Supporting Information for

Is a 1,4-Alkyl Shift Involved in the Biosynthesis of Ledol and Viridiflorol?

Young J. Hong and Dean J. Tantillo*

Department of Chemistry, University of California—Davis, Davis, CA 95616, USA

**djtantillo@ucdavis.edu*

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Gaussian Full Reference

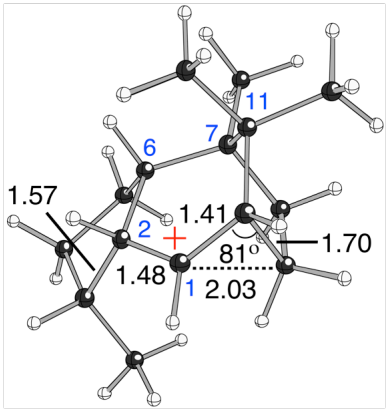
Gaussian 09, Revision D.01

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

Coordinates and Energies

Structures in Figure 1

C



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.4169016 hartrees (-367982.469923016 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.369290 (Hartree/Particle)

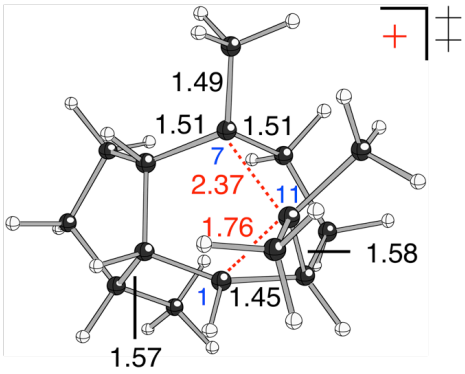
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.2996531 hartrees (-367908.895316781 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.067549	-0.383330	0.931668
2	6	0.864693	0.753420	-0.422916
3	6	-0.432839	0.961384	0.416791
4	6	-0.253272	-1.587295	0.683935
5	6	0.564592	-0.111949	-1.678622
6	6	0.464672	-1.571452	-1.215122
7	6	1.118559	-1.523681	0.352969
8	1	1.375002	-0.020657	-2.405635
9	6	1.454137	2.116201	-0.805351
10	1	2.361169	2.012194	-1.406413
11	1	1.699388	2.709723	0.081490
12	1	-0.347843	0.200613	-2.188835
13	1	-0.536243	-1.999970	-1.346132
14	1	1.139807	-2.299526	-1.671633
15	6	1.851207	-0.172662	0.397635
16	1	-0.707577	-2.568343	0.827512
17	1	1.705214	-2.424452	0.527481
18	1	0.737357	2.693823	-1.396493
19	1	-0.146434	1.548552	1.294216

20	1	-1.015740	-0.384678	2.040137
21	6	-2.597187	-0.379845	0.579193
22	6	3.232050	-0.333210	-0.276022
23	1	3.175801	-0.613507	-1.331025
24	1	3.801236	0.596826	-0.209383
25	1	3.813891	-1.103714	0.240604
26	6	2.099134	0.259658	1.859051
27	1	2.810105	-0.419413	2.339844
28	1	2.541408	1.259982	1.883456
29	1	1.197610	0.278089	2.475663
30	6	-1.615633	1.703384	-0.253289
31	1	-1.533155	2.786515	-0.133808
32	1	-1.660042	1.507093	-1.329789
33	6	-2.868179	1.136032	0.438603
34	1	-2.981760	1.587009	1.431812
35	1	-3.789128	1.339306	-0.115161
36	1	-3.159469	-0.795554	1.422022
37	6	-2.997964	-1.164972	-0.678775
38	1	-2.525322	-0.779473	-1.588597
39	1	-2.774685	-2.235113	-0.595066
40	1	-4.079116	-1.085427	-0.824760

TS (C-D2)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.3223816 hartrees (-367923.157677816 kcal/mol)
Imaginary Frequencies: 1 (-312.3124 1/cm)
Zero-point correction = 0.368638 (Hartree/Particle)

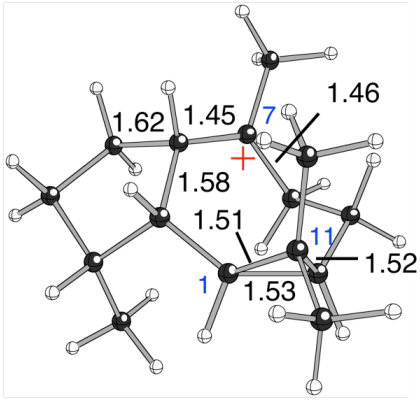
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.2007725 hartrees (-367846.846751475 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.947978	-0.522251	-0.964280
2	6	-0.412030	1.249585	0.170342
3	6	0.774113	0.986312	-0.727942
4	6	-0.306216	-1.277264	-0.572269
5	6	-0.360661	0.769411	1.604991
6	6	-0.774019	-0.724401	1.880469
7	6	-1.128360	-1.457373	0.610710
8	1	-0.973576	1.429166	2.222199
9	6	-1.110308	2.543736	-0.098163
10	1	-1.970886	2.735141	0.541943
11	1	-1.385349	2.660291	-1.150112
12	1	0.669152	0.900333	1.948909
13	1	0.043191	-1.246123	2.380483
14	1	-1.625474	-0.745036	2.565607
15	6	-1.885132	-0.518131	-0.408280
16	1	-0.526313	-2.046628	-1.306719
17	1	-1.576106	-2.443261	0.758086
18	1	-0.372497	3.335420	0.116821
19	1	0.563018	1.465232	-1.688692
20	1	1.010931	-0.652919	-2.049946
21	6	2.361170	-0.947842	-0.435260
22	6	-2.996480	0.298322	0.316626
23	1	-2.741881	0.713873	1.285626
24	1	-3.351339	1.100747	-0.333556
25	1	-3.825401	-0.403279	0.465518
26	6	-2.551925	-1.056738	-1.703169
27	1	-2.634052	-2.150186	-1.674044
28	1	-3.562282	-0.658234	-1.815443
29	1	-1.995730	-0.790093	-2.606667
30	6	2.163755	1.498653	-0.220497
31	1	2.422647	2.465828	-0.658408
32	1	2.175276	1.627844	0.865642
33	6	3.141730	0.376544	-0.637427
34	1	3.405861	0.493424	-1.694900
35	1	4.076281	0.402848	-0.068827
36	1	2.761940	-1.723186	-1.097014
37	6	2.455269	-1.482795	0.998987
38	1	2.186056	-0.735608	1.752028
39	1	1.826264	-2.366239	1.147994

40	1	3.486968	-1.783956	1.204445

D2



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.3992783 hartrees (-367971.411126033 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.367559 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.276005 hartrees (-367894.05589755 kcal/mol)

Coordinates (from last standard orientation):

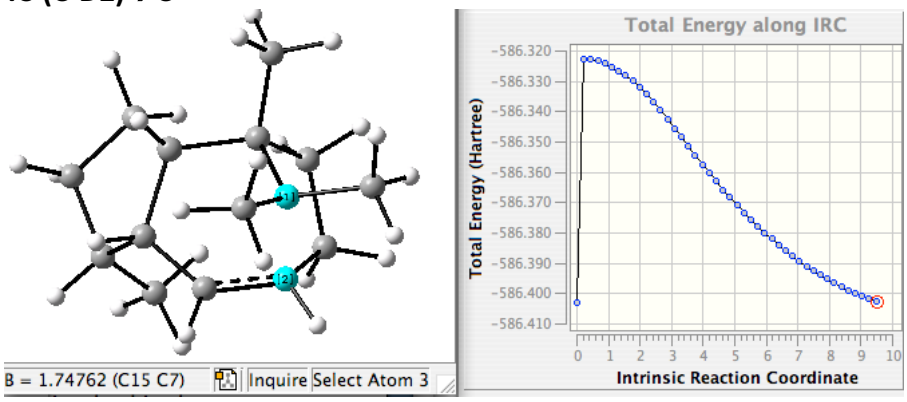
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.305650	-0.898611	-0.581167
2	6	0.931415	1.615154	0.076355
3	6	1.092878	0.456375	-0.783798
4	6	-1.030614	-0.970444	0.155310
5	6	0.416726	1.533870	1.437685
6	6	-1.172594	1.496152	1.232475
7	6	-1.720652	0.107609	1.001116
8	1	0.686350	2.410778	2.030165
9	6	1.288400	2.957169	-0.446052
10	1	0.527046	3.694080	-0.160301
11	1	1.453434	2.982659	-1.523324
12	1	0.693915	0.616295	1.956822
13	1	-1.569080	1.899525	2.168551
14	1	-1.465970	2.205627	0.452600
15	6	-2.333061	-0.356846	-0.314159
16	1	-1.162155	-1.963343	0.580555

17	1	-2.192047	-0.296914	1.894654
18	1	2.205448	3.286007	0.067766
19	1	1.015010	0.779863	-1.825513
20	1	0.081451	-1.180224	-1.619052
21	6	1.362277	-1.938985	-0.091907
22	6	-2.343269	0.570828	-1.519354
23	1	-1.441072	1.181371	-1.617337
24	1	-2.438186	-0.012040	-2.442304
25	1	-3.199912	1.252965	-1.476819
26	6	-3.585007	-1.219131	-0.221886
27	1	-3.562061	-1.872333	0.656105
28	1	-4.483504	-0.595752	-0.151661
29	1	-3.686528	-1.854755	-1.108984
30	6	2.653289	0.073131	-0.572387
31	1	3.269560	0.626816	-1.282924
32	1	2.992791	0.325530	0.436906
33	6	2.650426	-1.450242	-0.773993
34	1	2.629332	-1.677954	-1.845461
35	1	3.557120	-1.897570	-0.354694
36	1	1.075832	-2.922470	-0.482361
37	6	1.528742	-2.077454	1.429788
38	1	1.910196	-1.165308	1.902809
39	1	0.589589	-2.340600	1.923941
40	1	2.245801	-2.873705	1.651722

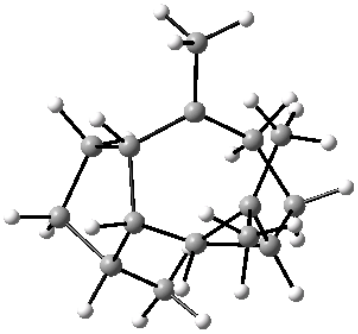
IRC Plots

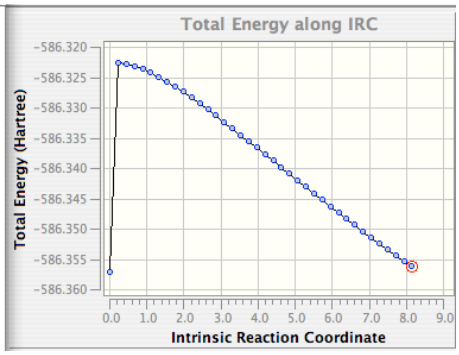
For structures in Figure 1

TS (C-D2)→C



TS (C-D2)→D2




Total Energy along IRC
Total Energy (Hartree)
-586.320
-586.325
-586.330
-586.335
-586.340
-586.345
-586.350
-586.355
-586.360
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
Intrinsic Reaction Coordinate