4.45930300	-0.54683500	-0.12846900
H	-5.08385400	0.34248500	-0.04225400
H	-4.75759300	-1.25555700	0.64475100
H	-4.67712200	-1.00860000	-1.09564800
Br	2.44917200	-0.59937300	-0.16155000



syn-9c/anti-9c

C	2.05499900	1.96049800	0.58852400
C	1.55295000	0.79405200	0.20636100

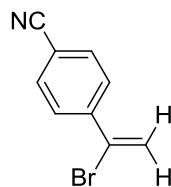
H	3.11625900	2.16256700	0.60515600
H	1.38840100	2.75084400	0.91214500
C	0.12281600	0.46086000	0.11400300
C	-0.77431900	1.42720900	-0.35259600
C	-0.37854600	-0.78282500	0.50584200
C	-2.13546300	1.16925300	-0.41028700
H	-0.40275600	2.38505200	-0.69072100
C	-1.73742400	-1.05163000	0.45733600
H	0.29463300	-1.54916200	0.86433200
C	-2.60525100	-0.07027300	-0.00115400
H	-2.81942900	1.92001300	-0.78084300
H	-2.11613800	-2.01392100	0.77240700
Cl	-4.31916600	-0.40681700	-0.07578800
Br	2.77769800	-0.61344500	-0.30106600



syn-9d/anti-9d

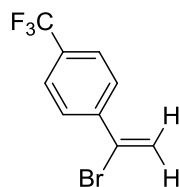
C	-2.32996000	1.92834500	-0.66637600
C	-1.81590300	0.77891800	-0.24918500
H	-3.39444800	2.10957300	-0.70617300
H	-1.67476100	2.72305200	-1.00189000
C	-0.37930500	0.47426300	-0.14879500
C	0.50488200	1.48508800	0.25141300
C	0.13224500	-0.78908800	-0.46320900
C	1.86585800	1.24968800	0.31808200
H	0.11990000	2.45536600	0.53168300
C	1.49141400	-1.03680600	-0.40537600
H	-0.53465200	-1.58325500	-0.76593100
C	2.34111100	-0.01124900	-0.01450000
H	2.54794300	2.02432000	0.63415200
H	1.88932900	-2.00784300	-0.65753400
N	3.77717500	-0.27138800	0.06010600
O	4.17877200	-1.39035900	-0.23263300
O	4.51554700	0.64058200	0.41060600

Br	-3.01742300	-0.63232800	0.28424400
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syn-9e/anti-9e

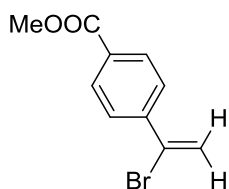
C	1.42181300	0.78672400	0.20250900
C	1.91628700	1.95799900	0.57973300
H	2.97711200	2.16138000	0.60767600
H	1.24578000	2.75028500	0.88994600
C	-0.00924500	0.45278900	0.11326100
C	-0.50333900	-0.79641100	0.50078900
C	-0.90632200	1.42342300	-0.34877900
C	-1.85818400	-1.06659400	0.45195300
H	0.17488600	-1.55993800	0.85433500
C	-2.26292900	1.16256600	-0.40643000
H	-0.53338000	2.38191500	-0.68211500
C	-2.74504200	-0.08606300	-0.00309500
H	-2.23542500	-2.03083600	0.76358200
H	-2.94950400	1.91355000	-0.77253900
Br	2.64615500	-0.62193300	-0.28916400
C	-4.14154200	-0.36319400	-0.06435800
N	-5.27165600	-0.58595000	-0.11169600



syn-9f/anti-9f

C	2.24363700	0.79140600	0.24558700
C	2.74419900	1.93971900	0.67996200
H	3.80416700	2.14933300	0.68622000
H	2.07956600	2.70536800	1.06170800
C	0.81258000	0.45014800	0.17819400
C	0.33786100	-0.82002900	0.51913100
C	-0.10462300	1.43022600	-0.21093100

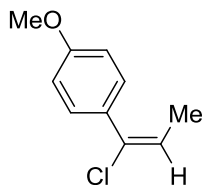
C	-1.01752600	-1.09575800	0.49454000
H	1.03089300	-1.59452600	0.81599500
C	-1.46363400	1.15608600	-0.24283000
H	0.24937900	2.40798400	-0.50735600
C	-1.92079200	-0.10604700	0.11411900
H	-1.37084100	-2.08033500	0.77115200
H	-2.15880900	1.92278700	-0.55410100
Br	3.46103000	-0.57449600	-0.37230600
C	-3.38123300	-0.43962600	0.05667500
F	-4.16145100	0.64800100	-0.09612000
F	-3.80479200	-1.07095100	1.17611300
F	-3.67182500	-1.27102800	-0.97570200



syn-9g/anti-9g

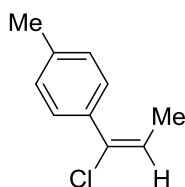
C	2.24432400	0.79124400	0.25175400
C	2.74387000	1.94804100	0.66651100
H	3.80432600	2.15466500	0.67716200
H	2.07938700	2.72257100	1.02987000
C	0.81454200	0.44915100	0.18050900
C	0.34023000	-0.83066500	0.48361700
C	-0.10685700	1.44060800	-0.17807100
C	-1.01518000	-1.10455900	0.45277400
H	1.03477200	-1.61340900	0.75383500
C	-1.46298200	1.16660200	-0.21263500
H	0.24580000	2.42595600	-0.45031600
C	-1.92946100	-0.10997800	0.10480400
H	-1.37555100	-2.09409400	0.69749100
H	-2.15895700	1.94219800	-0.49786800
Br	3.47137500	-0.58432200	-0.32546700
C	-3.37189900	-0.45335400	0.07411900
O	-3.81870600	-1.55106200	0.34107900
O	-4.14445800	0.58037000	-0.28189700
C	-5.56084500	0.33359000	-0.34551800

H	-6.00665800	1.28122400	-0.63504900
H	-5.77973200	-0.43179700	-1.08922500
H	-5.93588600	0.01813200	0.62747700



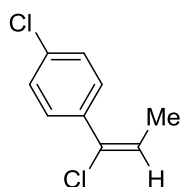
syn-11a

C	-2.91298600	0.86186600	0.29773000
C	-2.04127000	-0.09949000	0.00125700
H	-3.96900400	0.62104200	0.25373800
Cl	-2.68842000	-1.71297000	-0.38030300
C	-2.57257300	2.25386000	0.72121800
H	-2.83173300	2.97593000	-0.05972900
H	-3.15798900	2.52545300	1.60399000
H	-1.51691200	2.37589900	0.95726800
C	-0.57468500	-0.00497600	-0.06211500
C	0.24634900	-0.93238700	0.57860700
C	0.03603200	1.03584000	-0.77262400
C	1.63000600	-0.82386800	0.54166700
H	-0.19903700	-1.75510700	1.12249700
C	1.41250900	1.15459800	-0.82132000
H	-0.57663600	1.75064500	-1.30527300
C	2.21999600	0.22750600	-0.16001300
H	2.23169500	-1.55799900	1.05641300
H	1.88144900	1.95638000	-1.37699900
O	3.56291400	0.42255500	-0.26255500
C	4.43385500	-0.50267300	0.38304600
H	5.44307400	-0.15369700	0.17629000
H	4.26853100	-0.51366100	1.46311500
H	4.30958000	-1.51047000	-0.02081900



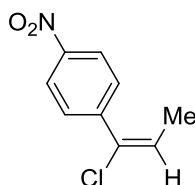
syn-11b

C	-2.46624500	1.00282700	-0.21303600
C	-1.66102100	-0.02892800	0.02808900
H	-3.53546300	0.83952500	-0.13899200
Cl	-2.40985200	-1.59850100	0.39813900
C	-2.03762700	2.37708000	-0.61258500
H	-0.98075400	2.43123000	-0.86714000
H	-2.62010300	2.70859000	-1.47670100
H	-2.23257600	3.09521500	0.19019100
C	-0.18854900	-0.04682900	0.03127600
C	0.52963900	-1.01012700	-0.68499600
C	0.52589300	0.91171500	0.75057300
C	1.91371900	-0.99471100	-0.69707100
H	-0.00264800	-1.77203000	-1.23950900
C	1.91565300	0.91853800	0.73720800
H	-0.00785100	1.64857500	1.33610700
C	2.63444500	-0.02894300	0.01210900
H	2.44805200	-1.74652600	-1.26654600
H	2.44770900	1.67051000	1.30783300
C	4.13614400	-0.02742100	-0.00839400
H	4.53663600	-0.97290600	0.36635500
H	4.54160300	0.77750600	0.60490100
H	4.51552300	0.09919800	-1.02586600

**syn-11c**

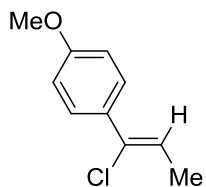
C	-2.82886700	1.00259800	-0.21282400
C	-2.02707700	-0.03197500	0.02637100
H	-3.89841100	0.84008300	-0.14191700
Cl	-2.77059700	-1.60143400	0.39248600
C	-2.39858600	2.37731800	-0.60717300
H	-1.34016100	2.43520400	-0.85422200
H	-2.97531100	2.70834500	-1.47519900
H	-2.60249100	3.09325300	0.19522300

C	-0.55377000	-0.04825400	0.02753600
C	0.16030200	-1.00710400	-0.69588300
C	0.15737200	0.90831700	0.75532100
C	1.54589600	-0.99971900	-0.71533100
H	-0.37085600	-1.76533000	-1.25549500
C	1.54540100	0.92481800	0.74830000
H	-0.37651000	1.64006400	1.34615800
C	2.22649200	-0.02883100	0.00746000
H	2.08987400	-1.73970300	-1.28567300
H	2.08736500	1.66609100	1.31892700
Cl	3.97563100	-0.01569400	-0.00971900

**syn-11d**

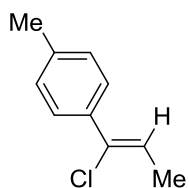
C	-3.08120300	0.98391800	-0.28715600
C	-2.28184400	-0.03558200	0.02016000
H	-4.15073500	0.81877500	-0.22161800
Cl	-3.01976600	-1.58019700	0.46999800
C	-2.65657500	2.33474800	-0.75871300
H	-1.59950100	2.38721000	-1.01155500
H	-3.23703600	2.61164500	-1.64280200
H	-2.86635500	3.09371000	0.00155900
C	-0.80901000	-0.04804000	0.02548100
C	-0.09538100	-1.07564000	-0.60201500
C	-0.10417800	0.97809800	0.66403100
C	1.28646500	-1.06902800	-0.61812400
H	-0.62741600	-1.88090000	-1.08868500
C	1.27965500	0.99609300	0.65888200
H	-0.64298400	1.75679800	1.18433700
C	1.95660600	-0.02775600	0.01198000
H	1.84028900	-1.85263800	-1.11254900
H	1.82639200	1.78230000	1.15682100
N	3.41724200	-0.01403700	-0.00158100
O	3.99429200	0.93603200	0.51305700

O 4.00162300 -0.95210400 -0.52935800



anti-11a

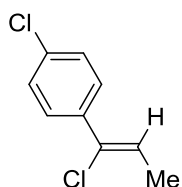
C	-2.68747800	1.05746000	0.36508900
C	-1.87841600	0.05263100	0.03111000
H	-2.19071500	1.97634600	0.66001700
C	-4.17516400	1.07975700	0.39876500
H	-4.55626700	1.90339000	-0.21272500
H	-4.61724600	0.15198600	0.04121200
H	-4.53247200	1.25922000	1.41780300
C	-0.40872200	0.12156400	-0.02154300
C	0.22411800	1.31383900	-0.40380700
C	0.39967000	-0.96153500	0.32211700
C	1.60082600	1.42127300	-0.41547900
H	-0.37277800	2.16122300	-0.71362600
C	1.78612500	-0.86802400	0.31401900
H	-0.05465000	-1.89892800	0.61220100
C	2.39426000	0.33059000	-0.05263800
H	2.08344300	2.34092700	-0.72055200
H	2.37415600	-1.72958300	0.59333100
O	3.74032700	0.52795900	-0.09837500
C	4.59555800	-0.56179000	0.23589600
H	5.61049200	-0.18352600	0.13522700
H	4.43250200	-0.89270600	1.26455000
H	4.45071800	-1.40080000	-0.44931200
Cl	-2.56863700	-1.52254200	-0.39680700



anti-11b

C	-2.22113800	1.14353400	0.32365900
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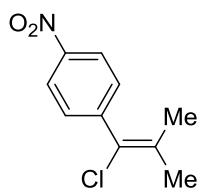
C	-1.47437100	0.08123500	0.02565800
H	-1.66987900	2.03431500	0.60774300
C	-3.70403800	1.26347600	0.32884200
H	-4.01811700	2.09215300	-0.31334600
H	-4.20025000	0.35675700	-0.01100900
H	-4.06545600	1.49754400	1.33516800
C	-0.00123600	0.05568500	0.00602300
C	0.71181700	1.18919600	-0.39872200
C	0.72677200	-1.06699000	0.40929000
C	2.09830400	1.20310000	-0.37648300
H	0.17591800	2.06207000	-0.74761900
C	2.11324900	-1.04540500	0.42861800
H	0.20539300	-1.96117600	0.72255400
C	2.82717900	0.08781800	0.03749500
H	2.62388100	2.09443700	-0.69873900
H	2.65119300	-1.92727000	0.75656600
C	4.32859800	0.09216800	0.02374900
H	4.72537500	1.09939900	0.15913900
H	4.71045600	-0.28293200	-0.93099100
H	4.73623200	-0.54637100	0.80913500
Cl	-2.25420700	-1.45387500	-0.38812900



anti-11c

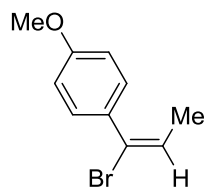
C	-2.59208400	1.15156100	0.32423500
C	-1.85573900	0.08220400	0.02562200
H	-2.03381900	2.04007000	0.60157300
C	-4.07351000	1.28062000	0.33935600
H	-4.38562800	2.10774200	-0.30567000
H	-4.57836500	0.37522900	0.00909800
H	-4.42459500	1.52441000	1.34694200
C	-0.38243800	0.04969300	0.00228000
C	0.33242900	1.18185700	-0.40425000
C	0.33705400	-1.08185500	0.39605000

C	1.71869000	1.19654700	-0.39520200
H	-0.19875900	2.05801400	-0.75024500
C	1.72380500	-1.08073100	0.40944400
H	-0.18762200	-1.97479500	0.70546900
C	2.40374100	0.06220500	0.01553800
H	2.25862400	2.07587300	-0.71806900
H	2.26802200	-1.96056300	0.72346800
Cl	4.15294800	0.06855100	0.02128100
Cl	-2.64313300	-1.44822600	-0.37903400



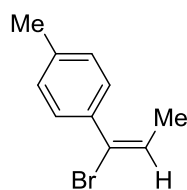
anti-11d

C	-2.84963900	1.14842300	0.35047900
C	-2.12024900	0.08085100	0.02271400
H	-2.28950700	2.03183000	0.63860400
C	-4.32895300	1.27406200	0.39622100
H	-4.64794000	2.14655100	-0.18141000
H	-4.84045500	0.39421100	0.01227200
H	-4.66179700	1.44633400	1.42490200
C	-0.64890300	0.04833200	-0.00006400
C	0.06779600	1.20790100	-0.33112500
C	0.06446900	-1.11458500	0.31525900
C	1.44899800	1.21712600	-0.32272800
H	-0.46158600	2.10429900	-0.62058400
C	1.44692900	-1.11846500	0.33080700
H	-0.46569700	-2.02260800	0.56202700
C	2.12465900	0.05074600	0.01353400
H	1.99841400	2.10860200	-0.58470600
H	1.99479300	-2.01299500	0.58550600
N	3.58247100	0.05240500	0.02407600
O	4.16346900	-0.96883600	0.37227200
O	4.16591900	1.07613100	-0.31319000
Cl	-2.91381300	-1.43620100	-0.40052000



syn-12a

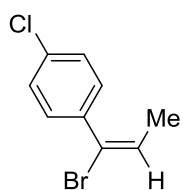
C	-2.08470100	1.70858900	-0.21490100
C	-1.50659300	0.52249400	-0.05373800
H	-3.16042800	1.78212700	-0.10569000
C	-1.37333400	2.97602800	-0.56736800
H	-0.33410600	2.80910300	-0.84504300
H	-1.88193800	3.46727400	-1.40159100
H	-1.39374300	3.68068600	0.27004800
C	-0.07300200	0.20290300	-0.09474700
C	0.81825500	0.88618200	0.73059400
C	0.44115200	-0.77408500	-0.95711400
C	2.18431800	0.62653500	0.69823000
H	0.44065600	1.63041300	1.41961300
C	1.79474400	-1.03964700	-1.00348100
H	-0.22959900	-1.32683500	-1.60189800
C	2.67766200	-0.34036900	-0.17465400
H	2.84218200	1.17396100	1.35662400
H	2.19252900	-1.78785000	-1.67697200
O	3.99133600	-0.67568700	-0.28750700
C	4.93894900	0.00940800	0.52714600
H	5.90973100	-0.40511700	0.26483900
H	4.93541800	1.08240600	0.32051700
H	4.74586000	-0.16373300	1.58878700
Br	-2.66026000	-1.00423400	0.31380300



syn-12b

C	-1.74061500	1.69061300	-0.25100500
C	-1.15239700	0.51476400	-0.05732800
H	-2.82212800	1.74416900	-0.20431800

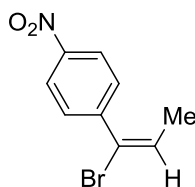
C	-1.03495800	2.97191400	-0.56141200
H	0.02380100	2.82849400	-0.76934400
H	-1.49881400	3.44960500	-1.42896300
H	-1.12720300	3.67675400	0.27083900
C	0.28876900	0.22048700	-0.02548800
C	0.86088800	-0.73762800	-0.86848300
C	1.12244100	0.91382300	0.85229000
C	2.22452600	-0.97465800	-0.84406200
H	0.23138100	-1.29506600	-1.55026800
C	2.49011500	0.66731300	0.87489500
H	0.69584700	1.64493600	1.52676300
C	3.06586100	-0.27683900	0.02827000
H	2.64783300	-1.71530700	-1.51293000
H	3.11715300	1.21592100	1.56766600
C	4.54181900	-0.55208800	0.05154100
H	4.74555900	-1.58203300	0.35675900
H	5.05828800	0.11209100	0.74478800
H	4.98375100	-0.41956200	-0.93924600
Br	-2.29222200	-1.03150300	0.25254300



syn-12c

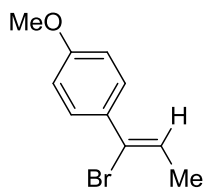
C	-2.13631000	1.65413600	-0.24983900
C	-1.50948900	0.49704700	-0.06459400
H	-3.21916300	1.66925100	-0.20603900
C	-1.47766600	2.96270900	-0.54670100
H	-0.41425000	2.86345500	-0.75637300
H	-1.95948500	3.43121700	-1.40930200
H	-1.59847800	3.65439100	0.29283900
C	-0.05729700	0.25669000	-0.03597600
C	0.54396000	-0.68167400	-0.87848900
C	0.74963000	0.98414100	0.84152800
C	1.91587700	-0.87631100	-0.86423400
H	-0.06439100	-1.26421400	-1.55755300

C	2.12489100	0.79625300	0.86995600
H	0.29790100	1.69863200	1.51644600
C	2.69472200	-0.13198900	0.01228200
H	2.37439900	-1.59746900	-1.52631800
H	2.74123500	1.36113800	1.55548800
Cl	4.42644600	-0.37757100	0.03858300
Br	-2.58745300	-1.09115400	0.23056800



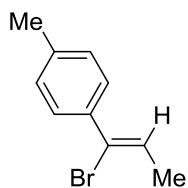
syn-12d

C	-2.39985000	1.62105000	-0.35084500
C	-1.75675900	0.48434200	-0.10151600
H	-3.48314200	1.61627900	-0.31368300
C	-1.76914100	2.92519700	-0.71542600
H	-0.70407100	2.84282100	-0.92321100
H	-2.26405100	3.33664000	-1.59918100
H	-1.90712600	3.65446900	0.08895200
C	-0.30053000	0.27077200	-0.06298800
C	0.30740900	-0.73116700	-0.82771900
C	0.49555100	1.08505500	0.74951800
C	1.67805200	-0.90618300	-0.80165000
H	-0.29732400	-1.37307600	-1.45322200
C	1.86921300	0.91972600	0.78810500
H	0.03266600	1.84352300	1.36484000
C	2.44195500	-0.07426600	0.00806700
H	2.15220900	-1.67138600	-1.39726400
H	2.48606800	1.54339700	1.41701900
N	3.89167800	-0.25397800	0.04152600
O	4.55435700	0.49878100	0.74463300
O	4.38148500	-1.14798100	-0.63704700
Br	-2.79913600	-1.10246300	0.28136500



anti-12a

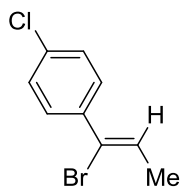
C	-2.08483400	1.59446400	0.42128200
C	-1.40237300	0.48832700	0.13482500
H	-1.47181100	2.45860900	0.66364200
Br	-2.35693700	-1.15962900	-0.24458700
C	-3.55551200	1.81574800	0.46240600
H	-3.82896200	2.65053200	-0.19021000
H	-4.12062900	0.93795800	0.15544400
H	-3.87280800	2.09397100	1.47239000
C	0.06307200	0.39108600	0.05064300
C	0.79646500	1.44968700	-0.50585700
C	0.77275700	-0.71160900	0.52533600
C	2.17624300	1.41286500	-0.56265300
H	0.27371000	2.30389100	-0.91530100
C	2.15990900	-0.76335800	0.47304400
H	0.23888000	-1.54974100	0.95221900
C	2.87022200	0.30476900	-0.07240300
H	2.73515900	2.22859900	-1.00308900
H	2.67024700	-1.63442600	0.85629300
O	4.22625600	0.35181300	-0.18014900
C	4.98157200	-0.77444200	0.25825700
H	6.02328200	-0.52668500	0.06654900
H	4.84228400	-0.95330800	1.32734900
H	4.71381100	-1.67214900	-0.30470800



anti-12b

C	-1.60924800	1.66529500	0.36114000
C	-1.00933500	0.50249000	0.11915900
H	-0.93687000	2.48994900	0.58218100

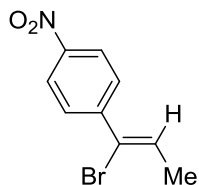
Br	-2.07615600	-1.08010900	-0.22803000
C	-3.05988800	1.99358100	0.38323200
H	-3.27049900	2.81664100	-0.30656900
H	-3.68693300	1.14662000	0.11231800
H	-3.35807900	2.33840100	1.37835800
C	0.44746700	0.29279300	0.07105400
C	1.26716800	1.26431200	-0.51233000
C	1.05937700	-0.83895600	0.61789100
C	2.64682900	1.11578000	-0.52806700
H	0.81824900	2.13633100	-0.96972800
C	2.43783000	-0.98020900	0.59875600
H	0.45255700	-1.61117600	1.07119200
C	3.25960800	-0.00822900	0.02456900
H	3.25656500	1.88294200	-0.99095100
H	2.88550400	-1.86365700	1.03902800
C	4.74942800	-0.19019600	-0.02921800
H	5.26431500	0.76589300	-0.13199600
H	5.03513000	-0.81084000	-0.88420200
H	5.12156400	-0.68676500	0.86870700



anti-12c

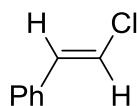
C	-1.97225000	1.65767400	0.36076300
C	-1.36690200	0.49870200	0.11390800
H	-1.30463100	2.48697800	0.57860400
Br	-2.41735100	-1.09103100	-0.23179500
C	-3.42441300	1.97504900	0.39368500
H	-3.64464200	2.79773200	-0.29341700
H	-4.04794700	1.12432500	0.12674500
H	-3.71634200	2.31731300	1.39147200
C	0.09253000	0.30443200	0.06447500
C	0.89939200	1.29106300	-0.51289700
C	0.71186900	-0.82858700	0.59929200
C	2.28050400	1.16562800	-0.53663500

H	0.44219900	2.16067700	-0.96520100
C	2.09109700	-0.96668200	0.58234800
H	0.11395600	-1.61236600	1.04321200
C	2.86525400	0.03541900	0.01485400
H	2.89143600	1.93241100	-0.99248300
H	2.55784000	-1.84459400	1.00684000
Cl	4.60556500	-0.13751400	-0.01880200



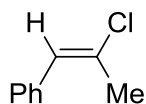
anti-12d

C	-2.22382100	1.64044700	0.42542300
C	-1.61662400	0.49110200	0.13466700
H	-1.55954900	2.46537700	0.66747700
Br	-2.65542600	-1.08684500	-0.26902800
C	-3.67538200	1.94884600	0.48090600
H	-3.90541000	2.77722000	-0.19630200
H	-4.29976900	1.09877800	0.21500200
H	-3.95245000	2.28375000	1.48513400
C	-0.15664500	0.31086100	0.08713300
C	0.64708300	1.34534400	-0.41372400
C	0.46140000	-0.86032000	0.54219300
C	2.02371800	1.22634700	-0.44199100
H	0.18626000	2.24054100	-0.80644000
C	1.83688800	-0.99408700	0.51742400
H	-0.13770000	-1.67227700	0.92800000
C	2.60300200	0.05374400	0.02410600
H	2.64073600	2.01846700	-0.83844500
H	2.31276800	-1.89275600	0.87946700
N	4.05394200	-0.08554100	-0.01835800
O	4.54471900	-1.16220800	0.29997800
O	4.72042700	0.88092900	-0.36989000



syn-13a

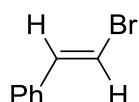
H	0.85968700	-1.56046600	-0.72588300
C	-0.20662600	-1.53022800	-0.53095700
C	-0.72105600	-2.43711100	0.29417300
C	-0.94918500	-0.47158100	-1.21843200
C	-0.24293900	0.40052500	-2.05534800
C	-2.33196900	-0.28445900	-1.08300600
C	-0.89085700	1.42422800	-2.73452900
H	0.82598900	0.27042400	-2.17158000
C	-2.97783700	0.73682000	-1.76068400
H	-2.91024000	-0.93905100	-0.44493800
C	-2.26168900	1.59713200	-2.59027600
H	-0.32354200	2.08604200	-3.37607800
H	-4.04618000	0.86442200	-1.64259000
H	-2.77031500	2.39343300	-3.11763400
H	-1.76240700	-2.51124700	0.56678400
Cl	0.25283500	-3.65610200	1.06137100



syn-13b

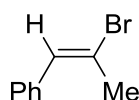
H	0.78545100	-1.57894300	-0.76746600
C	-0.22291500	-1.36507000	-0.43299200
C	-0.66844200	-2.02061700	0.63969300
C	-0.93924900	-0.33914600	-1.20225800
C	-0.20855500	0.73149600	-1.73452600
C	-2.31218300	-0.39998400	-1.46942500
C	-0.83318100	1.72686500	-2.47192900
H	0.85866100	0.78222500	-1.55690200
C	-2.93630500	0.59431700	-2.21150700
H	-2.89026100	-1.24468500	-1.12260900
C	-2.20279200	1.66546700	-2.70930900
H	-0.25020500	2.54962900	-2.86541900
H	-3.99800300	0.52515500	-2.41091700

H	-2.69103700	2.43827600	-3.28845700
Cl	0.38987200	-3.24378800	1.34980300
C	-1.94891500	-1.85823600	1.38476300
H	-2.45810600	-0.94641100	1.08054600
H	-2.61678000	-2.70590000	1.21240800
H	-1.75282400	-1.81107500	2.45676600



syn-14a

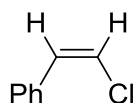
H	0.85796300	-1.55744400	-0.72792600
C	-0.20793900	-1.53080500	-0.53022900
C	-0.72475700	-2.43587100	0.29394800
C	-0.95028800	-0.47100900	-1.21865900
C	-0.24270800	0.40025300	-2.05517900
C	-2.33286400	-0.28369200	-1.08343000
C	-0.88983400	1.42416300	-2.73468700
H	0.82616800	0.26943000	-2.17082700
C	-2.97793400	0.73778800	-1.76143200
H	-2.91103800	-0.93836800	-0.44531500
C	-2.26068400	1.59750500	-2.59077800
H	-0.32208100	2.08568500	-3.37609500
H	-4.04622000	0.86612000	-1.64392900
H	-2.76870100	2.39399900	-3.11841400
Br	0.33413500	-3.77058200	1.13550700
H	-1.76466400	-2.51325400	0.56883900



syn-14b

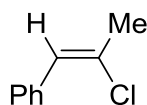
H	0.78210600	-1.58228200	-0.77429600
C	-0.22385600	-1.36873900	-0.43327800
C	-0.67269000	-2.01797900	0.64041100
C	-0.94062700	-0.34072000	-1.20252600
C	-0.20884600	0.73061600	-1.73127600
C	-2.31277500	-0.40265000	-1.47179000

C	-0.83264900	1.72671800	-2.46842100
H	0.85804600	0.78127700	-1.55173400
C	-2.93582900	0.59215800	-2.21413100
H	-2.89062500	-1.24833500	-1.12700500
C	-2.20171400	1.66441000	-2.70862000
H	-0.24957000	2.55046500	-2.85963700
H	-3.99698400	0.52269400	-2.41615100
H	-2.68932000	2.43769500	-3.28766700
C	-1.95114200	-1.85319100	1.38737200
H	-2.46081700	-0.94352100	1.07460700
H	-2.61925800	-2.70184700	1.22184100
H	-1.75824600	-1.79553700	2.45921300
Br	0.48391400	-3.36052300	1.41434900



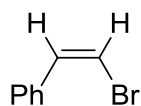
anti-13a

H	0.76752000	-1.52887000	-0.73203200
C	-0.29801000	-1.51803100	-0.52187300
C	-0.66416800	-2.48444100	0.32004500
C	-1.02500100	-0.45689600	-1.21451800
C	-0.27421800	0.39251800	-2.04257300
C	-2.40541800	-0.22480400	-1.11525700
C	-0.86971300	1.42991500	-2.74338100
H	0.79269400	0.22930900	-2.13212200
C	-2.99899600	0.81434300	-1.81784700
H	-3.01690300	-0.85430700	-0.49027700
C	-2.23890800	1.64597300	-2.63370300
H	-0.26590600	2.06907700	-3.37444900
H	-4.06552500	0.97543700	-1.72669900
H	-2.70955800	2.45411400	-3.17825100
Cl	-2.26619600	-2.81604400	0.91204200
H	0.05627400	-3.17916800	0.72332800



anti-13b

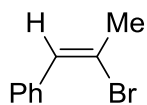
H	0.72416500	-1.40114800	-0.44336200
C	-0.35759600	-1.48488300	-0.39944000
C	-0.77453100	-2.54707100	0.29381000
C	-1.05808700	-0.43962900	-1.14742500
C	-0.31736500	0.25802900	-2.11428600
C	-2.39437200	-0.06405000	-0.95007400
C	-0.88995900	1.26647100	-2.87432200
H	0.72198000	-0.00443900	-2.26963900
C	-2.96369600	0.95174000	-1.70601600
H	-2.98738600	-0.55463600	-0.19551100
C	-2.22101200	1.61713000	-2.67541100
H	-0.29635400	1.78190000	-3.61833800
H	-3.99594900	1.22776200	-1.53213900
H	-2.67231400	2.40579200	-3.26321500
C	0.12784300	-3.51739000	0.98195400
H	-0.08304100	-3.54955400	2.05321700
H	-0.01955900	-4.52676100	0.59147000
H	1.16946800	-3.23234300	0.83852800
Cl	-2.47148600	-2.97578700	0.46395800



anti-14a

H	0.75422200	-1.52366600	-0.73342100
C	-0.31198100	-1.51598000	-0.52062800
C	-0.66459200	-2.48601100	0.32137700
C	-1.03362900	-0.45255300	-1.21619000
C	-0.27568800	0.39267600	-2.04239800
C	-2.41271500	-0.21340300	-1.12280000
C	-0.86389900	1.43204600	-2.74626900
H	0.79084800	0.22488400	-2.12823500
C	-2.99935700	0.82758500	-1.82827600
H	-3.03047600	-0.83869800	-0.49986500
C	-2.23250100	1.65481500	-2.64203500
H	-0.25481200	2.06775700	-3.37568700
H	-4.06545800	0.99322400	-1.74082000
H	-2.69715900	2.46465800	-3.18916500

H	0.06374000	-3.17489900	0.71840800
Br	-2.39666900	-2.89027700	0.99770800



anti-14b

H	0.72975300	-1.27834400	-0.25774800
C	-0.34188900	-1.43968600	-0.34661200
C	-0.75998200	-2.56235800	0.23602500
C	-1.04042000	-0.41289600	-1.12693100
C	-0.33602600	0.21240300	-2.16486200
C	-2.34858900	0.01095600	-0.86685300
C	-0.92860800	1.19675900	-2.94235200
H	0.68543400	-0.08772100	-2.36452400
C	-2.93733000	1.00392600	-1.63845800
H	-2.90176400	-0.42365200	-0.04854800
C	-2.23601300	1.59484600	-2.68393200
H	-0.36827700	1.65715700	-3.74584700
H	-3.94823000	1.32160300	-1.41714300
H	-2.70029800	2.36613200	-3.28458600
C	0.11064200	-3.50683300	0.99588300
H	-0.23143100	-3.60863700	2.02795100
H	0.09210100	-4.50249400	0.54792300
H	1.13832000	-3.14249000	1.00345800
Br	-2.58473800	-3.17350000	0.13018200

H-Cl

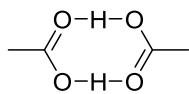
HCl

Cl	0.00000000	0.00000000	0.07428200
H	0.00000000	0.00000000	-1.21387400

H-Br

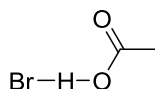
HBr

Br	0.00000000	0.00000000	0.04062900
H	0.00000000	0.00000000	-1.38636300



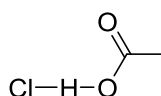
(AcOH)₂

C	1.92075600	-0.07267900	0.00009200
O	1.24967400	-1.10120000	-0.00027600
O	1.38657600	1.13326000	0.00021100
C	3.41401700	-0.07203500	0.00039300
H	0.38001300	1.08772700	-0.00014700
H	3.79194900	-1.09065700	0.00048400
H	3.77748500	0.46250400	-0.87936100
H	3.77716200	0.46256400	0.88023800
O	-1.38660100	-1.13330500	-0.00057000
O	-1.24961700	1.10113600	-0.00012600
C	-1.92075600	0.07265200	-0.00024300
C	-3.41401600	0.07208000	0.00002400
H	-0.38003800	-1.08782300	-0.00067000
H	-3.79191100	1.09071600	0.00027400
H	-3.77750600	-0.46231900	-0.87980300
H	-3.77718300	-0.46263100	0.87979500



Br⁻-AcOH (anion)

C	2.05526900	0.11802900	0.00002700
O	1.86026900	1.31488200	0.00000300
O	1.08615800	-0.79531100	0.00002000
H	0.17763100	-0.37239900	-0.00000200
C	3.42230200	-0.51577000	0.00007500
H	3.53417500	-1.15187200	0.87928000
H	3.53419700	-1.15197000	-0.87905700
H	4.18999400	0.25293400	0.00004400
Br	-1.96705500	0.12196800	-0.00003300



Cl⁻-AcOH (anion)

C	1.25715700	0.11797500	0.00001300
O	1.06834400	1.31763900	-0.00002200
O	0.29115000	-0.79178000	0.00001800
H	-0.63346100	-0.37483200	-0.00000600
C	2.62767100	-0.51220900	0.00006000
H	2.74233000	-1.14786400	0.87928600
H	2.74234800	-1.14796500	-0.87909100
H	3.39340200	0.25872600	0.00002600
Cl	-2.55492800	0.09492300	-0.00003600

3. Source Data of pKa Calculations.

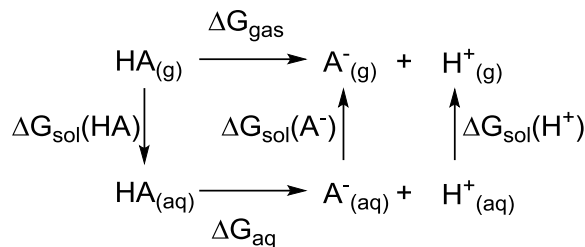


Figure S1. Proton-based thermodynamic cycle

In the First Principles approach, the direct use is made of the fundamental relationship between the pK_a value and the corresponding Gibbs Free Energy (ΔG_{aq} in kJ/mol) change for the dissociation reaction,

$$\Delta G_{\text{aq}} = -RT \ln K_a = -2.303 RT \log_{10} K_a = 2.303 RT (pK_a)$$

Followed by formula and Figure S1, the pK_a can be calculated from solution phase free energies ΔG_{aq} , which calculated from Gibbs energies of solvation ΔG_{SOLV} and gas phase free energies ΔG_{gas} . In order to get more accurate conclusion, combination of solvent molecule is necessary. Thus, in the calculation, the real structure of 'HX' is hydrogen halide combining with one molecule of acetic acid in connection to the hydrogen bond and hydrogen halide as the donor, while 'X⁻' is halide anion combining with one molecule of acetic acid in connection to the hydrogen bond and acetic acid as the donor. In order to get the highly accurate calculations, high levels of theory CBS-QB3 is used to calculate the gas phase Gibbs energy $G_{\text{CBS-QB3}}$ in a.u. calculation which is the smallest source of error. The $G_{\text{CBS-QB3}}(\text{H}^+)$ value is 270.29 kcal/mol. So the gas phase free energy $\Delta G_{\text{gas}} = G_{\text{CBS-QB3}}(\text{X}^-) + G_{\text{CBS-QB3}}(\text{H}^+) - G_{\text{CBS-QB3}}(\text{HX}) = 574.69$ kcal/mol. And the Gibbs energies of solvation ΔG_{SOLV} are calculated under M05-2X/6-31G* by the SMD solvation model, which is performed well in calculation of Gibbs energies of solvation and the value of $\Delta G_{\text{SOLV}}(\text{H}^+)$ is -10.67 kcal/mol which can be searched. And finally, $\Delta G_{\text{aq}} = \Delta G_{\text{gas}} + \Delta G_{\text{SOLV}}(\text{HX}) - \Delta G_{\text{SOLV}}(\text{H}^+) - \Delta G_{\text{SOLV}}(\text{X}^-) = 10.152$ kcal/mol. After all, we give out the pK_a of hydrogen chloride in acetic acid as 9.09 and the pK_a of hydrogen bromide in acetic acid as 7.44.

Table S1. Accurate values of Gibbs energies in a.u. The Gibbs energies of solvation $\Delta G_{\text{SOLV}}(\text{X})$ are calculated from G_{GAS} and G_{SMD} . $\Delta G_{\text{SOLV}}(\text{X}) = G_{\text{SMD}}(\text{X}) - G_{\text{GAS}}(\text{X})$

$G_{\text{CBS-QB3}}(\text{HCl})$	$G_{\text{GAS}}(\text{HCl})$	$G_{\text{SMD}}(\text{HCl})$	$\Delta G_{\text{SOLV}}(\text{HCl})$
-689.146842	-689.8106936	-689.8240749	-0.0133813
$G_{\text{CBS-QB3}}(\text{Cl}^-)$	$G_{\text{GAS}}(\text{Cl}^-)$	$G_{\text{SMD}}(\text{Cl}^-)$	$\Delta G_{\text{SOLV}}(\text{Cl}^-)$
-688.64867	-689.3049745	-689.3830536	-0.0780791
$G_{\text{CBS-QB3}}(\text{HBr})$	$G_{\text{GAS}}(\text{HBr})$	$G_{\text{SMD}}(\text{HBr})$	$\Delta G_{\text{SOLV}}(\text{HBr})$
-2802.26733	-2801.321384	-2801.334878	-0.0134943
$G_{\text{CBS-QB3}}(\text{Br}^-)$	$G_{\text{GAS}}(\text{Br}^-)$	$G_{\text{SMD}}(\text{Br}^-)$	$\Delta G_{\text{SOLV}}(\text{Br}^-)$
-2801.78224	-2800.825856	-2800.894531	-0.0686755

4. Source Data of Rates of Hydrohalogenations for Alkynes

To find out which *anti*-adducts and *syn*-adducts are the major products, we should calculate the ratios of their reaction rates K_{anti}/K_{syn} , rates can be calculated from rate constants k_{anti}/k_{syn} combined with the concentrations of alkynes and hydrogen halides or halide ions. An ordinary dynamics treatment is used. Depending on the transition state theory (TST), the reaction rate constant (k^{TST}) is:

$$k_{TST} = \sigma \frac{k_B T}{h} \left(\frac{1}{c^\ominus} \right)^{\Delta n} e^{-\Delta G^\ominus / RT}$$

In the formula, σ is the tunnel effect coefficient (here we suppose it to be 1); k_B is the Boltzmann constant; T represents the Kelvin temperature (298 K for room temperature 25 °C); h is the Planck constant; R is the ideal gas constant; $c^\ominus$ represents 1 mol/L; Δn is the number difference of the molecules from reactants to products in the rate-determining step; and $\Delta G^\ominus$ represents the Gibbs free energy in the transition state. In the calculation of K, the halide ions come from hydrogen halides, in the section 3 we discuss about the *pKa* of hydrogen chloride and bromide and their values are 9.09 and 7.44, respectively, which acidic are small enough to use the simple formula, that is $[X^-] = K_{a(HX)}^{0.5}[HX]^{0.5}$. The details calculation values of reaction rates are shown below (Table S2).

Table S2. Activation free energies and ratios of relative rate constants of hydrohalogenations of alkynes at 298 K. (note that $K_{syn} = k_{syn} [\text{alkyne}][HX]$; $K_{anti} = k_{anti}[\text{alkyne}][HX][X^-]$; and all of structures can be classified by two key substituents, H, Ar, and alkyl R); (Note that concentration in mol/L and energies in kcal/mol, data are obtained in Table S2 with $[HX] = 1$ mol/L used, K_{anti}/K_{syn} would increase along with increase of $[HX]$ or $[X^-]$)

Alkyne	HX-addition	$\Delta G(\text{syn})$	$\Delta G(\text{AdE3})$	K_{anti}/K_{syn}	favor
1a	HCl	43.5	25.3	>1000	<i>anti</i>
1b	HCl	36.3	19.6	>1000	<i>anti</i>
1c	HCl	35.8	24.6	716.1	<i>anti</i>
1d	HCl	36.2	23.3	>1000	<i>anti</i>
1a	HBr	43.7	22.2	>1000	<i>anti</i>
1b	HBr	35.1	15.9	>1000	<i>anti</i>
1c	HBr	35.6	20.5	>1000	<i>anti</i>
1d	HBr	33.2	18.9	>1000	<i>anti</i>
4a	HCl	28.0	22.8	0.028	<i>syn</i>
4b	HCl	31.5	23.8	1.936	<i>anti</i>
4c	HCl	31.9	23.0	14.70	<i>anti</i>
4d	HCl	29.4	20.4	17.41	<i>anti</i>
4e	HCl	29.2	25.8	0.001	<i>syn</i>
4a	HBr	27.8	16.6	>1000	<i>anti</i>
4b	HBr	30.4	15.9	>1000	<i>anti</i>
4c	HBr	27.8	15.9	>1000	<i>anti</i>
4d	HBr	29.9	16.1	>1000	<i>anti</i>
4e	HBr	23.6	18.8	0.614	<i>syn</i>
7a	HCl	15.9	15.3	<10 ⁻³	<i>syn</i>
7b	HCl	25.8	20.0	0.078	<i>syn</i>
7c	HCl	29.6	23.0	0.302	<i>syn</i>
7d	HCl	37.4	27.4	94.30	<i>anti</i>
7e	HCl	35.4	40.9	<10 ⁻³	<i>syn</i>

7f	HCl	35.5	25.8	56.80	<i>anti</i>
7g	HCl	33.2	24.8	6.317	<i>anti</i>
7a	HBr	14.0	9.9	0.193	<i>syn</i>
7b	HBr	24.0	12.2	>1000	<i>anti</i>
7c	HBr	28.9	16.6	>1000	<i>anti</i>
7d	HBr	37.5	23.5	>1000	<i>anti</i>
7e	HBr	35.2	20.8	>1000	<i>anti</i>
7f	HBr	35.2	19.1	>1000	<i>anti</i>
7g	HBr	33.5	19.1	>1000	<i>anti</i>
10a	HCl	20.8	19.5	<10 ⁻³	<i>syn</i>
10b	HCl	29.5	21.2	5.335	<i>anti</i>
10c	HCl	32.3	22.8	40.52	<i>anti</i>
10d	HCl	39.4	27.6	>1000	<i>anti</i>
10a	HBr	20.2	13.2	25.94	<i>anti</i>
10b	HBr	26.8	9.5	>1000	<i>anti</i>
10c	HBr	32.6	17.2	>1000	<i>anti</i>
10d	HBr	40.3	22.2	>1000	<i>anti</i>

5. Source Data of Distances of Key Bonds and Angles in Transition States

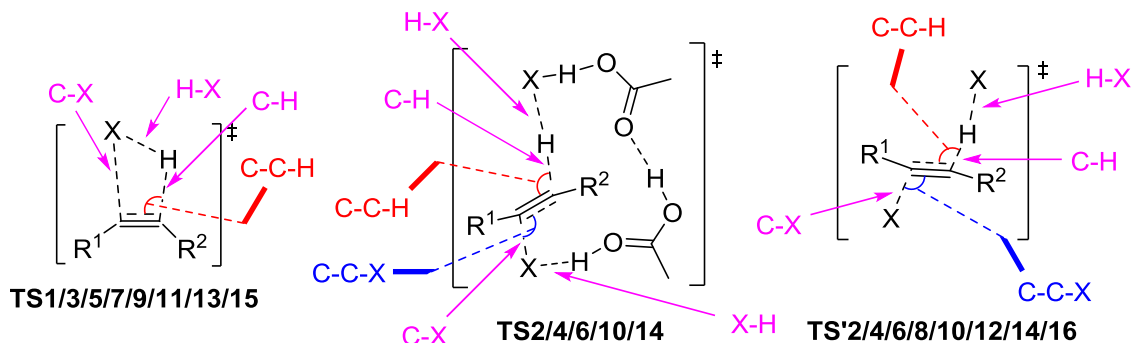


Figure S2. Schematic diagrams on names of the key bonds and angles

Table S3. Distances of key bonds and angles in transition states. Different types of transition states have different meanings in **Table S3**. The figures of transition states are shown in **Figure S2**, which figure out names of bonds and angles. (Note that bonds in Å and angles in °)

Structure	X	$\angle\text{C-C-H}$	$\angle\text{C-C-X}$	C-H	H-X	C-X	X-H
TS1a	Cl	91.2	-	1.20	1.95	2.76	-
TS1b	Cl	100.5	-	1.14	2.14	3.03	-
TS1c	Cl	105.9	-	1.14	2.11	3.05	-
TS1d	Cl	105.1	-	1.14	2.09	3.04	-
TS2a	Cl	108.0	115.6	1.35	1.59	2.63	1.79
TS2b	Cl	99.9	102.8	1.23	1.81	2.98	1.71
TS2c	Cl	106.5	104.0	1.24	1.75	2.95	1.71
TS2d	Cl	106.9	104.1	1.25	1.74	2.96	1.70
TS'2a	Cl	106.2	120.9	1.53	1.46	2.56	-
TS'2b	Cl	98.7	103.6	1.38	1.58	2.87	-
TS'2c	Cl	103.2	110.7	1.42	1.54	2.78	-
TS'2d	Cl	103.1	109.7	1.40	1.55	2.82	-
TS3a	Br	98.6	-	1.18	2.09	2.99	-
TS3b	Br	103.1	-	1.14	2.26	3.21	-
TS3c	Br	108.2	-	1.14	2.24	3.21	-
TS3d	Br	108.9	-	1.13	2.29	3.29	-
TS4a	Br	107.2	116.0	1.38	1.40	2.88	1.93
TS4b	Br	97.7	100.5	1.29	1.84	3.30	1.89
TS4c	Br	105.9	104.9	1.28	1.82	3.26	1.88
TS4d	Br	106.6	104.8	1.28	1.83	3.41	1.88
TS'4a	Br	105.7	120.3	1.49	1.63	2.85	-
TS'4b	Br	95.8	99.4	1.40	1.72	3.23	-
TS'4c	Br	102.3	108.1	1.40	1.70	3.16	-
TS'4d	Br	102.3	107.9	1.38	1.71	3.23	-
TS5a	Cl	114.3	-	1.11	2.31	3.23	-

TS5b	Cl	110.2	-	1.11	2.32	3.24	-
TS5c	Cl	111.1	-	1.11	2.33	3.24	-
TS5d	Cl	111.4	-	1.11	2.31	3.24	-
TS5e	Cl	110.8	-	1.11	2.30	3.22	-
TS6a	Cl	114.8	99.1	1.13	2.14	2.92	1.75
TS6b	Cl	107.4	103.1	1.14	2.07	2.89	1.76
TS6c	Cl	107.8	103.5	1.14	2.09	2.86	1.77
TS6d	Cl	108.5	103.5	1.14	2.10	2.82	1.76
TS'6a	Cl	107.7	104.2	1.38	1.56	3.00	-
TS'6b	Cl	102.5	99.8	1.35	1.60	3.03	-
TS'6c	Cl	103.1	97.8	1.35	1.60	3.06	-
TS'6d	Cl	102.4	97.8	1.36	1.59	3.08	-
TS'6e	Cl	98.3	108.1	1.32	1.64	3.01	-
TS7a	Br	114.9	-	1.11	2.41	3.36	-
TS7b	Br	110.5	-	1.11	2.41	3.36	-
TS7c	Br	111.5	-	1.11	2.41	3.37	-
TS7d	Br	112.8	-	1.10	2.51	3.45	-
TS7e	Br	112.6	-	1.10	2.51	3.44	-
TS'8a	Br	106.1	105.0	1.40	1.69	3.69	-
TS'8b	Br	98.8	96.5	1.41	1.69	3.40	-
TS'8c	Br	99.6	90.2	1.39	1.70	3.56	-
TS'8d	Br	98.7	101.5	1.38	1.71	3.48	-
TS'8e	Br	100.7	88.5	1.33	1.76	4.21	-
TS9a	Cl	116.3	-	1.10	2.44	3.32	-
TS9b	Cl	115.3	-	1.10	2.37	3.28	-
TS9c	Cl	114.5	-	1.11	2.31	3.24	-
TS9d	Cl	112.5	-	1.12	2.21	3.16	-
TS9e	Cl	113.0	-	1.11	2.24	3.19	-
TS9f	Cl	113.4	-	1.11	2.25	3.19	-
TS9g	Cl	113.6	-	1.11	2.26	3.21	-
TS10a	Cl	115.1	101.1	1.11	2.35	2.64	1.82
TS10b	Cl	114.6	99.4	1.12	2.23	2.82	1.78
TS10c	Cl	115.0	99.6	1.13	2.14	2.89	1.76
TS10d	Cl	112.1	101.3	1.20	1.83	3.16	1.68
TS10e	Cl	113.3	102.0	1.21	1.80	3.36	1.63
TS10f	Cl	114.1	100.5	1.15	1.99	3.10	1.71
TS10g	Cl	115.1	99.7	1.14	2.03	3.00	1.73
TS'10a	Cl	121.1	76.2	1.13	2.07	3.45	-
TS'10b	Cl	107.9	102.0	1.38	1.56	3.13	-
TS'10c	Cl	107.8	105.4	1.38	1.55	2.97	-
TS'10d	Cl	106.7	112.8	1.47	1.49	2.68	-
TS'10e	Cl	106.7	112.1	1.44	1.52	2.73	-
TS'10f	Cl	106.7	110.0	1.44	1.51	2.77	-

TS'10g	Cl	106.7	109.5	1.43	1.52	2.79	-
TS11a	Br	116.3	-	1.10	2.53	3.44	-
TS11b	Br	115.7	-	1.10	2.45	3.40	-
TS11c	Br	114.8	-	1.11	2.40	3.36	-
TS11d	Br	113.6	-	1.11	2.37	3.35	-
TS11e	Br	113.8	-	1.12	2.34	3.32	-
TS11f	Br	114.1	-	1.11	2.35	3.33	-
TS11g	Br	114.4	-	1.11	2.36	3.34	-
TS'12a	Br	104.4	101.2	1.48	1.63	4.01	-
TS'12b	Br	105.0	103.2	1.45	1.65	3.63	-
TS'12c	Br	105.8	103.9	1.41	1.67	3.51	-
TS'12d	Br	104.0	112.7	1.54	1.59	2.99	-
TS'12e	Br	106.0	107.6	1.40	1.68	3.24	-
TS'12f	Br	105.9	105.7	1.41	1.67	3.27	-
TS'12g	Br	105.2	105.1	1.43	1.66	3.25	-
TS13a	Cl	112.5	79.0	1.10	2.47	3.30	-
TS13b	Cl	111.0	77.4	1.10	2.36	3.27	-
TS13c	Cl	110.0	77.4	1.11	2.31	3.23	-
TS13d	Cl	107.4	77.9	1.12	2.21	3.14	-
TS14a	Cl	109.8	105.4	1.11	2.26	2.63	1.82
TS14b	Cl	108.3	104.0	1.13	2.16	2.78	1.79
TS14c	Cl	107.3	103.2	1.14	2.07	2.92	1.76
TS14d	Cl	104.1	103.5	1.20	1.84	2.92	1.73
TS'14a	Cl	102.8	92.7	1.36	1.59	3.37	-
TS'14b	Cl	101.8	100.7	1.36	1.58	3.05	-
TS'14c	Cl	102.9	100.7	1.35	1.60	3.00	-
TS'14d	Cl	102.4	106.8	1.43	1.53	2.69	-
TS15a	Br	112.3	77.8	1.10	2.53	3.43	-
TS15b	Br	111.5	76.9	1.11	2.45	3.40	-
TS15c	Br	110.5	76.9	1.11	2.41	3.36	-
TS15d	Br	108.7	77.1	1.12	2.33	3.29	-
TS'16a	Br	98.0	87.7	1.43	1.68	3.79	-
TS'16b	Br	98.6	89.4	1.40	1.70	3.63	-
TS'16c	Br	99.1	100.1	1.40	1.70	3.38	-
TS'16d	Br	100.4	103.0	1.41	1.69	3.10	-

6. Computed Energies and Charges

Table S4. Electronic energies (E_{gas} in Hartree), thermal corrections to Gibbs free energies ($\Delta G_{correction}$ in Hartree), Gibbs free energies in the gas phase ($G_{gas} = E_{gas} + \Delta G_{correction}$), solvation free energies (G_{uESE} in kcal/mol), Gibbs free energies about molecules converts from the gas-phase standard state to the solution-phase standard state of 1M $RT\ln(RT/p)$ in kcal/mol (for (HOAc)₂ is 8.75 mol/L because acetic acid is the solvent), free energies in solution (ΔG_{solv} in kcal/mol, $\Delta G_{solv} = G_{gas} + G_{uESE} + RT\ln(RT/p) = E_{gas} + \Delta G_{correction} + G_{uESE} + RT\ln(RT/p)$). Relative energies (ΔG) at 298 K are reported in kcal/mol.

Structure	$\Delta G_{correction}$	E_{gas}	G_{uESE}	ΔG_{solv}	ΔG
(AcOH) ₂	0.087627	-457.5258311	-7.210	-287050.1975	0.0
Br-AcOH	0.027144	-2801.551170	-56.201	1758038.6530	0.0
Cl-AcOH	0.027484	-688.5689848	-58.796	-432123.5832	0.0
HBr	-0.013312	-2573.307234	-1.821	-1614784.3070	0.0
HCl	-0.011292	-460.3371534	-1.880	-288873.2430	0.0
1a	0.010580	-77.18659818	-1.247	-48428.0802	0.0
1b	0.110126	-234.1578053	-4.239	-146869.6083	0.0
1c	0.031302	-116.4340971	-2.346	-73044.3739	0.0
1d	0.109940	-234.1518649	-4.090	-146865.8483	0.0
4a	0.079078	-307.8059362	-5.898	-193105.6888	0.0
4b	0.103311	-347.0532593	-7.039	-217719.7110	0.0
4c	0.128149	-386.2922380	-7.175	-242327.1128	0.0
4d	0.156186	-425.5333400	-8.020	-266934.5479	0.0
4e	0.182380	-464.7758047	-8.726	-291543.8559	0.0
7a	0.106514	-422.1540180	-7.884	-264845.0232	0.0
7b	0.102605	-347.0486867	-6.410	-217716.6557	0.0
7c	0.067271	-766.9397005	-6.373	-481224.6013	0.0
7d	0.077486	-512.0315406	-9.270	-321263.6688	0.0
7e	0.075115	-399.8977085	-8.830	-250899.6157	0.0
7f	0.075872	-644.4670091	-6.512	-404366.5045	0.0
7g	0.114706	-535.3489560	-9.644	-335872.5982	0.0
10a	0.133230	-461.4059179	-9.742	-289461.0764	0.0
10b	0.126040	-386.2958770	-7.462	-242331.0064	0.0
10c	0.090777	-806.1873088	-6.850	-505838.5947	0.0
10d	0.102092	-551.2797420	-10.396	-345877.9931	0.0
Int1a	0.006539	-537.5276875	-3.467	-337301.4729	-0.1
Int1b	0.113462	-694.5032909	-5.682	-435740.3536	2.9
Int1c	0.033119	-576.7767673	-4.182	-361914.6988	2.9
Int1d	0.112647	-694.4960876	-5.403	-435736.0658	3.0
Int2a	0.004895	-2650.497143	-3.451	-1663211.9510	0.4
Int2b	0.111875	-2807.472729	-5.758	-1761650.8780	3.0
Int2c	0.031381	-2689.746086	-4.224	-1687825.2090	3.5
Int2d	0.111075	-2807.464575	-5.689	-1761646.1940	4.0
Int3a	0.079915	-768.1485168	-7.685	-481976.5233	2.4

Int3b	0.105277	-807.3975540	-8.345	-506590.4318	2.5
Int3c	0.133127	-846.6371532	-8.865	-531196.7165	3.6
Int3d	0.158617	-885.8782277	-9.450	-555805.4729	2.3
Int3e	0.185420	-925.1212418	-9.755	-580414.3425	2.8
Int4a	0.077794	-2881.118457	-7.514	-1807887.4503	2.5
Int4b	0.104004	-2920.366951	-8.784	-1832501.096	2.9
Int4c	0.129966	-2959.606767	-8.758	-1857108.1554	3.3
Int4d	0.155262	-2998.847809	-9.643	-1881717.3130	1.5
Int4e	0.183619	-3038.090949	-9.929	-1906325.2680	2.9
Int5a	0.108925	-882.5019898	-10.003	-553718.5851	-0.3
Int5b	0.105312	-807.3914416	-8.375	-506586.6042	3.3
Int5c	0.068694	-1227.282041	-8.436	-770095.1933	2.7
Int5d	0.079578	-972.3732969	-11.525	-610133.6665	3.2
Int5e	0.076487	-860.2395184	-11.052	-539770.0658	2.8
Int5f	0.077259	-1104.809317	-8.277	-693236.8010	2.9
Int5g	0.115423	-995.6915228	-10.940	-624743.0084	2.8
Int6a	0.108301	-2995.471371	-10.377	-1879628.7670	0.6
Int6b	0.103370	-2920.360893	-8.581	-1832497.4890	3.5
Int6c	0.066092	-3340.251614	-8.422	-2096006.3490	2.6
Int6d	0.076694	-3085.343058	-11.639	-1936045.2450	2.7
Int6e	0.074072	-2973.209168	-11.169	-1865681.2830	2.6
Int6f	0.075421	-3217.779003	-8.353	-2019147.6370	3.2
Int6g	0.113662	-3108.660924	-11.674	-1950654.2760	3.3
Int7a	0.135199	-921.7504335	-11.157	-578332.0428	2.3
Int7b	0.131732	-846.6401596	-9.359	-531199.9724	4.3
Int7c	0.094512	-1266.531044	-9.314	-794709.0122	2.8
Int7d	0.104835	-1011.623101	-12.403	-634748.3404	2.9
Int8a	0.132581	-3034.719823	-11.314	-1904243.2640	2.1
Int8b	0.130692	-2959.609608	-9.471	-1857110.1960	5.1
Int8c	0.093601	-3379.500663	-9.467	-2120619.3020	3.6
Int8d	0.103028	-3124.592802	-12.559	-1960659.2470	3.1
TS1a	0.007090	-537.4393027	-15.640	-337257.8378	43.5
TS1b	0.114181	-694.4175939	-26.106	-435706.5506	36.3
TS1c	0.033901	-576.6915438	-25.223	-361881.7704	35.8
TS1d	0.112588	-694.4114869	-25.268	-435702.8800	36.2
TS2a	0.112196	-1455.345705	-20.811	-913192.5004	32.3
TS2b	0.228329	-1612.331679	-24.743	-1011633.8260	32.5
TS2c	0.146043	-1494.597758	-23.873	-937805.3787	35.7
TS2d	0.224421	-1612.320312	-23.267	-1011627.6700	34.9
TS'2a	0.002726	-997.315501	-52.680	-625874.5297	25.3
TS'2b	0.107537	-1154.292952	-60.695	-724321.6946	19.6
TS'2c	0.027664	-1036.562683	-57.276	-650491.4756	24.6
TS'2d	0.106491	-1154.283284	-58.701	-724314.2905	23.3
TS3a	0.005892	-2650.412964	-13.601	-1663168.6530	43.7
TS3b	0.112750	-2807.395327	-22.774	-1761618.7740	35.1

TS3c	0.032758	-2689.668491	-21.651	-1687793.0800	35.6
TS3d	0.111502	-2807.386324	-25.863	-1761616.9967	33.2
TS4a	0.117954	-5681.294697	-19.996	-3565013.3240	33.6
TS4b	0.225293	-5838.283239	-22.901	-3663460.7530	27.7
TS4c	0.145333	-5720.546984	-22.848	-3589630.1980	33.0
TS4d	0.221881	-5838.268168	-23.582	-3663454.1180	30.5
TS'4a	-0.001097	-5223.270545	-50.424	-3277703.7221	22.2
TS'4b	0.103642	-5380.251724	-56.764	-3376151.5968	15.9
TS'4c	0.024719	-5262.519450	-55.538	-3302321.7168	20.5
TS'4d	0.102835	-5380.239989	-56.818	-3376144.7935	18.9
TS5a	0.083827	-768.0672377	-35.534	-481950.9140	28.0
TS5b	0.111309	-807.3130122	-36.183	-506561.4338	31.5
TS5c	0.138320	-846.5528351	-36.753	-531168.4354	31.9
TS5d	0.163119	-885.7954912	-37.111	-555778.3909	29.4
TS5e	0.190124	-925.0398304	-37.354	-580387.9033	29.2
TS6a	0.201319	-1685.964335	-34.806	-1057866.0660	36.3
TS6b	0.228517	-1725.217157	-33.170	-1082478.9010	37.5
TS6c	0.254268	-1764.457551	-33.699	-1107087.0110	36.8
TS6d	0.278409	-1803.701610	-32.360	-1131696.5630	34.7
TS'6a	0.075265	-1227.925638	-68.069	-770550.0672	22.8
TS'6b	0.101876	-1267.176378	-67.611	-795167.6414	23.8
TS'6c	0.128634	-1306.416953	-68.760	-819775.8532	23.0
TS'6d	0.152380	-1345.659438	-68.640	-844385.8837	20.4
TS'6e	0.182922	-1384.902069	-66.609	-868989.8312	25.8
TS7a	0.082956	-2881.048662	-29.318	-1807862.2180	27.8
TS7b	0.109733	-2920.295042	-30.053	-1832473.6460	30.4
TS7c	0.135749	-2959.534908	-30.602	-1857081.2780	30.1
TS7d	0.161687	-2998.775326	-36.236	-1881694.3907	24.5
TS7e	0.187389	-3038.019297	-36.514	-1906304.5240	23.6
TS'8a	0.071609	-5453.882607	-67.900	-3422386.9490	16.6
TS'8b	0.096526	-5493.137932	-65.119	-3447001.6420	15.9
TS'8c	0.126334	-5532.377800	-65.546	-3471606.7730	18.2
TS'8d	0.150217	-5571.621065	-64.527	-3496216.3090	16.1
TS'8e	0.179214	-5610.862224	-65.124	-3520822.929	18.8
TS9a	0.114398	-882.4271375	-44.224	-553702.4012	15.9
TS9b	0.109809	-807.3113238	-38.945	-506564.0775	25.8
TS9c	0.072563	-1227.199835	-35.539	-770068.2834	29.6
TS9d	0.082444	-972.2869364	-33.329	-610099.4800	37.4
TS9e	0.079971	-860.1533469	-34.735	-539737.4891	35.4
TS9f	0.082673	-1104.723397	-33.052	-693204.2627	35.5
TS9g	0.118975	-995.6078439	-35.298	-624712.6281	33.2
TS10a	0.231284	-1800.324309	-39.523	-1129614.0070	27.7
TS10b	0.226934	-1725.209114	-36.774	-1082478.4520	34.9
TS10c	0.188534	-2145.097732	-34.812	-1345984.8930	36.4
TS10d	0.195750	-1890.188867	-32.093	-1186019.7840	40.6

TS10e	0.188737	-1778.059623	-29.537	-1115659.4070	36.9
TS10f	0.197026	-2022.622853	-32.567	-1269123.1080	40.1
TS10g	0.235707	-1913.504506	-35.678	-1200629.0920	40.2
TS'10a	0.108411	-1342.255499	-92.584	-842301.4131	15.3
TS'10b	0.097816	-1267.166508	-72.044	-795168.4292	20.0
TS'10c	0.063625	-1687.063358	-66.065	-1058673.3776	23.0
TS'10d	0.073659	-1432.167982	-56.403	-898708.0216	27.4
TS'10e	0.070976	-1320.031886	-43.656	-828330.4366	40.9
TS'10f	0.072794	-1564.597454	-59.420	-981812.3994	25.8
TS'10g	0.109871	-1455.476110	-64.572	-913319.5509	24.8
TS11a	0.112554	-2995.410399	-37.882	-1879615.3430	14.0
TS11b	0.108227	-2920.293675	-32.385	-1832476.0660	24.9
TS11c	0.071097	-3340.181555	-29.161	-2095979.9850	28.9
TS11d	0.078714	-3085.265671	-31.018	-1936014.7954	33.2
TS11e	0.078364	-2973.133640	-28.739	-1865648.7650	35.2
TS11f	0.081010	-3217.703824	-27.011	-2019115.6130	35.2
TS11g	0.118612	-3108.588720	-29.178	-1950623.3660	33.5
TS'12a	0.101058	-5568.239218	-72.511	-3494132.9970	9.9
TS'12b	0.093093	-5493.127633	-69.172	-3447001.3870	13.1
TS'12c	0.059642	-5913.021164	-65.307	-3710505.9020	16.6
TS'12d	0.070009	-5658.125345	-53.571	-3550537.9850	23.5
TS'12e	0.067401	-5545.984696	-60.046	-3480176.7180	20.8
TS'12f	0.067725	-5790.551884	-60.444	-3633645.2690	19.1
TS'12g	0.107158	-5681.431844	-65.155	-3565151.3180	19.1
TS13a	0.139541	-921.6727815	-44.121	-578313.5547	20.8
TS13b	0.136348	-846.5575970	-38.868	-531174.7760	29.5
TS13c	0.099038	-1266.446166	-35.934	-794679.5305	32.3
TS13d	0.107417	-1011.533746	-33.636	-634711.8816	39.4
TS14a	0.255112	-1839.576187	-36.489	-1154226.9670	30.8
TS14b	0.252958	-1764.461021	-35.847	-1107092.1590	35.5
TS14c	0.215491	-2184.350203	-33.398	-1370597.8810	37.4
TS14d	0.223369	-1929.442557	-31.953	-1210634.3960	40.3
TS'14a	0.131322	-1381.527440	-75.350	-866913.3377	19.5
TS'14b	0.125206	-1306.420243	-70.216	-819781.5244	21.2
TS'14c	0.089352	-1726.313689	-66.378	-1083287.5215	22.8
TS'14d	0.099511	-1471.420334	-55.484	-923322.1236	27.6
TS15a	0.140557	-3034.656161	-38.154	-1904225.1510	20.2
TS15b	0.134027	-2959.539787	-32.976	-1857087.7940	27.5
TS15c	0.099379	-3379.427867	-29.817	-2120590.3460	32.6
TS15d	0.107582	-3124.513533	-27.960	-1960622.0480	40.3
TS'16a	0.126405	-5607.491252	-70.157	-3518745.7820	13.2
TS'16b	0.121747	-5532.379228	-73.654	-3471618.6560	10.2
TS'16c	0.086240	-5952.273987	-63.811	-3735119.2540	17.2
TS'16d	0.096906	-5697.373176	-57.728	-3575153.6700	22.2
TS17a	0.080905	-768.060252	-18.558	-481931.3884	47.5

TS17b	0.108596	-807.313165	-25.550	-506552.599186	40.4
TS18a	0.196388	-1685.972849	-23.609	-1057863.3060	39.1
TS'18a	0.077187	-1227.942670	-54.088	-770550.0672	27.3
TS'18b	0.102659	-1267.191463	-57.103	-795166.1084	25.3
TS19a	0.078773	-2881.034159	-18.424	-1807844.8480	45.2
TS19b	0.107544	-2920.288134	-25.754	-1832466.386052	37.6
TS20a	0.195065	-5911.923312	-24.061	-3709690.7630	33.7
TS'20a	0.072876	-5453.896893	-52.367	-3422379.586	24.0
TS'20b	0.099152	-5493.147600	-55.471	-3446996.4125	21.2
<i>syn-2a/anti-2a</i>	0.017075	-537.5724898	-2.260	-337321.7683	-20.4
<i>syn-2b</i>	0.121136	-694.5385200	-5.009	-435756.9716	-14.1
<i>syn-2c/anti-2c</i>	0.043083	-576.8187519	-2.976	-361933.5860	-16.0
<i>syn-2d/anti-2d</i>	0.121738	-694.5370875	-4.711	-435755.3970	-16.3
<i>anti-2b</i>	0.121567	-694.5403966	-5.009	-435757.8788	-15.0
<i>syn-3a/anti-3a</i>	0.015301	-2650.543971	-2.644	-1663234.0000	-21.6
<i>syn-3b</i>	0.119795	-2807.510293	-5.567	-1761669.2880	-15.4
<i>syn-3c/anti-3c</i>	0.041312	-2689.790038	-3.375	-1687845.7080	-17.0
<i>syn-3d/anti-3d</i>	0.119625	-2807.508711	-5.172	-1761668.0080	-17.9
<i>anti-3b</i>	0.120483	-694.5405108	-5.448	-435759.0696	-16.2
<i>syn-5a/anti-5a</i>	0.090824	-768.1887045	-6.886	-481994.0970	-15.2
<i>syn-5b</i>	0.116645	-807.4302478	-8.019	-506603.4879	-10.5
<i>syn-5c</i>	0.142717	-846.6696253	-8.512	-531210.7222	-10.4
<i>syn-5d</i>	0.169248	-885.9113555	-9.118	-555819.2579	-11.5
<i>syn-5e</i>	0.195338	-925.1486955	-9.996	-580425.5873	-8.5
<i>syn-6a/anti-6a</i>	0.088975	-2881.160413	-7.438	-1807906.6861	-16.7
<i>syn-6b</i>	0.114897	-2920.402648	-8.360	-1832516.2370	-12.2
<i>syn-6c</i>	0.141411	-2959.641912	-9.001	-1857123.2710	-11.9
<i>syn-6d</i>	0.167237	-2998.883891	-9.499	-1881732.2968	-13.4
<i>Syn-6e</i>	0.193552	-3038.121411	-10.565	-1906338.7860	-10.6
<i>anti-5b</i>	0.116198	-807.4320811	-7.773	-506604.6728	-11.7
<i>anti-5c</i>	0.142820	-846.6712545	-8.594	-531211.7619	-11.4
<i>anti-5d</i>	0.169230	-885.9081356	-9.369	-555817.4997	-9.7
<i>anti-5e</i>	0.196055	-925.1506335	-9.824	-580426.1815	-9.1
<i>anti-6b</i>	0.114359	-2920.403849	-8.580	-1832517.5480	-13.5
<i>anti-6c</i>	0.140772	-2959.643275	-9.066	-1857124.5920	-13.2
<i>anti-6d</i>	0.167704	-2998.879503	-9.969	-1881729.7200	-10.9
<i>anti-6e</i>	0.194295	-3038.12205	-10.533	-1906338.6880	-10.5
<i>syn-8a/anti-8a</i>	0.119421	-882.5418722	-9.608	-553736.6303	-18.4
<i>syn-8b/anti-8b</i>	0.114358	-807.4316266	-7.588	-506605.3572	-15.5
<i>syn-8c/anti-8c</i>	0.078913	-1227.322453	-7.779	-770113.4829	-15.6
<i>syn-8d/anti-8d</i>	0.089236	-972.4144356	-11.043	-610152.9390	-16.0
<i>syn-8e/anti-8e</i>	0.086882	-860.2806985	-11.674	-1950654.2760	-15.9
<i>syn-8f/anti-8f</i>	0.088970	-1104.849802	-10.441	-539788.7728	-15.9
<i>syn-8g/anti-8g</i>	0.127617	-995.7318917	-7.913	-693254.4926	-14.7
<i>syn-9a/anti-9a</i>	0.118125	-2995.513517	-11.038	-624760.7864	-14.9

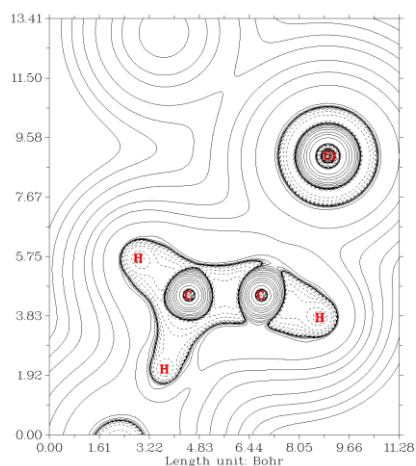
<i>syn-9b/anti-9b</i>	0.114086	-2920.403100	-8.250	-1832516.9190	-16.5
<i>syn-9c/anti-9c</i>	0.077060	-3340.294127	-8.231	-2096025.9530	-17.0
<i>syn-9d/anti-9d</i>	0.086877	-3085.386091	-11.451	-1936065.6710	-17.7
<i>syn-9e/anti-9e</i>	0.084707	-2973.252433	-10.806	-1865701.3960	-17.5
<i>syn-9f/anti-9f</i>	0.087296	-3217.821371	-8.335	-2019166.7540	-15.9
<i>syn-9g/anti-9g</i>	0.125273	-3108.703386	-11.670	-1950673.6320	-16.7
<i>syn-11a</i>	0.145681	-921.7831783	-10.507	-578345.3629	-11.0
<i>syn-11b</i>	0.141273	-846.6729394	-8.733	-531213.9290	-9.7
<i>syn-11c</i>	0.104822	-1266.564190	-8.716	-794722.7437	-10.9
<i>syn-11d</i>	0.114917	-1011.656087	-11.783	-634762.0923	-10.9
<i>syn-12a</i>	0.144011	-3034.755434	-11.027	-1904258.1510	-12.8
<i>syn-12b</i>	0.139806	-2959.645212	-9.168	-1857126.5150	-11.2
<i>syn-12c</i>	0.103075	-3379.536436	-9.128	-2120635.4660	-12.6
<i>syn-12d</i>	0.112918	-3124.628440	-12.164	-1960675.0090	-12.7
<i>anti-11a</i>	0.144200	-921.7849618	-10.543	-578347.4474	-13.1
<i>anti-11b</i>	0.139468	-846.6746687	-8.755	-531216.1688	-11.9
<i>anti-11c</i>	0.104255	-1266.565953	-8.778	-794724.2684	-12.4
<i>anti-11d</i>	0.113924	-1011.658271	-12.175	-634764.4784	-13.2
<i>anti-12a</i>	0.143342	-3034.756742	-11.118	-1904259.4820	-14.1
<i>anti-12b</i>	0.139503	-2959.646525	-9.301	-1857127.6630	-12.3
<i>anti-12c</i>	0.103130	-3379.537805	-9.375	-2120636.5380	-13.6
<i>anti-12d</i>	0.112991	-3124.629996	-12.574	-1960676.3500	-14.1
<i>syn-13a</i>	0.090481	-768.188128	-7.105	-481994.1693	-15.2
<i>syn-13b</i>	0.116944	-807.432322	-7.878	-506604.4606	-11.5
<i>syn-13c</i>	0.088807	-2881.160258	-7.643	-1807906.8991	-16.9
<i>syn-13d</i>	0.115377	-2920.403978	-8.370	-1832516.7803	-12.8
<i>anti-13a</i>	0.092691	-768.186696	-7.381	-481992.1601	-13.2
<i>anti-13b</i>	0.116234	-807.432338	-8.156	-506605.1944	-12.2
<i>anti-13c</i>	0.087404	-2881.157983	-7.936	-1807906.6447	-16.6
<i>anti-13d</i>	0.115031	-2920.403606	-8.595	-1832516.9886	-13.0

7. Calculation on Laplacian of Electron Density Analysis

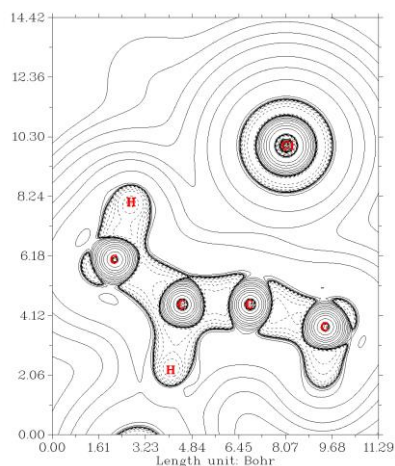
The Laplacian of the electron density is the trace of the Hessian matrix. The topology of Laplacian of electron density can be almost faithfully mapped onto the electron pairs of the VSEPR model.²⁴ The whole analyses are calculated by Multiwfn program.²⁵ The contour maps of electron density Laplacian of transition states in the selected hydrohalogenation of alkynes without contributions of unimportant atoms can help to find out whether two atoms contribute the covalent bond in the transition states. We lay out some analysis graphs of the selected transition states below. It is obvious that the C atom in the triple bond and the halogen atom in HX have almost no effect from the electron density, revealing that the hydrohalogenations proceed through intimate ion-pair mechanism with asynchronous concerted characteristic.

References

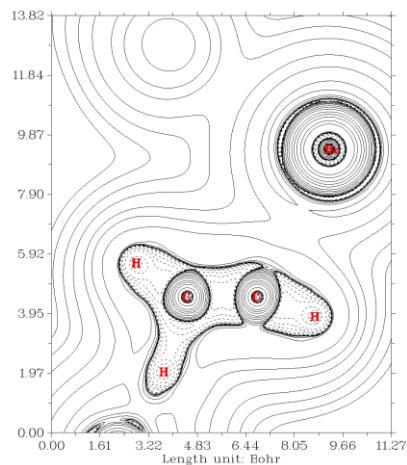
- 24 P. L. A Popelier, *Coord. Chem. Rev.*, 2000, 197, 169–189.
25 T. Lu and F. W. Chen, *J. Comput. Chem.*, 2012, 33, 580–592.



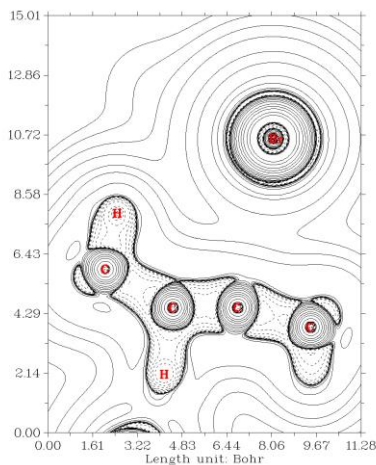
TS2a



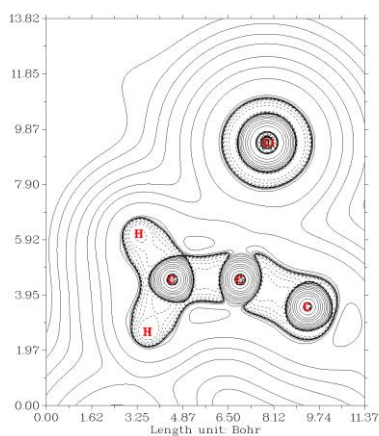
TS2b



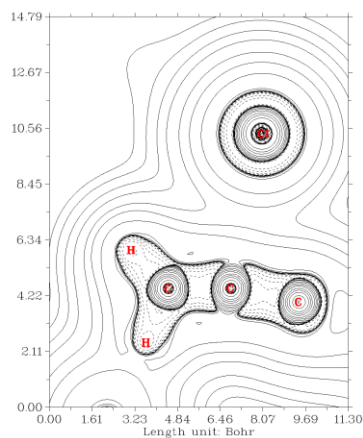
TS4a



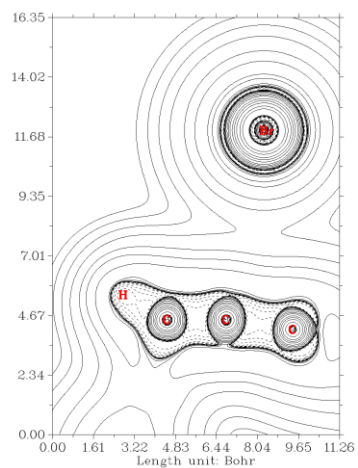
TS4b



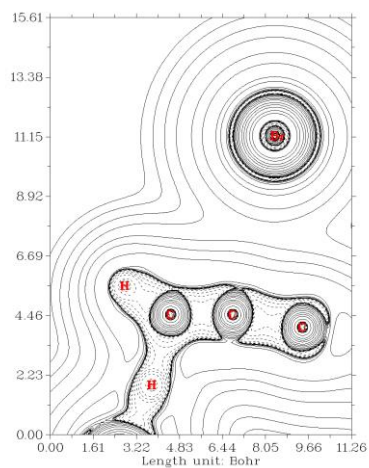
TS10a



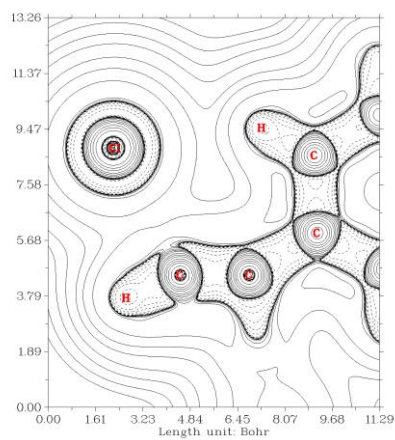
TS10b



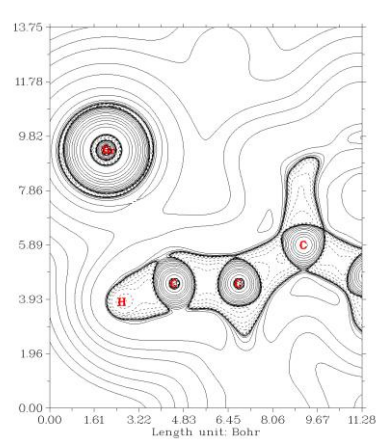
TS'12a



TS'12b



TS18a



TS20a

Figure S3. Electron localization function analyses and drawings in the contour maps without contributions of unimportant atoms.

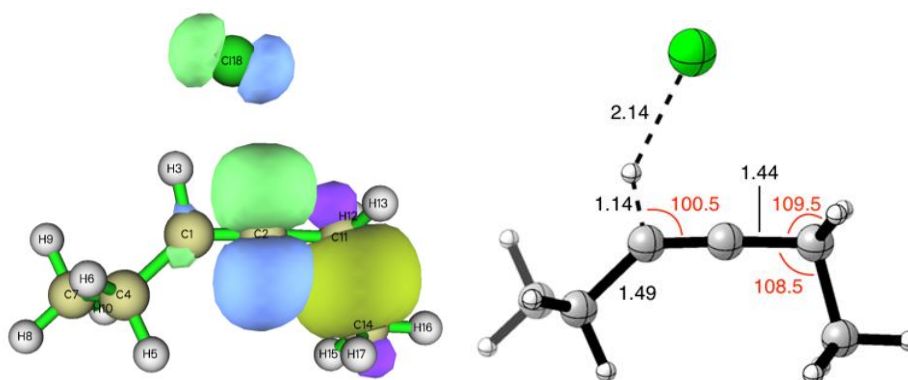
8. Calculations on Natural Bond Orbital (NBO) Methods Analysis

Natural bond orbital (NBO) methods refers to a suite of mathematical algorithms for analyzing electronic wavefunctions in the language of localized Lewis-like chemical bonds.²⁶ We use it to translate accurate calculations into chemical insights. Such insights are formulated in terms of commonly understood bonding concepts such as Lewis structures. In our works, some of hyperconjugations worth careful considering are presented and labeled in red in the following tables. Generally, the low bond energy reveals that the bond is more stable in great bond order. For example, in TS1b, the bond order of C2-C11 increases due to decrease of its bond energy (-0.78737 a.u.), while the bond order of C11-C14 decreases because the bond energy of C11-C14 increases (-0.63118 a.u.), revealing that the hyperconjugation exists between the alkenic carbocation and the methyl group. Of course, the bond energies are also impacted by steric hindrance in some cases. Whole picture are drawn by Multiwfn²⁷ program and CYLview program.

References

- 26 E. D. Glendening, C. R. Landis and F. Weinhold, WIREs. Comput. Mol. Sci. 2012, 2, 1-42.
 27 T. Lu and F. W. Chen, J. Comput. Chem., 2012, 33, 580–592.
 28 Legault, C. Y, CYLview20, Université de Sherbrooke, 2020 (<http://www.cylview.org>).

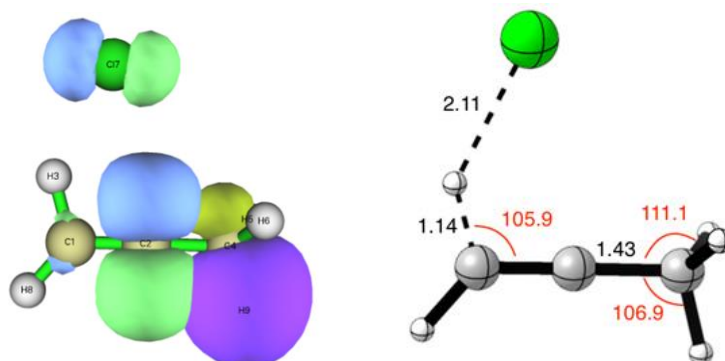
1. TS1b



Natural Bond Orbitals	Occupancy	Energy	Principal Delocalizations
1. BD (1) C 1 - C 2	1.98418	-0.88800	167(v),275(g),90(v),274(g),276(g),91(v)
2. BD (2) C 1 - C 2	1.96071	-0.34432	285(v),284(v),279(v),280(v),168(v),92(v)
3. BD (1) C 1 - H 3	1.80789	-0.50380	277(v),276(v),59(v),272(g),278(v),274(g),91(v),66(v)
4. BD (1) C 1 - C 4	1.94601	-0.68060	276(v),277(v),272(g),274(g),281(v),60(v),59(v)
5. BD (1) C 2 - C 11	1.98923	-0.78737	34(v),275(v),272(g),288(v),33(v),35(v),274(v),203(v)
6. BD (1) C 2 - Cl 18	1.95134	-0.21555	274(v),286(v),275(v)
7. BD (1) C 4 - H 5	1.98092	-0.53958	274(v),282(v),33(v)
8. BD (1) C 4 - H 6	1.96855	-0.53157	273(v),272(v),283(v),35(v),126(v)
9. BD (1) C 4 - C 7	1.97952	-0.64117	273(v),272(v)
10. BD (1) C 7 - H 8	1.98349	-0.52346	275(v),92(v)
11. BD (1) C 7 - H 9	1.98958	-0.52406	278(v)
12. BD (1) C 7 - H 10	1.99025	-0.52593	279(v)
13. BD (1) C 11 - H 12	1.95288	-0.54458	273(v),272(v),277(v),289(v),60(v)
14. BD (1) C 11 - H 13	1.95515	-0.54531	273(v),272(v),277(v),287(v),61(v)
15. BD (1) C 11 - C 14	1.92504	-0.63118	277(v) ,272(v),59(v),276(g)

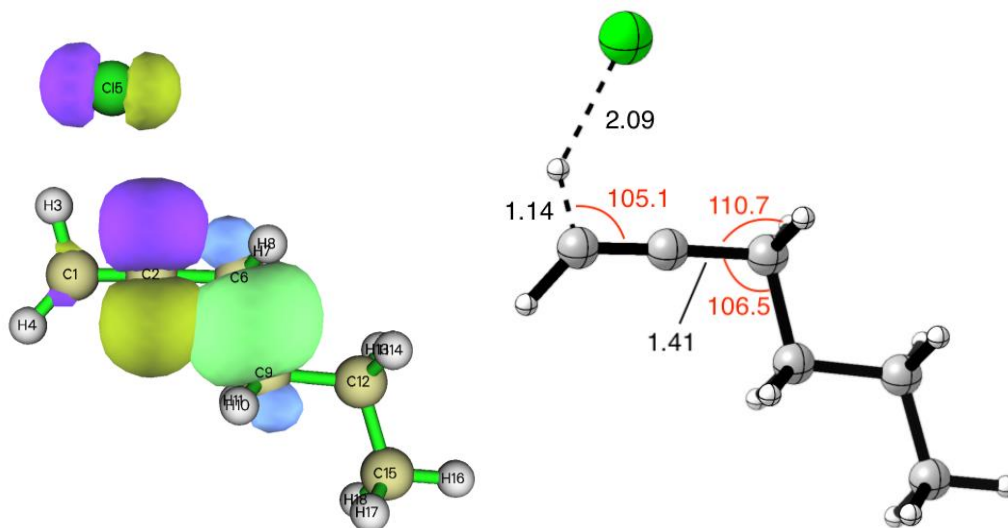
16. BD (1) C 14 - H 15	1.99165	-0.55496	285(v),277(r),171(v)
17. BD (1) C 14 - H 16	1.97798	-0.54551	276(v),277(r)
18. BD (1) C 14 - H 17	1.99181	-0.55505	284(v),277(r)

2. TS1c



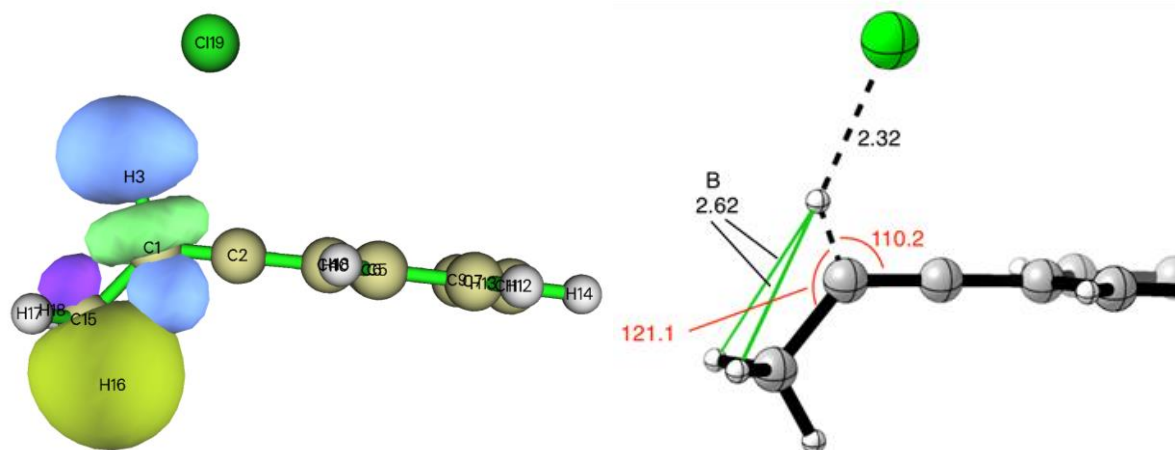
Natural Bond Orbitals	Occupancy	Energy	Principal Delocalizations
1. BD (1) C 1 - C 2	1.99131	-0.90822	78(v),155(g),156(g),154(g),48(g)
2. BD (2) C 1 - C 2	1.97433	-0.36033	158(v),159(v),79(v)
3. BD (1) C 1 - H 3	1.83431	-0.53319	157(v),156(v),47(v),152(g),154(g)
4. BD (1) C 1 - H 8	1.93539	-0.60291	157(v),156(v),48(v),152(g),47(v)
5. BD (1) C 2 - C 4	1.99436	-0.81907	21(v),22(v),152(g),155(v),154(v)
6. BD (1) C 2 - Cl 7	1.93697	-0.22576	154(v),155(v),160(v),157(g)
7. BD (1) C 4 - H 5	1.95708	-0.57128	153(v),152(v),157(v),49(v)
8. BD (1) C 4 - H 6	1.95708	-0.57128	153(v),152(v),157(v),49(v)
9. BD (1) C 4 - H 9	1.90834	-0.56451	157(v) ,152(v),47(v)

3. TS1d



Natural Bond Orbitals	Occupancy	Energy	Principal Delocalizations
1. BD (1) C 1 - C 2	1.99085	-0.89876	123(v),275(g),277(g),274(g),126(v)
2. BD (2) C 1 - C 2	1.97313	-0.35095	278(v),279(v),124(v)
3. BD (1) C 1 - H 3	1.83026	-0.52145	276(v),277(v),59(v),272(g),274(g)
4. BD (1) C 1 - H 4	1.93641	-0.59594	276(v),277(v),272(g),60(v),59(v)
5. BD (1) C 2 - Cl 5	1.93865	-0.21825	274(v),275(v),280(v),276(g)
6. BD (1) C 2 - C 6	1.98926	-0.79881	33(v),283(v),34(v),272(g),275(v),160(v),85(r)
7. BD (1) C 6 - H 7	1.95172	-0.55062	273(v),272(v),276(v),281(v),61(v)
8. BD (1) C 6 - H 8	1.95172	-0.55062	273(v),272(v),276(v),282(v),61(v)
9. BD (1) C 6 - C 9	1.91138	-0.61937	276(v) ,272(v),286(v),59(v),277(g),195(v)
10. BD (1) C 9 - H 10	1.98322	-0.54631	284(v),278(v),276(r)
11. BD (1) C 9 - H 11	1.98322	-0.54631	285(v),279(v),276(r)
12. BD (1) C 9 - C 12	1.97518	-0.64097	287(v),277(v),125(v)
13. BD (1) C 12 - H 13	1.97930	-0.52396	281(v),288(v)
14. BD (1) C 12 - H 14	1.97930	-0.52396	282(v),289(v)
15. BD (1) C 12 - C 15	1.98635	-0.63476	280(v),159(v)
16. BD (1) C 15 - H 16	1.98640	-0.52240	283(v),195(v)
17. BD (1) C 15 - H 17	1.98997	-0.52519	284(v)
18. BD (1) C 15 - H 18	1.98997	-0.52519	285(v)

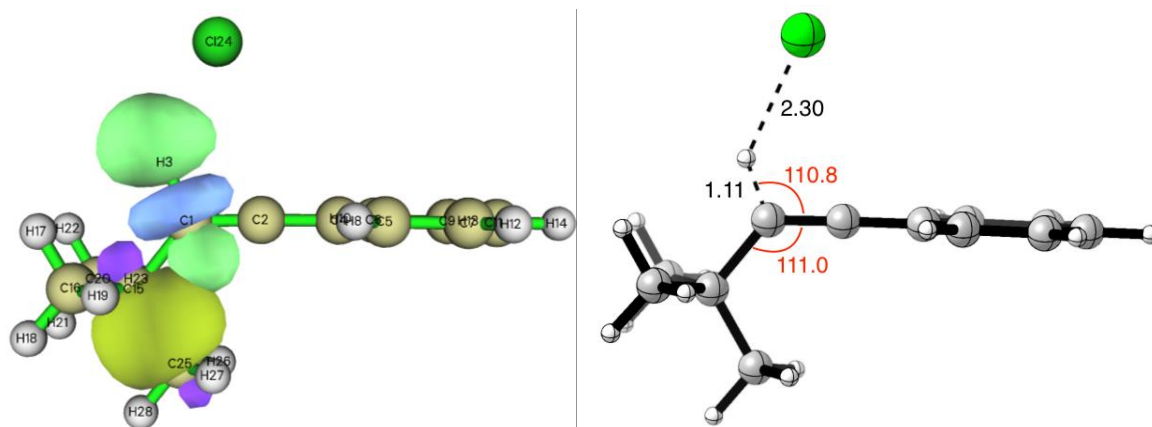
4. TS5b



Natural Bond Orbitals	Occupancy	Energy	Principal Delocalizations
1. BD (1) C 1 - C 2	1.98769	-0.86355	100(v),353(g),352(g),351(g),281(v),...
2. BD (2) C 1 - C 2	1.95791	-0.3255	354(v),355(v),369(v),370(v),101(v),...
3. BD (1) C 1 - H 3	1.88773	-0.51826	37(v),353(v),349(g),68(v),368(v),...
4. BD (1) C 1 - C 15	1.95273	-0.67279	37(v),353(v),349(g),68(v),351(g),...
5. BD (1) C 2 - C 4	1.98205	-0.81302	42(v),349(g),355(g),354(g),357(v),...
6. BD (1) C 4 - C 5	1.97051	-0.73249	349(v),353(g),363(v),350(v),361(v),...
7. BD (1) C 4 - C 6	1.97052	-0.73249	349(v),353(g),366(v),350(v),359(v),...
8. BD (2) C 4 - C 6	1.51997	-0.28761	37(v),358(v),365(v),356(g),128(v),68(v)
9. BD (1) C 5 - C 7	1.98371	-0.76423	353(v),367(v),362(g),99(v),354(g),...

10. BD (2) C 5 - C 7	1.65168	-0.29975	365(v),356(v),241(v)
11. BD (1) C 5 - H 8	1.97945	-0.56693	355(v),362(v),99(v),177(v)
12. BD (1) C 6 - C 9	1.98371	-0.76423	353(v),367(v),364(g),99(v),355(g),...
13. BD (1) C 6 - H 10	1.97945	-0.56693	354(v),364(v),99(v),208(v)
14. BD (1) C 7 - C 11	1.98396	-0.75162	359(v),366(v),357(g),364(g),126(v),...
15. BD (1) C 7 - H 12	1.97634	-0.56088	354(v),364(v),125(v),239(v),203(r)
16. BD (1) C 9 - C 11	1.98396	-0.75162	361(v),363(v),360(g),362(g),178(v),...
17. BD (2) C 9 - C 11	1.58411	-0.2952	356(v),358(v),179(v)
18. BD (1) C 9 - H 13	1.97634	-0.56088	355(v),362(v),151(v),239(v),234(r)
19. BD (1) C 11 - H 14	1.97848	-0.56482	357(v),360(v),208(v),177(v),275(g),...
20. BD (1) C 15 - H 16	1.99097	-0.54232	351(v) ,43(v)
21. BD (1) C 15 - H 17	1.97580	-0.53376	350(v),349(v)
22. BD (1) C 15 - H 18	1.97580	-0.53376	350(v),349(v)

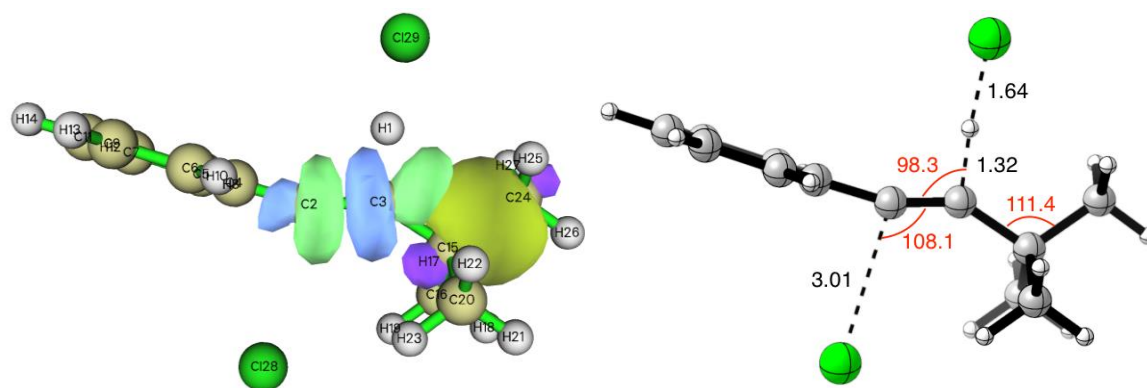
5. TS5e



Natural Bond Orbitals	Occupancy	Energy	Principal Delocalizations
1. BD (1) C 1 - C 2	1.98549	-0.85815	112(v),473(g),472(g),292(v),471(g),...
2. BD (2) C 1 - C 2	1.95749	-0.32008	474(v),476(v),488(v),489(v),113(v),...
3. BD (1) C 1 - H 3	1.88586	-0.51206	49(v),473(v),490(v),469(g),292(v),...
4. BD (1) C 1 - C 15	1.92658	-0.63593	49(v),473(v),469(g),492(v),494(v),...
5. BD (1) C 2 - C 4	1.98228	-0.80828	54(v),469(g),474(g),476(g),477(v),...
6. BD (1) C 4 - C 5	1.97044	-0.72947	469(v),473(g),484(v),470(v),481(v),...
7. BD (2) C 4 - C 5	1.52277	-0.28498	49(v),480(v),483(v),475(g),165(v),...
8. BD (1) C 4 - C 6	1.97043	-0.72947	469(v),473(g),486(v),470(v),478(v),...
9. BD (1) C 5 - C 7	1.98361	-0.7614	473(v),487(v),482(g),111(v),474(g),...
10. BD (1) C 5 - H 8	1.97929	-0.56488	476(v),482(v),111(v),189(v)
11. BD (1) C 6 - C 9	1.98361	-0.7614	473(v),487(v),485(g),111(v),476(g),...
12. BD (2) C 6 - C 9	1.65126	-0.29749	483(v),475(v),253(v)
13. BD (1) C 6 - H 10	1.9793	-0.56488	474(v),485(v),111(v),220(v)
14. BD (1) C 7 - C 11	1.98393	-0.74917	478(v),486(v),477(g),485(g),138(v),...
15. BD (2) C 7 - C 11	1.58709	-0.29318	475(v),480(v),222(v),143(v)
16. BD (1) C 7 - H 12	1.97644	-0.55933	474(v),485(v),137(v),251(v),215(r),...

17. BD (1) C 9 - C 11	1.98393	-0.74917	481(v),484(v),479(g),164(v),482(g),...
18. BD (1) C 9 - H 13	1.97645	-0.55933	476(v),482(v),163(v),251(v),246(r),...
19. BD (1) C 11 - H 14	1.97833	-0.56293	477(v),479(v),189(v),220(v),287(g),...
20. BD (1) C 15 - C 16	1.96925	-0.61671	470(v),469(v),497(v),496(v),56(v),...
21. BD (1) C 15 - C 20	1.96925	-0.61671	470(v),469(v),498(v),493(v),56(v),...
22. BD (1) C 15 - C 25	1.9803	-0.62555	471(v) ,491(v),495(v),472(g)
23. BD (1) C 16 - H 17	1.98785	-0.51218	490(v),293(v),294(v)
24. BD (1) C 16 - H 18	1.9828	-0.5125	472(v),296(v)
25. BD (1) C 16 - H 19	1.9883	-0.51371	489(v),295(v),292(v)
26. BD (1) C 20 - H 21	1.9828	-0.5125	472(v),296(v)
27. BD (1) C 20 - H 22	1.98785	-0.51218	490(v),293(v),294(v)
28. BD (1) C 20 - H 23	1.9883	-0.51371	488(v),295(v),292(v)
29. BD (1) C 25 - H 26	1.98733	-0.5195	488(v),49(r),293(v)
30. BD (1) C 25 - H 27	1.98733	-0.5195	489(v),49(r),293(v)
31. BD (1) C 25 - H 28	1.98684	-0.51798	472(v),292(v)

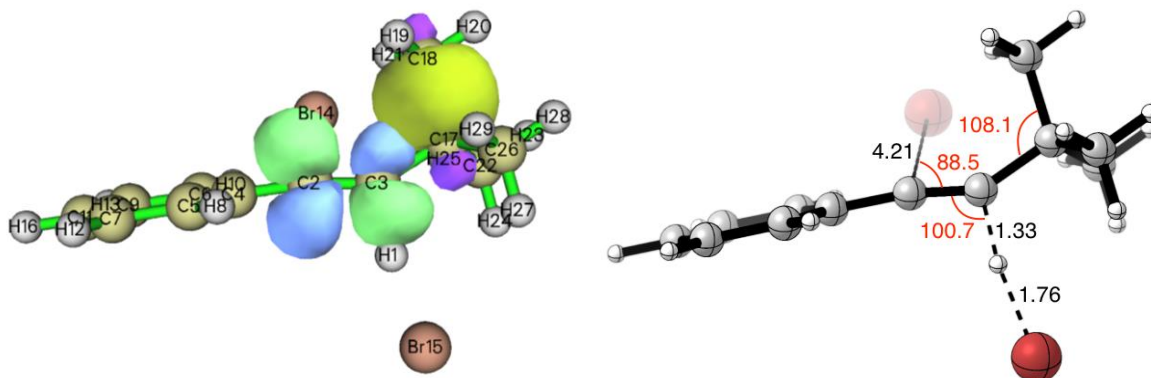
6. TS'6e



Natural Bond Orbitals	Occupancy	Energy	Principal Delocalizations
1. BD (1) C 2 - C 3	1.98364	-0.72443	54(r),121(v),510(g),509(g),302(v),...
2. BD (2) C 2 - C 3	1.96348	-0.18137	511(v),512(v),526(v),525(v),122(v),...
3. BD (3) C 2 - C 3	1.66314	-0.19301	54(r),513(v),63(r),508(g),527(v),...
4. BD (1) C 2 - C 4	1.97772	-0.62877	506(g),510(v),514(v),517(v),508(g),...
5. BD (1) C 3 - C 15	1.94995	-0.53369	54(r),506(g),531(v),529(v),535(v),...
6. BD (1) C 4 - C 5	1.97147	-0.59952	506(v),509(g),518(v),507(v),512(g),...
7. BD (1) C 4 - C 6	1.97164	-0.59951	506(v),509(g),516(v),511(g),507(v),...
8. BD (2) C 4 - C 6	1.58626	-0.14832	508(v),522(v),148(v),231(v)
9. BD (1) C 5 - C 7	1.98203	-0.61915	509(v),511(g),519(g),120(v),260(v),...
10. BD (2) C 5 - C 7	1.65928	-0.16116	522(v),513(v),262(v)
11. BD (1) C 5 - H 8	1.97877	-0.42635	512(v),519(v),120(v),198(v)
12. BD (1) C 6 - C 9	1.98203	-0.61896	509(v),524(v),512(g),521(g),120(v),...
13. BD (1) C 6 - H 10	1.97874	-0.42592	511(v),521(v),120(v),229(v)
14. BD (1) C 7 - C 11	1.983	-0.61811	523(v),516(v),514(g),521(g),147(v),...
15. BD (1) C 7 - H 12	1.97728	-0.43298	511(v),521(v),146(v),260(v),286(g),...

16. BD (1) C 9 - C 11	1.98301	-0.61808	520(v),518(v),517(g),519(g),173(v),...
17. BD (2) C 9 - C 11	1.65825	-0.16519	513(v),515(v),200(v),174(v),
18. BD (1) C 9 - H 13	1.97727	-0.43279	512(v),519(v),172(v),260(v),291(g),...
19. BD (1) C 11 - H 14	1.97833	-0.43666	514(v),517(v),229(v),198(v),296(g),...
20. BD (1) C 15 - C 16	1.96654	-0.47869	508(v),507(v),534(v),532(v),506(v),...
21. BD (1) C 15 - C 20	1.96631	-0.47962	508(v),507(v),536(v),528(v),506(v),...
22. BD (1) C 15 - C 24	1.98208	-0.49061	506(v) ,530(v),533(v),54(r)
23. BD (1) C 16 - H 17	1.98838	-0.38285	526(v),301(v),304(v)
24. BD (1) C 16 - H 18	1.9838	-0.38319	510(v),306(v)
25. BD (1) C 16 - H 19	1.98793	-0.37282	527(v),303(v),450(r),451(r),54(r)
26. BD (1) C 20 - H 21	1.98393	-0.38472	510(v),306(v)
27. BD (1) C 20 - H 22	1.98841	-0.38434	525(v),301(v),304(v)
28. BD (1) C 20 - H 23	1.98799	-0.37454	527(v),303(v),452(r),54(r),450(r),...
29. BD (1) C 24 - H 25	1.98871	-0.38681	525(v),303(v),308(v),54(r),480(r)
30. BD (1) C 24 - H 26	1.98704	-0.39129	510(v),305(v)
31. BD (1) C 24 - H 27	1.98863	-0.38703	526(v),303(v),308(v),54(r)

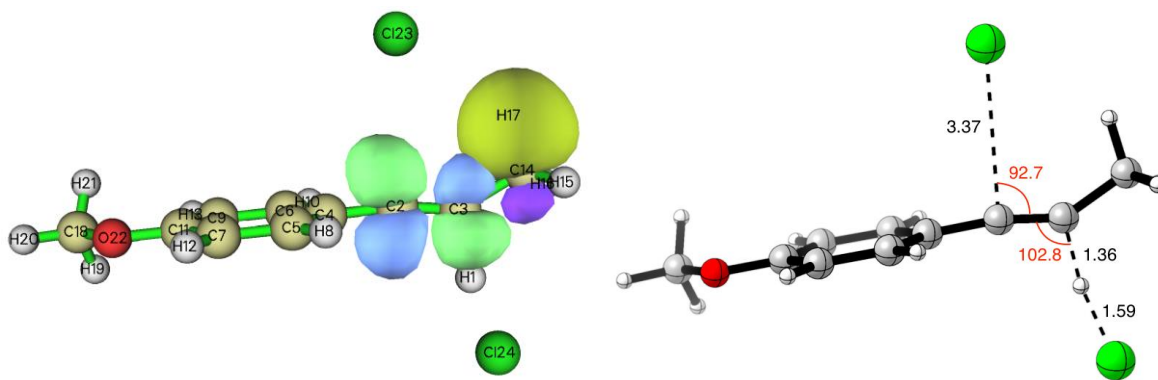
7. TS'8e



Natural Bond Orbitals	Occupancy	Energy	Principal Delocalizations
2. BD (1) C 2 - C 3	1.9817	-0.75327	527(r),...
3. BD (2) C 2 - C 3	1.96269	-0.20562	535(v),...
4. BD (3) C 2 - C 3	1.66909	-0.21558	527(r),...
5. BD (1) C 2 - C 4	1.97707	-0.65469	528(g),...
6. BD (1) C 3 - C 17	1.94601	-0.55824	527(r),...
7. BD (1) C 4 - C 5	1.97323	-0.62243	528(v),...
8. BD (2) C 4 - C 5	1.60334	-0.17615	530(v),...
9. BD (1) C 4 - C 6	1.97055	-0.61145	528(v),...
10. BD (1) C 5 - C 7	1.98269	-0.64404	531(v),...
11. BD (1) C 5 - H 8	1.97776	-0.45166	535(v),...
12. BD (1) C 6 - C 9	1.98216	-0.62965	531(v),...
13. BD (2) C 6 - C 9	1.61734	-0.17086	542(v),...
14. BD (1) C 6 - H 10	1.97524	-0.41961	533(v),...
15. BD (1) C 7 - C 11	1.98327	-0.63732	537(v),...

16. BD (2) C 7 - C 11	1.64441	-0.18476	534(v),...
17. BD (1) C 7 - H 12	1.97736	-0.45332	533(v),...
18. BD (1) C 9 - C 11	1.9841	-0.6341	543(v),...
19. BD (1) C 9 - H 13	1.97709	-0.44071	541(v),...
20. BD (1) C 11 - H 16	1.97863	-0.45372	536(v),...
21. BD (1) C 17 - C 18	1.96594	-0.49677	530(v),...
22. BD (1) C 17 - C 22	1.96805	-0.49165	529(v),...
23. BD (1) C 17 - C 26	1.97484	-0.5052	528(v),...
24. BD (1) C 18 - H 19	1.98882	-0.39833	548(v),...
25. BD (1) C 18 - H 20	1.98394	-0.39705	532(v),...
26. BD (1) C 18 - H 21	1.98783	-0.38659	549(v),...
27. BD (1) C 22 - H 23	1.98311	-0.38842	532(v),...
28. BD (1) C 22 - H 24	1.98758	-0.38622	547(v),...
29. BD (1) C 22 - H 25	1.98687	-0.37686	378(v),...
30. BD (1) C 26 - H 27	1.98849	-0.40402	380(v),...
31. BD (1) C 26 - H 28	1.98502	-0.40676	382(v),...
32. BD (1) C 26 - H 29	1.9891	-0.40720	378(v),...

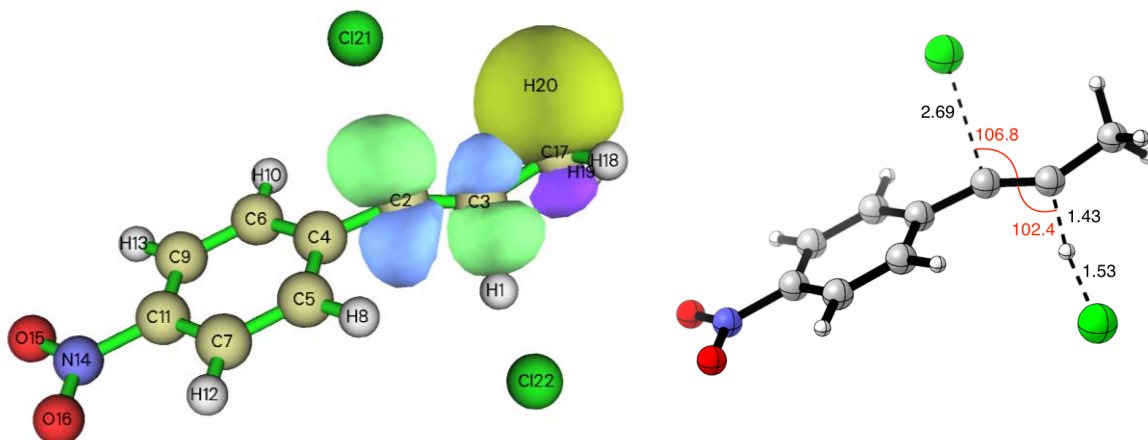
8. TS'14a



1. BD (1) C 2 - C 3	1.98398	-0.7307	48(r),...
2. BD (2) C 2 - C 3	1.96183	-0.18014	462(v),...
3. BD (3) C 2 - C 3	1.67758	-0.18343	48(r),...
4. BD (1) C 2 - C 4	1.97734	-0.63694	456(g),...
5. BD (1) C 3 - C 14	1.9668	-0.55737	48(r),...
6. BD (1) C 4 - C 5	1.97172	-0.6022	456(v),...
7. BD (1) C 4 - C 6	1.97175	-0.60556	456(v),...
8. BD (2) C 4 - C 6	1.59826	-0.15504	458(v),...
9. BD (1) C 5 - C 7	1.98034	-0.6376	474(v),...
10. BD (2) C 5 - C 7	1.71192	-0.1751	472(v),...
11. BD (1) C 5 - H 8	1.97657	-0.4344	462(v),...
12. BD (1) C 6 - C 9	1.97871	-0.63438	474(v),...
13. BD (1) C 6 - H 10	1.97846	-0.43353	461(v),...
14. BD (1) C 7 - C 11	1.97558	-0.62369	481(v),...

15. BD (1) C 7 - H 12	1.97496	-0.44189	471(v),...
16. BD (1) C 9 - C 11	1.98233	-0.63479	468(v),...
17. BD (2) C 9 - C 11	1.64329	-0.18344	463(v),...
18. BD (1) C 9 - H 13	1.97435	-0.45258	469(v),...
19. BD (1) C 11 - O 22	1.99147	-0.85033	335(v),...
20. BD (1) C 14 - H 15	1.97452	-0.38957	457(v),...
21. BD (1) C 14 - H 16	1.97642	-0.38884	457(v),...
22. BD (1) C 14 - H 17	1.97217	-0.37603	458(v),...
23. BD (1) C 18 - H 19	1.99438	-0.47358	374(v),...
24. BD (1) C 18 - H 20	1.99129	-0.47197	474(v),...
25. BD (1) C 18 - H 21	1.99435	-0.4725	374(v),...
26. BD (1) C 18 - O 22	1.99196	-0.75469	469(v),...

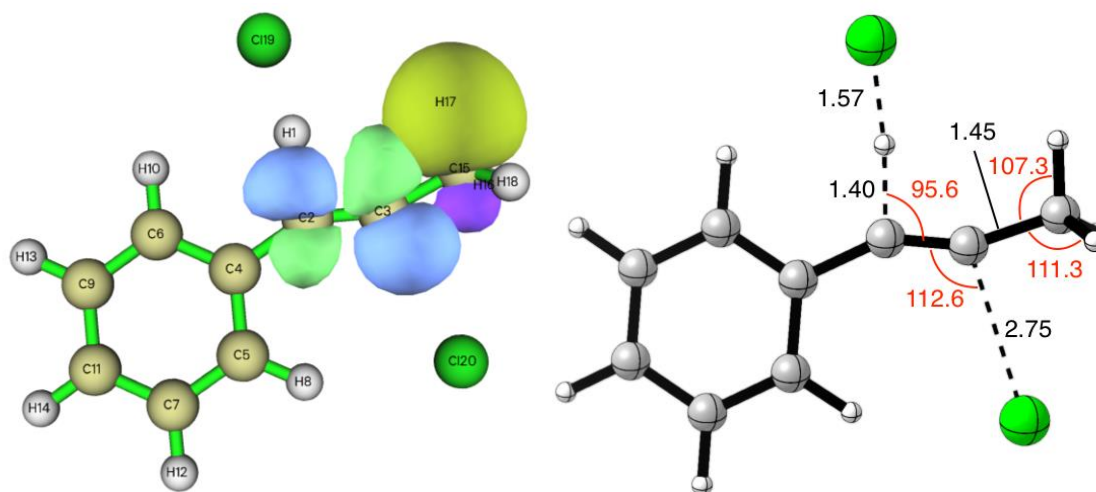
9. TS'14d



1. BD (1) C 2 - C 3	1.9855	-0.73491	48(r),...
2. BD (2) C 2 - C 3	1.92901	-0.18591	476(v),...
3. BD (3) C 2 - C 3	1.71265	-0.19706	48(r),...
4. BD (1) C 2 - C 4	1.97823	-0.62957	474(v),...
5. BD (1) C 3 - C 17	1.97468	-0.57519	48(r),...
6. BD (1) C 4 - C 5	1.96845	-0.61655	470(v),...
7. BD (2) C 4 - C 5	1.5838	-0.16716	484(v),...
8. BD (1) C 4 - C 6	1.97407	-0.61633	470(v),...
9. BD (1) C 5 - C 7	1.97704	-0.63692	488(v),...
10. BD (1) C 5 - H 8	1.9786	-0.43918	477(v),...
11. BD (1) C 6 - C 9	1.97758	-0.63522	488(v),...
12. BD (2) C 6 - C 9	1.65254	-0.17495	484(v),...
13. BD (1) C 6 - H 10	1.97518	-0.42674	475(v),...
14. BD (1) C 7 - C 11	1.9796	-0.64782	486(g),...
15. BD (2) C 7 - C 11	1.65047	-0.19193	490(v),...
16. BD (1) C 7 - H 12	1.97416	-0.44976	486(v),...
17. BD (1) C 9 - C 11	1.97954	-0.64422	483(g),...
18. BD (1) C 9 - H 13	1.97443	-0.44681	483(v),...

19. BD (1) C 11 - N 14	1.98866	-0.72305	478(v),...
20. BD (1) N 14 - O 15	1.99643	-1.00104	260(v),...
21. BD (2) N 14 - O 15	1.98658	-0.3739	53(v),...
22. BD (1) N 14 - O 16	1.99643	-1.00078	260(v),...
23. BD (1) C 17 - H 18	1.97548	-0.40724	471(v),...
24. BD (1) C 17 - H 19	1.97457	-0.40703	471(v),...
25. BD (1) C 17 - H 20	1.97447	-0.39844	472(v),...

10. TS'18b



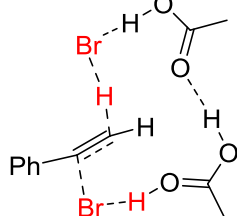
Natural Bond Orbitals	Occupancy	Energy	Principal Delocalizations
2. BD (1) C 2 - C 3	1.98314	-0.71801	385(r),...
3. BD (2) C 2 - C 3	1.92021	-0.17538	393(v),...
4. BD (3) C 2 - C 3	1.70887	-0.19081	385(r),...
5. BD (1) C 2 - C 4	1.96567	-0.57991	385(r),...
6. BD (1) C 3 - C 15	1.9907	-0.60218	389(v),...
7. BD (1) C 4 - C 5	1.97145	-0.58088	388(v),...
8. BD (1) C 4 - C 6	1.97859	-0.5911	386(v),...
9. BD (2) C 4 - C 6	1.62927	-0.1414	402(v),...
10. BD (1) C 5 - C 7	1.98045	-0.59668	389(v),...
11. BD (2) C 5 - C 7	1.65501	-0.14293	402(v),...
12. BD (1) C 5 - H 8	1.9771	-0.39309	392(v),...
13. BD (1) C 6 - C 9	1.98138	-0.60158	389(v),...
14. BD (1) C 6 - H 10	1.97853	-0.40931	391(v),...
15. BD (1) C 7 - C 11	1.98344	-0.60265	403(v),...
16. BD (1) C 7 - H 12	1.97773	-0.41559	391(v),...
17. BD (1) C 9 - C 11	1.98317	-0.60552	400(v),...
18. BD (2) C 9 - C 11	1.68454	-0.15442	393(v),...
19. BD (1) C 9 - H 13	1.97802	-0.42051	392(v),...
20. BD (1) C 11 - H 14	1.97861	-0.42373	397(v),...

21. BD (1) C 15 - H 16	1.96939	-0.39657	387(v),...
22. BD (1) C 15 - H 17	1.95041	-0.39550	388(v),...
23. BD (1) C 15 - H 18	1.96934	-0.39665	387(v),...

Figure S4. Hyperconjugations described by Natural Bond Orbital (NBO) Methods analyses

9. Coordinates of Cyclic Transition States in *anti*-Hydrobromination in Gas Phase

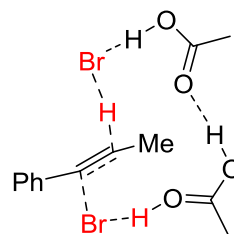
Coordinates of all cyclic transition states **TS8g**, **TS12g**, and **TS16g** in the *anti*-additions in hydrobrominations of 1-arylalk-1-ynes in gas phase are provided as following. These transition states cannot be located on the optimization in acetic acid solution.



TS8ga

H	-0.16061300	1.31195200	-2.16995300
H	0.86215700	-2.11295000	0.11186500
C	2.81772100	-1.59005700	0.21647600
O	1.60325900	-1.32819100	0.45330500
O	3.68697900	-0.65561700	0.25560200
H	3.23211600	0.30028900	0.32172800
C	3.27874500	-2.96978800	-0.09509100
H	4.30787300	-2.96036900	-0.44025500
H	3.19324900	-3.57941900	0.80689000
H	2.60964900	-3.41359400	-0.83392100
C	1.72164500	1.94325400	1.01024300
O	2.53344600	1.53609600	0.17862300
O	0.76592700	2.77669000	0.71652700
H	0.71400000	2.97100500	-0.27763200
C	1.74257000	1.50172600	2.44473800
H	1.06491600	2.09474200	3.05214300
H	1.44283300	0.45236200	2.48263200
H	2.75791800	1.57021000	2.83359200
C	-1.11796100	-0.22663300	-1.20822700
C	-0.22992600	0.12511200	-2.02068100
H	0.50223200	-0.43449000	-2.57699700
C	-2.16978000	-0.25180800	-0.29737900
C	-1.91201200	-0.12245200	1.08139400
C	-3.49507400	-0.38466900	-0.75388300
C	-2.96104700	-0.11739000	1.97700800
H	-0.88906900	-0.03556600	1.41555300
C	-4.53590400	-0.38141100	0.15432000

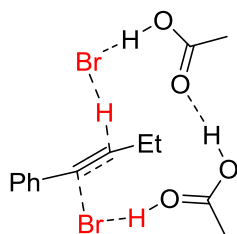
H	-3.67735500	-0.48993100	-1.81383900
C	-4.27020900	-0.24890400	1.51526000
H	-2.76878900	-0.01563900	3.03637400
H	-5.55552900	-0.48238700	-0.19151400
H	-5.08924600	-0.24909500	2.22270600
Br	-0.35201400	-3.19878300	-0.62778100
Br	0.20604800	3.21806200	-2.33384000



TS8gb

H	0.26567200	1.22161500	1.96027500
H	-0.85359300	-2.03476500	-0.49566800
C	-2.78072000	-1.49299200	-0.52781100
O	-1.56559500	-1.24784700	-0.79931400
O	-3.61955400	-0.53604900	-0.48836500
H	-3.13161200	0.42067000	-0.49513300
C	-3.26067900	-2.87575500	-0.26828000
H	-4.26838500	-2.86090400	0.13496000
H	-3.24415500	-3.43301300	-1.20751900
H	-2.56243100	-3.37767500	0.40377200
C	-1.62997000	2.06328400	-1.09162800
O	-2.41290900	1.59552400	-0.25932400
O	-0.67360600	2.88212100	-0.77621900
H	-0.58294800	3.01445100	0.22975700
C	-1.69536100	1.70916700	-2.54797800
H	-1.08325800	2.37958200	-3.14438200
H	-1.33039200	0.68632200	-2.66416900
H	-2.72959100	1.73424500	-2.88861200
C	1.07188400	-0.32215600	1.02707700

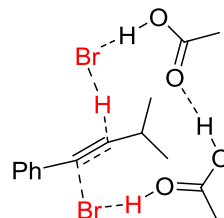
C	0.14443100	0.04047400	1.79115800
C	2.20005700	-0.29630100	0.20028700
C	2.06910600	0.05385300	-1.15569300
C	3.47022600	-0.59824300	0.72231800
C	3.18727500	0.10973700	-1.96434500
H	1.08700900	0.27772800	-1.54534600
C	4.58161400	-0.54420400	-0.09727100
H	3.55704000	-0.87521000	1.76329000
C	4.44137600	-0.19149200	-1.43736500
H	3.08947500	0.38532600	-3.00568200
H	5.55952400	-0.77579000	0.30247400
H	5.31468600	-0.15105400	-2.07534800
C	-1.04329300	-0.51287400	2.48486300
H	-0.96205200	-0.32748900	3.55645500
H	-1.93532400	0.01058200	2.13747800
H	-1.11773900	-1.58320500	2.29813800
Br	-0.02662100	3.13915100	2.25878200
Br	0.35448300	-3.16584500	0.29335200



TS8gc

H	0.12852900	1.27571600	1.75611300
H	-0.73766700	-2.01713400	-0.76383500
C	-2.66305400	-1.49192300	-0.94413300
O	-1.43408500	-1.23777400	-1.12782200
O	-3.51259400	-0.54351000	-0.97934500
H	-3.03748200	0.41579400	-0.96275800
C	-3.14922800	-2.87593000	-0.70336500
H	-4.18359200	-2.86539300	-0.37430500
H	-3.06037100	-3.44358600	-1.63226700
H	-2.49739500	-3.36407900	0.02316700
C	-1.49283800	2.07126700	-1.43850700
O	-2.35318400	1.60959600	-0.68386000

O	-0.57760800	2.90151400	-1.03852300
H	-0.59183500	3.04541900	-0.03153200
C	-1.40730000	1.69911700	-2.88926000
H	-0.74224000	2.36708100	-3.42907200
H	-1.02608400	0.67774500	-2.95441300
H	-2.40178100	1.71201300	-3.33325000
C	1.04676400	-0.25870600	0.90652500
C	0.04450600	0.09636500	1.57225600
C	2.24725200	-0.24435400	0.18958700
C	2.24572600	0.08341700	-1.17841200
C	3.46215200	-0.53700500	0.83441700
C	3.43547700	0.12603300	-1.87831100
H	1.30528100	0.30007700	-1.66328800
C	4.64616500	-0.49615000	0.12297900
H	3.44968400	-0.79659600	1.88337700
C	4.63376300	-0.16584300	-1.23004400
H	3.43698400	0.38370400	-2.92878400
H	5.58156200	-0.72086600	0.61721600
H	5.56354200	-0.13583500	-1.78315600
C	-1.19560000	-0.47377000	2.17210700
H	-2.04046500	0.07430200	1.74827900
H	-1.25809200	-1.52187900	1.87627000
C	-1.20743300	-0.33121100	3.69452700
H	-1.12103000	0.71556000	3.98537700
H	-2.14178200	-0.72469800	4.09713700
H	-0.38199300	-0.88649500	4.14126500
B	-0.24025700	3.18799000	2.04787900
Br	0.41324000	-3.13314600	0.11654600

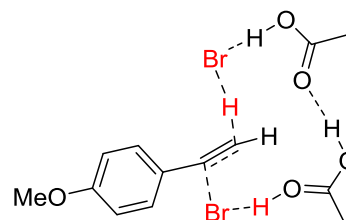


TS8gd

H	-0.02683700	1.21429700	1.77450500
H	0.74185600	-0.04028500	-2.17323900

C	2.44409100	-0.98570400	-1.69869600
O	1.18330300	-0.87287000	-1.60317600
O	3.07681200	-1.67285400	-0.83530300
H	2.46961800	-1.88378800	0.02948300
C	3.20250700	-0.33840800	-2.80099600
H	4.27105100	-0.42965400	-2.63424100
H	2.92587500	-0.80832300	-3.74677000
H	2.89641800	0.70696900	-2.87344500
C	0.63970000	-2.45386900	1.33361300
O	1.71768500	-1.86702900	1.19992000
O	-0.23528900	-2.12310600	2.23167300
H	0.01650800	-1.27842800	2.74414300
C	0.24653300	-3.62039200	0.47472600
H	-0.78793000	-3.90396400	0.64486900
H	0.40089400	-3.36558600	-0.57369100
H	0.89816800	-4.46356700	0.71042800
C	-0.87279700	1.10919800	-0.00589700
C	0.09158300	1.57424600	0.65322200
C	-2.09160700	0.49452900	-0.31596100
C	-2.13517000	-0.83623300	-0.76973700
C	-3.29145400	1.20642100	-0.13643700
C	-3.35073200	-1.43877400	-1.02366100
H	-1.20797700	-1.36592500	-0.92360300
C	-4.50368400	0.59290300	-0.39402100
H	-3.24648700	2.22964200	0.20850600
C	-4.53428700	-0.72628000	-0.83697700
H	-3.38537300	-2.46251600	-1.37143000
H	-5.42641100	1.13858600	-0.25067000
H	-5.48480000	-1.20243200	-1.03977000
C	1.30111500	2.43667900	0.43257100
C	1.10576400	3.77006800	1.16115100
H	0.99855800	3.61115900	2.23525400
H	1.97346800	4.41049600	0.99323900
H	0.21987500	4.29090800	0.79685500
C	2.57241700	1.72821000	0.90204900
H	3.43707700	2.36585100	0.70983400
H	2.52707600	1.51082000	1.96907300
H	2.72172700	0.78301400	0.38272700

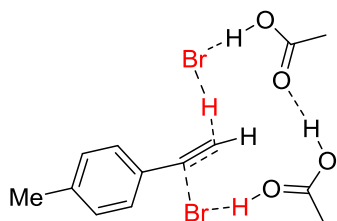
H	1.34896700	2.61302700	-0.64414100
Br	0.14278500	0.60357300	3.68134500
Br	-0.01843900	1.48895200	-2.85306700



TS12ga

H	-0.99640700	-1.42409300	-1.65639100
H	-0.87282000	2.30042300	0.21240500
C	-2.76417300	2.17392700	0.84049900
O	-1.56587300	1.74227900	0.84513200
O	-3.69875800	1.42480400	1.25555900
H	-3.37322100	0.38091200	1.36669800
C	-3.08887700	3.54811400	0.37206800
H	-4.16308400	3.67565000	0.28228900
H	-2.68478000	4.26813200	1.08673700
H	-2.58020500	3.73325500	-0.57571700
C	-2.04566000	-1.34977800	1.96044800
O	-2.95841700	-0.89790900	1.25669000
O	-1.35016700	-2.38646300	1.62622300
H	-1.56358700	-2.73178500	0.67671200
C	-1.65774900	-0.71820200	3.26620900
H	-0.92845000	-1.32455700	3.79534700
H	-1.23589300	0.26753900	3.06076000
H	-2.54631200	-0.57557800	3.88085200
C	0.41219800	-0.02746300	-1.18719700
C	-0.69655300	-0.31292100	-1.72681500
Br	-1.64970300	-3.38179200	-1.26367200
Br	0.26635300	3.01263400	-1.06539100
C	1.62766200	-0.10375600	-0.54245300
C	1.71119800	0.03737700	0.86455500
C	2.80837700	-0.33984800	-1.27559900
C	2.91685100	-0.06801600	1.50032500
H	0.80782800	0.23483300	1.42176600

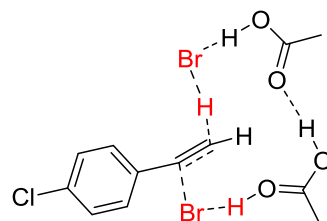
C	4.02456500	-0.44486500	-0.63946400
H	2.74394600	-0.43865000	-2.34990200
C	4.08669500	-0.30808700	0.75539400
H	3.00353500	0.03211500	2.57307800
H	4.91578500	-0.63087900	-1.21819900
O	5.21644100	-0.39057100	1.46762700
C	6.45348600	-0.62662000	0.79602300
H	6.67385300	0.17840500	0.09235600
H	7.20947500	-0.64903200	1.57522100
H	6.43568300	-1.58474300	0.27304300
H	-1.39500700	0.35588100	-2.20328200



TS12gb

H	-0.89648100	-1.43386700	-1.58651000
H	-0.29251600	2.32995900	0.19447700
C	-2.22024700	2.50203700	0.75253900
O	-1.11481900	1.88320100	0.80136600
O	-3.28672000	1.91731800	1.13070900
H	-3.13390400	0.86677400	1.27937900
C	-2.30902000	3.90894900	0.27761200
H	-3.34554400	4.20103700	0.14120300
H	-1.83182800	4.55836500	1.01456300
H	-1.73545900	4.01325100	-0.64484800
C	-2.07659100	-1.07492100	1.95307200
O	-2.89975200	-0.51356900	1.22588400
O	-1.52079100	-2.20770800	1.64667800
H	-1.76286700	-2.52386300	0.70719500
C	-1.62385800	-0.48873400	3.25893600
H	-1.03463100	-1.20121000	3.82900300
H	-1.01999100	0.39550400	3.04486700
H	-2.49009900	-0.16653100	3.83578000
C	0.68812200	-0.22644500	-1.11339600

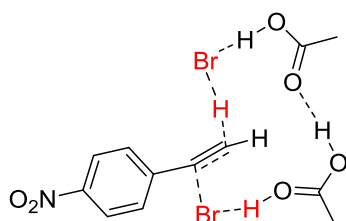
C	-0.43629400	-0.35232600	-1.66448400
B	-1.86644500	-3.16510800	-1.29077600
B	0.98806800	2.86215100	-0.97471000
C	1.88206400	-0.44807300	-0.44548100
C	1.95006500	-0.31561700	0.95696400
C	3.03565900	-0.82912300	-1.15812900
C	3.13192700	-0.56598800	1.61413400
H	1.06504100	-0.01237900	1.49616200
C	4.21229700	-1.07330500	-0.48220200
H	2.98055600	-0.92613800	-2.23311500
H	3.17880100	-0.46899700	2.69137300
H	5.09500900	-1.37054300	-1.03341600
C	4.28342700	-0.94311100	0.90873200
C	5.57294100	-1.17590800	1.63577000
H	6.05892400	-0.22088900	1.85628700
H	5.40495200	-1.68061700	2.58790900
H	6.26579200	-1.77075900	1.04206600
H	-1.05411800	0.37780800	-2.16004400



TS12gc

H	-1.02453900	-1.53797100	-1.61246200
H	-0.82336200	2.30190300	0.18858900
C	-2.71671200	2.17907400	0.89478800
O	-1.53419300	1.73018200	0.85391600
O	-3.65928200	1.44083000	1.33672100
H	-3.34515000	0.43484700	1.46173000
C	-3.04827800	3.56070800	0.45454200
H	-4.12379200	3.69672800	0.39934700
H	-2.61852000	4.26796200	1.16702800
H	-2.56748100	3.75665600	-0.50517300
C	-1.95392900	-1.35651400	2.02381200
O	-2.90261600	-0.91690700	1.37325600

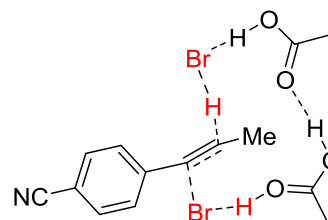
O	-1.25546400	-2.38781500	1.64635900
H	-1.52542400	-2.72250500	0.72729200
C	-1.49907200	-0.73363000	3.31166100
H	-0.73799300	-1.33716000	3.79767900
H	-1.09640700	0.25686000	3.09065000
H	-2.35466500	-0.60169800	3.97342200
C	0.38138500	-0.09403800	-1.22819100
C	-0.73629900	-0.38104600	-1.72027700
Br	-1.68990200	-3.34423000	-1.30375900
Br	0.27097800	3.01706500	-1.03922200
C	1.62930100	-0.14459300	-0.61898700
C	1.74433500	0.00865600	0.77688100
C	2.78674500	-0.36587000	-1.38992100
C	2.97716000	-0.06688100	1.38470800
H	0.85421200	0.19437600	1.35862400
C	4.02254300	-0.43930800	-0.78251700
H	2.69380400	-0.47560700	-2.46090200
H	3.07916400	0.04705700	2.45398200
H	4.91751000	-0.61036900	-1.36259900
C	4.10931400	-0.28866100	0.60004600
C	5.65841500	-0.37761200	1.36364400
H	-1.49416200	0.22530000	-2.18633800



TS12gd

H	-0.95067500	-1.57425800	-1.65517300
H	-1.27313500	2.15523100	0.46154500
C	-3.17687800	1.79843900	1.05295200
O	-1.95802000	1.46695600	1.03226200
O	-4.05970400	0.93413800	1.38535200
H	-3.64471400	-0.02604300	1.46214100
C	-3.62938200	3.17382100	0.71643800
H	-4.70869000	3.20601000	0.60509400

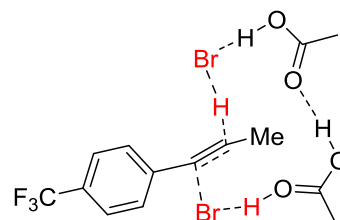
H	-3.31814700	3.84825900	1.51721300
H	-3.12001600	3.50876300	-0.18844200
C	-2.00660200	-1.63698000	1.97026600
O	-3.00112400	-1.33044800	1.31754100
O	-1.13064000	-2.51518400	1.55286900
H	-1.32746300	-2.83474400	0.62080000
C	-1.66260000	-1.01992700	3.29225700
H	-1.03956400	-1.68524700	3.88451700
H	-1.10679500	-0.09947500	3.09827100
H	-2.56975800	-0.76195700	3.83443400
C	0.17323800	0.09498400	-1.19021800
C	-0.92732200	-0.31118000	-1.60626000
Br	-1.27418200	-3.35607600	-1.50869900
Br	-0.19792700	3.06250900	-0.65331000
C	1.48617600	0.10265200	-0.68621200
C	1.73052800	-0.42884000	0.59109700
C	2.54833200	0.60282700	-1.45675600
C	3.01920000	-0.46362800	1.08901000
H	0.90926300	-0.83078200	1.16553300
C	3.83392700	0.57922400	-0.95587100
H	2.34331800	1.02418400	-2.42973700
H	3.23992100	-0.87449400	2.06192000
H	4.66916800	0.96278400	-1.52090100
C	4.04668800	0.04697600	0.30965300
N	5.42347000	0.02189500	0.84733800
O	6.31326200	0.45425800	0.13447000
O	5.58037800	-0.42934000	1.96981000
H	-1.88085900	0.10608500	-1.86923300



TS12ge

H	1.38954300	1.48356700	-1.77656500
H	1.45116300	-2.21462100	0.37436800

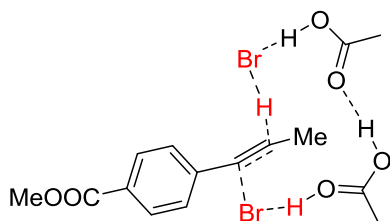
C	3.26897100	-1.83073700	1.18747800
O	2.05513600	-1.51404700	1.03127100
O	4.10260200	-0.95901100	1.60966800
H	3.68283000	0.00828400	1.61905100
C	3.76739900	-3.20392000	0.90843900
H	4.85220500	-3.23058400	0.93549200
H	3.35826000	-3.88407600	1.65845200
H	3.38050700	-3.53651500	-0.05611700
C	2.07661700	1.69878600	1.92790000
O	3.10133400	1.30525300	1.37284000
O	1.29920400	2.61017900	1.41208600
H	1.59235300	2.87949200	0.48545700
C	1.60695100	1.15701300	3.24600500
H	0.76788100	1.72706900	3.63415000
H	1.30733900	0.11691900	3.10185600
H	2.43176100	1.16715600	3.95784800
C	0.16517800	-0.11674400	-1.35566600
C	1.27014200	0.25825600	-1.79957500
Br	1.80651700	3.30322700	-1.62816800
Br	0.53282400	-3.13496600	-0.85014000
C	-1.13181900	-0.13473200	-0.82983900
C	-1.32707200	-0.12965300	0.56243400
C	-2.24142000	-0.13526500	-1.69032200
C	-2.60540800	-0.11703100	1.07828400
H	-0.46651800	-0.14631600	1.21339700
C	-3.52031200	-0.12595600	-1.16615700
H	-2.08194400	-0.14797800	-2.75875900
H	-2.76274300	-0.11664200	2.14736100
H	-4.37783200	-0.13093400	-1.82297800
C	-3.69992200	-0.11880800	0.21390700
C	-5.09120500	-0.06461600	0.79235500
F	-6.01380200	-0.54670700	-0.05781800
F	-5.18477100	-0.77087600	1.93490600
F	-5.44449400	1.20579100	1.08482100
H	2.15338300	-0.23897200	-2.15838200



TS12gf

H	1.53073800	1.64546700	-1.57459100
H	1.32884600	-2.28948900	0.12808800
C	3.19424000	-2.15594200	0.91413100
O	2.01095200	-1.72001700	0.83264000
O	4.11110500	-1.41194200	1.40501800
H	3.77498000	-0.42512700	1.54439000
C	3.56397000	-3.52568700	0.46868900
H	4.64277600	-3.64459900	0.45061300
H	3.12095200	-4.24835300	1.15731000
H	3.12086600	-3.71710000	-0.50984200
C	2.29366200	1.31354500	2.10654700
O	3.28296000	0.93827600	1.48050700
O	1.55937500	2.32488300	1.72829800
H	1.85280600	2.69444000	0.83903500
C	1.81015800	0.63380000	3.35331600
H	1.08425600	1.24485400	3.88228000
H	1.34479500	-0.31151400	3.06501400
H	2.65631400	0.40413800	3.99911200
C	0.19880500	0.08538200	-1.36084100
C	1.34393300	0.42507000	-1.71853500
Br	2.05083500	3.38460400	-1.21743200
Br	0.30045000	-2.99042600	-1.15287300
C	-1.11838700	0.10330400	-0.88644000
C	-1.36343100	0.08619500	0.49789200
C	-2.19532600	0.15998300	-1.78738000
C	-2.65628800	0.13140600	0.97111500
H	-0.52764300	0.03728600	1.17908000
C	-3.48980600	0.19876500	-1.31364700
H	-1.99612200	0.16438400	-2.84914900
H	-2.85597600	0.12362700	2.03302200
H	-4.32531200	0.24022000	-1.99760000

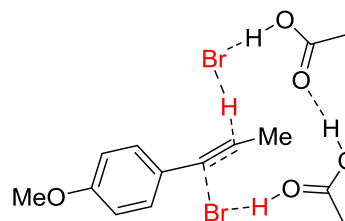
C	-3.72523600	0.18412200	0.06673300
H	2.22309600	-0.08022100	-2.07474000
C	-5.06477800	0.22426500	0.55835700
N	-6.14491000	0.25727300	0.95778500



TS12gg

H	1.59129300	1.57907800	-1.64066300
H	1.33379800	-2.30918500	0.08788700
C	3.16841800	-2.15986700	0.94555400
O	1.98589400	-1.73216200	0.81938800
O	4.06271200	-1.41003700	1.46625300
H	3.72043200	-0.41786000	1.58131600
C	3.56076200	-3.52970900	0.51831300
H	4.63979400	-3.64488100	0.54507800
H	3.09137200	-4.25322000	1.18816700
H	3.15971600	-3.72342300	-0.47776300
C	2.24459400	1.34695900	2.05761400
O	3.25119000	0.93852000	1.47983200
O	1.55464200	2.36999200	1.63794600
H	1.88909000	2.71778600	0.75000000
C	1.69938400	0.69631100	3.29523000
H	0.89776000	1.28407600	3.73297700
H	1.32240100	-0.29191300	3.02415900
H	2.50336900	0.55673500	4.01721800
C	0.21368600	0.07424100	-1.39092000
C	1.35469600	0.39601900	-1.78987100
Br	2.18632900	3.35358600	-1.28590100
Br	0.35886200	-3.02187900	-1.22260900
C	-1.08407100	0.09751300	-0.87687700
C	-1.29620400	-0.04802200	0.50644100
C	-2.18067900	0.29307100	-1.73639800
C	-2.57511300	0.01043100	1.01684800

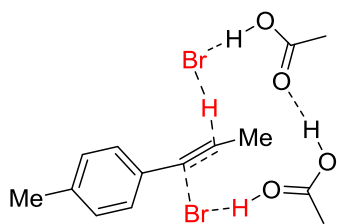
H	-0.44676200	-0.21269100	1.15164500
C	-3.45718200	0.34703100	-1.21651500
H	-2.00699400	0.39741700	-2.79772000
H	-2.74725100	-0.09761300	2.07691400
H	-4.31516600	0.49746400	-1.85587900
C	-3.66071000	0.20625300	0.15763700
H	2.18193500	-0.15612900	-2.19994100
C	-5.06493100	0.27164400	0.65988600
O	-6.02585800	0.43892200	-0.04923100
O	-5.13793500	0.12322900	1.99235100
C	-6.46074200	0.17334700	2.55200300
H	-6.32952600	0.03714000	3.62126000
H	-6.92442800	1.13541600	2.33910100
H	-7.07749400	-0.62095900	2.13418500



TS16ga

H	-0.84545900	-1.37400200	-1.59490000
H	-0.82424300	2.37957700	0.25007200
C	-2.76300900	2.31151300	0.66121200
O	-1.57992100	1.85301900	0.80502300
O	-3.75063800	1.58051800	0.96099800
H	-3.45950800	0.50995600	1.08449100
C	-2.99763700	3.69357400	0.16461400
H	-4.04554400	3.83645300	-0.07993200
H	-2.69750700	4.40034500	0.94142300
H	-2.35166700	3.88199200	-0.69479400
C	-2.28318600	-1.24537000	1.79406400
O	-3.08251000	-0.75296400	0.98217700
O	-1.61914600	-2.32375200	1.55122600
H	-1.73212400	-2.66788100	0.58201500
C	-2.00674800	-0.61174600	3.12534800
H	-1.45356200	-1.28679700	3.77174400

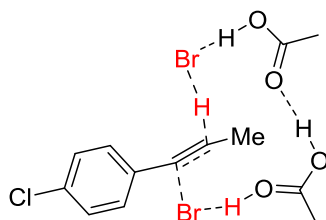
H	-1.41773400	0.29193400	2.95535500
H	-2.94262400	-0.31472300	3.59712100
C	0.43175000	0.06208900	-1.14657300
C	-0.68368600	-0.22844600	-1.67050000
Br	-1.60669700	-3.30658100	-1.35016900
Br	0.44046600	3.04038400	-0.98680700
C	1.66023100	-0.08166700	-0.52001800
C	1.75693100	-0.07057000	0.89046000
C	2.83286000	-0.25725300	-1.27746200
C	2.96722900	-0.24422000	1.50717500
H	0.85945100	0.07585500	1.47319100
C	4.05441300	-0.43002000	-0.66300900
H	2.76203000	-0.25351800	-2.35593800
C	4.12866900	-0.42438100	0.73657200
H	3.05951600	-0.24671200	2.58422300
H	4.93931800	-0.56818000	-1.26459800
O	5.26559500	-0.58418500	1.43062200
C	6.49074300	-0.77141600	0.72626700
H	6.71731400	0.09386100	0.09980600
H	7.25510300	-0.87930300	1.49030300
H	6.45459000	-1.67422300	0.11297100
C	-1.81946900	0.49605900	-2.29686900
H	-2.72862300	0.28691500	-1.73047100
H	-1.61555300	1.56452900	-2.33290400
H	-1.98190400	0.11381900	-3.30559800



TS16gb

H	-0.86180600	-1.34877200	-1.54318200
H	-0.03579800	2.41765000	0.13231400
C	-1.95789400	2.79865100	0.50150900
O	-0.91501700	2.09675100	0.69446000
O	-3.09522100	2.32190000	0.80550100

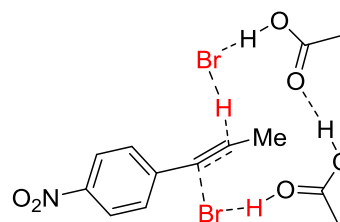
H	-3.04738000	1.25341100	0.99806100
C	-1.87761500	4.17343100	-0.05841400
H	-2.86643100	4.53667400	-0.32018200
H	-1.42422600	4.82967400	0.68759400
H	-1.20625500	4.17124000	-0.91897100
C	-2.26174300	-0.73127800	1.80702600
O	-2.94129900	-0.11407000	0.97824500
O	-1.82202100	-1.93144500	1.59976200
H	-2.00912500	-2.26796900	0.65053200
C	-1.86784400	-0.13418300	3.12578300
H	-1.45037900	-0.88617400	3.78902100
H	-1.12122700	0.64042800	2.93870700
H	-2.73190200	0.34184000	3.58789500
C	0.68615700	-0.19712200	-1.11376000
C	-0.44631700	-0.25000500	-1.66294600
Br	-2.01745800	-2.98203200	-1.30406800
Br	1.35332400	2.73090200	-1.05685500
C	1.84510500	-0.56837100	-0.43363900
C	1.89115800	-0.52117400	0.97344200
C	2.97709500	-1.00990500	-1.14009900
C	3.02925200	-0.91335100	1.64089300
H	1.02260400	-0.17286400	1.51314600
C	4.11201900	-1.39680700	-0.45571500
H	2.94401700	-1.03701000	-2.22006800
H	3.05556400	-0.88028100	2.72301600
H	4.97909600	-1.73766700	-1.00663400
C	4.15996500	-1.35429200	0.94007400
C	5.39550500	-1.76433300	1.68453000
H	5.81163600	-0.91770300	2.23627800
H	5.16889900	-2.54377700	2.41531700
H	6.16348000	-2.13985700	1.01012900
C	-1.39797300	0.65687000	-2.35205700
H	-2.33622200	0.67643600	-1.79518600
H	-0.97122400	1.65484100	-2.43722600
H	-1.62586400	0.26310400	-3.34324800



TS16gc

H	-0.98094700	-1.47027700	-1.56710600
H	-0.64617100	2.39161600	0.14275600
C	-2.56818400	2.44050100	0.69690100
O	-1.41536400	1.91460700	0.77219000
O	-3.58608800	1.77512500	1.07354700
H	-3.35018200	0.73937500	1.22711300
C	-2.76514800	3.82463900	0.19246700
H	-3.81958700	4.02627600	0.03205900
H	-2.35842400	4.52539000	0.92480900
H	-2.18377900	3.95892800	-0.72155000
C	-2.17006700	-1.11655900	1.91395000
O	-3.00998000	-0.61584000	1.16038000
O	-1.54270600	-2.21861400	1.63564900
H	-1.74948700	-2.56409500	0.70055200
C	-1.77560200	-0.48415600	3.21585800
H	-1.19282600	-1.16816700	3.82601400
H	-1.17834600	0.40314700	2.99451800
H	-2.66571900	-0.15996200	3.75344800
C	0.37501600	-0.06363300	-1.23995900
C	-0.77698300	-0.29133300	-1.68272400
Br	-1.78096700	-3.23178100	-1.30127600
Br	0.54333000	2.95798000	-1.13713700
C	1.63975900	-0.23834900	-0.67246600
C	1.78662100	-0.26687600	0.72613900
C	2.77433100	-0.40006100	-1.48729400
C	3.02725500	-0.46224000	1.29514100
H	0.91366400	-0.13581800	1.34812200
C	4.01827400	-0.59038500	-0.92155000
H	2.66041700	-0.36697000	-2.56134700
H	3.14931800	-0.49231800	2.36802700
H	4.89585400	-0.71548100	-1.53886000

C	4.13592000	-0.61989200	0.46607100
C	5.69668200	-0.85765100	1.17854700
C	-1.94675200	0.42994200	-2.23909500
H	-2.80973900	0.25899300	-1.59377600
H	-1.72351200	1.49256900	-2.32352600
H	-2.19640700	0.02313300	-3.21959300



TS16gd

H	-1.06736000	-1.63715900	-1.46196700
H	-1.07674800	2.35792700	0.02310200
C	-2.98069500	2.30423600	0.63113100
O	-1.79259900	1.86919000	0.70099100
O	-3.93504500	1.59107200	1.08833200
H	-3.61089100	0.61009500	1.31482200
C	-3.30178000	3.63113000	0.04581500
H	-4.36960400	3.72528100	-0.12516600
H	-2.96852400	4.40636500	0.73967400
H	-2.72952700	3.76700700	-0.87337400
C	-2.19389400	-1.07842500	2.07704300
O	-3.12429400	-0.74182300	1.34479500
O	-1.45150400	-2.12502300	1.83537800
H	-1.66144700	-2.55247800	0.94625100
C	-1.78446300	-0.31180000	3.29732200
H	-1.31831300	-0.96674800	4.02924200
H	-1.05361800	0.44024400	2.99017300
H	-2.64123600	0.19880400	3.73109600
C	0.10344000	-0.04085800	-1.27924500
C	-1.03561600	-0.39003200	-1.64666000
Br	-1.58610900	-3.35667600	-1.06151500
Br	0.03575100	2.92038500	-1.33014000
C	1.40757000	-0.14496500	-0.74700700
C	1.57936200	-0.70510600	0.52911500

C	2.52577600	0.26903600	-1.48708600	N	5.29168900	-0.58042700	0.86692200
C	2.85047000	-0.85905400	1.05236600	O	6.23168900	-0.22225500	0.17684000
H	0.71691200	-1.04025900	1.08606200	O	5.38662400	-1.05127700	1.98881700
C	3.79388300	0.13077800	-0.96017700	C	-2.33706100	0.10863600	-2.13369900
H	2.37885000	0.71970000	-2.45719900	H	-2.27854800	1.18659100	-2.28469400
H	3.01176600	-1.29783900	2.02483100	H	-2.59642700	-0.37916700	-3.07381000
H	4.66991600	0.44800100	-1.50425100	H	-3.11565500	-0.14552400	-1.41301200
C	3.93537700	-0.43212000	0.30214900				