Supplemental Information for:

Product rearrangement from altering a single residue in the rice *syn*-copalyl diphosphate synthase

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Materials and Methods

All reagents were purchased from Fisher Scientific unless noted otherwise. Enzymes were characterized in a previously described modular metabolic engineering system in *E. coli*.[1] To increase carbon flux through the isoprenoid precursor pathway, a compatible plasmid (pIRS) was co-transformed into *E. coli*.[2] This system increases metabolic flux to yield more of the diterpene precursor, GGPP (**1**), produced by a GGPP synthase, which is co-expressed with OsCPS4 in pGG/DEST constructs created via recombination into the DESTination cassette by the Gateway cloning system (Invitrogen).[2] The recombinant enzymes used in this study were derived from a previously described pseudo-mature construct for OsCPS4.[3]

Mutants were generated by whole-plasmid PCR amplification with overlapping mutagenic primers of the previously described pENTR/SD/d-TOPO (Invitrogen) based clone of pseudo-mature OsCPS4,[3] each of which was verified by complete gene sequencing prior to transfer by directional recombination to the pGG-Dest expression vector. The constructs were transformed into the C41 OverExpress strain of *Escherichia coli* (Lucigen), along with pIRS, and heterologously expressed, much as previously described for other class II diterpene cyclases.[4-6] Briefly, the recombinant mutant clones were grown in liquid NZY media (10 g casein, 10 g NaCl, 5 g yeast extract, 1 g $MgSO_4$ (anhydrous) in 1 L H_2O, and pH adjusted to 7.0) at 37 °C to OD_{600} = 0.6, then transferred to 16 °C for an hour and induced with 0.5 mM IPTG. At the time of induction, cultures were supplemented with phosphate buffer (pH 7.0) to 100 mM, sodium pyruvate to 50 mM, and $MgCl_2$ to 1 mM (final concentrations), as previously described.[2] After 3 days fermentation at 16 °C, dephosphorylated enzymatic products were extracted by addition of equal volume of hexanes and gentle swirling, the organic solvent was separated out and then dried under N_2, with the residue resuspended in fresh hexanes and analyzed by GC-MS. Note that dephosphorylation of the class II diterpene cyclases products reported here relied on the activity of endogenous phosphatases from *E. coli*. Compound analysis by GC-MS was carried out as previously described.[7] Briefly, using a 3900 GC with Saturn 2100T ion trap MS (Varian), equipped with a HP-5MS column (Agilent, 0.25 µm, 0.25 ID, 30 m) with a He flow rate of 1.2 mL/min, and the following oven temperature program: 50 °C for 3 min, 15 °C/min to 300 °C, hold 3 min. Samples (1 µL) were injected via splitless injection at 250 °C.

Given the somewhat surprising production of *syn*-CPP (**2**) by OsCPS4:H501Y, the absolute stereochemistry of this product was investigated by further co-expression of a subsequently acting class I diterpene synthase that is selective for **2**. Namely, the rice *syn*-stemarene/stemodene synthase OsKLS8.[8] This analysis indicated that OsCPS4:H501Y does selectively produce **2** – i.e., rather than the enantiomeric *ent-syn*-CPP – as OsKSL8 readily reacts with the product of this mutant (data not shown).

The dephosphorylated product of the OsCPS4:H501D mutant (**3'**) was purified much as previously described for other class II diterpene cyclase products.[4-6] To obtain sufficient quantities of the compound, 8 L of the relevant bacterial culture were grown as described above. After extraction, the phases were separated in a separatory funnel, and the pooled hexanes dried by rotary evaporation. The resulting extract was redissolved in 10 mL of fresh hexanes and fractionated over silica (4 g) using a Reveleris automated flash chromatography system (Grace, Deerfield, IL) with a 15 mL/min flow rate, 5 mL injections, and UV detection at 200 nm, with the following stepwise gradient: 0%, 5%, 15%, 25% ethyl acetate (in hexane) for 1 minute each, and a final wash with 100% ethyl acetate for 3 minutes. The resulting fractions were analyzed by GC-MS (as described above). Those containing **3'** were dried under N2 and dissolved in 5 mL of 50% acetonitrile/dH_2O. **3'** was then further purified via HPLC using an Agilent 1200 system equipped with an Agilent Poroshell 120 EC-C18 (4.6 x 100 mm, 4 µm) column at a flow rate of 1 mL/min. The column was pre-equilibrated, sample injected and washed with 50% acetonitrile/dH2O (0 - 2 minutes), eluted with 50 - 100% acetonitrile (2 - 7 minutes), and followed by a 100% acetonitrile wash (7 - 23 minutes), with peak based fraction collection. Again, those containing **3'** were identified by GC-MS analysis. The final yield of pure **3'** was estimated to be ~3.0 mg by GC-FID (flame ionization detection) analysis using a Agilent 6890N GC equipped with HP-5 column and the same temperature program described above, with comparison to a standard curve generated for the diterpene cembrene, as previously described.[2]

The HPLC fractions containing pure **3'** were pooled, dried under N_2 and dissolved in 0.5 mL $CDCl_3$ (Aldrich). NMR spectra were acquired on a Bruker AVIII-800 spectrometer equipped with a 5-mm HCN cryogenic probe, using TopSpin 3.2 software. Analysis was carried out at 25 °C. Chemical shifts were calculated by reference to those known for $CDCl_3$ signals offset from TMS (^{13}C 77.23 ppm, ^{1}H 7.24 ppm). All spectra were acquired using standard programs from the TopSpin 3.2 software, with collection of 1D ^{1}H-NMR, and 2D double-quantum filtered correlation spectroscopy (DQF-COSY), heteronuclear single-quantum coherence (HSQC), heteronuclear multiple-bond correlation (HMBC), HMQC-COSY and NOESY (800 MHz), as well as 1D ^{13}C-NMR (201 MHz), spectra. Observed HMBC correlations were used to propose a partial structure, while COSY correlations between protonated carbons were used to complete the structure, which was further verified by HSQC correlations. Observed correlations from NOESY spectrum were used to assign the relative stereochemistry of chiral carbons and also verify the configuration of the *exo*-cyclic double bond.

Quantum Chemical Calculations

Calculations were performed with GAUSSIAN03[9] and GAUSSIAN09.[10] Geometries were optimized using the B3LYP method with the basis set of 6-31+G(d,p) in the absence and 6-31G(d) in the presence of theozymes.[11] All stationary points were characterized as minima or transition state structures using frequency calculations at the same level. All reported energies include zero-point energy corrections (unscaled) from the frequency calculations at the same level. Intrinsic reaction coordinate (IRC) calculations were used for further characterization of transition state structures.[12] mPW1PW91[13] single point energies are also shown, since it is known that B3LYP underestimates the relative energies of cyclic structures versus acyclic isomers.[13] The validity of this computational approach for examining terpene-forming carbocation rearrangements is well-established.[14] Structural images were created with *Ball&Stick*.[15]

References

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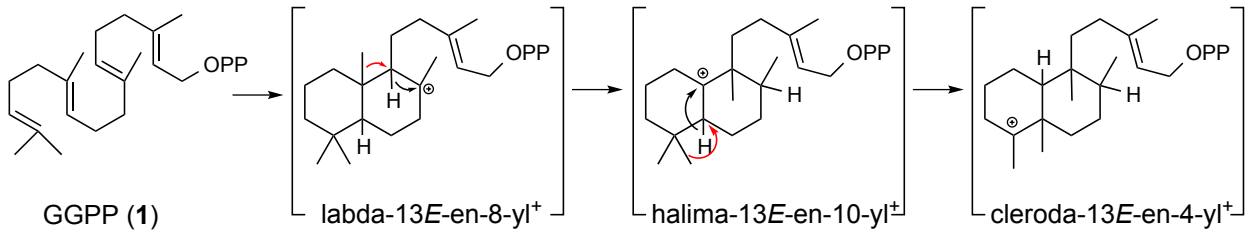
Scheme S1: Cyclization of **1** to a labdaenyl$^+$ intermediate, which can undergo sequential 1,2-shifts of a hydride (C9 → C8) and methyl (C10 → C9), with the latter (red arrow) creating a structurally distinct halimaenyl$^+$ intermediate that can, in turn, also undergo sequential 1,2-shifts of a hydride (C5 → C10) and methyl (C4 → C5), again with the latter (red arrow) creating the structurally distinct clerodanenyl$^+$ intermediate.



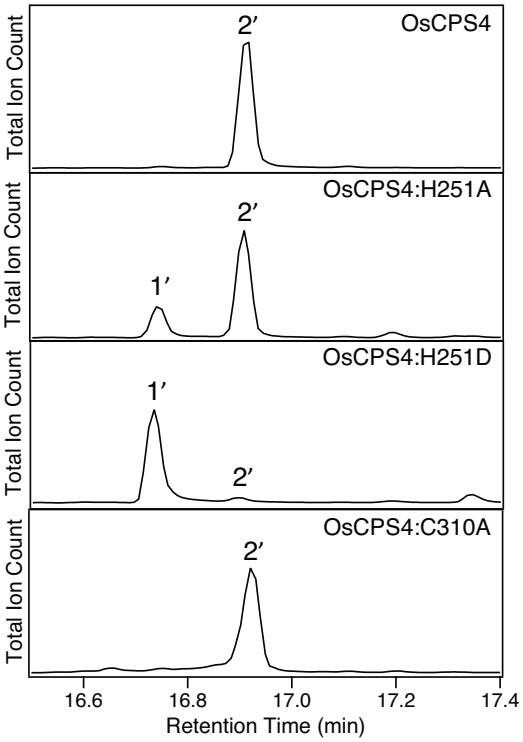


Figure S1: GC-MS chromatograms for dephorphorylated products from OsCPS4 mutants (as indicated) corresponding to the catalytic general base dyad conserved in CPSs from gibberellin phytohormone biosynthesis. Product numbering as in text, with prime' notation indicating that these are dephosphorylated derivatives.

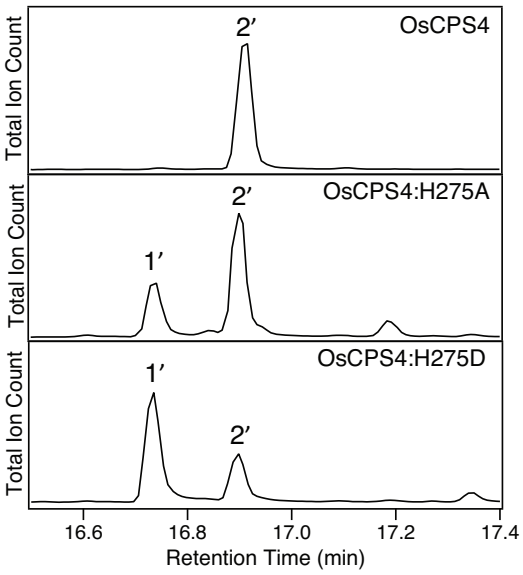


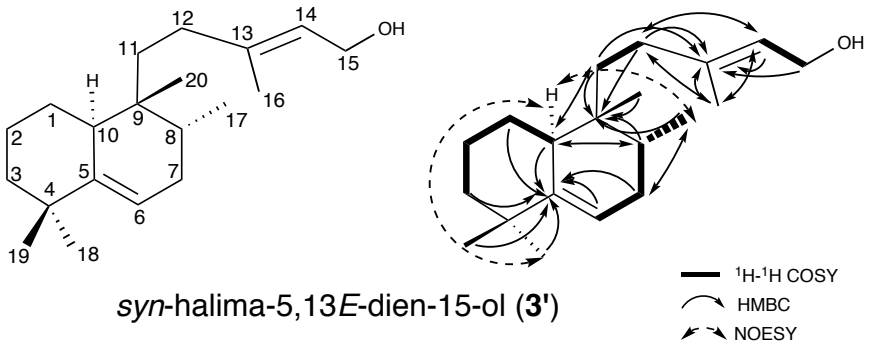
Figure S2: GC-MS chromatograms for dephorphorylated products from OsCPS4 mutants (as indicated) of putative active site histidine (H275) identified by molecular modeling (see Figure 1). Product numbering as in text, with prime' notation indicating that these are dephosphorylated derivatives.

Table S1: ^{1}H and ^{13}C NMR assignments for *syn*-halima-5,13*E*-dien-15-ol (**3'**) in $CDCl_3$

Note: The chemical shift values of C11 and C20 were determined by HSQC and HMBC, respectively, due to low ^{13}C signal.

Position	*syn*-halima-5,13*E*-dien-15-ol (3')	
	δ_H	δ_C
1 a	1.75 (1H, m)	29.2
b	1.05 (1H, m)	
2	1.60 (2H, m)	23.3
3 a	1.43 (1H, m)	42.4
b	1.18 (1H, m)	
4		36.9
5		146.9
6	5.32 (1H, t, J = 3.4 H)	114.7
7 a	2.05 (1H, d, J = 12.0 Hz)	31.3
b	1.68 (1H, m)	
8	1.63 (1H, m)	33.2
9		36.2
10	1.98 (1H, d, J = 12.6 Hz)	41.2
11 a	1.42 (1H, m)	32.2
b	1.26 (1H, m)	
12	1.92 (2H, m)	33.9
13		141.6
14	5.39 (1H, tq, J = 6.99, 1.18 Hz)	123.2
15	4.12 (2H, d, J = 6.99 Hz)	59.8
16	1.66 (3H, s)	16.7
17	0.78 (3H,d, J = 6.8 Hz)	14.8
18	1.04 (3H, s)	29.7
19	1.02 (3H, s)	27.1
20	0.81 (3H, s)	22.4

Figure S3: ^{1}H spectra obtained for *syn*-halima-5,13*E*-dien-15-ol (**3'**) purified as the dephosphorylated product of the OsCPS4:H501D mutant. Carbon numbering and HMBC correlation and NOESY Nuclear Overhauser Effect correlations used to assign configurations.



syn-halima-5,13*E*-dien-15-ol (**3'**)

Figure S4: ^{1}H Spectrum of *syn*-halima-5,13*E*-dien-15-ol (**3'**).

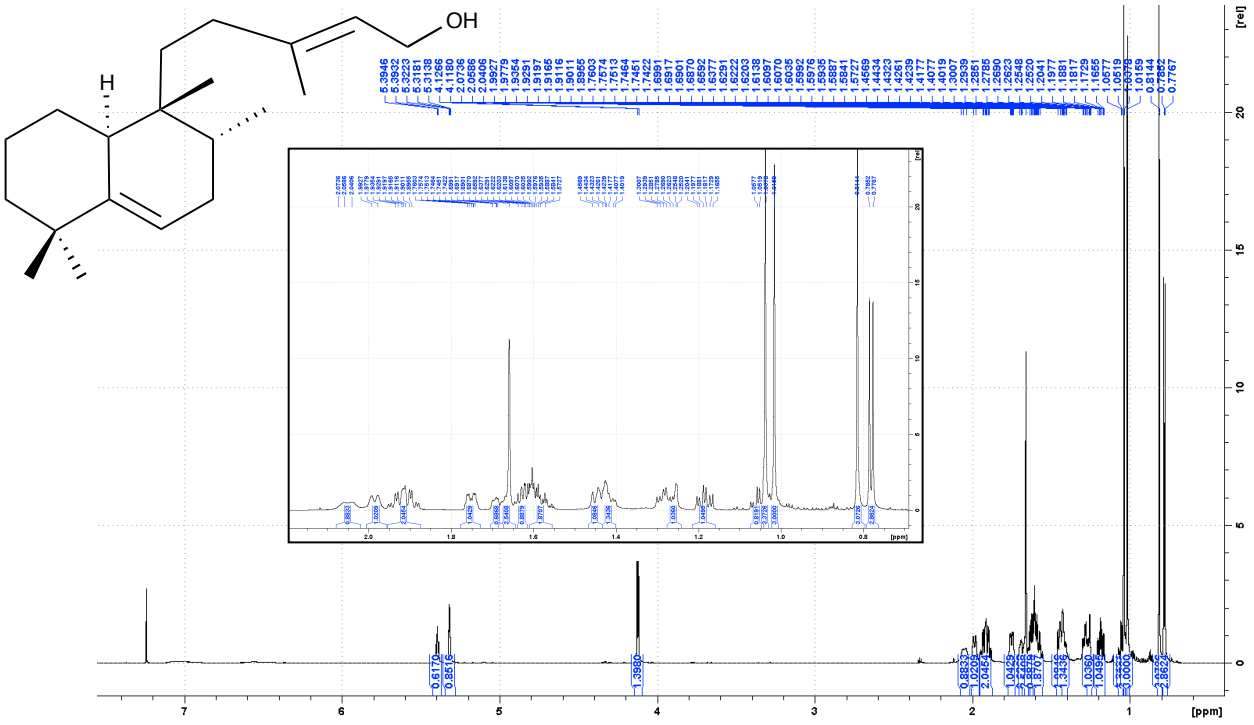


Figure S5: ^{13}C Spectrum of *syn*-halima-5,13*E*-dien-15-ol (**3'**).

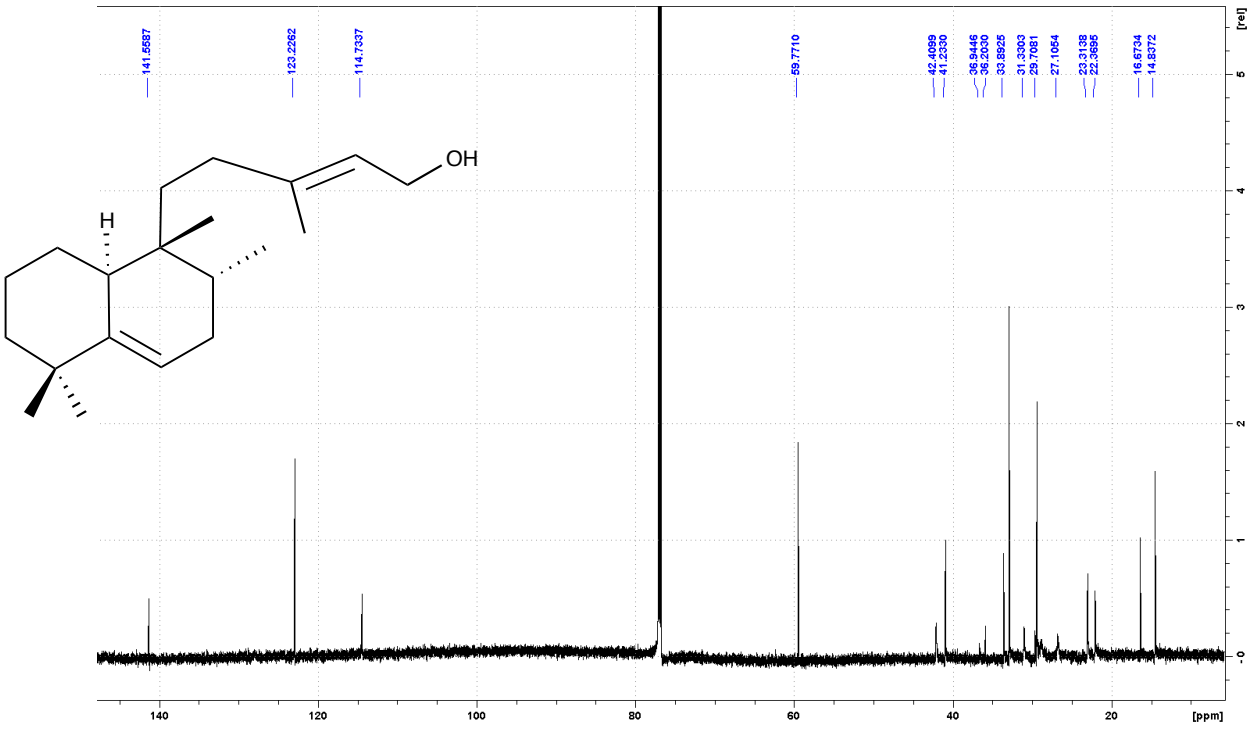


Figure S6. Carbocationic rearrangements of GGPP (monophosphate instead of diphosphate is used in the calculations, B3LYP/6-31+G(d,p)). Computed energies (in kcal/mol) from B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p) in normal texts and mpw1pw91/6-31+G(d,p)//B3LYP/6-31+G(d,p) in brackets are shown. All energies include zero point energy corrections from frequency calculations using the B3LYP/6-31+G(d,p) method.

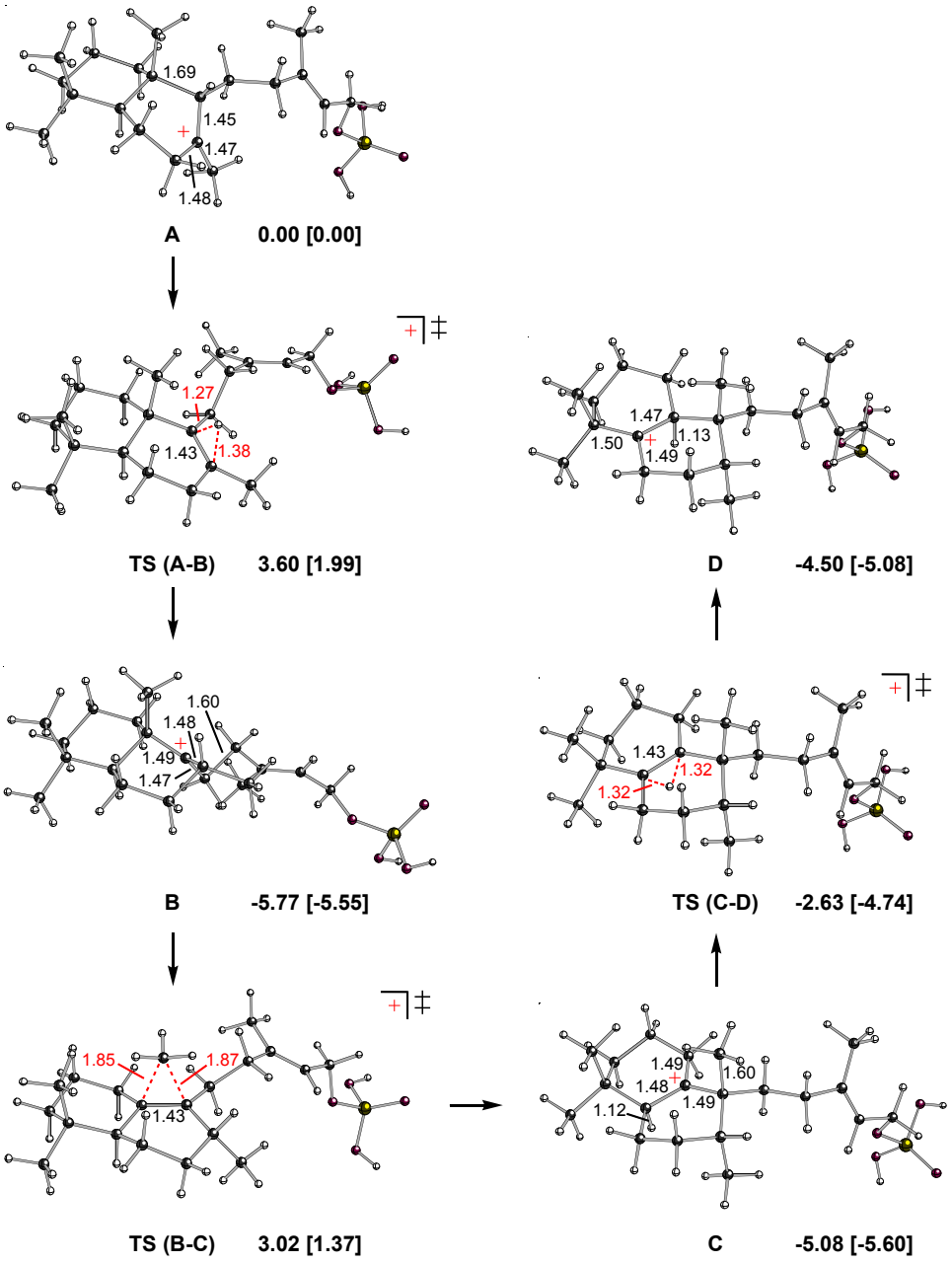
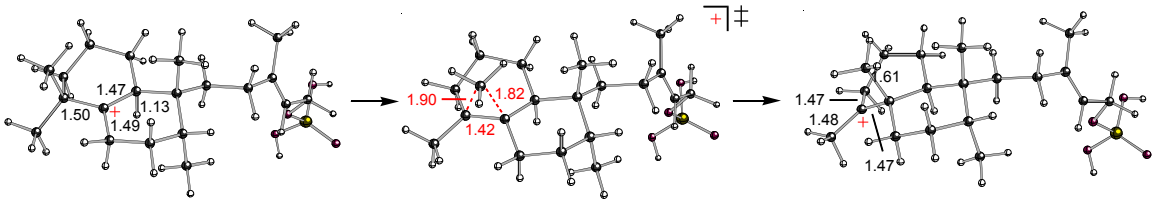
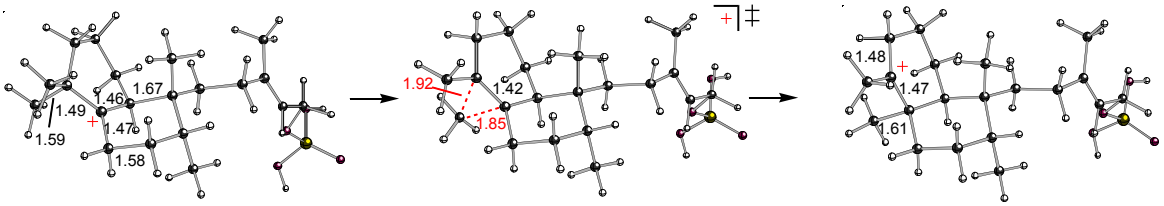


Figure S7. Conversion of cation **D** to cation **E** (monophosphate instead of diphosphate is used in the calculations, B3LYP/6-31+G(d,p)). Computed energies (in kcal/mol) from B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p) in normal texts and mpw1pw91/6-31+G(d,p)//B3LYP/6-31+G(d,p) in brackets are shown. All energies include zero point energy corrections from frequency calculations using the B3LYP/6-31+G(d,p) method.



D **-4.50 [-5.08]** **TS (D-E)** **7.00 [5.28]** **E** **3.61 [3.05]**

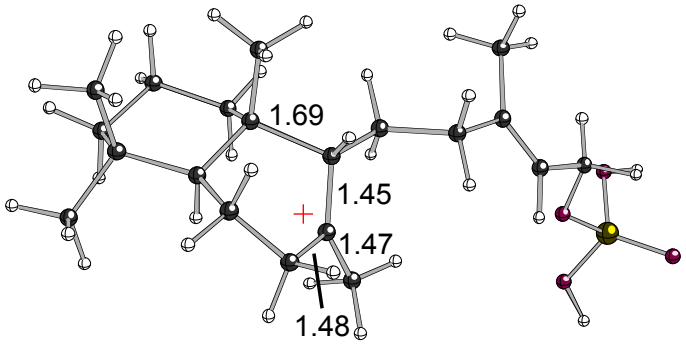
Figure S8. Conversion of cation **D'** (conformational isomer of **D**) to cation **F** via alternative geminal methyl shift (monophosphate instead of diphosphate is used in the calculations, B3LYP/6-31+G(d,p)). Computed energies (in kcal/mol) from B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p) in normal texts and mpw1pw91/6-31+G(d,p)//B3LYP/6-31+G(d,p) in brackets are shown. All energies include zero point energy corrections from frequency calculations using the B3LYP/6-31+G(d,p) method.



D' **-2.65 [-2.49]** **TS (D'-F)** **5.76 [4.35]** **F** **1.61 [0.89]**

Coordinates and Energies for structures shown in Figures 3 & S6 – S8.
Computed structures where selected distances are shown in Å.

A



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1425.9464979 hartrees (-894795.686897229 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.537617 (Hartree/Particle)

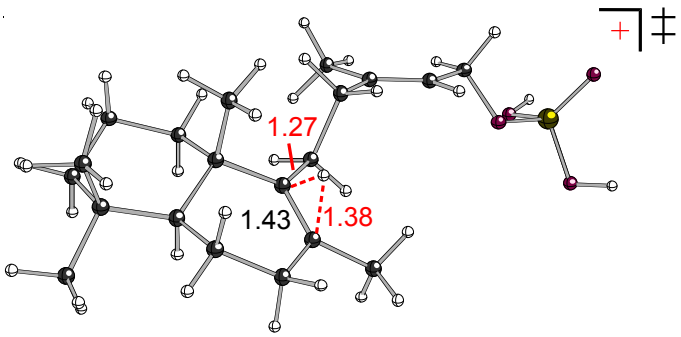
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1425.6967572 hartrees (-894638.972110572 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.577265	-2.194328	-0.379519
2	6	-2.034815	1.347250	-1.105870
3	6	1.665291	0.104610	-0.828716
4	6	1.635672	-1.341756	-0.947168
5	1	-0.406050	-1.724482	-0.344609
6	6	0.375132	0.819158	-0.410404
7	6	-0.663139	0.879996	-1.558950
8	6	3.056959	0.589661	-0.002443
9	1	-0.064267	0.339221	0.470789
10	1	1.961324	0.434952	-1.838555
11	1	0.536230	-3.179925	-0.849952
12	1	0.622481	1.837442	-0.102591
13	6	2.783150	-1.986962	-1.625945
14	1	2.476151	-2.075272	-2.686107
15	1	2.883365	-3.021852	-1.277089
16	6	4.100775	-1.196839	-1.475603
17	1	4.202259	-0.427611	-2.248522
18	1	4.930318	-1.890854	-1.620155
19	6	4.081044	-0.580211	-0.062387
20	1	3.635361	-1.361981	0.578581

21	6	2.745317	0.870073	1.480414
22	1	2.047596	1.705503	1.589379
23	1	2.271611	-0.008854	1.938127
24	6	5.453368	-0.326188	0.647000
25	6	5.114086	0.092390	2.106881
26	1	4.764052	-0.800678	2.643890
27	1	6.035654	0.406667	2.610746
28	6	4.050997	1.190371	2.246005
29	1	4.448456	2.155628	1.914557
30	1	3.801524	1.321435	3.304765
31	6	3.466175	1.885753	-0.731052
32	1	3.889363	1.691761	-1.720881
33	1	2.599278	2.540832	-0.858892
34	1	4.203113	2.451062	-0.164117
35	6	6.376028	0.702010	-0.042400
36	1	6.046535	1.734521	0.076530
37	1	7.378491	0.636566	0.392273
38	1	6.476835	0.500600	-1.114630
39	6	6.228195	-1.663120	0.715655
40	1	7.071307	-1.564037	1.406618
41	1	5.599918	-2.483803	1.081901
42	1	6.644685	-1.953561	-0.253980
43	1	-0.763481	-0.105807	-2.029786
44	1	-0.275637	1.553185	-2.337957
45	6	-3.064170	0.485280	-1.156073
46	6	-4.486634	0.724597	-0.758790
47	1	-4.647781	1.701196	-0.298081
48	1	-2.885597	-0.520913	-1.535073
49	1	-5.150362	0.627177	-1.626560
50	1	0.875930	-2.364595	0.673359
51	6	-2.119875	2.781559	-0.643343
52	1	-3.113874	3.058493	-0.291159
53	1	-1.416520	2.981358	0.173906
54	1	-1.856899	3.463086	-1.462609
55	8	-4.832291	-0.307896	0.208314
56	8	-6.231876	-1.698628	1.689430
57	15	-6.379114	-0.560518	0.560196
58	8	-7.303464	-0.886641	-0.551860
59	8	-6.729599	0.790246	1.374898
60	1	-6.720535	-2.497176	1.440163
61	1	-7.681225	0.972033	1.392766

TS (A-B)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1425.9394739 hartrees (-894791.279266989 kcal/mol)
Imaginary Frequencies: 1 (-339.1941 1/cm)
Zero-point correction = 0.536331 (Hartree/Particle)

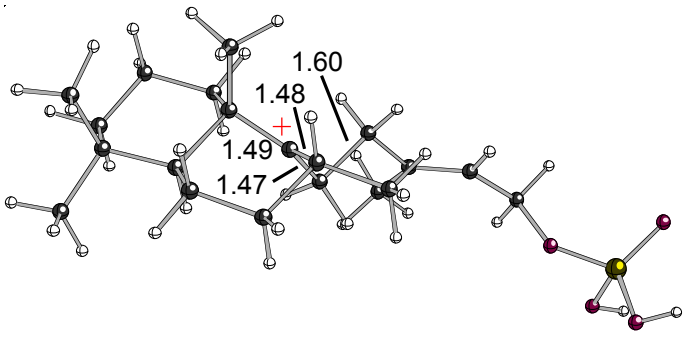
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1425.6923079 hartrees (-894636.180130329 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.481613	2.895755	-0.247092
2	6	-1.811990	-1.308666	0.525706
3	6	1.604644	0.602752	0.097723
4	6	1.683134	2.024299	0.035360
5	1	-0.432952	2.554915	0.239548
6	6	0.274286	-0.073969	-0.227870
7	6	-0.446922	-0.791661	0.947313
8	6	2.903055	-0.251723	0.310318
9	1	-0.418983	0.649987	-0.656287
10	1	1.442982	1.267887	1.166982
11	1	0.677174	3.925741	0.055511
12	1	0.483612	-0.793293	-1.022460
13	6	2.985500	2.764680	0.168756
14	1	2.864996	3.573968	0.899269
15	1	3.072288	3.279863	-0.802211
16	6	4.231407	1.917760	0.433294
17	1	4.376859	1.790627	1.510152
18	1	5.100383	2.474367	0.076592
19	6	4.119893	0.559779	-0.271825
20	1	3.826382	0.771295	-1.314015
21	6	2.780472	-1.586585	-0.475932
22	1	1.981120	-2.204537	-0.054206
23	1	2.508866	-1.370293	-1.517846

24	6	5.486825	-0.203186	-0.417304
25	6	5.226001	-1.561832	-1.114638
26	1	4.976970	-1.372972	-2.168772
27	1	6.155253	-2.143053	-1.120625
28	6	4.094406	-2.380016	-0.489660
29	1	4.359990	-2.706283	0.522198
30	1	3.938514	-3.297662	-1.067217
31	6	3.000988	-0.560993	1.830436
32	1	3.157429	0.338631	2.433835
33	1	2.087774	-1.043577	2.188059
34	1	3.824670	-1.239171	2.043891
35	6	6.245634	-0.413324	0.912454
36	1	5.767254	-1.130576	1.582092
37	1	7.246966	-0.800392	0.698120
38	1	6.378097	0.523541	1.463191
39	6	6.409208	0.619959	-1.348339
40	1	7.293347	0.028842	-1.607674
41	1	5.906236	0.885744	-2.285387
42	1	6.770329	1.540547	-0.879417
43	1	-0.563456	-0.088183	1.781031
44	1	0.167719	-1.622295	1.311668
45	6	-2.911158	-0.654016	0.934738
46	6	-4.338904	-0.974989	0.621772
47	1	-4.450975	-1.824119	-0.055605
48	1	-2.791643	0.222320	1.571590
49	1	-4.898706	-1.180093	1.542182
50	1	0.298154	2.889227	-1.329196
51	6	-1.799971	-2.550808	-0.332079
52	1	-2.787538	-2.817778	-0.709235
53	1	-1.140912	-2.433022	-1.201014
54	1	-1.419877	-3.407106	0.239777
55	8	-4.902970	0.207064	-0.012436
56	8	-6.612517	1.721270	-0.955091
57	15	-6.497637	0.310417	-0.189108
58	8	-7.338735	0.172600	1.023255
59	8	-6.745073	-0.799350	-1.336622
60	1	-7.143069	2.351180	-0.444748
61	1	-7.665062	-1.102496	-1.364799

B



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1425.9578709 hartrees (-894802.823568459 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.539794 (Hartree/Particle)

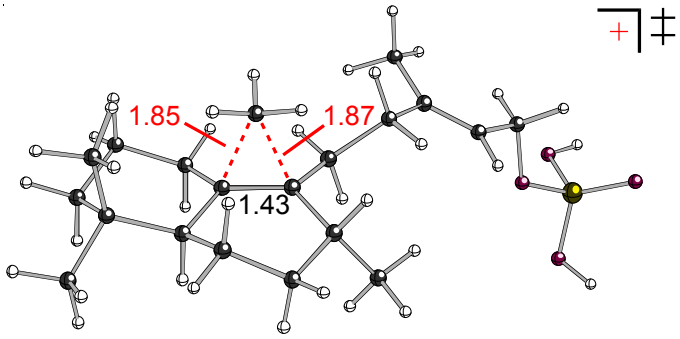
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1425.707782 hartrees (-894645.89028282 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.089406	2.546281	-0.734782
2	6	1.657525	-1.399354	-0.314931
3	6	-1.649051	0.486077	-0.439182
4	6	-1.494987	1.934292	-0.698089
5	1	0.530050	2.099259	-1.516386
6	6	-0.556702	-0.234659	0.232108
7	6	0.330690	-0.948403	-0.890681
8	6	-2.971994	-0.131707	-0.729382
9	1	0.095950	0.450974	0.773971
10	1	-2.030258	2.208502	-1.609958
11	1	-0.180873	3.612014	-0.960795
12	1	-0.919394	-1.004979	0.913088
13	6	-2.347264	2.555016	0.499971
14	1	-2.323200	3.638737	0.346029
15	1	-1.825861	2.349671	1.442349
16	6	-3.771724	2.014285	0.531658
17	1	-4.340158	2.404669	-0.317618
18	1	-4.264616	2.397863	1.430363
19	6	-3.803617	0.479805	0.562669
20	1	-3.224910	0.160254	1.441800
21	6	-3.001387	-1.681771	-0.653807
22	1	-2.527763	-2.082922	-1.556972
23	1	-2.415859	-2.039214	0.199085
24	6	-5.224140	-0.164883	0.774192

25	6	-5.103176	-1.707432	0.743257
26	1	-4.540985	-2.035571	1.629476
27	1	-6.105911	-2.137874	0.842798
28	6	-4.415067	-2.257266	-0.506723
29	1	-5.017211	-2.059740	-1.400202
30	1	-4.337757	-3.347468	-0.436126
31	6	-3.533531	0.322292	-2.106769
32	1	-4.347597	-0.332165	-2.413061
33	1	-3.915706	1.342710	-2.118409
34	6	-6.286694	0.319053	-0.235221
35	1	-6.093950	-0.002609	-1.259505
36	1	-7.261933	-0.087419	0.051272
37	1	-6.384601	1.408704	-0.236003
38	6	-5.703946	0.231488	2.193223
39	1	-6.615582	-0.324513	2.434980
40	1	-4.958620	-0.010494	2.959181
41	1	-5.945963	1.295308	2.270292
42	1	0.502619	-0.259432	-1.720978
43	1	-0.235369	-1.800673	-1.276942
44	6	2.780147	-0.797997	-0.745318
45	6	4.192340	-1.100082	-0.349864
46	1	4.269405	-1.844500	0.445322
47	1	2.698183	0.005928	-1.475699
48	1	4.762349	-1.450053	-1.219518
49	1	0.441517	2.460849	0.217055
50	6	1.589959	-2.521027	0.691193
51	1	2.572086	-2.814520	1.062137
52	1	0.986566	-2.241951	1.564349
53	1	1.122190	-3.409671	0.249293
54	8	4.767814	0.146699	0.121156
55	8	6.506432	1.763927	0.811261
56	15	6.370076	0.284127	0.197114
57	8	7.138291	0.031261	-1.044495
58	8	6.693965	-0.702766	1.432928
59	1	6.977124	2.353699	0.203450
60	1	7.621040	-0.984540	1.450653
61	1	-2.756001	0.242246	-2.873417

TS (B-C)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1425.9426356 hartrees (-894793.263265356 kcal/mol)
Imaginary Frequencies: 1 (-278.8232 1/cm)
Zero-point correction = 0.538573 (Hartree/Particle)

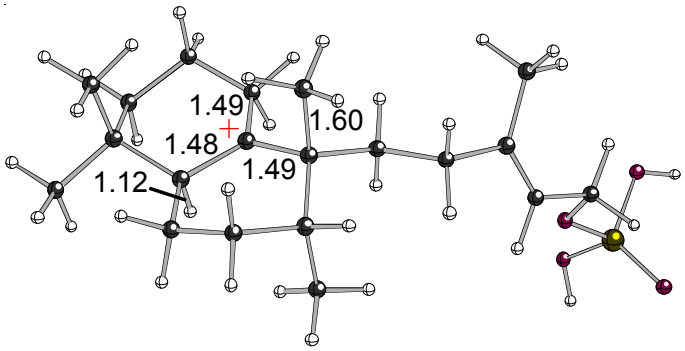
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1425.6955364 hartrees (-894638.206046364 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.376799	2.410689	-0.015408
2	6	1.913927	-1.110631	-1.173070
3	6	-1.687601	0.246581	-0.338775
4	6	-1.546450	1.726528	-0.764453
5	1	0.603214	1.998752	-0.258064
6	6	-0.368330	-0.512929	-0.211515
7	6	0.539121	-0.531379	-1.470223
8	6	-2.899555	-0.258211	0.218992
9	1	0.175083	-0.025931	0.606847
10	1	-1.287731	1.725904	-1.830560
11	1	-0.367379	3.468249	-0.293980
12	1	-0.538338	-1.536870	0.115707
13	6	-2.814696	2.583649	-0.555768
14	1	-2.805903	3.402501	-1.281829
15	1	-2.758152	3.054198	0.433935
16	6	-4.121015	1.803011	-0.636152
17	1	-4.281668	1.418726	-1.650109
18	1	-4.956364	2.476732	-0.434714
19	6	-4.123822	0.660761	0.391085
20	1	-3.911990	1.117429	1.373517
21	6	-2.913852	-1.512600	1.081857
22	1	-2.139513	-2.221310	0.789482
23	1	-2.632550	-1.155104	2.084653

24	6	-5.522052	-0.044128	0.580701
25	6	-5.374269	-1.229799	1.562783
26	1	-5.156977	-0.839295	2.567092
27	1	-6.335717	-1.749652	1.638848
28	6	-4.274314	-2.213163	1.166471
29	1	-4.507937	-2.699339	0.211434
30	1	-4.200254	-3.018453	1.904146
31	6	-2.679438	-0.773449	-1.547023
32	1	-3.757890	-0.761087	-1.690537
33	1	-2.250857	-0.190078	-2.360696
34	6	-6.156562	-0.530246	-0.742175
35	1	-5.610035	-1.350386	-1.219133
36	1	-7.162581	-0.911504	-0.540184
37	1	-6.263430	0.279313	-1.469824
38	6	-6.492614	0.974815	1.220867
39	1	-7.428841	0.474729	1.487948
40	1	-6.076387	1.406202	2.138350
41	1	-6.749232	1.794363	0.543832
42	1	0.655923	0.477342	-1.873459
43	1	0.054991	-1.131520	-2.252587
44	6	2.973690	-0.285815	-1.142684
45	6	4.402642	-0.634912	-0.867271
46	1	4.554146	-1.691206	-0.636214
47	1	2.817067	0.774349	-1.339300
48	1	5.032809	-0.366278	-1.723694
49	1	-0.515594	2.361160	1.069866
50	6	1.964490	-2.603999	-0.955421
51	1	2.955091	-2.960426	-0.672043
52	1	1.270201	-2.921412	-0.167551
53	1	1.670979	-3.134365	-1.870747
54	8	4.815799	0.154753	0.283035
55	8	6.332280	1.215539	1.925138
56	15	6.385403	0.349747	0.569905
57	8	7.218975	0.916277	-0.517015
58	8	6.790790	-1.136964	1.054512
59	1	6.743956	2.083658	1.800614
60	1	7.744034	-1.298809	0.990248
61	1	-2.280980	-1.782285	-1.522134

C



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1425.9550974 hartrees (-894801.083169474 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.538127 (Hartree/Particle)

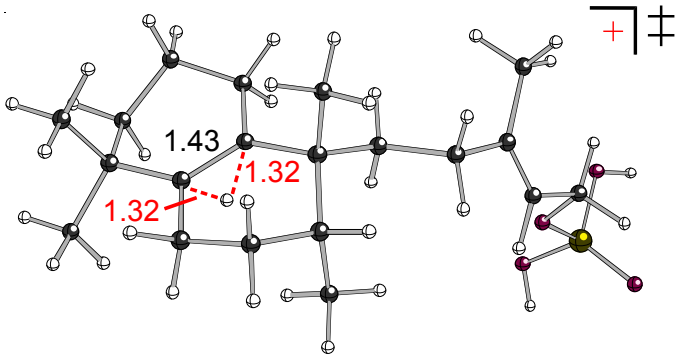
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1425.7061913 hartrees (-894644.892102663 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.256150	-1.116349	-2.330251
2	6	1.990860	-1.566494	1.023750
3	6	-1.828224	-0.979669	0.191878
4	6	-1.974989	-1.779965	-1.139799
5	1	-0.175073	-1.061751	-2.185689
6	6	-0.331235	-0.693931	0.541451
7	6	0.591234	-1.935093	0.553060
8	6	-2.709856	0.215563	0.260247
9	1	0.071384	0.028314	-0.176692
10	1	-1.497014	-2.749503	-0.964096
11	1	-1.432296	-1.701380	-3.237922
12	1	-0.263756	-0.218927	1.522892
13	6	-3.453860	-2.039567	-1.448795
14	1	-3.902011	-2.643400	-0.653072
15	1	-3.538307	-2.639377	-2.360286
16	6	-4.239707	-0.736176	-1.627904
17	1	-5.303424	-0.944895	-1.502806
18	1	-4.132730	-0.377007	-2.655496
19	6	-3.842031	0.425047	-0.674063
20	1	-3.292598	1.172636	-1.299232
21	6	-2.393729	1.293973	1.237261
22	1	-1.788590	0.905871	2.058211
23	1	-1.688117	1.930351	0.666245

24	6	-5.068974	1.262063	-0.117415
25	6	-4.537984	2.502027	0.633114
26	1	-4.051960	3.177295	-0.085163
27	1	-5.388201	3.056634	1.044731
28	6	-3.559545	2.153704	1.750066
29	1	-4.067263	1.618523	2.559336
30	1	-3.146090	3.061394	2.199196
31	6	-2.481248	-1.801235	1.398591
32	1	-3.573285	-1.795287	1.410855
33	1	-2.163980	-2.839324	1.269023
34	6	-5.931511	0.387869	0.817366
35	1	-5.375515	0.022286	1.686852
36	1	-6.776256	0.974661	1.191815
37	1	-6.349358	-0.480272	0.300527
38	6	-5.926774	1.751277	-1.301753
39	1	-6.732948	2.389449	-0.926827
40	1	-5.336698	2.346141	-2.008240
41	1	-6.393976	0.931733	-1.853108
42	1	0.650211	-2.370772	-0.447679
43	1	0.177402	-2.706354	1.214810
44	6	2.943261	-1.318427	0.109549
45	6	4.365345	-0.925022	0.355737
46	1	4.611437	-0.841125	1.416190
47	1	2.687693	-1.404412	-0.946378
48	1	5.048971	-1.644371	-0.110440
49	1	-1.610454	-0.098488	-2.529402
50	6	2.182913	-1.521596	2.520347
51	1	3.127968	-1.066763	2.820081
52	1	1.378371	-0.957625	3.008457
53	1	2.153250	-2.535903	2.939069
54	8	4.561679	0.375949	-0.271002
55	8	5.746452	2.360896	-1.139153
56	15	6.056383	0.910522	-0.511872
57	8	6.982529	0.063498	-1.300730
58	8	6.521842	1.211430	1.006711
59	1	6.132402	2.442600	-2.023988
60	1	7.486469	1.230283	1.096447
61	1	-2.118202	-1.431251	2.358632

TS (C-D)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1425.9497501 hartrees (-894797.727685251 kcal/mol)
Imaginary Frequencies: 1 (-363.0034 1/cm)
Zero-point correction = 0.536672 (Hartree/Particle)

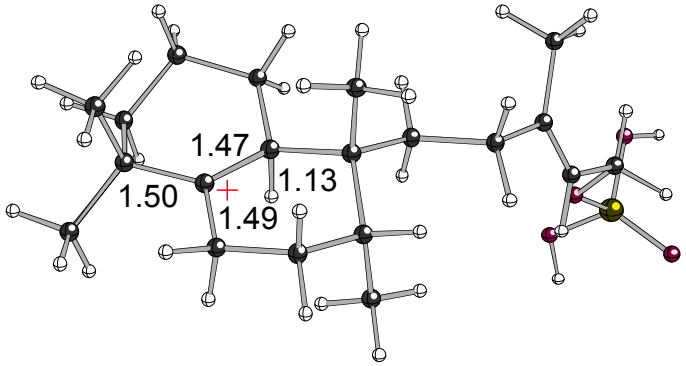
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1425.7033613 hartrees (-894643.116249363 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.231049	-0.731509	-2.373138
2	6	1.979780	-1.799415	0.763743
3	6	-1.882834	-1.242169	0.106375
4	6	-1.998344	-1.648307	-1.399462
5	1	-0.153472	-0.752995	-2.202323
6	6	-0.399715	-0.973192	0.509606
7	6	0.580646	-2.146102	0.275431
8	6	-2.760078	-0.009779	0.426224
9	1	-0.021859	-0.098036	-0.031172
10	1	-1.553588	-2.645743	-1.479063
11	1	-1.403935	-1.061578	-3.402114
12	1	-0.361204	-0.715464	1.571176
13	6	-3.475335	-1.764570	-1.804347
14	1	-3.977722	-2.527120	-1.202274
15	1	-3.554478	-2.096005	-2.844156
16	6	-4.199100	-0.423312	-1.654348
17	1	-5.283074	-0.569226	-1.653345
18	1	-4.003909	0.223083	-2.517745
19	6	-3.861048	0.362416	-0.398191
20	1	-2.652378	0.862121	-0.563523
21	6	-2.471981	0.732886	1.723880
22	1	-2.249844	-0.027724	2.477820

23	1	-1.534813	1.287535	1.593546
24	6	-4.812468	1.517615	-0.025042
25	6	-4.178411	2.441892	1.039333
26	1	-3.396186	3.053676	0.566806
27	1	-4.943808	3.142761	1.386333
28	6	-3.583058	1.666117	2.210929
29	1	-4.360498	1.088073	2.721441
30	1	-3.170985	2.352159	2.956460
31	6	-2.465556	-2.375539	1.009839
32	1	-3.555697	-2.439095	0.962945
33	1	-2.067432	-3.339737	0.684091
34	6	-6.111761	0.870175	0.533254
35	1	-5.924367	0.216364	1.389209
36	1	-6.782483	1.669533	0.861865
37	1	-6.643579	0.291740	-0.225987
38	6	-5.166234	2.366507	-1.267601
39	1	-5.798019	3.202916	-0.955562
40	1	-4.271704	2.789469	-1.738523
41	1	-5.722204	1.803949	-2.021108
42	1	0.623087	-2.400423	-0.787548
43	1	0.224759	-3.039649	0.802849
44	6	2.901521	-1.389444	-0.123362
45	6	4.312738	-0.977462	0.151646
46	1	4.588503	-1.064095	1.204453
47	1	2.623138	-1.334191	-1.175555
48	1	5.012730	-1.571344	-0.447374
49	1	-1.540109	0.321257	-2.324342
50	6	2.208060	-1.957980	2.247756
51	1	3.155037	-1.535326	2.585636
52	1	1.410041	-1.477213	2.826733
53	1	2.198447	-3.020475	2.523481
54	8	4.435547	0.421180	-0.246550
55	8	5.507611	2.586059	-0.760165
56	15	5.897203	1.068350	-0.386243
57	8	6.865852	0.420100	-1.302479
58	8	6.353489	1.133701	1.163688
59	1	5.885554	2.836785	-1.616187
60	1	7.316276	1.186903	1.258646
61	1	-2.182902	-2.239414	2.056939

D



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1425.9541985 hartrees (-894800.519100735 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.538146 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1425.7053813 hartrees (-894644.383819563 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.222892	-0.961950	-2.364948
2	6	1.991201	-1.656227	0.945329
3	6	-1.850731	-1.101050	0.172090
4	6	-1.967892	-1.726671	-1.253949
5	1	-0.146144	-0.924113	-2.189734
6	6	-0.365110	-0.816785	0.539825
7	6	0.593138	-2.028762	0.475434
8	6	-2.646957	0.267768	0.223023
9	1	0.035095	-0.030861	-0.111844
10	1	-1.512531	-2.721545	-1.192453
11	1	-1.377198	-1.459481	-3.327518
12	1	-0.328560	-0.411551	1.555229
13	6	-3.443654	-1.932789	-1.622130
14	1	-3.915482	-2.656118	-0.951068
15	1	-3.529594	-2.351512	-2.629542
16	6	-4.228694	-0.616816	-1.576941
17	1	-5.307279	-0.768951	-1.681393
18	1	-3.972825	0.000185	-2.460879
19	6	-3.955247	0.305655	-0.447327
20	1	-2.181764	0.898559	-0.587807
21	6	-2.457462	1.079655	1.538408
22	1	-2.304130	0.370939	2.354793

23	1	-1.520048	1.633607	1.444520
24	6	-4.970767	1.353606	-0.125585
25	6	-4.365357	2.519043	0.687235
26	1	-3.707869	3.102433	0.028348
27	1	-5.180033	3.189464	0.979045
28	6	-3.595939	2.043556	1.915129
29	1	-4.284761	1.558882	2.614716
30	1	-3.182446	2.902421	2.451113
31	6	-2.469451	-2.063775	1.219124
32	1	-3.562379	-2.100650	1.166784
33	1	-2.105140	-3.082848	1.063004
34	6	-6.023599	0.557979	0.745836
35	1	-5.582258	0.028847	1.592955
36	1	-6.723437	1.301279	1.139577
37	1	-6.582432	-0.156847	0.138706
38	6	-5.696497	1.919107	-1.370735
39	1	-6.423985	2.663424	-1.036075
40	1	-4.993125	2.422404	-2.041980
41	1	-6.242133	1.163364	-1.938481
42	1	0.648829	-2.412716	-0.547836
43	1	0.206819	-2.843774	1.100217
44	6	2.936132	-1.367994	0.034883
45	6	4.351101	-0.955898	0.288453
46	1	4.607385	-0.928654	1.349307
47	1	2.676394	-1.427933	-1.021843
48	1	5.047718	-1.626965	-0.227246
49	1	-1.562414	0.075595	-2.484669
50	6	2.191879	-1.648630	2.441596
51	1	3.137146	-1.198987	2.748462
52	1	1.387724	-1.099542	2.946241
53	1	2.166016	-2.673585	2.833890
54	8	4.512739	0.387465	-0.260420
55	8	5.641854	2.455041	-1.004024
56	15	5.990046	0.973659	-0.474347
57	8	6.933529	0.206654	-1.323067
58	8	6.462374	1.188848	1.057166
59	1	6.014198	2.599426	-1.886560
60	1	7.427137	1.223394	1.139406
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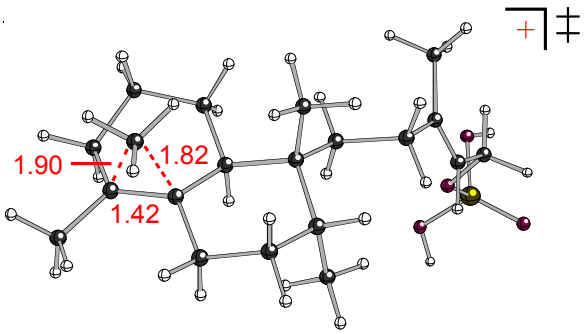
TS (D-E)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1425.9365051 hartrees (-894789.416315301 kcal/mol)
Imaginary Frequencies: 1 (-299.4242 1/cm)
Zero-point correction = 0.538782 (Hartree/Particle)

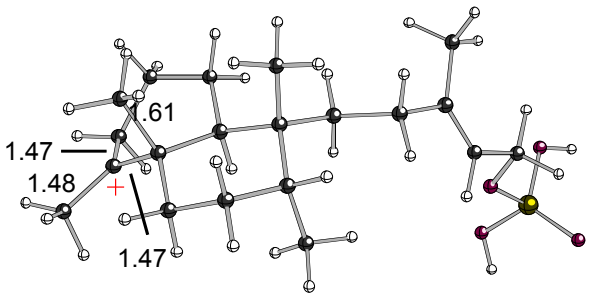
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1425.6895007 hartrees (-894634.418584257 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.087857	-0.845879	-2.369747
2	6	1.947193	-1.691964	0.931184
3	6	-1.890520	-1.074644	0.120215
4	6	-1.967724	-1.603224	-1.354305
5	1	-0.025012	-0.932959	-2.137944
6	6	-0.409747	-0.848910	0.557682
7	6	0.547613	-2.059953	0.461432
8	6	-2.611424	0.331110	0.218357
9	1	0.020047	-0.031533	-0.033244
10	1	-1.603299	-2.637106	-1.332575
11	1	-1.234264	-1.264986	-3.370597
12	1	-0.403703	-0.502799	1.595779
13	6	-3.429645	-1.656505	-1.838272
14	1	-4.009106	-2.373986	-1.247347
15	1	-3.463901	-2.022800	-2.869660
16	6	-4.105553	-0.282640	-1.794431
17	1	-5.142527	-0.359672	-2.125609
18	1	-3.612567	0.391013	-2.508861
19	6	-3.999910	0.420627	-0.444176
20	1	-2.045753	0.977161	-0.472243
21	6	-2.485578	0.997540	1.623720
22	1	-2.337449	0.230554	2.386894
23	1	-1.567756	1.590807	1.621221

24	6	-4.829724	1.533580	-0.159944
25	6	-4.413622	2.521001	0.904587
26	1	-3.770661	3.241977	0.374581
27	1	-5.283157	3.088494	1.250991
28	6	-3.656595	1.893283	2.073090
29	1	-4.365503	1.321667	2.682378
30	1	-3.285112	2.687565	2.725953
31	6	-2.529874	-2.122605	1.063299
32	1	-3.576509	-2.336054	0.832760
33	1	-2.002399	-3.075828	0.976480
34	6	-5.387140	-0.112382	0.608838
35	1	-4.795805	-0.707729	1.298294
36	1	-6.029093	0.532210	1.214766
37	1	-5.997583	-0.700827	-0.068885
38	6	-5.930577	2.002718	-1.077308
39	1	-6.739441	2.469379	-0.510055
40	1	-5.498909	2.777743	-1.724292
41	1	-6.344917	1.230601	-1.723795
42	1	0.597078	-2.425699	-0.568586
43	1	0.170308	-2.888025	1.073984
44	6	2.892207	-1.397463	0.022617
45	6	4.305020	-0.979986	0.278496
46	1	4.559861	-0.953734	1.339778
47	1	2.632795	-1.452773	-1.034317
48	1	5.007237	-1.643878	-0.238532
49	1	-1.313688	0.224403	-2.431706
50	6	2.149907	-1.690282	2.427502
51	1	3.099144	-1.249324	2.734954
52	1	1.350726	-1.136282	2.934422
53	1	2.116165	-2.716203	2.816681
54	8	4.460704	0.366802	-0.267321
55	8	5.580814	2.438486	-1.025838
56	15	5.932564	0.974643	-0.449787
57	8	6.914979	0.203463	-1.249307
58	8	6.353049	1.240738	1.088803
59	1	5.947586	2.552753	-1.915073
60	1	7.313609	1.305788	1.197226
61	1	-2.469971	-1.826006	2.115263

E



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1425.9414643 hartrees (-894792.528262893 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.538332 (Hartree/Particle)

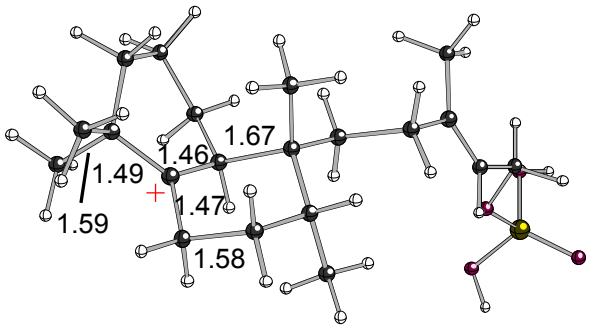
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1425.6926086 hartrees (-894636.368822586 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.191107	-0.526343	-2.373431
2	6	1.923970	-1.819086	0.684212
3	6	-1.940095	-1.124874	0.071476
4	6	-2.035859	-1.440384	-1.461580
5	1	-0.121222	-0.634983	-2.186832
6	6	-0.450612	-0.943441	0.505287
7	6	0.511542	-2.118326	0.205524
8	6	-2.681011	0.239633	0.367128
9	1	-0.038498	-0.041124	0.038124
10	1	-1.652033	-2.458767	-1.595531
11	1	-1.362768	-0.788949	-3.422633
12	1	-0.424055	-0.765719	1.585081
13	6	-3.504927	-1.459457	-1.924282
14	1	-4.058176	-2.253955	-1.411812
15	1	-3.554434	-1.706564	-2.990590
16	6	-4.200836	-0.109535	-1.718627
17	1	-5.244303	-0.187190	-2.041318
18	1	-3.727082	0.639025	-2.364087
19	6	-4.127734	0.381315	-0.244230
20	1	-2.100226	0.989199	-0.189283
21	6	-2.622294	0.666469	1.857668
22	1	-2.845890	-0.183508	2.507230
23	1	-1.594237	0.955270	2.081989
24	6	-4.621599	1.759398	-0.080103
25	6	-4.089669	2.598768	1.005407

26	1	-3.235377	3.094930	0.492492
27	1	-4.775606	3.410811	1.263970
28	6	-3.560540	1.838865	2.230940
29	1	-4.426740	1.485158	2.798615
30	1	-3.048662	2.553653	2.879667
31	6	-2.525119	-2.310424	0.878394
32	1	-3.596181	-2.457174	0.737643
33	1	-2.041743	-3.242743	0.574940
34	6	-5.274940	-0.359660	0.599626
35	1	-5.069631	-0.356518	1.667644
36	1	-6.271162	0.058595	0.427983
37	1	-5.297917	-1.389051	0.240473
38	6	-5.595216	2.363011	-1.014254
39	1	-6.162819	3.179867	-0.565663
40	1	-4.993719	2.793964	-1.835143
41	1	-6.256168	1.636066	-1.488703
42	1	0.534972	-2.328339	-0.867652
43	1	0.152551	-3.029857	0.698625
44	6	2.843982	-1.397379	-0.200015
45	6	4.267533	-1.030372	0.070824
46	1	4.567009	-1.199563	1.106825
47	1	2.551555	-1.295595	-1.244778
48	1	4.942786	-1.587202	-0.588746
49	1	-1.426419	0.537869	-2.264354
50	6	2.170051	-2.034958	2.158005
51	1	3.137715	-1.660954	2.495015
52	1	1.398720	-1.543068	2.762629
53	1	2.121278	-3.104891	2.398825
54	8	4.412286	0.395292	-0.222497
55	8	5.511635	2.577874	-0.567615
56	15	5.880339	1.022740	-0.355234
57	8	6.805214	0.455100	-1.366198
58	8	6.400597	0.929168	1.174000
59	1	5.882322	2.903254	-1.401276
60	1	7.367906	0.935364	1.227748
61	1	-2.347817	-2.197196	1.952084

D'



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1425.9525172 hartrees (-894799.464068172 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.539414 (Hartree/Particle)

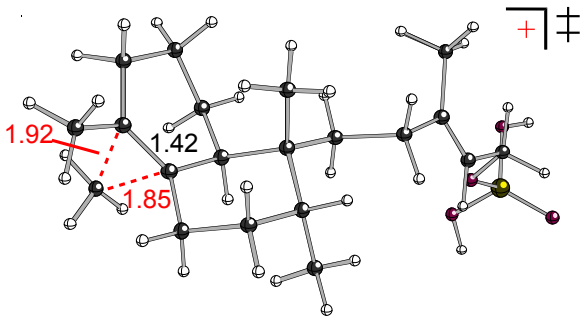
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1425.7025211 hartrees (-894642.589015461 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.922807	2.584811	-0.060701
2	6	1.872734	-0.650375	-1.680588
3	6	-1.863528	0.232885	-0.752890
4	6	-1.887557	1.782209	-0.953738
5	1	0.118597	2.297880	-0.214263
6	6	-0.424204	-0.330282	-0.657533
7	6	0.487292	-0.058554	-1.884628
8	6	-2.580164	-0.071479	0.725134
9	1	0.072868	0.064692	0.234532
10	1	-1.567187	1.943733	-1.992247
11	1	-1.001925	3.650192	-0.296896
12	1	-0.482629	-1.413818	-0.523128
13	6	-3.315171	2.339437	-0.863370
14	1	-3.941836	1.976393	-1.681819
15	1	-3.314158	3.431255	-0.928330
16	6	-3.997728	1.967996	0.508451
17	1	-5.014035	2.356643	0.538275
18	1	-3.409494	2.448305	1.299448
19	6	-3.924423	0.503996	0.664055
20	1	-1.968510	0.571308	1.369798
21	6	-2.522858	-1.506051	1.280319
22	1	-1.526129	-1.923594	1.130331
23	1	-2.624119	-1.410689	2.367145
24	6	-5.142797	-0.343615	0.741701

25	6	-4.897431	-1.801164	0.270788
26	1	-5.768063	-2.389734	0.575730
27	1	-4.918294	-1.788005	-0.822852
28	6	-3.598294	-2.482385	0.757789
29	1	-3.193701	-3.080289	-0.064103
30	1	-3.824525	-3.195731	1.555441
31	6	-2.621578	-0.474424	-1.894233
32	1	-3.670609	-0.177664	-1.970114
33	1	-2.154424	-0.235182	-2.853320
34	6	-6.373398	0.226987	0.001214
35	1	-6.169424	0.379735	-1.062929
36	1	-7.190310	-0.495693	0.078152
37	1	-6.733211	1.166215	0.426792
38	6	-5.450941	-0.308847	2.297231
39	1	-6.353063	-0.912921	2.437003
40	1	-4.653162	-0.739576	2.903647
41	1	0.576898	1.017754	-2.059052
42	1	0.039517	-0.492367	-2.786473
43	6	2.881011	0.156116	-1.307907
44	6	4.303621	-0.221721	-1.042372
45	1	4.499294	-1.287182	-1.177907
46	1	2.676657	1.217965	-1.172976
47	1	4.980799	0.347805	-1.689810
48	1	-1.130908	2.477135	1.010264
49	6	1.991549	-2.133868	-1.934219
50	1	2.947527	-2.550053	-1.613906
51	1	1.201688	-2.690791	-1.415851
52	1	1.876037	-2.348246	-3.004614
53	8	4.585674	0.127833	0.344962
54	8	5.896993	0.520090	2.401595
55	15	6.111351	0.201933	0.837464
56	8	7.031931	1.120481	0.125382
57	8	6.524694	-1.360256	0.790967
58	1	6.317737	1.358485	2.643473
59	1	7.484546	-1.483057	0.741960
60	1	-2.588159	-1.560692	-1.779815
61	1	-5.658870	0.705585	2.646186

TS (D'-F)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1425.9388943 hartrees (-894790.915562193 kcal/mol)
Imaginary Frequencies: 1 (-264.8401 1/cm)
Zero-point correction = 0.539190 (Hartree/Particle)

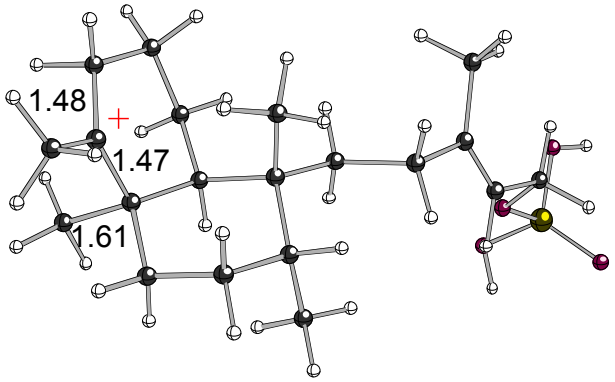
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1425.6913941 hartrees (-894635.606711691 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.244235	2.314069	-1.447616
2	6	-1.875816	0.712119	1.644075
3	6	1.898556	0.615783	0.454719
4	6	2.073105	2.042667	-0.176186
5	1	0.171581	2.222722	-1.266289
6	6	0.394109	0.253861	0.617082
7	6	-0.471514	1.252851	1.421693
8	6	2.555031	-0.447796	-0.536488
9	1	-0.064865	0.118529	-0.369075
10	1	1.724053	2.755126	0.580505
11	1	1.426077	3.337156	-1.792200
12	1	0.326651	-0.717843	1.117186
13	6	3.563500	2.351432	-0.414436
14	1	4.103221	2.405321	0.536629
15	1	3.673048	3.333743	-0.885594
16	6	4.235035	1.308134	-1.331962
17	1	5.291189	1.548583	-1.462568
18	1	3.770768	1.354238	-2.323147
19	6	4.025839	-0.089971	-0.775685
20	1	2.041972	-0.277719	-1.490887
21	6	2.378342	-1.945578	-0.206440
22	1	1.339378	-2.150743	0.056103
23	1	2.553685	-2.520708	-1.125018
24	6	5.062058	-0.845199	-0.173743

25	6	4.781484	-2.075063	0.675529
26	1	5.359458	-2.908002	0.256677
27	1	5.265797	-1.870075	1.638689
28	6	3.307182	-2.464020	0.896814
29	1	2.979694	-2.084535	1.866004
30	1	3.230120	-3.553437	0.957853
31	6	2.566430	0.604934	1.853847
32	1	3.659344	0.563870	1.815613
33	1	2.309943	1.512494	2.407664
34	6	6.491102	-0.366715	-0.070827
35	1	6.598779	0.136215	0.898050
36	1	7.181926	-1.214210	-0.072329
37	1	6.792079	0.337289	-0.844887
38	6	4.780258	-1.214861	-2.034387
39	1	5.142388	-2.226251	-1.858458
40	1	3.831774	-1.292157	-2.564827
41	1	-0.531977	2.210689	0.896575
42	1	-0.005510	1.453257	2.394521
43	6	-2.868852	1.092409	0.822938
44	6	-4.297847	0.654347	0.861562
45	1	-4.518933	-0.011184	1.698298
46	1	-2.641623	1.797228	0.023413
47	1	-4.968408	1.519805	0.911016
48	1	1.486323	1.647227	-2.281905
49	6	-2.024272	-0.236646	2.809376
50	1	-2.984042	-0.754774	2.827826
51	1	-1.238104	-1.001304	2.796174
52	1	-1.917574	0.305801	3.757855
53	8	-4.565625	-0.061795	-0.383595
54	8	-5.854738	-1.226327	-2.145612
55	15	-6.079983	-0.421927	-0.767533
56	8	-7.067282	0.682378	-0.835912
57	8	-6.409846	-1.574193	0.318260
58	1	-6.283717	-0.769064	-2.883995
59	1	-7.363024	-1.685567	0.451371
60	1	2.225500	-0.241224	2.454971
61	1	5.504895	-0.612632	-2.573126

F



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1425.945061 hartrees (-894794.78522811 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.538746 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1425.6964724 hartrees (-894638.793395724 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.209558	2.650235	-0.117722
2	6	1.820795	-0.511375	-1.701667
3	6	-1.934030	0.173621	-0.624816
4	6	-2.064930	1.697662	-0.976431
5	1	-0.142448	2.439328	-0.211851
6	6	-0.434649	-0.250363	-0.571850
7	6	0.415034	0.054277	-1.828702
8	6	-2.567017	-0.082538	0.803426
9	1	0.050619	0.217818	0.292138
10	1	-1.710885	1.807746	-2.008270
11	1	-1.363871	3.682314	-0.449244
12	1	-0.386516	-1.329733	-0.395449
13	6	-3.545655	2.127285	-0.969447
14	1	-4.095878	1.607320	-1.762717
15	1	-3.623628	3.194563	-1.204154
16	6	-4.200783	1.879981	0.392785
17	1	-5.249156	2.193072	0.381683
18	1	-3.716724	2.516371	1.140314
19	6	-4.056516	0.421888	0.897019
20	1	-2.011493	0.568656	1.487476
21	6	-2.441058	-1.511030	1.380369
22	1	-1.417119	-1.873137	1.269164

23	1	-2.601254	-1.461802	2.462658
24	6	-5.036537	-0.550960	0.393919
25	6	-4.835286	-2.006274	0.578854
26	1	-5.456366	-2.208319	1.476115
27	1	-5.380223	-2.541217	-0.209610
28	6	-3.404878	-2.538995	0.769874
29	1	-3.041920	-2.873004	-0.204209
30	1	-3.442424	-3.433914	1.397969
31	6	-2.633584	-0.644503	-1.737209
32	1	-3.729330	-0.644739	-1.658196
33	1	-2.412913	-0.228933	-2.724789
34	6	-6.340250	-0.129780	-0.167792
35	1	-6.155431	0.230607	-1.192535
36	1	-7.061365	-0.947026	-0.219396
37	1	-6.765388	0.726100	0.364667
38	6	-4.519197	0.450402	2.438694
39	1	-4.540272	-0.526142	2.919652
40	1	-3.774853	1.072344	2.942916
41	1	0.477559	1.133921	-1.992032
42	1	-0.066557	-0.373392	-2.717443
43	6	2.823897	0.295915	-1.317157
44	6	4.258857	-0.069408	-1.109071
45	1	4.479084	-1.108235	-1.362557
46	1	2.600682	1.344066	-1.119689
47	1	4.913779	0.584705	-1.695926
48	1	-1.450468	2.616187	0.949556
49	6	1.963096	-1.977458	-2.033670
50	1	2.934717	-2.391076	-1.760261
51	1	1.196876	-2.573466	-1.523044
52	1	1.820875	-2.139585	-3.110124
53	8	4.555466	0.133293	0.306715
54	8	5.889772	0.361564	2.378201
55	15	6.083785	0.177019	0.789209
56	8	6.992286	1.157475	0.146870
57	8	6.509707	-1.373232	0.615860
58	1	6.272647	1.200169	2.675569
59	1	7.470518	-1.481521	0.554429
60	1	-2.305208	-1.686431	-1.748299
61	1	-5.496784	0.926809	2.539754
