Supporting Information

Secondary Orbital Interactions in the Propagation Steps of Lipid Peroxidation

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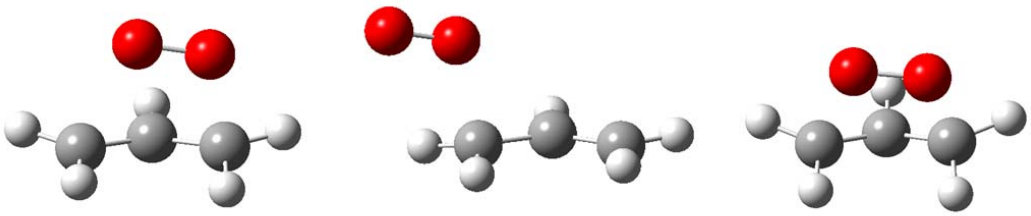

Relative Energies[a] (kcal/mol)

	syn TS	*anti* TS	concerted TS
UMP(2)/6-311+G(3df,2p)	0.0	+18.3[b]	+2.9
UCCSD(T)/6-311+G(3df,2p)[c]	0.0	+8.1[b]	+7.9
ROCCSD(T)/6-311+G(3df,2p)[c]	0.0	+4.0	+8.0

[a]Zero point energy-corrected. [b]Badly spin-contaminated Hartee-Fock wavefunction, $\langle S^2 \rangle$ = 1.68; hence the CCSD(T) calculation was also carried out with a spin-restricted reference wavefunction. [c]Calculated at the UMP2 stationary points.

Figure S1. Relevant MP2-calculated transitions structures for the degenerated rearrangement of the allylperoxyl radical. The *syn* TS for C-O bond fragmentation is found to be significantly lower in energy at all levels of theory compared to the *anti* TS and concerted TS structures originally identified by Olivella and Sole (manuscript ref. 16). See below for cartesian coordinates, electronic energies and thermochemical corrections for these structures. ROCCSD(T) calculations were performed with the Gaussian 09 suite of programs (Gaussian 09, Gaussian, Inc., Wallingford, CT, 2009).

Table S1. Cartesian Coordinates for Relevant Structures in the Manuscript.

Methylperoxyl

O	-1.18428200	-0.27715700	-0.00000200
O	-0.15717600	0.54091000	0.00000400
C	1.09413400	-0.18224200	0.00000300
H	1.87037200	0.57875600	-0.00047400
H	1.14843800	-0.79732200	0.89552700
H	1.14805000	-0.79800100	-0.89508600

Propene

C	-0.13393200	-0.45293300	0.00000300
C	-1.27784100	0.21996600	-0.00000700
H	-1.29946200	1.30355800	0.00002300
C	1.23074500	0.16224800	-0.00000800
H	1.80375900	-0.15366200	-0.87567200
H	1.17958600	1.25107300	-0.00092200
H	1.80309900	-0.15217900	0.87663300
H	-0.16652800	-1.53898600	0.00000100
H	-2.23428700	-0.28548600	0.00001100

Methylperoxyl + Propene *syn* TS

C	1.68859300	-0.21593500	0.50458200
C	2.20854500	-0.99667000	-0.46087600
H	2.38490900	-0.61679500	-1.45932100
O	-1.17816900	1.09624800	-0.36325500
O	-1.44721400	-0.23768200	-0.62821600
C	1.28178800	1.15708700	0.32590200
H	1.25598500	1.77745500	1.21725100
H	1.68301500	1.66740700	-0.54590500
H	0.00159700	1.11952900	0.00324200
H	1.52126400	-0.65419500	1.48404800
C	-2.09977100	-0.81359000	0.49825400
H	-3.02292000	-0.27621700	0.71739300
H	-2.31926400	-1.84087700	0.21033200
H	-1.44603900	-0.80122000	1.37210500
H	2.46959200	-2.02896100	-0.27455200

Methylperoxyl + Propene *anti* TS

C	-2.21894600	-0.08222900	-0.42198300
C	-3.12045800	-0.06632700	0.57574500
H	-3.00291300	0.58523100	1.43288100
O	0.90498900	-0.82811800	0.24769900
O	2.02427300	-0.39892900	-0.45143800
C	-1.00925800	0.70742300	-0.45343000
H	-0.62479500	0.96781100	-1.43687300
H	-0.95111200	1.52052500	0.26539500
H	-0.02791800	-0.09422400	-0.08362400
H	-2.38049300	-0.76059400	-1.25381000
C	2.78204500	0.47638200	0.37524900
H	3.06222400	-0.02261500	1.30330700
H	3.67079600	0.72313200	-0.20431600
H	2.21679500	1.38424300	0.59690500
H	-3.99698300	-0.69862900	0.55655900

1,3-Pentadiene

C	-1.10978400	0.41667800	0.00006500
C	0.05219200	-0.24397600	0.00004800
H	0.04305500	-1.33258700	0.00007300
H	-1.08559500	1.50498200	0.00002300
C	1.35625400	0.39316600	-0.00001500
H	1.35947500	1.48094600	-0.00005700
C	2.52108300	-0.25913700	-0.00001900
H	2.56338500	-1.34302500	0.00001600
H	3.46686500	0.26711800	-0.00006100
C	-2.46350500	-0.21577900	-0.00004300
H	-3.04305000	0.09087100	0.87711500
H	-3.04308900	0.09128800	-0.87701400
H	-2.39849000	-1.30530800	-0.00030800

Methylperoxyl + 1,3-Pentadiene *syn* TS

C	-0.55337500	1.00262800	0.63700600
O	2.37311800	0.43705300	-0.69674900
O	1.87542100	-0.85006700	-0.57403500
C	-1.55589800	0.49986900	-0.13457100
H	-1.63138500	0.82368000	-1.17006400
H	-0.48701300	0.65340000	1.66554500
C	2.42447200	-1.45529700	0.59230100
H	2.01943400	-2.46792200	0.61086800
H	3.51411600	-1.48326200	0.52703800
H	2.12087800	-0.91203500	1.49092800
C	-2.53757500	-0.43639400	0.33291000
H	-2.45083600	-0.75619100	1.36878900
C	-3.53557100	-0.92881900	-0.41796900
H	-3.65832900	-0.63796400	-1.45519900
H	-4.25140100	-1.63480000	-0.01788700
C	0.46120100	1.91042000	0.18268500
H	0.94041800	2.51753500	0.94800000
H	1.44485500	1.17933400	-0.23175700
H	0.23143100	2.46789600	-0.72416100

Methylperoxyl + 1,3-Pentadiene *anti* TS

C	0.50683600	1.48174300	-0.42224000
C	-0.08843800	2.50585600	0.19798200
H	-0.22500200	2.51721800	1.27413000
O	-0.92073600	-1.40888600	-0.19355100
O	-2.00489300	-0.66621400	-0.60582100
C	0.99517000	0.26859200	0.23910400
H	0.05189700	-0.56297700	0.02740400
H	1.00874000	0.33341700	1.32851600
H	0.62028700	1.51843900	-1.50312000
C	-2.87849400	-0.44367900	0.49963400
H	-3.72860700	0.10286600	0.09032400
H	-3.20396800	-1.39740100	0.91893700
H	-2.38113600	0.15470300	1.26628800
H	-0.44766200	3.36725100	-0.35043500
C	2.16482600	-0.41384000	-0.32770200
H	2.27326700	-0.36093600	-1.40850400
C	3.05961300	-1.10947000	0.37883500
H	2.98933700	-1.19580300	1.45765100
H	3.89080300	-1.61118000	-0.09988700

1,4-Pentadiene

C	0.00000000	0.65954800	-0.00001100
H	0.30959400	1.31030900	-0.82541900
H	-0.30959600	1.31033700	0.82537400
C	1.17488600	-0.17804700	0.42993900
H	0.99616700	-0.83603700	1.27738900
C	-1.17488500	-0.17806300	-0.42993200
H	-0.99616400	-0.83608500	-1.27735600
C	2.36876300	-0.17400600	-0.14899900
H	3.17480100	-0.80447700	0.20644700
C	-2.36876400	-0.17400100	0.14900300
H	-3.17480000	-0.80448400	-0.20642100
H	2.58642800	0.46390700	-0.99960500
H	-2.58643000	0.46394400	0.99958500

Methylperoxyl + 1,4-Pentadiene TS

C	0.50683600	1.48174300	-0.42224000
C	-0.08843800	2.50585600	0.19798200
H	-0.22500200	2.51721800	1.27413000
O	-0.92073600	-1.40888600	-0.19355100
O	-2.00489300	-0.66621400	-0.60582100
C	0.99517000	0.26859200	0.23910400
H	0.05189700	-0.56297700	0.02740400
H	1.00874000	0.33341700	1.32851600
H	0.62028700	1.51843900	-1.50312000
C	-2.87849400	-0.44367900	0.49963400
H	-3.72860700	0.10286600	0.09032400
H	-3.20396800	-1.39740100	0.91893700
H	-2.38113600	0.15470300	1.26628800
H	-0.44766200	3.36725100	-0.35043500
C	2.16482600	-0.41384000	-0.32770200
H	2.27326700	-0.36093600	-1.40850400
C	3.05961300	-1.10947000	0.37883500
H	2.98933700	-1.19580300	1.45765100
H	3.89080300	-1.61118000	-0.09988700

Allyl

C	0.00000000	1.22435900	-0.19547600
H	0.00000000	1.29284800	-1.27557300
H	0.00000000	2.15024300	0.36068300
C	0.00000000	0.00000000	0.44137300
H	0.00000000	0.00000000	1.52725300
C	0.00000000	-1.22435900	-0.19547600
H	0.00000000	-1.29284800	-1.27557300
H	0.00000000	-2.15024300	0.36068300

O_2

O	0.00000000	0.00000000	0.60162900
O	0.00000000	0.00000000	-0.60162900

Allyl +O_2 *syn* TS

C	1.29134700	-1.02245700	0.20856000
H	0.97591600	-1.18218400	1.23018600
C	1.22027700	0.21065600	-0.36833800
H	1.55043300	0.32905000	-1.39428700

C	0.55781100	1.27124200	0.23858100
H	0.42547200	2.21709800	-0.26571100
H	0.31886800	1.24285300	1.29143700
O	-1.51157500	0.39373300	-0.06303700
O	-1.41168200	-0.82995900	-0.06400900
H	1.69875800	-1.87365800	-0.31806800

Allyl +O_2 *anti* TS

C	2.26824900	-0.55102900	0.16839100
H	2.14679300	-0.90330600	1.18482900
H	3.10767200	-0.93928400	-0.39036400
C	1.40281100	0.34116700	-0.37568800
H	1.56298500	0.66133900	-1.39963800
C	0.27589100	0.85059300	0.29480000
H	0.13082100	0.64453900	1.34554500
O	-1.33475400	-0.52868900	-0.19733700
O	-2.45652000	-0.09220300	0.05504300
H	-0.29978500	1.65946100	-0.12704100

Allyl-O_2 complex

C	1.09157400	-1.21670300	0.22029200
H	0.74182200	-1.27688900	1.24170100
C	1.33888800	-0.00002500	-0.37724100
H	1.70149400	-0.00017200	-1.40007400
C	1.09144800	1.21682200	0.21991300
H	1.26375700	2.14782700	-0.30004600
H	0.74183400	1.27731300	1.24134700
O	-1.67778700	0.60613900	-0.05344200
O	-1.67778200	-0.60623600	-0.05423800
H	1.26418000	-2.14787400	-0.29926800

Allylperoxyl Conformation 1 (gauche, away)

C	-2.24312000	-0.12268500	-0.20381300
H	-2.55720400	0.88791900	-0.43548000
C	-1.00935500	-0.39523500	0.19825200
H	-0.71028800	-1.41272700	0.42345600
C	0.04494400	0.64223700	0.38792700
H	0.42244800	0.67225500	1.40982900
H	-0.29044500	1.63096500	0.07884200
O	1.20465900	0.36958200	-0.46783400
O	1.96648800	-0.57272500	0.03511400
H	-2.98849900	-0.89917200	-0.30908300

Allylperoxyl Conformation 2 (anti)

C	-2.30881200	0.16228000	-0.28049100
H	-2.31331100	1.17711200	-0.65925400
C	-1.22158200	-0.37569500	0.25523800
H	-1.23978400	-1.39530000	0.62440200
C	0.06473800	0.35774900	0.41428400
H	0.40407500	0.39120200	1.45009100
H	0.02306100	1.36823100	0.00948600
O	1.10013700	-0.36982600	-0.33070000
O	2.29443200	0.11748100	-0.09504800
H	-3.23665900	-0.38849100	-0.35292700

Allylperoxyl Conformation 3 (gauche, toward)

C	2.01768800	-0.50079700	0.10478500
H	1.96380800	-0.88644400	1.11523400
C	1.08427800	0.30511500	-0.38215800
H	1.15215400	0.67392000	-1.39988800
C	-0.09536600	0.76342800	0.40471900
H	-0.18271100	1.85060300	0.41970300
H	-0.09682000	0.37185700	1.42000600
O	-1.35484900	0.34473600	-0.22618700
O	-1.61347100	-0.92144700	-0.00271900
H	2.87053100	-0.80272800	-0.48789000

Pentadienyl

C	0.00000000	2.45530800	0.22657700
H	0.00000000	2.53677800	1.30745200
H	0.00000000	3.37795000	-0.33794100
C	0.00000000	1.24407200	-0.39048500
H	0.00000000	1.22069100	-1.47823200
C	0.00000000	0.00000000	0.27100800
H	0.00000000	0.00000000	1.35828800
C	0.00000000	-1.24407200	-0.39048500
H	0.00000000	-1.22069100	-1.47823200
C	0.00000000	-2.45530800	0.22657700
H	0.00000000	-2.53677800	1.30745200
H	0.00000000	-3.37795000	-0.33794100

Pentadienyl + O_2 *syn* TS (terminal addition)

C	-3.00101400	0.52183900	0.20522200
H	-2.91168400	0.94505900	1.19936800
H	-3.93496400	0.68557500	-0.31616700
C	-1.99443500	-0.16760300	-0.35403900
H	-2.12111700	-0.57028000	-1.35582500
C	-0.73671400	-0.41488200	0.28773800
H	-0.60550100	-0.01878300	1.29055200
C	0.28554600	-1.14151200	-0.26947700
H	0.15854200	-1.52831300	-1.27662800
C	1.53927100	-1.23140100	0.32391300
H	2.34183800	-1.78106500	-0.14806100
H	1.66482300	-1.00601700	1.37436200
O	2.27201100	0.71296100	-0.10827700
O	1.33450500	1.52143600	-0.13269100

Pentadienyl + O_2 *anti* TS (terminal addition)

C	3.50340000	-0.64982100	0.13038500
H	3.44658200	-1.14665600	1.09240900
H	4.43981300	-0.72438700	-0.40645200
C	2.45494000	0.02560100	-0.37157800
H	2.55255300	0.50839800	-1.34074900
C	1.19394700	0.15815500	0.29015500
H	1.08810000	-0.32523300	1.25875100
C	0.12527400	0.85357000	-0.21351900
H	0.23329500	1.32915500	-1.18472800
C	-1.11721900	0.93993800	0.42457700
H	-1.86890200	1.63021300	0.07054100
H	-1.22498000	0.59383600	1.44417600

O	-2.24660400	-0.66972900	-0.27801200
O	-3.45696000	-0.55901900	-0.03374600

Pentadienyl + O_2 TS (central addition)

C	-1.95909700	-1.21415200	0.29488700
H	-2.12070200	-0.81025900	1.28624200
H	-2.81000400	-1.67396700	-0.19097800
C	-0.75005800	-1.17209700	-0.29214500
H	-0.62339100	-1.58096300	-1.29043400
C	0.33912600	-0.44541700	0.26500300
H	0.29514000	-0.21535300	1.32372200
C	1.64274600	-0.41648800	-0.34919000
H	1.70736900	-0.76797200	-1.37534800
C	2.74214800	0.04529400	0.25831900
H	3.69963100	0.07172100	-0.24543000
H	2.71370300	0.40990800	1.27899800
O	-0.31460900	1.43946000	-0.12977000
O	-1.55425800	1.53354600	-0.10123300

Pentadienyl-O_2 complex

C	2.84315600	-0.75476600	0.21601100
H	2.71088100	-1.14255800	1.21955300
H	3.73343600	-1.05968700	-0.31739900
C	1.92882100	0.07524400	-0.34566000
H	2.10854800	0.43452900	-1.35659100
C	0.74571200	0.51692300	0.28614200
H	0.55053600	0.17274600	1.29821500
C	-0.18065300	1.39459600	-0.30567200
H	0.03672600	1.73333300	-1.31626400
C	-1.32749100	1.82217300	0.28614700
H	-2.01183300	2.48827800	-0.22167300
H	-1.59070200	1.51669800	1.29181700
O	-2.38236900	-1.11740100	-0.09332400
O	-1.31698800	-1.69114300	-0.08410900

Pentadienylperoxyl Conformation 1 (gauche, away)

C	-1.30483400	0.73134400	0.40148200
H	-1.09985300	1.75170700	0.07657800
H	-1.81713000	0.73515600	1.36487500
O	-2.97887300	-0.77582800	-0.10259800
O	-2.28898800	0.23642800	-0.57555800
C	-0.08348000	-0.11578500	0.39866100
H	-0.22037100	-1.15038900	0.69983500
C	1.12875500	0.33259200	0.05751000
H	1.24382300	1.37126100	-0.24652200
C	2.33455600	-0.47398300	0.06862300
H	2.22081700	-1.51281600	0.36726400
C	3.54253700	-0.01473000	-0.26376300
H	3.69350100	1.01585900	-0.56602700
H	4.41690700	-0.65221000	-0.24583800

Pentadienylperoxyl Conformation 2 (anti)

C	1.27671900	-0.17157500	0.59146200
H	1.21318100	-1.25952200	0.63969100
H	1.76229900	0.20750900	1.49273000

O	3.42125900	-0.18492900	-0.25898600
O	2.18247300	0.15980600	-0.52335200
C	-0.03823800	0.46568300	0.32906700
H	-0.05568100	1.55177200	0.30478200
C	-1.16913000	-0.22291100	0.14434900
H	-1.13520000	-1.31038100	0.16527300
C	-2.47013800	0.37876000	-0.07824100
H	-2.50553300	1.46476500	-0.10345000
C	-3.59387200	-0.31953000	-0.25151900
H	-3.59563400	-1.40388700	-0.23192500
H	-4.54533800	0.16816600	-0.41910700

Pentadienylperoxyl Conformation 3 (gauche, toward)

C	-3.35342300	0.49338500	0.12669200
H	-3.31943200	1.01436500	1.07726400
H	-4.30057900	0.49183700	-0.39695100
C	-2.27563500	-0.11352800	-0.37388400
H	-2.34573400	-0.62516200	-1.33032000
C	-0.98189200	-0.13801400	0.28161300
H	-0.91028900	0.37920100	1.23586400
C	0.10171400	-0.74861600	-0.20833300
H	0.04996500	-1.26139300	-1.16492800
C	1.41383400	-0.76978700	0.48697400
H	1.83586100	-1.77493500	0.55152200
H	1.37130000	-0.31478500	1.47594200
O	2.44544700	-0.04048800	-0.27721200
O	2.32846800	1.25926700	-0.13863400

Bis-allylic Pentadienylperoxyl

C	1.65170100	-1.73672400	-0.28308300
H	1.67673500	-1.63844100	-1.36245200
H	2.32499000	-2.46105800	0.15826400
C	0.83640600	-1.00479700	0.46337400
H	0.83142900	-1.11403900	1.54438600
C	-0.11650900	0.00141900	-0.09477800
H	-0.07491100	0.02724900	-1.18362100
C	-1.51638700	-0.16138400	0.40302400
H	-1.63988500	-0.16800900	1.48244000
C	-2.56652300	-0.31216300	-0.39201900
H	-3.56351100	-0.44919700	0.00769200
H	-2.46879300	-0.31083900	-1.47212500
O	0.30774600	1.36805600	0.35340100
O	1.33998200	1.80647300	-0.32261300

Table S2. Electronic Energies and Enthalpy Corrections to 298 K for Relevant Structures in the Manuscript. Values in hartree.

Structure	E_e, B3LYP	H_{corr}, B3LYP	E_e, CCSD(T)
	All calculations with a 6-311+G(3df,2p) Basis Set		
Methylperoxyl	-190.291585	0.047628	-189.941364
Propene	-117.95371	0.084365	-117.674232
Methylperoxyl + Propene *syn* TS	-308.218467	0.127376	-307.583074
Methylperoxyl + Propene *anti* TS	-308.218046	0.127367	-307.581238
	All calculations with a 6-311+G(2df,p) Basis Set		
Methylperoxyl	-190.2887348	0.047592	-189.9268296
1,3-Pentadiene	-195.3805552	0.119870	-194.9100025
Methylperoxyl + 1,3-Pentadiene *syn* TS	-385.6469338	0.163046	-384.805959
Methylperoxyl + 1,3-Pentadiene *anti* TS	-385.6463308	0.162995	-384.8035367
1,4-Pentadiene	-195.3675335	0.119977	-194.899837
Methylperoxyl + 1,4-Pentadiene TS	-385.6379645	0.163017	-384.801748

Structure	E_e, B3LYP	H_{corr}, B3LYP	E_e, CCSD(T)
	All calculations with a 6-311+G(3df,2p) Basis Set		
Allyl	-117.3065024	0.070714	-117.025725
O_2	-150.3794885	0.007056	-150.128249
Allyl +O_2 *syn* TS	-267.6864505	0.07945	-267.158972
Allyl +O_2 *anti* TS	-267.6823199	0.079083	-267.150373
Allyl-O_2 complex	-267.6875032	0.079609	-267.156486
Allylperoxyl Conformation 1 (gauche, away)	-267.7129621	0.082946	-267.188690
Allylperoxyl Conformation 2 (anti)	-267.7127773	0.082908	-267.188300
Allylperoxyl Conformation 3 (gauche, toward)	-267.7124376	0.082940	-267.188334

All calculations with a 6-311+G(2df,p) Basis Set

Pentadienyl	-194.743334	0.106456	-194.116828
O_2	-150.378488	0.007039	-150.044794
Pentadienyl + O_2 *syn* TS (terminal addition)	-345.117813	0.115205	-344.159612
Pentadienyl + O_2 *anti* TS (terminal addition)	-345.114456	0.114813	-344.152637
Pentadienyl + O_2 TS (central addition)	-345.116715	0.115457	-344.161630
Pentadienyl-O_2 complex	-345.122592	0.115035	-344.164276
Pentadienylperoxyl Conformation 1 (gauche, away)	-345.138839	0.118435	-344.185216
Pentadienylperoxyl Conformation 2 (anti)	-345.138796	0.118383	-344.185205
Pentadienylperoxyl Conformation 3 (gauche, toward)	-345.138394	0.118428	-344.185105
Bis-allylic Pentadienylperoxyl	-345.127677	0.117675	-344.179094

Table S3. Cartesian Coordinates for MP2-Calculated TS Structures for the Degenerate Allylperoxyl Rearrangement.

Allyl +O_2 *syn* TS

C	1.24203300	-0.91124000	0.21131200
H	0.96011500	-1.06588000	1.24402300
C	1.14452800	0.32148700	-0.35196800
H	1.46529800	0.46691100	-1.37622100
C	0.28827400	1.24802000	0.24143100
H	0.08126400	2.20108100	-0.22871400
H	0.13999400	1.21123100	1.31445900
O	-1.38109900	0.28651200	-0.08020800
O	-1.16894300	-0.91420700	-0.07645500
H	1.70466000	-1.74138200	-0.30489100

Allyl +O_2 *anti* TS

H	-1.50335000	0.71159800	-1.37462500
C	-1.33797600	0.35335600	-0.36592200
C	-2.18122100	-0.52727700	0.15979200
C	-0.16928300	0.80946700	0.31100700
O	1.21045300	-0.48383400	-0.20087100
O	2.33936500	-0.14005800	0.03467700
H	-3.03548500	-0.89128400	-0.39027700
H	0.37584400	1.66133500	-0.06398100
H	-2.03781500	-0.90527100	1.16305500
H	-0.06685800	0.60148300	1.36611200

Concerted TS

H	1.50282200	0.40599100	-1.33713100
C	1.17862100	0.30331300	-0.31083400
C	0.25519300	1.21193100	0.22491300
C	0.99188600	-0.93113000	0.22879300
O	-1.02707700	-0.89079200	-0.11191400
O	-1.26083000	0.33674100	-0.08360700
H	0.04375900	2.15097600	-0.27231300
H	1.34183900	-1.83035800	-0.26226800
H	0.11416000	1.23385200	1.30052500
H	0.74648700	-1.03274400	1.27812400

Table S4. Electronic Energies and Thermochemical Corrections for the MP2-Calculated TS Structures for the Degenerate Allylperoxyl Rearrangement. Values in hartree.

Structure	E_e, MP2	*ZPE*, MP2	E_e, CCSD(T)
	All calculations with a 6-311+G(3df,2p) Basis Set		
Allyl +O_2 *syn* TS	-267.0734562	0.076025	-267.158700 (U) -267.158939 (RO)
Allyl +O_2 *anti* TS	-267.0430313	0.074768	-267.144539 (U) -267.151382 (RO)
Concerted TS	-267.072691	0.079999	-267.150048 (U) -267.150188 (RO)