

Supplementary information for

Trajectory surface hopping molecular dynamics simulations for retinal protonated Schiff-base photoisomerization

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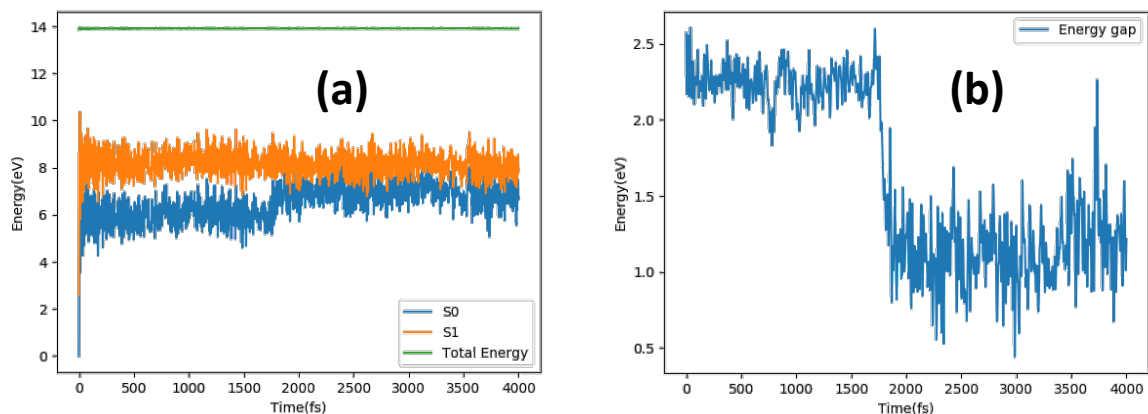


Fig. S1 One resonance trajectory evolution starting from Franck-Condon region on S₁ state at all-trans isomer up to 4000fs simulation. (a) Potential energy surfaces and (b) energy gap between S₁ and S₀ states.

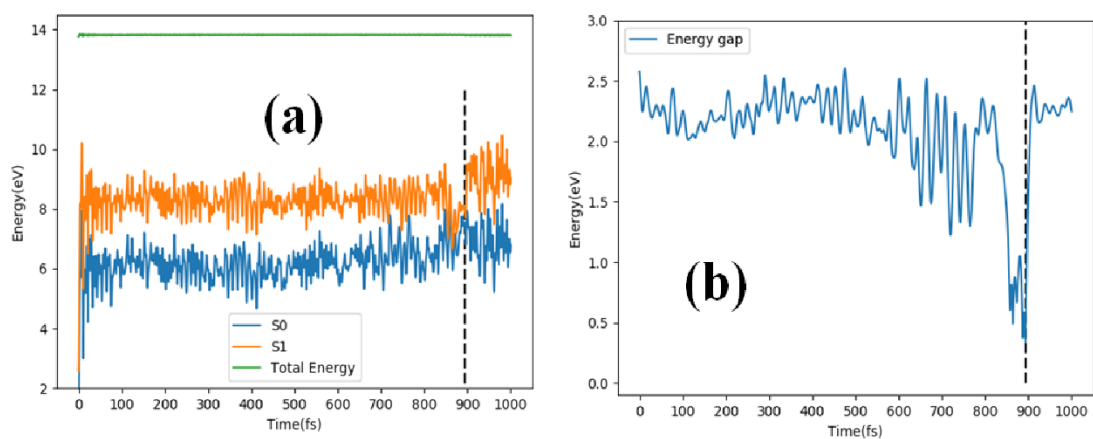
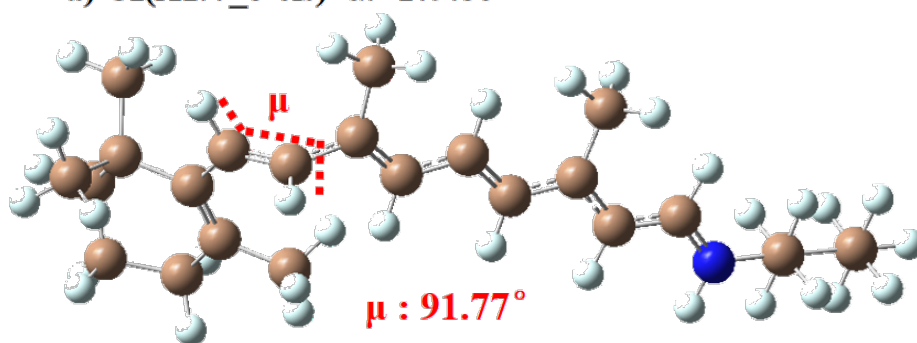
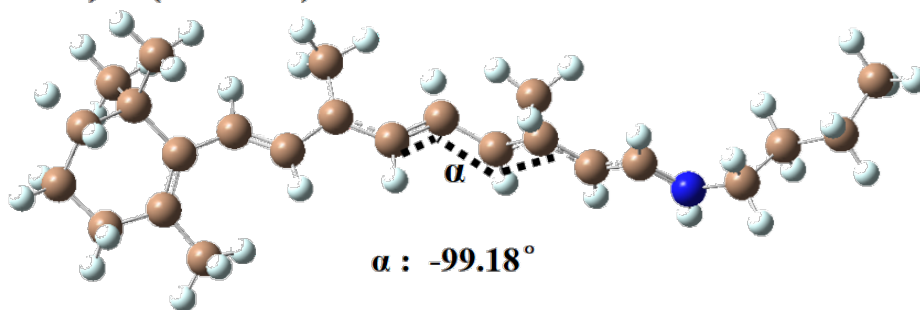


Fig. S2 One hopping trajectory evolution starting from 11-cis Franck-Condon region on S₁ state up to 1000fs simulation (hop is taken place at 900fs). (a) Potential energy surfaces and (b) energy gap between S₁ and S₀ states.

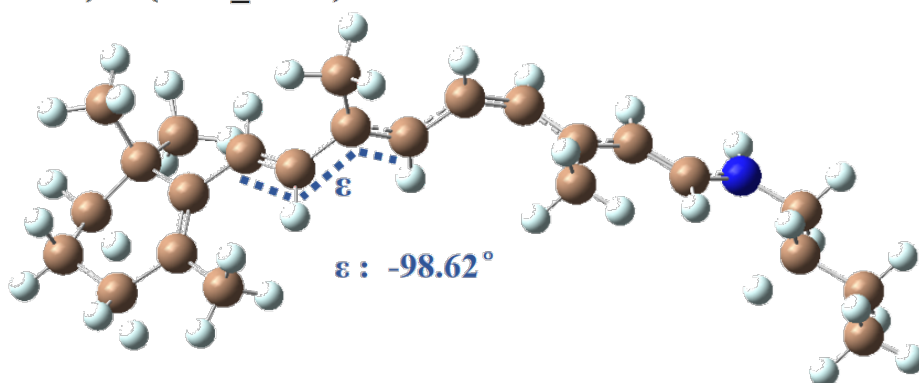
a) CI(AT/7_8-cis) α : -179.86°



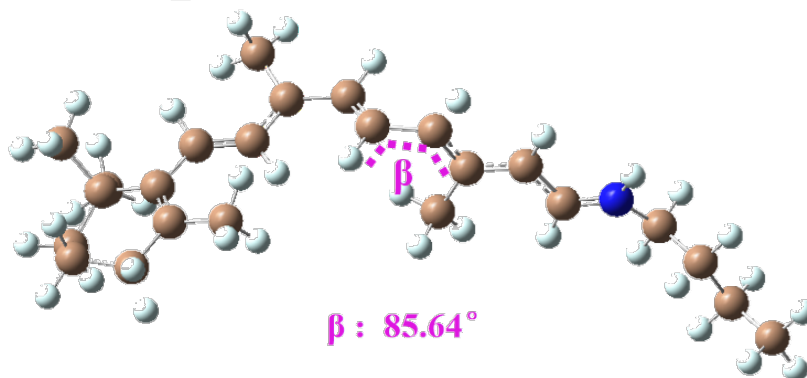
b) CI(AT/11-cis)



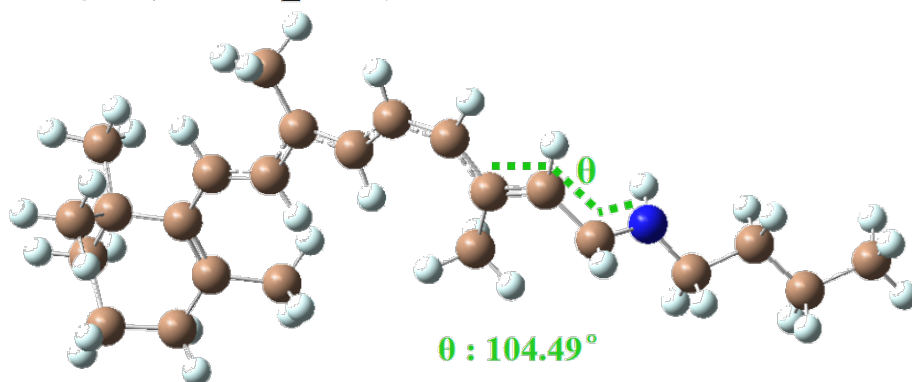
c) CI(AT/8_11-cis) α : -88.74°



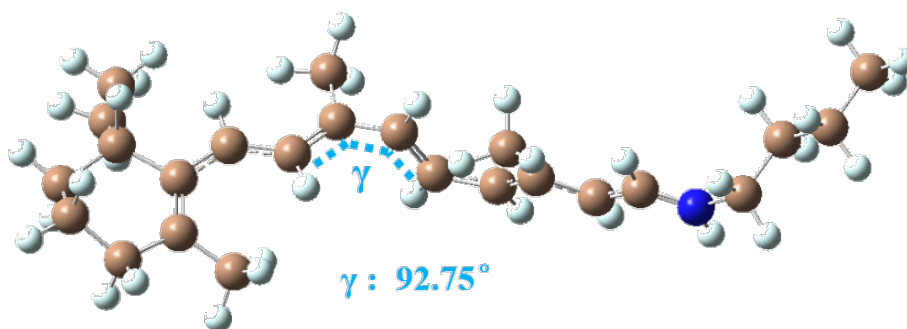
d) CI(AT/9_11-cis) α : -80.25°



e) CI(11-cis/11_14-cis) α : 1.97°



f) CI(11-cis/9_11-cis) α : 23.55°



g) CI(AT/9-cis) α : 178.61°

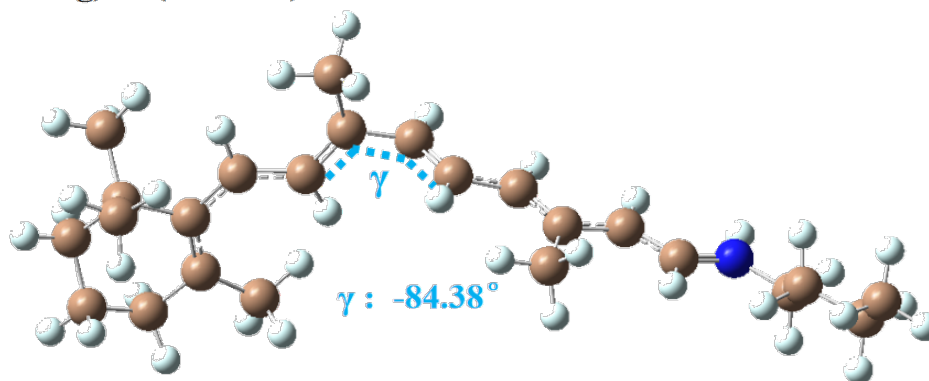
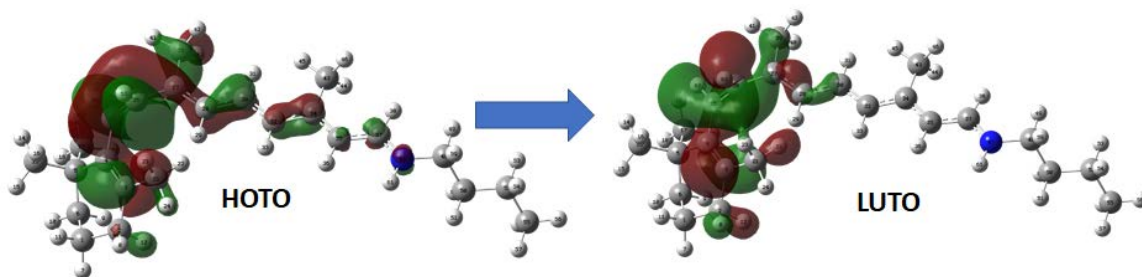


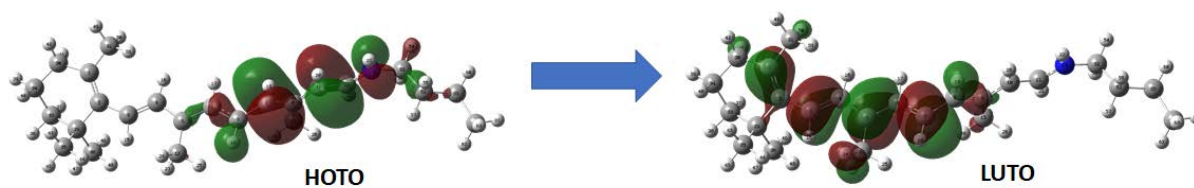
Fig. S3 Conical intersection structures for (a) CI(all-trans/7_8-cis), (b) CI(all-trans/11-cis), (c) CI(all-trans/8_11-cis), (d) CI(all-trans/9_11-cis), (e) CI(11-cis/11_14-cis), (f) CI(11-cis/9_11-cis), and (g) CI(all-trans/9-cis). The α dihedral angle is shown for all seven CIs plus each CI has its own important dihedral angle. All seven dihedral angles are defined in Fig.1

a) CI(AT/7_8-cis) α : -179.86°

μ : 91.77°

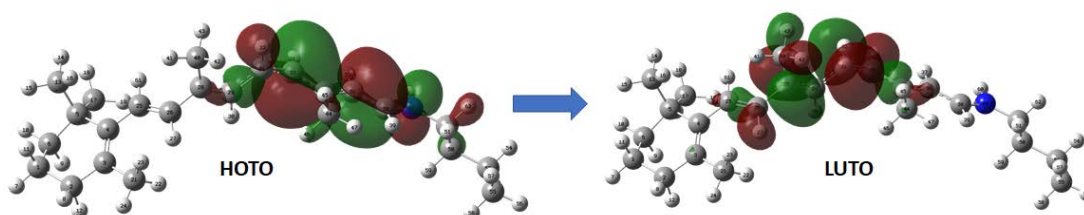


b) CI(AT/11-cis) α : -99.18°



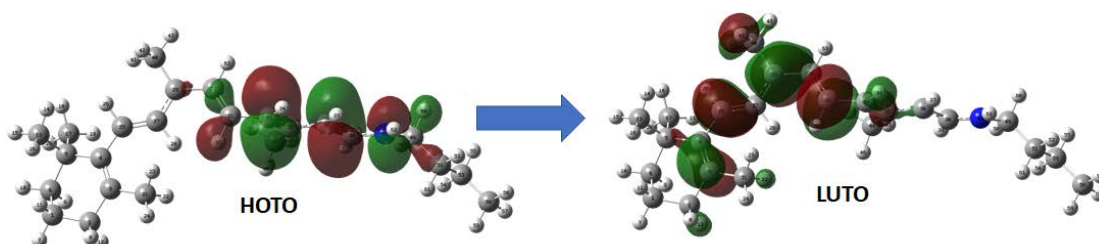
c) CI(AT/8_11-cis) α : -88.74°

ϵ : -98.62°



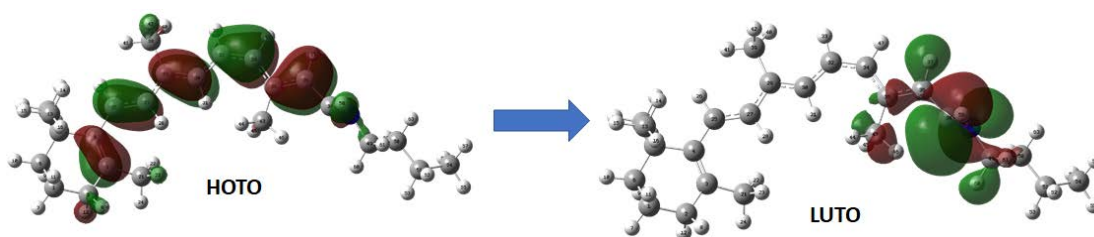
d) CI(AT/9_11-cis) α : -80.25°

β : 85.64°



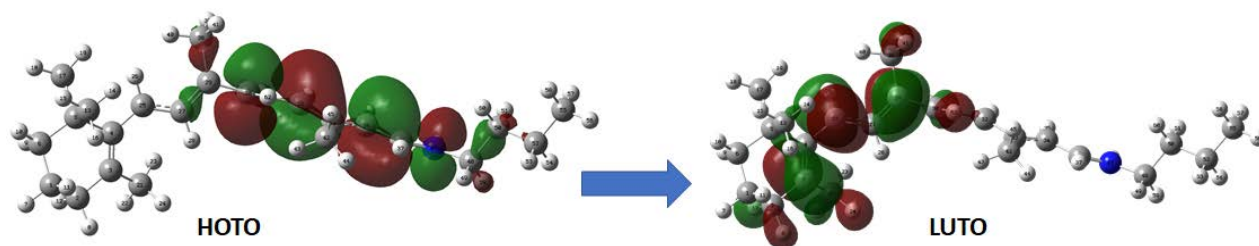
e) CI(11-cis/11_14-cis) α : 1.97°

θ : 104.49°



f) CI(11-cis/9_11-cis) α : 23.55°

γ : 92.75°



g) CI(AT/9-cis) α : 178.61°

γ : -84.38°

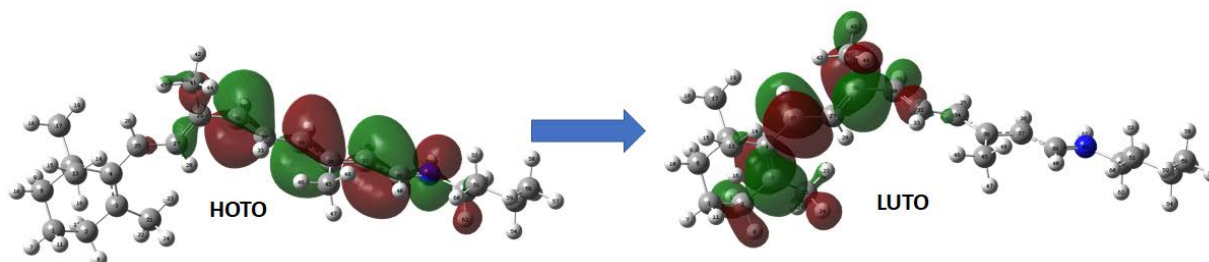


Fig. S4 Calculated natural transition orbitals of $S_0 \rightarrow S_1$ at representative conical intersections corresponding to dominant HOMO (HOTO) to LUMO (LUTO) transition with percentage contribution for (a) 86.4% at CI(all-trans/7_8-cis), (b) 93.5% at CI(all-trans/11-cis), (c) 93.5% at CI(all-trans/8_11-cis), (d) 94.5% at CI(all-trans/9_11-cis), (e) 81.6% at CI(11-cis/11_14-cis), (f) 94.8% at CI(11-cis/9_11-cis), and (g) 94.8% at CI(all-trans/9-cis). The α dihedral angle plus the other important dihedral angles are defined in Fig.S3.

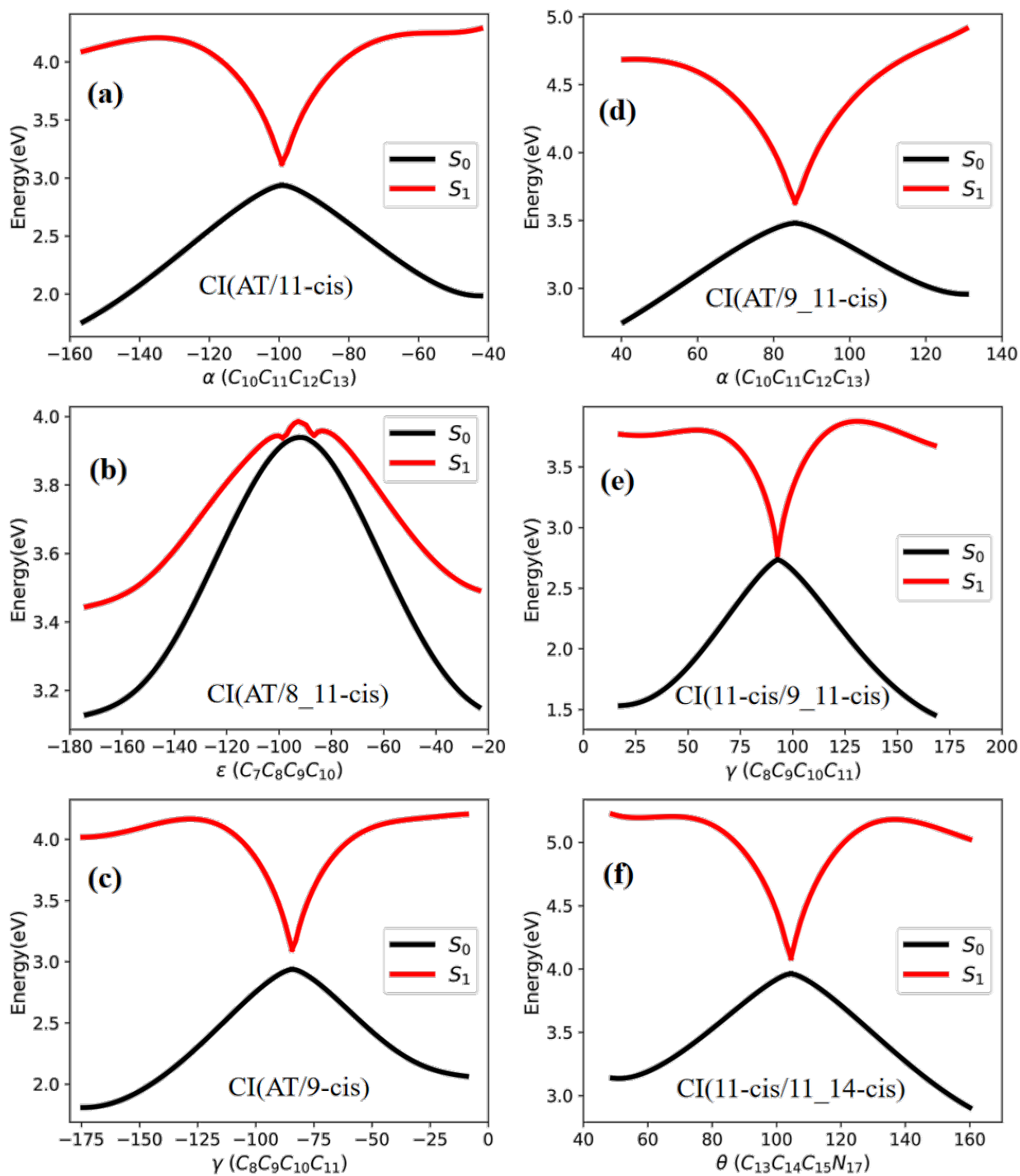


Fig. S5 Scanned potential energy surfaces along minimum energy path for each conical intersection with respect to specific dihedral angle. (a) CI(all-trans/11-cis), (b) CI(all-trans/8_11-cis), (c) CI(all-trans/9-cis), (d) CI(all-trans/9_11-cis), (e) CI(11-cis/9_11-cis), and (f) CI(11-cis/11_14-cis).

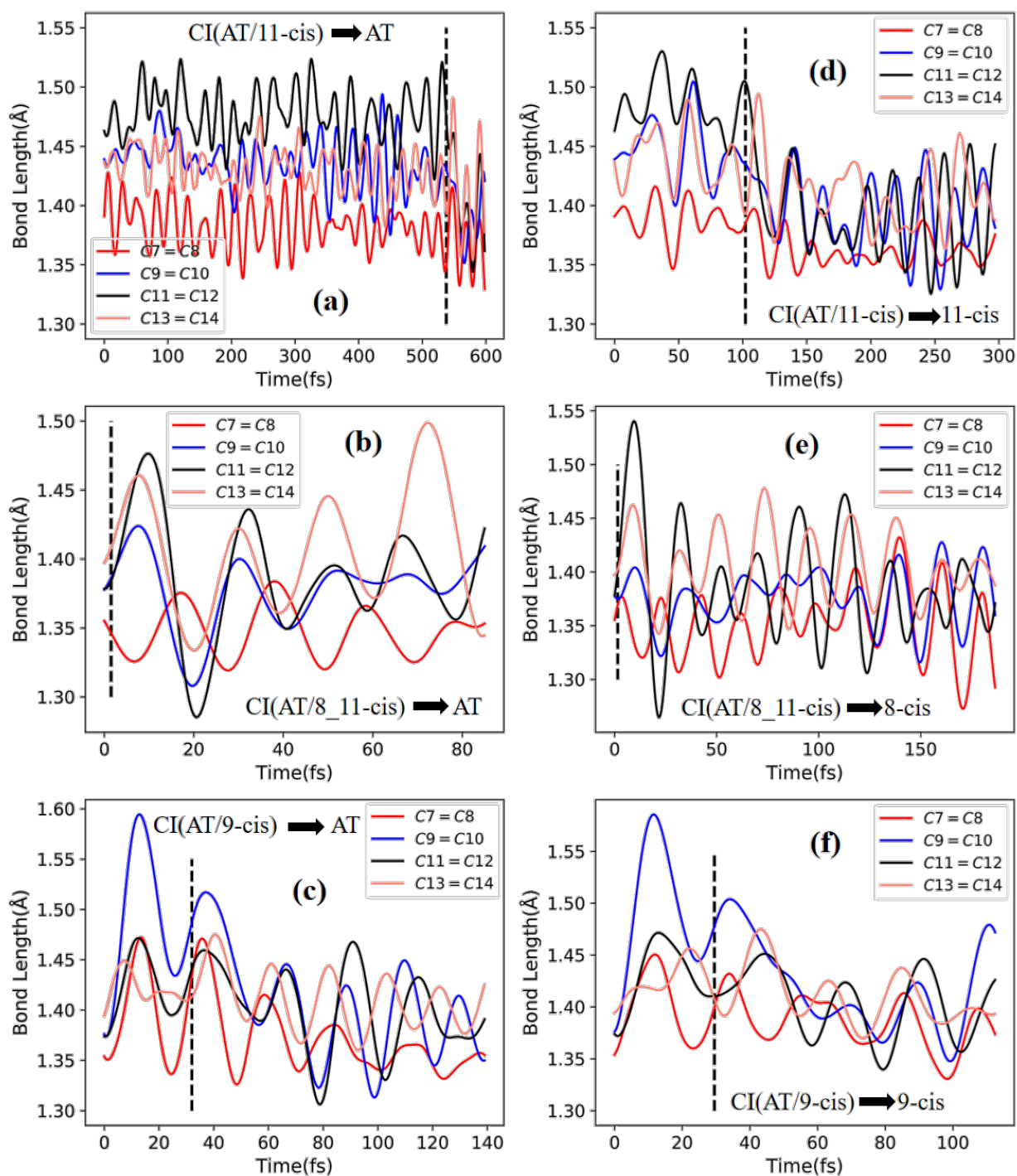


Fig. S6 Four CC double bonds (C7=C8, C9=C10, C11=C12 and C13=C14) vary as function of time for typical trajectory corresponding to (a) Fig.5a, (b) Fig.5b, (c) Fig.5c, (d) Fig.6a, (e) Fig.6b, and Fig. 6c in the text. respectively.

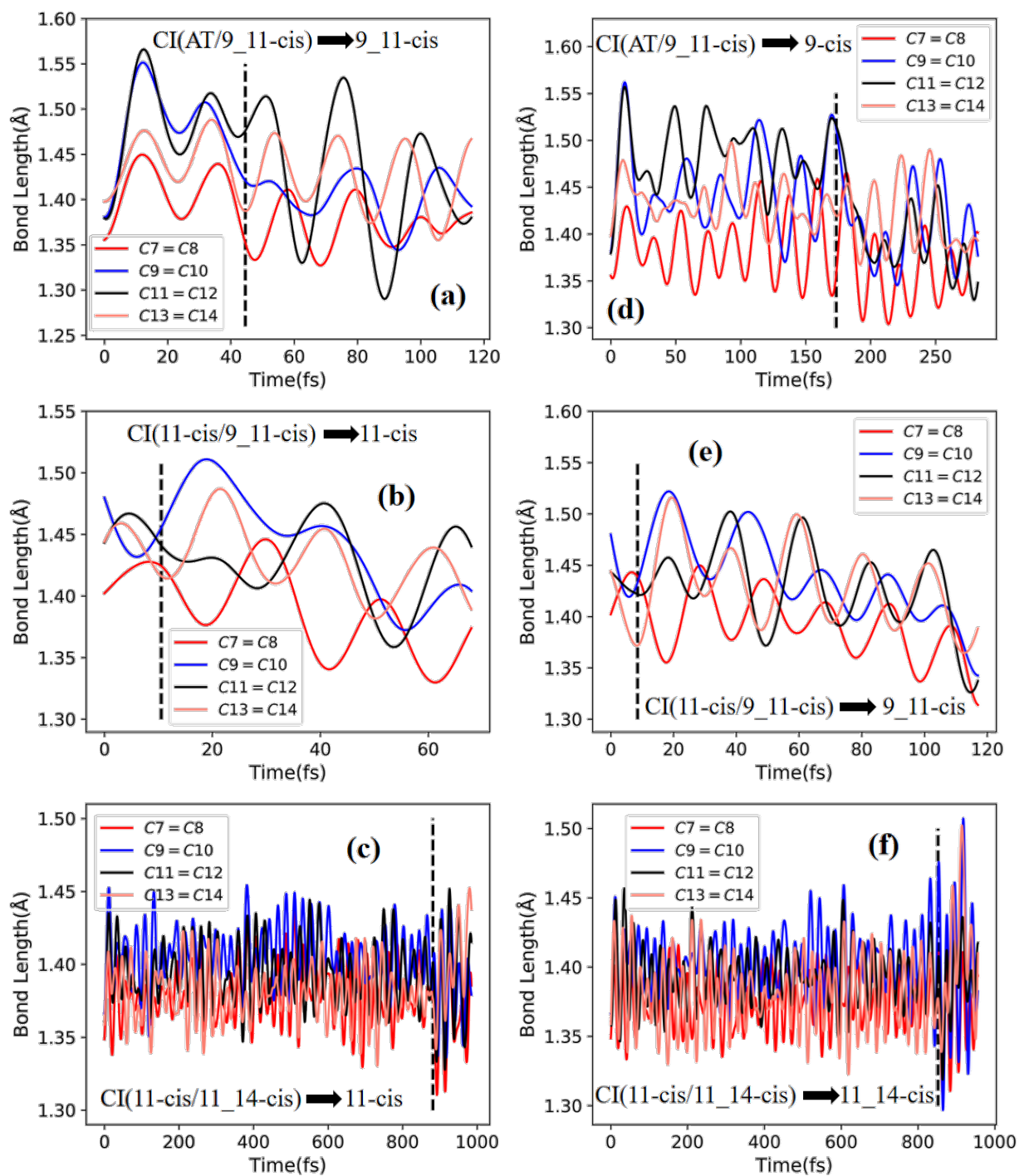


Fig. S7 Four CC double bonds (C7=C8, C9=C10, C11=C12 and C13=C14) vary as function of time for typical trajectory corresponding to (a) Fig.7a, (b) Fig.7b, (c) Fig.7c, (d) Fig.8a, (e) Fig.8b, and Fig. 8c in the text, respectively.

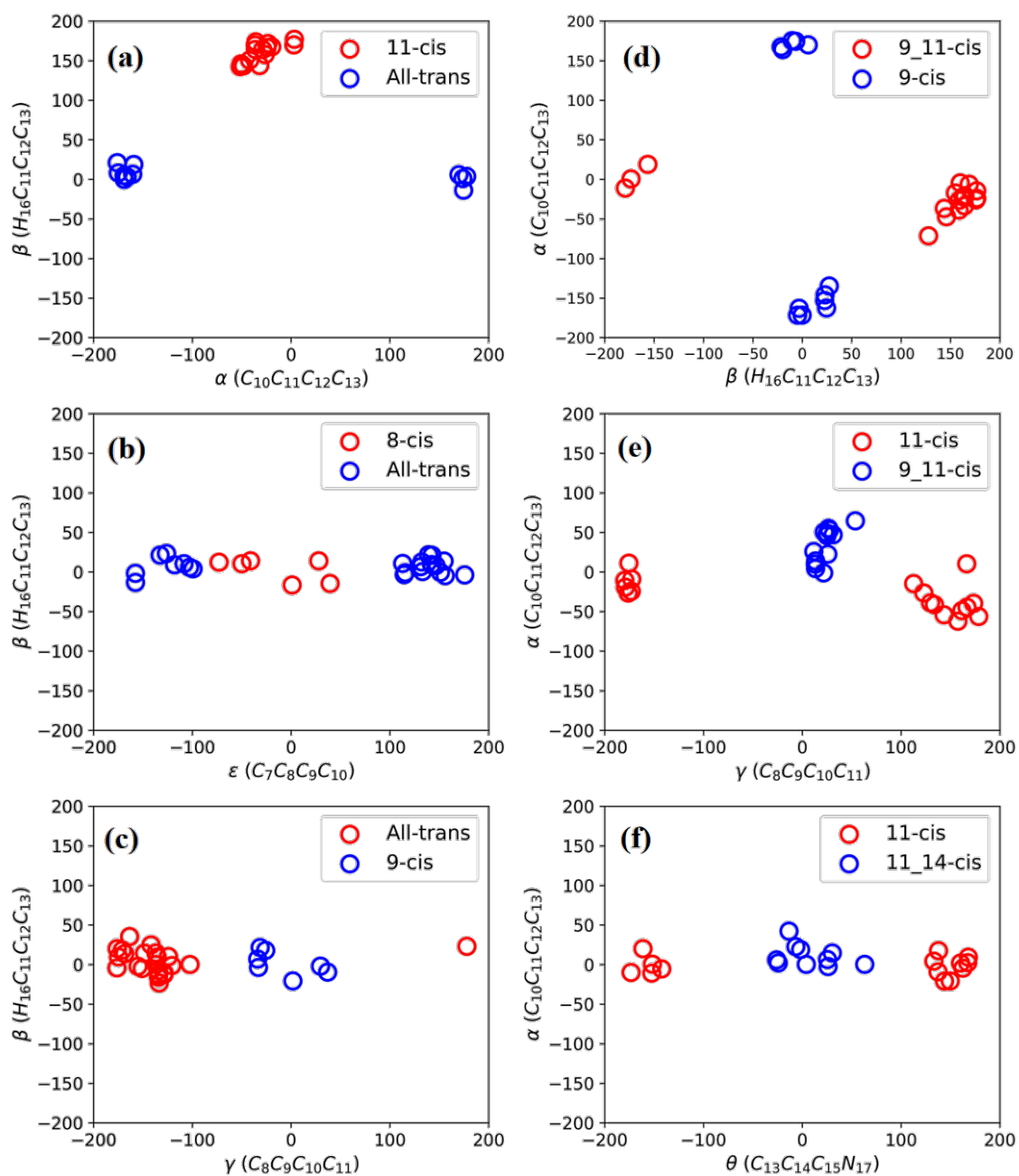


Fig. S8 The distribution of final products on S_0 state in terms of two characteristic dihedral angles for sampling trajectories corresponding to (a) Fig.3a, (b) Fig.3b, (c) Fig.3c, (d) Fig.3d, (e) Fig.3e, and (f) Fig.3f in the text, respectively.

Table S1 Cartesian coordinates for ground state geometries listed in Table 1.**Table S1.1: All-trans**

C	-9.37200100	-2.86344100	-1.53813700
C	-7.98770800	-2.77473500	-0.90882500
C	-7.54862000	-1.37129200	-0.56091900
C	-8.16364500	-0.27741600	-1.06781300
C	-9.39652500	-0.35755600	-1.98944200
C	-9.53294900	-1.77017800	-2.58206400
H	-9.51579500	-3.85028200	-1.98858200
H	-7.93576600	-3.39734300	-0.00839700
H	-8.76727100	-1.90474000	-3.35740900
H	-10.50326900	-1.84883900	-3.08512200
H	-10.13806200	-2.76252700	-0.76157300
H	-7.23764700	-3.19637900	-1.59529600
C	-10.66625000	0.00591100	-1.19730700
H	-10.60738600	1.01107700	-0.76685000
H	-11.53996100	-0.01119900	-1.85725300
H	-10.84640600	-0.69200700	-0.37568300
C	-9.24931700	0.62373000	-3.16549400
H	-10.08435800	0.49734500	-3.86222800
H	-9.25173200	1.66940600	-2.84179800
H	-8.32082800	0.44375900	-3.71665800
C	-6.38922900	-1.33818800	0.40038200
H	-5.44748900	-1.57066100	-0.11365200
H	-6.26937100	-0.37849200	0.90279600
H	-6.51925700	-2.10978600	1.16577500
C	-7.75560700	1.08809400	-0.73940500
H	-8.57492400	1.79082400	-0.60407500
C	-6.49678300	1.57558100	-0.66301100
H	-5.66027800	0.91736500	-0.87676800
C	-6.15971200	2.94520700	-0.35366100
C	-4.83050900	3.29243100	-0.35784200
H	-4.11342200	2.50981600	-0.59537900
C	-4.29293900	4.57038400	-0.08392800
H	-4.97990200	5.37397500	0.16081600
C	-2.94829200	4.84701100	-0.11040300
H	-2.26502800	4.03796400	-0.35692200
C	-2.37451100	6.11240600	0.16010100
C	-0.98784500	6.22786700	0.09137500
H	-0.42360200	5.33490300	-0.16717400
C	-0.26338500	7.39053400	0.32855100
H	-0.76094900	8.31811400	0.59230500
C	-7.26604200	3.91444500	-0.04841100
H	-7.95039400	3.98896800	-0.89943600
H	-7.85234900	3.56704300	0.80740100
H	-6.91017000	4.91837700	0.17737000
C	-3.26790500	7.27247100	0.50829700
H	-3.97540500	7.46333700	-0.30356200
H	-3.85057800	7.04620800	1.40577300
H	-2.72847400	8.19927100	0.69501400
N	1.05051600	7.47743900	0.26294200
C	1.84033600	8.68921500	0.48265100
H	1.15141000	9.47333100	0.80863100
C	2.60162200	9.11867600	-0.76789300
H	3.24670100	8.29539900	-1.10190500
C	3.45339100	10.36358600	-0.51892100
H	2.80787200	11.18299300	-0.17876500
H	4.15639900	10.16500100	0.29948200
C	4.22315100	10.80015100	-1.76179400
H	4.82238900	11.69126500	-1.55831300
H	4.90274500	10.01293300	-2.10388300
H	3.54337300	11.03684800	-2.58667000
H	2.53354900	8.50041600	1.30931700
H	1.88694400	9.30679900	-1.57781300
H	1.56817400	6.64160000	0.01013900

Table S1.2: 7_8-cis

C	-2.52380200	-1.99186000	-2.70048500
C	-3.38547300	-1.25208900	-1.68132200
C	-3.34674300	-1.86446100	-0.29841000
C	-2.87221500	-3.11114200	-0.06708300
C	-2.39254000	-4.05421700	-1.19548900
C	-2.77642600	-3.49172200	-2.58093100
H	-2.75085200	-1.64341400	-3.71299900
H	-3.08050200	-0.19966800	-1.60552600
H	-3.84289300	-3.68427400	-2.75863400
H	-2.22381900	-4.04605100	-3.34791400
H	-1.46316600	-1.77259600	-2.52399700
H	-4.43099500	-1.22855200	-2.02318000
C	-0.85956000	-4.21879200	-1.09444400
H	-0.50812900	-4.95031000	-1.82964000
H	-0.33936200	-3.27412700	-1.28146100
H	-0.56855700	-4.57338400	-0.10022700
C	-3.03853600	-5.45175100	-1.06875100
H	-2.80292300	-6.03975000	-1.96126700
H	-2.66261500	-6.00907600	-0.20627500
H	-4.12848900	-5.38090900	-0.99269200
C	-3.91275300	-0.96193600	0.76496400
H	-4.14915000	-1.48595700	1.69102600
H	-3.20720800	-0.15532800	1.00472200
H	-4.82724600	-0.48259900	0.39857300
C	-2.86787000	-3.71978800	1.27625500
H	-3.40458500	-4.66507700	1.32876700
C	-2.31541000	-3.33293900	2.45170400
H	-2.54329300	-3.97048200	3.30305400
C	-1.43248200	-2.22359200	2.79054800
C	-0.77049400	-1.47272500	1.85063600
H	-0.93393200	-1.71314200	0.80668300
C	0.12634100	-0.40965000	2.12242300
H	0.28650800	-0.12331800	3.15666400
C	0.80162400	0.27703100	1.14068700
H	0.63771000	-0.01727100	0.10778100
C	1.71034200	1.34280900	1.36846000
C	2.32526400	1.92989400	0.26061200
H	2.06834300	1.53276400	-0.71769900
C	3.24219800	2.97510300	0.30524900
H	3.54150300	3.41461500	1.25017500
C	-1.26566500	-2.02654800	4.27482600
H	-0.61079600	-1.20100000	4.54704800
H	-2.24171500	-1.85160100	4.74019100
H	-0.86115800	-2.93810600	4.72903800
C	1.98338400	1.79630700	2.77931800
H	2.66915300	2.63890400	2.84031400
H	1.05452900	2.09774300	3.27162800
H	2.41603500	0.98042300	3.36593300
N	3.81870800	3.51142800	-0.76171100
C	4.77455100	4.62978200	-0.73933000
H	4.99713900	4.85432800	0.30778200
C	4.23397300	5.87029400	-1.45260600
H	3.97227000	5.61390100	-2.48804800
C	5.25293400	7.01658700	-1.45674400
H	5.51870500	7.27096800	-0.42243800
H	6.17834600	6.67944800	-1.94121700
C	4.72413100	8.26184500	-2.17092800
H	5.46562900	9.06470900	-2.16047800
H	4.48258300	8.04502900	-3.21665100
H	3.81681800	8.63943500	-1.68818100
H	5.70702100	4.29702400	-1.20750400
H	3.30800800	6.19574900	-0.96322600
H	3.57720300	3.14801500	-1.67717900

Table S1.3: **8_11-cis**

C	-5.09899000	-4.00267200	-2.21874200
C	-4.13592500	-4.89730300	-1.44669300
C	-3.24545600	-4.14497800	-0.48527500
C	-3.09115900	-2.79422600	-0.53946300
C	-3.72678000	-1.92504600	-1.65022600
C	-4.33249600	-2.80393900	-2.76630000
H	-5.56802200	-4.56504600	-3.03185400
H	-4.68357900	-5.66216300	-0.88072000
H	-3.52227600	-3.16930600	-3.41213400
H	-4.97608200	-2.17629200	-3.39259900
H	-5.90906300	-3.66823800	-1.56016700
H	-3.49716800	-5.45582200	-2.14814300
C	-4.82355900	-1.03270700	-1.02910300
H	-5.24696000	-0.36636300	-1.78800900
H	-5.63600000	-1.63147700	-0.60804100
H	-4.41735400	-0.41206000	-0.22322700
C	-2.66926400	-1.01537300	-2.31675300
H	-2.33329400	-0.20541100	-1.66209000
H	-1.79694100	-1.59359000	-2.63863400
H	-3.10698900	-0.54513800	-3.20300400
C	-2.53474500	-5.05884100	0.47999700
H	-1.62449400	-4.62559500	0.89542900
H	-3.18752000	-5.34003900	1.31643800
H	-2.27007100	-5.99131500	-0.02996400
C	-2.31065300	-2.05035400	0.44498100
H	-1.82962600	-1.15069700	0.07084300
C	-2.20164800	-2.30184900	1.77524100
H	-2.79592400	-3.09778400	2.20987200
C	-1.42185100	-1.51891000	2.71396300
C	-0.38022900	-0.71432700	2.29419400
H	-0.12613000	-0.76127400	1.24660700
C	0.36100700	0.13779600	3.14652200
H	0.05392000	0.12953100	4.18800500
C	1.41464600	0.99988700	2.90039300
H	1.77349700	1.53590100	3.77373200
C	2.11258400	1.30352500	1.70310700
C	3.14978000	2.24075700	1.79441400
H	3.34150900	2.67015200	2.77392400
C	3.95556200	2.66683400	0.74649700
H	3.82192600	2.27896500	-0.25713000
C	-1.84215600	-1.66689700	4.15143600
H	-1.98014300	-2.72616300	4.38937300
H	-1.13494300	-1.25701900	4.87000000
H	-2.81188600	-1.18134900	4.31173600
C	1.75701500	0.64436400	0.40034700
H	1.85277700	-0.44197900	0.48413000
H	0.71899800	0.86329700	0.13254600
H	2.38193300	0.96369900	-0.43150600
N	4.93423900	3.55621700	0.86852800
C	5.78732100	4.03611700	-0.22887100
H	6.83077100	3.81542200	0.02058400
C	5.60933800	5.53238700	-0.49241900
H	4.56320700	5.73290200	-0.75367700
C	6.53193200	6.02998000	-1.61187200
H	7.57526800	5.81746000	-1.34520900
H	6.32549600	5.46635600	-2.53109500
C	6.36581000	7.52686000	-1.88041600
H	7.03135400	7.85830500	-2.68154000
H	5.33953200	7.76350800	-2.17980900
H	6.59927600	8.11658600	-0.98789400
H	5.53627100	3.45615300	-1.12173900
H	5.81942000	6.09453400	0.42748100
H	5.10789700	3.96264100	1.78106400

Table S1.4: **9_11-cis**

C	-7.02185500	-2.42257100	-1.79077400
C	-5.62320500	-3.01985200	-1.93052700
C	-4.59836200	-2.43733500	-0.98042100
C	-4.80693100	-1.27265000	-0.31255900
C	-6.12267700	-0.46789500	-0.41848200
C	-6.92461100	-0.90688000	-1.66161600
H	-7.63355600	-2.69623700	-2.65606600
H	-5.65811800	-4.10665400	-1.79133300
H	-6.43639100	-0.50253100	-2.55865000
H	-7.92074200	-0.45275000	-1.61321100
H	-7.51992000	-2.84624800	-0.91136700
H	-5.25553100	-2.86740300	-2.95761300
C	-6.97043900	-0.67861200	0.85599500
H	-6.43332800	-0.36948700	1.75884700
H	-7.88506400	-0.07921700	0.79982900
H	-7.25416500	-1.72648000	0.98196300
C	-5.81852600	1.03797700	-0.57240100
H	-5.34127900	1.45994600	0.31749100
H	-5.16255200	1.21943300	-1.42964400
H	-6.75085300	1.58800400	-0.73614200
C	-3.36072600	-3.29103000	-0.85012600
H	-2.67680000	-3.12833100	-1.69396700
H	-2.80683000	-3.10703600	0.07081400
H	-3.63467400	-4.35002700	-0.87500700
C	-3.83875500	-0.69938500	0.62096500
H	-4.27929800	-0.22649400	1.49512600
C	-2.49046800	-0.63676100	0.48358300
H	-2.05274400	-1.02857900	-0.42474600
C	-1.60646300	-0.03820100	1.45689200
C	-0.23713700	0.06530800	1.28879700
H	0.30240500	0.53427500	2.09742600
C	0.48043800	-0.39159700	0.15551000
H	-0.12156100	-0.85529300	-0.62029600
C	1.82638100	-0.35815000	-0.15604100
C	2.94040200	0.15140900	0.56352700
C	4.19570000	0.02556100	-0.04271400
H	4.22800300	-0.45212300	-1.01807700
C	5.40374500	0.45535700	0.49371700
H	5.44582000	0.93890600	1.46320900
C	-2.19601300	0.50760300	2.73132700
H	-2.72184000	-0.27285800	3.29005300
H	-1.42401900	0.92444600	3.37919400
H	-2.92195300	1.30027400	2.52167900
C	2.77491600	0.79435400	1.91124000
H	3.71110900	1.14202100	2.34375100
H	2.10555800	1.65676300	1.84255800
H	2.32948200	0.08853600	2.61835600
N	6.57961200	0.31772500	-0.10598700
C	7.86725300	0.78156200	0.43277400
H	7.68761200	1.15498200	1.44509200
C	8.50368600	1.86794700	-0.43594100
H	8.63330800	1.49072300	-1.45929400
C	9.86302900	2.31662800	0.11446400
H	9.73542600	2.69052600	1.13872500
H	10.53279800	1.44961500	0.18166000
C	10.51140100	3.40001300	-0.74940100
H	11.47705300	3.70451200	-0.33785700
H	10.68212400	3.04196600	-1.76996500
H	9.87776800	4.29103600	-0.80804300
H	8.53814500	-0.08007000	0.51697700
H	7.82435900	2.72665200	-0.49883100
H	6.60895900	-0.12149100	-1.01949400
H	2.08014900	-0.79594600	-1.11669800

Table S1.5: 11-cis

C	-10.30725300	-2.77289500	-1.36216900
C	-8.87453100	-3.02944200	-0.91295700
C	-8.08914500	-1.78023500	-0.58707500
C	-8.49450500	-0.55084800	-0.98171100
C	-9.81433000	-0.30330400	-1.73855400
C	-10.33789400	-1.61517700	-2.34693300
H	-10.72421600	-3.67658800	-1.81698400
H	-8.85942000	-3.69642700	-0.04345100
H	-9.72067400	-1.87342800	-3.21753000
H	-11.35334200	-1.44814900	-2.72326000
H	-10.93256100	-2.54728000	-0.49150600
H	-8.32721800	-3.56925800	-1.70083400
C	-10.86396200	0.28829000	-0.77934700
H	-10.52758100	1.23007700	-0.33334400
H	-11.79126200	0.50189500	-1.32117000
H	-11.09814100	-0.39654000	0.03963400
C	-9.58906000	0.68510300	-2.89603400
H	-10.50822300	0.78777500	-3.48186500
H	-9.31390500	1.68501500	-2.54584500
H	-8.79934900	0.33399300	-3.56792800
C	-6.84782200	-2.05891000	0.21977700
H	-6.05447200	-2.47606600	-0.41421400
H	-6.44932800	-1.17743200	0.72171600
H	-7.06203500	-2.81637200	0.98038700
C	-7.75017100	0.66941400	-0.67189600
H	-8.36558800	1.52694600	-0.40926400
C	-6.41394400	0.86063100	-0.75097700
H	-5.78448100	0.04480200	-1.09352500
C	-5.73650400	2.10139000	-0.45329200
C	-4.37204400	2.13757500	-0.63610200
H	-3.92068900	1.22129400	-0.99092600
C	-3.54933200	3.26401000	-0.39543800
H	-4.06676000	4.14512200	-0.02883000
C	-2.19199900	3.46341700	-0.53686400
C	-1.16116600	2.59750100	-0.98480600
C	0.13170900	3.12093300	-1.00793000
H	0.25985400	4.15072600	-0.68338100
C	1.27462800	2.44048800	-1.41163900
H	1.22799500	1.41022200	-1.74903100
C	-6.55249200	3.26695000	0.02792000
H	-7.30026200	3.53894200	-0.72376000
H	-7.09423700	2.99964800	0.93987100
H	-5.96258400	4.15608300	0.24080100
C	-1.45456100	1.18957600	-1.41277900
H	-1.89953500	0.62891200	-0.58573100
H	-2.17374600	1.18811000	-2.23666000
H	-0.57385100	0.64222300	-1.74468800
N	2.48536800	2.96265400	-1.42683200
C	3.71206800	2.26933600	-1.82015700
H	3.42447400	1.28158100	-2.19082600
C	4.70450500	2.15061800	-0.66737600
H	4.93657900	3.15237200	-0.28256800
C	5.99829600	1.45796400	-1.09581900
H	5.76362700	0.45961700	-1.48581700
H	6.45068500	2.01457100	-1.92585500
C	7.00067500	1.33837800	0.04821100
H	7.91500400	0.83938800	-0.28283100
H	7.28040600	2.32378400	0.43459300
H	6.58669100	0.75849400	0.87942100
H	4.15940100	2.81422300	-2.65836100
H	4.23601700	1.59826500	0.15576900
H	2.59108500	3.92188000	-1.11179500
H	-1.85069700	4.45676700	-0.25981700

Table S1.6: **11_14-cis**

C	-5.64286100	-4.03301600	-0.16229600
C	-4.22055900	-4.03416700	0.39380500
C	-3.62981400	-2.65587200	0.60056700
C	-4.16750900	-1.54273000	0.03449200
C	-5.45330700	-1.57557000	-0.82368100
C	-5.75359600	-3.01515100	-1.29136900
H	-5.90554000	-5.03363100	-0.51937700
H	-4.18341800	-4.58151600	1.34284300
H	-5.04459800	-3.28446600	-2.08596400
H	-6.75279500	-3.03513900	-1.74076100
H	-6.35324500	-3.79150600	0.63638900
H	-3.55560800	-4.58634600	-0.28919700
C	-6.64444300	-1.02922200	-0.00512300
H	-6.84185000	-1.64316300	0.87718000
H	-6.46835800	-0.00396900	0.33700300
H	-7.54794200	-1.01553000	-0.62349200
C	-5.27600600	-0.70710900	-2.08798500
H	-6.15543800	-0.80914900	-2.73195700
H	-5.16489100	0.35571200	-1.85195300
H	-4.39809100	-1.02321000	-2.66025000
C	-2.41912000	-2.65932700	1.50099300
H	-1.51375800	-2.94021500	0.94645800
H	-2.23432400	-1.69475300	1.97479700
H	-2.54331900	-3.40690300	2.28993700
C	-3.62661800	-0.20121600	0.23533300
H	-4.37747600	0.58299500	0.29569200
C	-2.32385100	0.17691300	0.28599400
H	-1.54911100	-0.56686500	0.13529700
C	-1.86669000	1.53323900	0.48165800
C	-0.50501500	1.76707800	0.42957300
H	0.11729000	0.90013200	0.24750700
C	0.11869800	3.01653000	0.65717100
H	-0.53473800	3.81220900	1.00239400
C	1.44861300	3.39115600	0.58534000
C	2.57794200	2.70050000	0.07686400
C	3.83408000	3.27780900	0.30905200
H	3.83423300	4.23479200	0.81758100
C	5.11065200	2.80999500	-0.00126400
H	5.93311600	3.48751600	0.21089400
C	-2.88631200	2.61332700	0.71677700
H	-3.54675400	2.70709000	-0.15183500
H	-3.51590200	2.36802200	1.57675600
H	-2.44700500	3.59285400	0.89286600
C	2.43374200	1.45598900	-0.75760600
H	2.56698900	0.54548000	-0.15822600
H	1.45043900	1.40127900	-1.22111000
H	3.16258300	1.44656100	-1.57277400
N	5.50333400	1.63891400	-0.49588200
C	6.90823200	1.27983100	-0.75435900
H	7.01219200	1.02521200	-1.81455400
C	7.37908600	0.11780100	0.12130300
H	7.28044000	0.39638700	1.17744900
C	8.83046300	-0.27523100	-0.18087000
H	8.92197300	-0.54372400	-1.24124300
H	9.48237000	0.59368200	-0.02329400
C	9.31069200	-1.43986300	0.68704100
H	10.34644900	-1.70079600	0.45541400
H	9.26061400	-1.18691600	1.75114200
H	8.69792000	-2.33281100	0.52491000
H	7.51628700	2.17042200	-0.57285600
H	6.72736000	-0.75201800	-0.03979400
H	4.82573200	0.90891900	-0.66359500
H	1.66855200	4.37500400	0.98876400

Table S1.7: 9-cis

C	-3.92342300	-5.96214600	0.60419700
C	-2.75744200	-5.80210300	-0.36538100
C	-2.48860600	-4.36723500	-0.75829300
C	-3.38342000	-3.37058800	-0.53410700
C	-4.79447800	-3.62662100	0.04532600
C	-5.10428400	-5.13830100	0.10217300
H	-4.19934100	-7.01742700	0.69323800
H	-1.83672800	-6.22208800	0.06122500
H	-5.37289100	-5.48485500	-0.90497800
H	-5.98720600	-5.28897000	0.73315200
H	-3.62621500	-5.62925200	1.60574200
H	-2.94757000	-6.38487700	-1.27969400
C	-4.87708000	-3.01777200	1.46233000
H	-4.64208300	-1.94822900	1.44560500
H	-5.88776700	-3.13455800	1.86716300
H	-4.17559700	-3.50144800	2.14823900
C	-5.88227400	-2.97250700	-0.83673600
H	-6.86780500	-3.31382100	-0.50475000
H	-5.88505300	-1.88085600	-0.76706200
H	-5.76475400	-3.25647700	-1.88741700
C	-1.16673500	-4.19906200	-1.46589200
H	-0.99971700	-5.05439700	-2.13000700
H	-1.10979200	-3.28896300	-2.06335500
H	-0.33034100	-4.19480900	-0.75430000
C	-3.09387500	-1.96652500	-0.83098800
H	-3.93265800	-1.38594700	-1.20174600
C	-1.92076400	-1.31829700	-0.62842800
H	-1.10156000	-1.87039400	-0.18487000
C	-1.70210400	0.07881600	-0.93353900
C	-0.51442400	0.72803400	-0.67409100
H	-0.45157000	1.77792200	-0.94513400
C	0.64373400	0.16668200	-0.08170600
H	0.61817800	-0.87965700	0.20581400
C	1.79413100	0.88263300	0.14887200
H	1.80890100	1.92921900	-0.14247100
C	2.97528600	0.36597600	0.74289300
C	4.05866800	1.22972300	0.90761100
H	3.93169400	2.25407000	0.56740300
C	5.28622900	0.89040200	1.47142700
H	5.47279300	-0.11312000	1.82878700
C	-2.81716600	0.86990000	-1.56448000
H	-2.51695400	1.90277100	-1.74445900
H	-3.12005200	0.43266500	-2.52109700
H	-3.70301300	0.88467400	-0.92068300
C	3.01864900	-1.07802900	1.17162600
H	2.83485000	-1.73620000	0.31744400
H	3.97035000	-1.37329300	1.60902000
H	2.24173500	-1.27954600	1.91489200
N	6.29201900	1.74156400	1.61160100
C	7.61991800	1.46439400	2.19651900
H	8.37196000	1.70371200	1.43676000
C	7.81522900	0.03243800	2.68066400
H	7.06977000	-0.21443300	3.44775300
C	9.21899000	-0.16357600	3.27221400
H	9.97059500	0.08684700	2.51319200
H	9.36496500	0.54077200	4.10065400
C	9.44532900	-1.59290500	3.76728400
H	10.44924700	-1.70807700	4.18337900
H	8.72827300	-1.85913700	4.55091700
H	9.33847600	-2.31627500	2.95214600
H	7.76495900	2.15971600	3.03051900
H	7.67946200	-0.67166800	1.84947200
H	6.15354900	2.69245900	1.28781400

Table S1.8: 8-cis

C	-5.37161800	2.14417800	-5.02582800
C	-5.47640200	1.39365600	-3.70864600
C	-4.15890800	1.16470600	-3.01704800
C	-2.95429600	1.38549700	-3.61661800
C	-2.84248600	1.79039600	-5.09929300
C	-4.19572200	1.59194900	-5.81295200
H	-6.30136000	2.04109400	-5.59314000
H	-6.14564800	1.91186100	-3.00990300
H	-4.35687700	0.51863800	-5.97936000
H	-4.13419800	2.05445400	-6.80384200
H	-5.23922500	3.21483000	-4.83682400
H	-5.93989500	0.40798400	-3.86856200
C	-2.42639900	3.26812000	-5.23968500
H	-1.47984600	3.49191800	-4.74399500
H	-2.31267200	3.52350900	-6.29836400
H	-3.17732700	3.93734600	-4.81136000
C	-1.83883500	0.88920600	-5.84466200
H	-0.80198700	1.03999500	-5.54242700
H	-2.07973700	-0.16787400	-5.69416200
H	-1.89783700	1.09458400	-6.91834300
C	-4.34175800	0.69913800	-1.59046900
H	-4.26587300	1.53767800	-0.88811800
H	-5.34049500	0.27258000	-1.46722600
H	-3.62584100	-0.06408600	-1.27794200
C	-1.77096700	1.23104100	-2.78668900
C	-0.48556200	1.60569100	-3.01232900
H	-0.22693100	2.13895700	-3.91774100
C	0.60694600	1.42103600	-2.08565200
C	0.54403400	0.54728100	-1.02318600
H	-0.34673800	-0.06454900	-0.91484000
C	1.54896900	0.34999600	-0.05656500
H	2.45868100	0.93569200	-0.13689200
C	1.44200300	-0.54374400	0.98573100
H	0.52896600	-1.12897300	1.06458600
C	2.43318700	-0.76512700	1.96522600
C	2.17620100	-1.71400900	2.95725600
H	1.22005700	-2.23068800	2.91717100
C	3.04035400	-2.05700500	3.98699100
H	4.01099200	-1.58227700	4.08683600
C	1.82340400	2.24732600	-2.40012200
H	2.67233000	2.06894100	-1.74218500
H	2.14753700	2.04469100	-3.42648500
H	1.57282000	3.31270100	-2.35525500
C	3.72006200	0.01483200	1.91019900
H	3.51710300	1.08807500	1.96390600
H	4.41121700	-0.22596100	2.71584700
H	4.23917900	-0.17505100	0.96642300
N	2.78199900	-2.96389200	4.91197900
C	3.66219600	-3.32702800	6.02158400
C	3.05105300	-2.99621300	7.37995100
H	2.84677400	-1.92012700	7.43020000
C	3.96233700	-3.41262500	8.53454400
H	4.16678300	-4.48828000	8.46621100
H	4.93121300	-2.90790600	8.43245100
C	3.35868300	-3.09100700	9.89837300
H	4.02895900	-3.39698000	10.70569500
H	3.17418500	-2.01736300	10.00722000
H	2.40557600	-3.61020200	10.04215900
H	2.08291900	-3.50505800	7.47670900
H	1.88395900	-3.43491300	4.87509900
H	-1.96269800	0.79373400	-1.81402500
H	4.60540700	-2.79239100	5.87876200
H	3.88201000	-4.39772400	5.94990200

Table S2 Cartesian coordinates for transition state geometries listed in Table 1, and it is called rotation state if imaginary frequency (in parentheses) is more than one.

Table S2.1: **RS(AT/7_8-cis)(-576.7 -250.5 -222.0 -201.67 -170.9 -143.8 -137.2 -51.7 -39.5 -13.9)**

C	-1.77796125	1.74695258	-5.83451714
C	-1.77796125	1.74695258	-4.31003880
C	-0.39688182	1.74695258	-3.69468419
C	0.71259051	1.43703046	-4.40553943
C	0.67522943	1.05594280	-5.90124099
C	-0.76261656	0.73296682	-6.34409373
H	-2.77848787	1.51190665	-6.21064029
H	-2.33581502	2.60931074	-3.92442958
H	-1.03558383	-0.26110810	-5.96586530
H	-0.78631563	0.66956460	-7.43783084
H	-1.53238904	2.74846734	-6.20688775
H	-2.31625640	0.86272356	-3.93655618
C	1.23821062	2.22026527	-6.74175105
H	2.18218582	1.94124051	-7.22152351
H	0.53705361	2.50341796	-7.53347398
H	1.42751968	3.10340316	-6.12462825
C	1.53140608	-0.19822903	-6.16673464
H	1.39605297	-0.52158168	-7.20376079
H	2.60007298	-0.01383525	-6.02169885
H	1.23425340	-1.02639490	-5.51530813
C	-0.40095575	2.11590070	-2.23471442
H	-0.03408523	1.29958511	-1.60528867
H	0.21134738	2.99890681	-2.03066232
H	-1.42248594	2.34121965	-1.91092895
C	2.05585316	1.42066873	-3.81293387
C	2.45530497	1.75501520	-2.56365022
C	2.60398082	0.88834746	-1.41014706
C	1.63523959	0.85683397	-0.43699689
H	0.76593805	1.49252337	-0.57566043
C	1.66079784	0.07517411	0.74229798
H	2.50949993	-0.58102670	0.90523784
C	0.66637848	0.10508543	1.69011764
H	-0.18037263	0.76516855	1.52089099
C	0.65689016	-0.65877865	2.88371644
C	-0.42750935	-0.50896296	3.74791899
H	-1.20690451	0.18919055	3.45314832
C	-0.59319233	-1.17508631	4.95738572
H	0.14716475	-1.88422156	5.31185621
C	3.86874741	0.07663652	-1.34522131
H	3.67314195	-0.99603514	-1.39862830
H	4.52644387	0.33461725	-2.18136528
H	4.42448685	0.26668930	-0.42450617
C	1.80275659	-1.59087144	3.17689187
H	1.48514712	-2.63466443	3.18290721
H	2.58064036	-1.48999350	2.41478242
H	2.26364572	-1.38520484	4.14424627
N	-1.62763469	-1.01281349	5.76437851
C	-1.83873009	-1.71799265	7.03325003
H	-0.94241756	-2.31223042	7.23211715
C	-3.08145877	-2.60580053	7.00341813
H	-3.96020050	-1.99631711	6.75394799
C	-3.31449140	-3.30780356	8.34401290
H	-2.43374942	-3.91230631	8.59562561
H	-3.40986905	-2.55524231	9.13686480
C	-4.55746424	-4.19574519	8.32729029
H	-4.70182454	-4.68612502	9.29333195
H	-5.45824071	-3.61166440	8.11239564
H	-4.47554877	-4.97770101	7.56537463
H	-1.91959806	-0.97250372	7.83149936
H	-2.97566707	-3.34901606	6.20411123
H	-2.35785282	-0.36710062	5.48261306
H	2.83709929	1.09523388	-4.46764499
H	2.69068653	2.78707227	-2.40759335

Table S2.2:TS(AT/11-cis imaginary frequency:-418.01)

C	5.53277672	1.50442163	-0.18572056
C	5.31165070	0.15216561	-0.01651356
C	4.06794070	-0.49233739	-0.31939656
C	2.77502868	0.01919561	-0.28570056
C	1.60838668	-0.68696539	-0.61197256
C	0.35086166	-0.01321839	-0.42342156
C	-0.87547734	-0.51470839	-0.74420257
C	-2.11758136	0.23455561	-0.55426757
C	-3.26987538	-0.25124839	0.00964344
C	-4.43281838	0.59236561	0.04943344
C	-5.66366540	0.19861861	0.51691344
C	1.61031568	-2.08048841	-1.16139356
C	-3.34379637	-1.64767141	0.57273344
N	-6.75424540	0.98824063	0.58310444
H	4.15593570	-1.55315141	-0.53170356
H	2.62564668	1.02701863	0.08075644
H	0.39941366	0.98505863	0.00546944
H	-0.94871936	-1.51034741	-1.17734856
H	-2.12312936	1.26184662	-0.91662057
H	-4.32115238	1.60550863	-0.33019656
H	-5.81842938	-0.81419041	0.87515844
H	-6.67783740	1.94488463	0.26074344
H	1.02088566	-2.12985641	-2.08447058
H	1.15034767	-2.78091441	-0.45385456
H	2.60829368	-2.44591041	-1.39739758
H	-3.99783538	-2.29007141	-0.02830556
H	-3.73944038	-1.63688841	1.59351146
H	-2.35905836	-2.11555341	0.61134245
C	6.43586672	-0.81175739	0.44073244
C	6.85809472	2.14770763	0.13184444
C	4.51018770	2.47054763	-0.71862056
C	-8.07578142	0.54555061	1.02775944
C	7.59711972	-0.02985339	1.09118846
C	8.02821574	1.17689061	0.26915044
C	6.95368072	-1.61178841	-0.77543157
C	5.90698072	-1.79999941	1.50396045
H	7.28352272	0.30833361	2.08809546
H	8.43486574	-0.71902939	1.24339146
H	8.87574274	1.68274163	0.74116244
H	8.36766374	0.86179662	-0.72373356
H	6.73179872	2.70861163	1.07403846
H	7.07406672	2.90890163	-0.62660856
H	7.39236173	-0.95813640	-1.53370458
H	6.15164372	-2.18261341	-1.25498257
H	7.71827073	-2.32627141	-0.45405356
H	5.44746471	-1.26686739	2.34207446
H	6.73971972	-2.39217041	1.89635846
H	5.17258370	-2.50303541	1.10100745
H	5.00520171	3.31925265	-1.19662956
H	3.89540470	2.88710763	0.09181844
H	3.83446570	2.01754963	-1.44612058
C	-9.07648842	0.39962461	-0.12468656
H	-7.95154942	-0.41148639	1.54396546
H	-8.45710542	1.26159961	1.76490446
C	-10.46157544	-0.03685739	0.36711544
H	-9.16190142	1.35654063	-0.65655256
H	-8.68835542	-0.32906939	-0.84710157
C	-11.46802744	-0.18216439	-0.77609356
H	-10.37335844	-0.99121640	0.90281745
H	-10.83578244	0.69374861	1.09607645
H	-12.44672146	-0.49456239	-0.40213256
H	-11.13430944	-0.92960541	-1.50347058
H	-11.60103944	0.76600461	-1.30748957

Table S2.3:RS(AT/8_11-cis)(-1128.7 -402.3 -258.1 -224.0 -206.8 -200.1 -168.1 -79.0 -52.6 -43.0 -28.5 -24.0)

C	-5.30985333	1.75896045	-5.02928865
C	-5.30985333	1.75896045	-3.50545104
C	-3.93006449	1.75896045	-2.88937376
C	-2.81752756	1.45178990	-3.60324243
C	-2.86241209	1.05393157	-5.09468798
C	-4.30184047	0.73595816	-5.53437096
H	-6.31185496	1.53117507	-5.40548799
H	-5.86515833	2.62246036	-3.11914787
H	-4.58115153	-0.25449859	-5.15059212
H	-4.32586759	0.66678144	-6.62763142
H	-5.05650912	2.75813681	-5.40133065
H	-5.84954297	0.87574646	-3.13065285
C	-2.29248597	2.20304329	-5.95098302
H	-1.40787916	1.87865498	-6.50902698
H	-3.03361233	2.55177917	-6.67666686
H	-2.00099888	3.05689206	-5.33198945
C	-2.02072925	-0.21393073	-5.34609030
H	-1.29334650	-0.05698530	-6.14881798
H	-1.47467468	-0.52439552	-4.44943032
H	-2.66843386	-1.04228820	-5.65025426
C	-3.94497218	2.11460601	-1.42512840
H	-3.57375665	1.29838202	-0.79839375
H	-3.34778320	3.00474200	-1.20720651
H	-4.97150551	2.32735056	-1.10914908
C	-1.47310598	1.49846429	-3.03263547
C	-1.12909529	1.78152801	-1.75274927
H	-1.90796923	2.03355010	-1.04075240
C	0.22483499	1.81014958	-1.24289778
C	0.72435319	0.71505133	-0.57253384
H	0.04770401	-0.11743174	-0.42228065
C	2.03838702	0.59544764	-0.06395884
H	2.69978981	1.44189559	-0.22017623
C	2.58836361	-0.47489403	0.60818036
H	3.09630799	-1.21654949	-0.00206351
C	2.57774128	-0.73220648	2.00173020
C	3.20860674	-1.89723473	2.44515544
H	3.66527994	-2.53268367	1.69068542
C	3.30305961	-2.31370162	3.76747044
H	2.87085293	-1.72874962	4.57218344
C	1.01167374	3.06797720	-1.48694949
H	0.43789434	3.75164205	-2.12042569
H	1.24583647	3.59819843	-0.56251838
H	1.95168653	2.86198492	-2.00440268
C	1.91000916	0.22570298	2.94940982
H	2.36204972	1.21830364	2.86803628
H	0.84885084	0.32650390	2.70356660
H	1.97517887	-0.07766196	3.99265540
N	3.90680595	-3.42389313	4.16008306
C	4.02352290	-3.88611139	5.54729222
C	3.31138811	-2.95817364	6.53005318
H	3.73146162	-1.94796433	6.44547867
C	3.43760780	-3.44989845	7.97471304
H	3.02296923	-4.46307651	8.05140262
H	4.49945809	-3.52930948	8.24029753
C	2.72847780	-2.52941353	8.96671634
H	2.83248243	-2.90063909	9.98944039
H	3.14527310	-1.51746469	8.93542373
H	1.65862195	-2.45798770	8.74530842
H	2.25131413	-2.88318295	6.25636820
H	4.33279121	-4.01316367	3.45258414
H	-0.66699154	1.28437772	-3.70289399
H	5.05971880	-3.93828680	5.80897102
H	3.59691238	-4.86442738	5.62345843

Table S2.4:RS(AT/9_11-cis)(-148.6 -113.6 -62.9 -32.3 -13.1 -12.2)

C	-4.12249943	2.13198030	-5.51010235
C	-4.12249943	2.13198030	-3.98406317
C	-2.74399009	2.13198030	-3.36005323
C	-1.62894471	1.81740042	-4.06677691
C	-1.65583136	1.48770463	-5.57553285
C	-3.08860599	1.13926041	-6.02513799
H	-5.11917744	1.87820606	-5.88416430
H	-4.68453323	2.99245587	-3.60295254
H	-3.34185581	0.13668541	-5.65508992
H	-3.10880887	1.08457188	-7.11941015
H	-3.89862752	3.13860781	-5.88058467
H	-4.65897433	1.24497704	-3.61226160
C	-1.12856373	2.69191217	-6.38459378
H	-0.10753816	2.96256947	-6.09577163
H	-1.10997271	2.44710164	-7.45171955
H	-1.75578675	3.57631247	-6.24716028
C	-0.76769931	0.26187332	-5.87142996
H	0.19988436	0.55623118	-6.28994871
H	-0.57829189	-0.32278594	-4.96565350
H	-1.25774332	-0.39157875	-6.60035953
C	-2.75433497	2.53094149	-1.90547538
H	-3.06579328	1.69242468	-1.26842496
H	-1.78616837	2.88221815	-1.54805647
H	-3.48575204	3.32862271	-1.74372953
C	-0.28663472	1.82280883	-3.48704497
H	0.49209522	2.19331945	-4.14933772
C	0.09122347	1.36214094	-2.26970752
H	-0.66039205	0.91158057	-1.63346843
C	1.44798654	1.39111644	-1.77487448
C	1.78705602	0.86531117	-0.54419722
C	1.17904396	1.20151410	0.68951627
H	0.38100422	1.93639117	0.64632803
C	1.45324699	0.72725026	1.95532881
H	1.66392476	1.48366327	2.70589863
C	1.50030818	-0.61178223	2.42307643
C	1.80815578	-0.80592367	3.77259352
H	1.99093849	0.08170613	4.37248962
C	1.90317886	-2.03577414	4.41337751
H	1.73460363	-2.96248299	3.87587550
C	2.51844960	2.01343939	-2.63076458
H	2.60137386	1.49292262	-3.59051154
H	2.28534409	3.05995597	-2.84979424
H	3.49569716	1.98057452	-2.14891192
C	1.22857646	-1.76259226	1.49501080
H	0.22673467	-1.67611357	1.06463950
H	1.94311357	-1.76063540	0.66681688
H	1.29269789	-2.73553879	1.97852137
N	2.20097729	-2.18993575	5.69473135
C	2.28710219	-3.47504750	6.40014140
H	2.16600673	-4.26813856	5.65676451
C	1.23640465	-3.60385517	7.50275537
H	1.34520992	-2.77184847	8.21128543
C	1.35936779	-4.93180898	8.25711270
H	1.25525625	-5.76353738	7.54847162
H	2.36604179	-5.01463895	8.68624046
C	0.31613732	-5.06977247	9.36582774
H	0.42277211	-6.02388429	9.88819967
H	0.41903194	-4.27073637	10.10728303
H	-0.70016370	-5.02276546	8.96125148
H	3.29435032	-3.57184722	6.81926904
H	0.23619325	-3.51473892	7.06202496
H	2.36283649	-1.35949695	6.25429495
H	2.57588852	0.14275170	-0.52072163

Table S2.5:TS(11-cis/11_14-cis imaginary frequency:-329.09)

C	-6.74610233	2.49527477	0.05367479
C	-5.41717932	2.85117577	-0.60980721
C	-4.47859232	1.67424577	-0.78543321
C	-4.64313332	0.50704376	-0.11850821
C	-5.82705033	0.24744976	0.83901879
C	-6.49710333	1.57691177	1.24513880
H	-7.26374033	3.40606378	0.37176779
H	-5.59430933	3.31271577	-1.58876822
H	-5.84740732	2.09466577	1.96397980
H	-7.43289633	1.35251177	1.77011380
H	-7.40221733	2.00163777	-0.67238321
H	-4.89863532	3.61793277	-0.01282621
C	-6.86193833	-0.67412424	0.15473779
H	-6.42092833	-1.63259025	-0.13763721
H	-7.68546934	-0.88955124	0.84395879
H	-7.27825733	-0.21248924	-0.74422321
C	-5.33102233	-0.43687224	2.13045380
H	-6.16149333	-0.54196724	2.83655380
H	-4.92882632	-1.43641825	1.94031880
H	-4.54787632	0.15792776	2.61132780
C	-3.37523131	1.94344277	-1.77983922
H	-2.60353531	2.59532077	-1.34868722
H	-2.88711131	1.03490777	-2.13225322
H	-3.77860832	2.47401277	-2.64886822
C	-3.74448931	-0.64685724	-0.28007221
H	-4.24386532	-1.61069625	-0.35089221
C	-2.39600231	-0.62869424	-0.28286021
H	-1.88319331	0.31882076	-0.14361821
C	-1.53373631	-1.79714925	-0.42759821
C	-0.18219030	-1.60530725	-0.37177821
H	0.14394270	-0.58487324	-0.22257721
C	0.81286870	-2.63549725	-0.49377921
H	0.41875870	-3.63535626	-0.64698521
C	2.17220071	-2.59053725	-0.45174221
C	3.09070571	-1.47785725	-0.26950221
C	4.42161672	-1.75068625	-0.25012121
H	4.77689172	-2.76661725	-0.41272921
C	5.48914473	-0.76258925	-0.10596921
C	-2.19202331	-3.13597225	-0.62664621
H	-2.83963531	-3.37314826	0.22390479
H	-2.82549731	-3.12153326	-1.51904322
H	-1.48418931	-3.95518226	-0.73795022
C	2.59516871	-0.06187824	-0.11563121
H	1.99692271	0.23109776	-0.98218321
H	1.96022371	0.03922176	0.76878679
H	3.41314172	0.65719876	-0.02042921
H	2.67447771	-3.54634526	-0.57327821
N	5.99637773	-0.45807824	1.04309779
C	7.11521673	0.47891476	1.33016979
C	7.71587974	1.14634176	0.10124279
C	8.86138374	2.09150477	0.49991679
H	8.48207874	2.84831077	1.19769279
H	9.62971374	1.52374577	1.03910580
C	9.48766374	2.77916278	-0.71425921
H	10.29818775	3.44464077	-0.40801621
H	9.90503375	2.04766477	-1.41368222
H	8.74988474	3.38114877	-1.25451422
H	5.93400472	-0.27584024	-0.97285221
H	5.58543373	-0.91618724	1.85707180
H	7.87409874	-0.10104624	1.86505480
H	6.72153973	1.22812976	2.02439380
H	8.10621974	0.39069176	-0.59236221
H	6.95088073	1.72375977	-0.43362521

Table S2.6: TS(11-cis/9_11-cis imaginary frequency:-467.16)

C	7.08185431	1.87003504	0.96826975
C	5.99075031	2.43362304	0.06820275
C	4.85861630	1.49105604	-0.21449225
C	4.94261130	0.13944303	0.08591175
C	6.26454131	-0.51499197	0.57420275
C	7.44704331	0.47340503	0.47912275
H	7.95452232	2.52829204	0.94961075
H	5.56202830	3.35868904	0.47751475
H	7.78059332	0.53814803	-0.56533325
H	8.28550132	0.06343603	1.05036576
H	6.73646631	1.83759204	2.00753576
H	6.41788331	2.73038504	-0.90374926
C	6.08862531	-0.97685697	2.03751076
H	5.25736630	-1.68340698	2.13802676
H	6.99561431	-1.48179498	2.38310176
H	5.89055731	-0.13601597	2.70808076
C	6.62132931	-1.73650998	-0.30264525
H	7.62143732	-2.08843898	-0.03308925
H	5.94446930	-2.58418298	-0.15965525
H	6.63297131	-1.47492498	-1.36512426
C	3.69702630	2.15740304	-0.89050725
H	4.04416030	3.04052305	-1.43278526
H	3.16827729	1.50979904	-1.58960126
H	2.97203530	2.51805604	-0.14839025
C	3.84282430	-0.74816598	-0.02915525
H	4.11396030	-1.79628798	0.03619575
C	2.46639829	-0.49772797	-0.12319225
H	2.08468129	0.50803803	-0.03875525
C	1.51311629	-1.49284098	-0.27259725
C	0.08112528	-1.11940298	-0.27071725
C	-0.60722572	-0.84967597	-1.40385425
C	-1.99001973	-0.48878597	-1.60543426
C	-2.91485873	-0.01620897	-0.71454325
C	-4.25942774	0.23262003	-1.17849826
H	-4.44100674	0.04847703	-2.23493726
C	-5.30483174	0.63961603	-0.41053025
H	-5.18335774	0.80822103	0.65482075
C	1.80249629	-2.94637899	-0.44650525
H	1.42144729	-3.25790498	-1.42773225
H	2.85153929	-3.23207998	-0.37864625
H	1.22272928	-3.52118099	0.28401675
C	-2.56594773	0.26989103	0.72489075
H	-1.53928373	0.63376303	0.81236576
H	-3.21565274	1.03364104	1.15455075
H	-2.65560573	-0.62838497	1.34779276
H	-2.32551173	-0.60148597	-2.63261826
N	-6.56759775	0.87464503	-0.85584825
C	-7.69257376	1.20702903	0.01364475
H	-7.28901275	1.64774204	0.93208075
C	-8.57900376	0.00591603	0.35698775
H	-8.95329576	-0.44403397	-0.57228325
C	-9.76082976	0.38820703	1.25427075
H	-9.38248476	0.84142904	2.18045976
H	-10.35985277	1.16196303	0.75596675
C	-10.65202177	-0.80741397	1.59652276
H	-11.48689677	-0.50999597	2.23715276
H	-11.07033177	-1.25820297	0.69031275
H	-10.08561877	-1.58275298	2.12343776
H	-8.29235776	1.98653704	-0.46962725
H	-7.96754075	-0.76098697	0.84985875
H	-6.76527775	0.73166603	-1.83555526
H	-0.39064572	-1.13793397	0.70725275
H	-0.04646372	-0.93465597	-2.33645626

Table S2.7:RS(AT/9-cis)(-797.3 -712.9 -201.3 -177.2 -120.4 -93.5 -64.5 -46.5 -28.6 -4.3)

C	-4.88380134	-2.09136164	-5.04490700
C	-4.88380134	-2.09136164	-3.52083736
C	-3.50306449	-2.09136164	-2.90593911
C	-2.39187610	-2.39798112	-3.61973097
C	-2.43602892	-2.79677753	-5.11084932
C	-3.87564453	-3.11441870	-5.55017983
H	-5.88594147	-2.31963058	-5.42063049
H	-5.43951817	-1.22768702	-3.13490316
H	-4.15458055	-4.10486219	-5.16637797
H	-3.89995841	-3.18359276	-6.64343066
H	-4.63052749	-1.09233873	-5.41775093
H	-5.42356378	-2.97472461	-3.14665972
C	-1.86572726	-1.64775797	-5.96722655
H	-0.84093061	-1.39793315	-5.67285129
H	-1.84433252	-1.93758509	-7.02299342
H	-2.46647814	-0.73883476	-5.87478054
C	-1.59331949	-4.06418247	-5.36062569
H	-1.74396776	-4.40652860	-6.38942734
H	-0.52054962	-3.88898031	-5.23481081
H	-1.89046949	-4.87604450	-4.68913028
C	-3.51747887	-1.74322060	-1.43911270
H	-4.16882971	-2.43692895	-0.89389452
H	-2.53044074	-1.77315501	-0.97757531
H	-3.93724641	-0.74226366	-1.28402972
C	-1.04547452	-2.35482102	-3.04824739
H	-0.24451612	-2.62350188	-3.73156626
C	-0.70531917	-2.02294392	-1.78053152
H	-1.49177341	-1.75173428	-1.08520567
C	0.64865568	-2.00394155	-1.27501029
C	0.90175799	-1.64808229	0.02994596
H	0.96350156	-2.45000995	0.76099457
C	1.09408454	-0.33632492	0.52469225
H	1.03918135	0.49006715	-0.17668811
C	1.34755011	-0.05756386	1.84581165
H	1.40134721	-0.89096709	2.54138319
C	1.54753437	1.23943387	2.38181284
C	1.79602222	1.35101315	3.74922836
H	1.82128877	0.43064885	4.32727561
C	2.01380229	2.54150205	4.43614798
H	2.00144371	3.49344030	3.91937649
C	1.77507636	-2.38078339	-2.19766536
H	2.34268542	-3.22211380	-1.79326241
H	1.39125705	-2.68016337	-3.17772765
H	2.47166486	-1.55478490	-2.35646947
C	1.48631765	2.43608152	1.46945685
H	1.24031841	2.12554608	0.44994145
H	0.72610205	3.15182115	1.78527386
H	2.43802498	2.96860277	1.42906115
N	2.24549681	2.61537946	5.73544226
C	2.49370904	3.83948854	6.51140055
C	3.65998217	4.66842352	5.98412075
H	4.57584266	4.06306223	5.98141688
C	3.88880806	5.92125202	6.83651572
H	2.97307454	6.52549735	6.84652904
H	4.07580744	5.62388875	7.87584039
C	5.05512695	6.76585223	6.32646156
H	5.19792470	7.65242112	6.94936671
H	5.99081399	6.19731581	6.33760779
H	4.88016083	7.10489972	5.30016566
H	3.46500513	4.96386657	4.94568074
H	2.27128947	1.74780005	6.26075566
H	1.60962546	4.44190756	6.49171470
H	2.69951759	3.56583019	7.52513325

Table S3 Cartesian coordinates for representative conical intersection geometries listed in Table 1.

Table S3.1: CI(AT/7_8-cis)

C	-1.77728132	1.74565161	-5.83595447
C	-1.77974299	1.74633915	-4.30964572
C	-0.39541811	1.74775533	-3.69425507
C	0.70846195	1.43341718	-4.40554751
C	0.67546127	1.05462882	-5.90446362
C	-0.76056754	0.73702549	-6.34452279
H	-2.77586756	1.51473141	-6.20996385
H	-2.34483856	2.60360875	-3.92413483
H	-1.04402509	-0.26584956	-5.95364564
H	-0.78956315	0.66246582	-7.44147708
H	-1.54147270	2.74688747	-6.18690172
H	-2.31195628	0.86850094	-3.93905126
C	1.23837309	2.21961101	-6.74227784
H	2.17100020	1.94337665	-7.22929810
H	0.52906260	2.50535829	-7.53780797
H	1.42257969	3.12152415	-6.11844390
C	1.53614630	-0.19625747	-6.16746381
H	1.39347157	-0.53418437	-7.20898949
H	2.60705693	-0.02376175	-6.01768331
H	1.23095811	-1.02341057	-5.52425011
C	-0.40121279	2.11712296	-2.23222604
H	-0.03182402	1.29259570	-1.61101689
H	0.20586994	3.00403658	-2.02137854
H	-1.42001045	2.33455948	-1.92189298
C	2.05586139	1.42212118	-3.81250282
C	2.45647651	1.75297420	-2.55958165
C	2.60157194	0.88703840	-1.41025268
C	1.63412368	0.85518496	-0.43801942
H	0.75827916	1.49886546	-0.57077924
C	1.66262621	0.07622620	0.74065467
H	2.51388311	-0.57995150	0.89646922
C	0.66661380	0.10319246	1.68787392
H	-0.18337398	0.76650055	1.51918455
C	0.65677290	-0.65749046	2.88217441
C	-0.42622406	-0.50791569	3.74996972
H	-1.20080262	0.20515076	3.44917481
C	-0.59545307	-1.17783418	4.96147458
H	0.14578201	-1.89569781	5.31706730
C	3.86860517	0.07768609	-1.34586424
H	3.68399691	-0.99513585	-1.39405167
H	4.52618361	0.34136159	-2.17558095
H	4.42088430	0.25817629	-0.43035103
C	1.80122740	-1.59111144	3.17585902
H	1.48303729	-2.63941505	3.18394132
H	2.58145885	-1.48921084	2.41677700
H	2.26193114	-1.38010806	4.14561230
N	-1.62739991	-1.01240161	5.76574449
C	-1.83938509	-1.71737219	7.03407574
H	-0.93247030	-2.31090308	7.23385730
C	-3.08145896	-2.60758250	7.00357062
H	-3.95995354	-1.98463721	6.75623802
C	-3.31630450	-3.30746222	8.34455443
H	-2.43313657	-3.91436346	8.59965813
H	-3.41348983	-2.56419422	9.13147097
C	-4.55665884	-4.19356412	8.32614067
H	-4.69444276	-4.68353780	9.29576986
H	-5.44852605	-3.61305654	8.09858402
H	-4.47702864	-4.97183403	7.55835744
H	-1.90393662	-0.97056093	7.84509534
H	-2.97882003	-3.35230062	6.20406172
H	-2.35680587	-0.36516615	5.47671795
H	2.85780882	1.10336428	-4.48362803
H	2.69300107	2.79111305	-2.40745176

Table S3.2:CI(AT/11-cis)

C	5.56905604	1.53135275	0.14969875
C	5.19682039	0.22549775	0.07277330
C	3.91606361	-0.31047235	-0.34990621
C	2.66671948	0.16197162	-0.17197787
C	1.53996202	-0.63532433	-0.63705128
C	0.22387669	-0.07708137	-0.59462461
C	-0.92241877	-0.60446520	-1.15597612
C	-2.19783191	0.13577138	-1.14522835
C	-3.26478091	-0.05967486	-0.23612955
C	-4.45475210	0.60782145	-0.53153591
C	-5.58697186	0.56400280	0.34825497
C	1.77777917	-1.95030583	-1.29842602
C	-3.14255325	-0.99232813	0.96875349
N	-6.72002849	1.17710212	0.06912690
H	3.99478276	-1.31615996	-0.82502018
H	2.36833656	1.08066063	0.32802129
H	0.14663835	0.88909090	-0.05973759
H	-0.73499048	-1.49557645	-1.86324393
H	-2.39694474	0.89099866	-1.84029957
H	-4.52686338	1.24186523	-1.39766140
H	-5.59489765	-0.01162467	1.27028293
H	-6.72072389	1.72332507	-0.79643589
H	2.29091570	-2.67040123	-0.69953376
H	2.38184471	-1.92150584	-2.18906603
H	0.82926293	-2.46875381	-1.55837340
H	-4.01067377	-1.63910307	1.07054648
H	-3.06261665	-0.40754087	1.91306217
H	-2.28082319	-1.61632314	0.87737330
C	6.24741851	-0.91615956	0.28222717
C	6.93354563	1.95584629	0.54845714
C	4.63074279	2.68070544	0.03677403
C	-7.99708089	1.06648030	0.82819635
C	7.40292928	-0.37599022	1.09813280
C	8.01934337	0.91944602	0.49297922
C	6.74316362	-1.50583761	-1.05317852
C	5.68515938	-2.04528226	1.13920612
H	7.13410029	-0.13813660	2.12866987
H	8.25280548	-1.13263459	1.11140661
H	8.87534401	1.27183971	1.10187588
H	8.43479879	0.73645596	-0.50254678
H	6.86205285	2.21516444	1.57802737
H	7.25092176	2.87038145	0.02734433
H	7.21019792	-0.78483248	-1.71219601
H	5.90985181	-1.99002230	-1.56672253
H	7.44987491	-2.33443604	-0.88872339
H	5.28147964	-1.67440157	2.08340833
H	6.49573927	-2.77253836	1.38147302
H	4.88397360	-2.57391528	0.66493173
H	5.14865410	3.60155588	-0.31385895
H	4.27542422	2.91779867	1.05191927
H	3.74180888	2.48967426	-0.59772137
C	-8.94822491	0.17580231	-0.04269404
H	-7.81623336	0.57972462	1.76070278
H	-8.42553558	2.03242740	1.06235866
C	-10.31512873	-0.04490815	0.68497781
H	-9.15581898	0.68874783	-1.01324283
H	-8.48736326	-0.78426723	-0.26202686
C	-11.13236650	-1.31963880	0.16479779
H	-10.15112548	-0.19735336	1.75781775
H	-10.90604262	0.87405437	0.57291363
H	-12.04334662	-1.28776929	0.73309534
H	-10.58030406	-2.22967795	0.37306524
H	-11.37343899	-1.28694949	-0.90388464

Table S3.3:CI(AT/8_11-cis)

C	-5.31536688	1.74337479	-5.02486053
C	-5.31212058	1.75795259	-3.50687485
C	-3.94061449	1.76122012	-2.89440613
C	-2.80855147	1.46283542	-3.59674319
C	-2.85990425	1.05855132	-5.09605023
C	-4.30420146	0.74766274	-5.53247853
H	-6.31064045	1.57463968	-5.42822237
H	-5.89739079	2.63296230	-3.14561704
H	-4.60950114	-0.25658640	-5.10236721
H	-4.29710035	0.65605298	-6.65653419
H	-5.03825145	2.76709115	-5.39713576
H	-5.84674733	0.81075079	-3.11461848
C	-2.29182987	2.18974359	-5.95717233
H	-1.43193386	1.85417150	-6.52521815
H	-3.04498265	2.53437166	-6.68458877
H	-2.01211456	3.07635231	-5.30620120
C	-2.01987017	-0.21014767	-5.35442432
H	-1.28689455	-0.03977972	-6.09583524
H	-1.49302846	-0.52615568	-4.44994336
H	-2.66714347	-1.03793442	-5.68276994
C	-3.94752108	2.12256924	-1.41607912
H	-3.57010585	1.30663045	-0.84261264
H	-3.33994073	3.01343594	-1.20281847
H	-4.97869413	2.29820822	-1.15757565
C	-1.47031205	1.50159032	-3.02880209
C	-1.12614172	1.77816411	-1.75674687
H	-1.91739300	2.02480645	-1.02018071
C	0.23904657	1.81412874	-1.24152150
C	0.72218606	0.70316514	-0.56818494
H	0.03569386	-0.14139177	-0.39539505
C	2.04361013	0.59582954	-0.06639296
H	2.67365064	1.42648322	-0.16196339
C	2.58777820	-0.48070477	0.61143945
H	3.07843410	-1.22449165	0.01220451
C	2.57980805	-0.73109282	1.99595051
C	3.20221392	-1.91050857	2.44706048
H	3.69735741	-2.55055295	1.66907695
C	3.31247789	-2.30861060	3.75693205
H	2.87664125	-1.70367223	4.56446338
C	1.01157007	3.07204251	-1.48210695
H	0.44015304	3.73233062	-2.13461944
H	1.23247674	3.57837358	-0.53811340
H	1.95229432	2.88524399	-1.96076976
C	1.91180955	0.22503097	2.95702049
H	2.35785466	1.20220178	2.82516216
H	0.85087118	0.28919085	2.67942832
H	1.97895308	-0.09338182	3.97187509
N	3.90423150	-3.42973003	4.16839239
C	4.02175702	-3.87111045	5.54817867
C	3.31479800	-2.95461682	6.52295484
H	3.72552383	-1.95552823	6.43521365
C	3.43581434	-3.43586034	7.96498090
H	3.05860027	-4.45746217	8.07677952
H	4.48150156	-3.51953980	8.20858228
C	2.72306245	-2.52718533	8.97343424
H	2.87153437	-2.93605725	9.95973450
H	3.11535351	-1.54389549	8.97358722
H	1.64523874	-2.48800390	8.72126123
H	2.21640821	-2.90130060	6.22874096
H	4.34823537	-4.01852641	3.45291026
H	-0.66867788	1.30955231	-3.67421837
H	5.05609284	-3.93605218	5.81400251
H	3.58915865	-4.88561731	5.61621620

Table S3.4:CI(AT/9_11-cis)

C	-4.13411262	2.15380344	-5.29770960
C	-4.09853177	1.94770234	-3.79841282
C	-2.65605756	1.92548709	-3.29327127
C	-1.55734568	1.77265453	-4.05204000
C	-1.66077145	1.55713415	-5.57088302
C	-3.12736021	1.22909757	-5.99349431
H	-5.16962208	1.95601817	-5.66939913
H	-4.72050599	2.73519130	-3.29790912
H	-3.35188031	0.20785974	-5.69528912
H	-3.25321615	1.31658276	-7.09617237
H	-3.93669769	3.19308496	-5.50631886
H	-4.66055045	0.99621766	-3.53586538
C	-1.25911423	2.82552039	-6.38133807
H	-0.24496187	3.11208959	-6.19835438
H	-1.34804723	2.57463327	-7.46040275
H	-1.91463818	3.68378097	-6.15660545
C	-0.76220213	0.38707264	-6.15008499
H	0.19324715	0.80507801	-6.54036280
H	-0.49847425	-0.43334508	-5.49158434
H	-1.23458328	-0.07459748	-7.03384039
C	-2.59677046	2.09072950	-1.76476837
H	-2.42203519	1.12064343	-1.28878739
H	-1.72452071	2.66787758	-1.47617408
H	-3.44316939	2.55721411	-1.29831429
C	-0.19566779	1.71223835	-3.51239948
H	0.51864628	2.08120467	-4.25970458
C	0.33237862	1.36457723	-2.31090752
H	-0.36325896	1.10352404	-1.49293158
C	1.68195208	1.29089893	-1.88487330
C	2.03278627	1.12710825	-0.42334169
C	1.12904400	1.26396561	0.58888738
H	0.01339223	1.41368262	0.42670230
C	1.40360935	0.89809025	2.03386410
H	1.79468347	1.66532538	2.78256029
C	1.33028637	-0.43130187	2.47432191
C	1.75919705	-0.72606994	3.79488647
H	2.09996378	0.06011426	4.41721209
C	1.65527293	-2.00115536	4.42485161
H	1.27101500	-2.85406577	3.89013473
C	2.70525510	1.63804852	-2.90142237
H	2.49193149	1.25730674	-3.89792755
H	2.78641919	2.72729697	-3.05687587
H	3.70567425	1.30058485	-2.60174785
C	0.75573714	-1.51531477	1.54666397
H	1.02762241	-2.55004027	1.78450073
H	-0.34583010	-1.46363445	1.46555165
H	1.06720928	-1.33235717	0.52783613
N	1.97616724	-2.10048046	5.69412917
C	2.18386229	-3.34763691	6.36488719
H	1.88486021	-4.09709352	5.66306383
C	1.37646394	-3.54600742	7.67827612
H	1.80328440	-2.97126191	8.50705916
C	1.30828969	-5.04021292	8.03126311
H	0.83527948	-5.56551109	7.19214116
H	2.33961109	-5.40979227	8.12520356
C	0.51826951	-5.22543520	9.33055644
H	0.38991584	-6.25731592	9.66400203
H	0.95677979	-4.67290534	10.17521918
H	-0.50981497	-4.85836081	9.20667618
H	3.28174026	-3.44285781	6.51968166
H	0.32110854	-3.12538167	7.56128068
H	2.14956432	-1.32131732	6.32544792
H	3.11928631	1.13573772	-0.10631009

Table S3.5: CI(11-cis/11_14-cis)

C	-6.41344290	2.18909648	-1.40255360
C	-4.98242328	2.63739299	-1.11561125
C	-4.14328246	1.68384800	-0.37881528
C	-4.59789402	0.51577951	0.16013683
C	-6.09666330	0.25434649	0.17583306
C	-6.91045118	1.52384329	-0.07150240
H	-7.09924719	2.99150670	-1.55418239
H	-4.43994170	2.92607708	-2.01079568
H	-6.71863482	2.25989129	0.71097991
H	-7.98375999	1.35495476	-0.09492952
H	-6.44475955	1.48621726	-2.22671641
H	-5.08591524	3.55714437	-0.46787659
C	-6.47545133	-0.80725936	-0.82388152
H	-5.91693875	-1.73534502	-0.55277536
H	-7.57155647	-0.98751812	-0.82606054
H	-6.08609754	-0.52376065	-1.83203055
C	-6.49357269	-0.24941873	1.59362084
H	-7.55841152	-0.50053447	1.66694419
H	-5.96690412	-1.23136465	1.75387802
H	-6.16604342	0.42162270	2.37272728
C	-2.72586458	2.19455023	-0.19553122
H	-2.21129643	1.91726023	0.72522381
H	-2.06438103	1.90059941	-1.04990716
H	-2.77818202	3.29548893	-0.18212521
C	-3.76506346	-0.58899534	0.60520955
H	-4.30244875	-1.36476221	1.14710428
C	-2.39798606	-0.77526496	0.46338672
H	-1.83675856	-0.04361208	-0.09420661
C	-1.58010853	-1.85982299	0.89071470
C	-0.26395244	-1.76960075	0.44162134
H	0.01843218	-0.85846762	-0.14136912
C	0.77390486	-2.67671595	0.59564227
H	0.56658370	-3.57467292	1.14632797
C	2.11083071	-2.55527207	0.19363597
C	2.87536770	-1.53849916	-0.43782947
C	4.22108609	-1.80256419	-0.55637301
H	4.56396239	-2.77068592	-0.09506037
C	5.19690572	-0.81038878	-1.12010496
C	-2.13849352	-3.09272471	1.57021619
H	-1.52300163	-3.44200126	2.42809117
H	-3.16486857	-2.95452776	1.91101848
H	-2.14214988	-4.03771530	0.87333832
C	2.35441082	-0.23225995	-0.98248029
H	1.46215397	-0.33265306	-1.62697564
H	2.01415421	0.42884009	-0.07874541
H	3.11639621	0.33673085	-1.52241366
H	2.71376984	-3.39542546	0.55406890
N	6.02309821	-0.15264187	-0.20078263
C	6.80230871	0.98635336	-0.63658583
C	7.96162698	1.20599975	0.32308882
C	8.87129783	2.36457952	-0.02338521
H	9.16426026	2.28125412	-1.08935426
H	8.34328338	3.32962376	-0.07326973
C	10.15741462	2.44977301	0.86225431
H	10.70553264	3.36650830	0.63105465
H	9.94959772	2.47521848	1.97549237
H	10.82637749	1.61235950	0.67931499
H	5.65891790	-1.19196618	-2.03922305
H	5.73965578	-0.15546405	0.78690929
H	6.23138514	1.94171173	-0.69423864
H	7.31751918	0.77696613	-1.59003409
H	7.55716048	1.33556810	1.34170359
H	8.58855631	0.28631185	0.36854673

Table S3.6: CI(11-cis/9_11-cis)

C	7.13784036	1.84663927	1.00743654
C	6.05138502	2.44191236	0.11219683
C	4.87161935	1.52963836	-0.17508902
C	4.90171284	0.19688602	0.06921521
C	6.25228393	-0.44693631	0.54852077
C	7.47792701	0.49402054	0.42056081
H	8.01788839	2.50415955	1.03941456
H	5.68264895	3.39805700	0.51274146
H	7.76977290	0.62259772	-0.62646630
H	8.29884446	-0.01558728	0.92965335
H	6.76409404	1.75225139	2.03526270
H	6.52205535	2.70078897	-0.84963539
C	6.10258315	-0.92408220	2.05111043
H	5.28123951	-1.63074241	2.19516621
H	7.02586783	-1.40595162	2.37681320
H	5.92533237	-0.08045634	2.71940093
C	6.61615297	-1.75318918	-0.28017855
H	7.64106231	-2.07356730	-0.08155777
H	5.95703814	-2.59554492	-0.02833488
H	6.51691462	-1.56955100	-1.35639999
C	3.70227393	2.15027858	-0.86220817
H	4.10188030	2.89709267	-1.55816067
H	3.15101679	1.42577946	-1.45123770
H	3.01983271	2.68532270	-0.19316073
C	3.82674080	-0.75103755	-0.03820525
H	4.13435824	-1.79042347	0.08456540
C	2.42325649	-0.53004771	-0.14075317
H	2.06349880	0.47974241	-0.08070874
C	1.48526805	-1.50514864	-0.30169355
C	0.07930298	-1.13090393	-0.28804908
C	-0.58840851	-0.84171421	-1.44455624
C	-1.98769708	-0.53051534	-1.59218483
C	-2.96990543	-0.00601586	-0.67430122
C	-4.25146765	0.17217913	-1.24990462
H	-4.43630271	-0.11455464	-2.28149829
C	-5.34746780	0.63494065	-0.43486435
H	-5.14219902	0.66878736	0.63884339
C	1.75688811	-3.03274539	-0.46127610
H	1.38014223	-3.47708825	-1.39424197
H	2.83428394	-3.14860504	-0.46825367
H	1.38690709	-3.62771147	0.38338962
C	-2.51924151	0.26617526	0.74493490
H	-1.49610311	0.65226766	0.76073103
H	-3.14677970	1.00037979	1.24615168
H	-2.55124035	-0.64806975	1.34432777
H	-2.37161073	-0.61535594	-2.60513746
N	-6.56067732	0.90713672	-0.80107097
C	-7.72171394	1.22909778	0.02139337
H	-7.33629203	1.64361820	0.96256128
C	-8.58962292	0.00207658	0.35310211
H	-8.97461337	-0.43526899	-0.58360698
C	-9.76834745	0.40872112	1.24155289
H	-9.39438494	0.89275207	2.15640230
H	-10.36205981	1.15906279	0.70841744
C	-10.64209644	-0.80559325	1.60390954
H	-11.47285192	-0.55234678	2.26778890
H	-11.05825513	-1.22268337	0.68144936
H	-10.03541233	-1.58096093	2.07954821
H	-8.24404920	2.03628118	-0.49643542
H	-7.94885830	-0.76121806	0.81552260
H	-6.77869254	0.89075366	-1.80733844
H	-0.44255067	-1.14085603	0.66744145
H	-0.00812405	-0.97925144	-2.36071573

Table S3.7: CI(AT/9-cis)

C	-4.93013175	-2.12479353	-5.02657595
C	-4.90695115	-2.10755716	-3.51490926
C	-3.57376063	-2.02505024	-2.89340077
C	-2.40469190	-2.40567922	-3.56543296
C	-2.46279875	-2.82646698	-5.09636262
C	-3.89380117	-3.11183676	-5.53489669
H	-5.94692758	-2.38631989	-5.34288855
H	-5.51004383	-1.29972438	-3.10204009
H	-4.11544701	-4.11931348	-5.15280711
H	-3.99486076	-3.16314667	-6.62512825
H	-4.72627402	-1.12885249	-5.42116722
H	-5.36323023	-3.04153123	-3.16376488
C	-1.84094559	-1.68275796	-5.93556447
H	-0.85265244	-1.37507175	-5.57251192
H	-1.75894231	-2.00444886	-6.96862044
H	-2.50038277	-0.81038219	-5.89518794
C	-1.63640790	-4.08890266	-5.39862442
H	-1.77751287	-4.36304637	-6.44543189
H	-0.56531074	-4.01774543	-5.18385512
H	-2.07241876	-4.86979007	-4.79241172
C	-3.84736147	-1.62606179	-1.44546655
H	-4.84783512	-1.96896593	-1.10131933
H	-3.13407199	-2.00689724	-0.65632872
H	-3.78288111	-0.51318156	-1.36219075
C	-1.05572476	-2.41411806	-3.04825286
H	-0.26363568	-2.85122452	-3.67085951
C	-0.53916354	-1.98718852	-1.78047923
H	-1.20961841	-1.60475436	-1.05707738
C	0.74256234	-2.07994171	-1.34388433
C	0.96828969	-1.69817812	0.07527474
H	0.90751473	-2.48376519	0.80122223
C	1.15270820	-0.46167923	0.47477110
H	1.22612207	0.35717625	-0.22426534
C	1.32080587	-0.03221662	1.83985468
H	1.28207393	-0.80392436	2.58266043
C	1.54522738	1.25972948	2.31493526
C	1.77072764	1.41964012	3.70040291
H	1.72561957	0.52119102	4.35185026
C	2.06960525	2.58007802	4.43232219
H	2.15470764	3.50224373	3.87313241
C	2.07434040	-2.31530062	-2.23564178
H	2.76171787	-3.11141581	-1.92968930
H	1.69531184	-2.58240394	-3.24061895
H	2.63505606	-1.39102179	-2.30635164
C	1.52490298	2.50465689	1.49202912
H	1.37990520	2.26985817	0.44109894
H	0.70618671	3.16322409	1.78102341
H	2.47099221	3.03773896	1.56084409
N	2.21261550	2.59902774	5.73395904
C	2.50537963	3.81816205	6.54375332
C	3.55859896	4.73268643	5.93820872
H	4.42087606	4.08144357	5.76875432
C	3.86266246	5.91285879	6.86537866
H	3.01526168	6.61873558	6.84714998
H	3.96005690	5.55797094	7.90438059
C	5.09146286	6.67890135	6.37686199
H	5.25386979	7.53878819	7.02718011
H	5.98631761	6.06120909	6.39728052
H	4.94012409	7.04116279	5.36739229
H	3.25001004	5.10979117	4.96338517
H	2.11774872	1.75068008	6.27546718
H	1.59095173	4.34142322	6.70608836
H	2.80303442	3.45547523	7.50481615