Supporting Information

Investigation of Stepwise and Concerted Pathways for (4+2) and (4+3) type Transannular Cycloaddition Reactions involving Furanoxonium Ion Intermediates using DFT Calculations. Implications for the Origin of Plumarellide and Rameswaralide and related Polycyclic Metabolites isolated from Corals.

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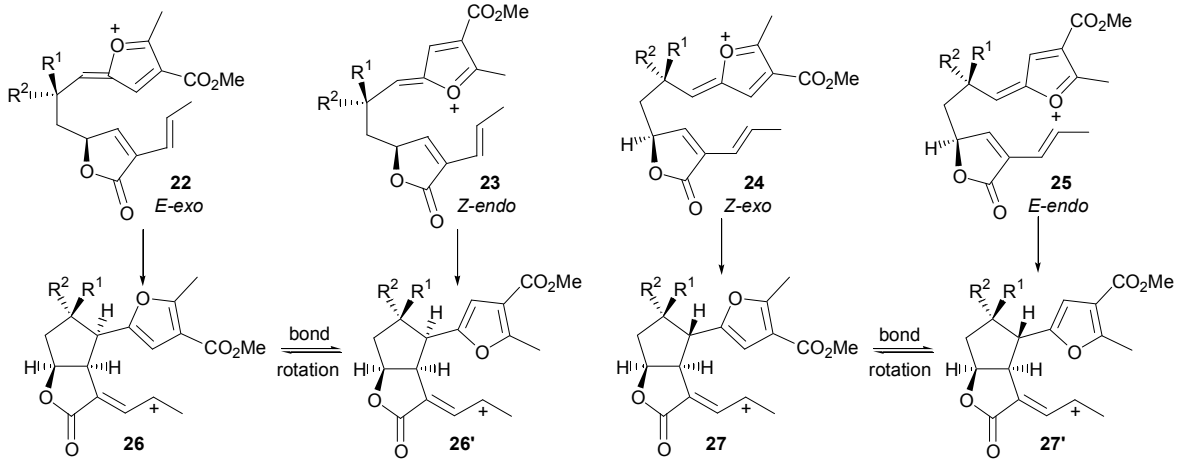
Computational Methodology

All calculations apart from gCP-D3 corrections were carried out using Gaussian 09 revB.01.[1] Default settings were used except that the UltraFine integration grid was used for calculations involving BMK and M06-2X. Initial structure searches were preformed using B3LYP/6-31G(d), and all resulting structures were further optimized at the B3LYP/6-31+G(d,p) level of theory.[2] Selected structures were also optimized using M06-2X/6-31+G(d,p).[3] BMK/6-311+G(d,p)[4] single-point energies were computed for all B3LYP/6-31+G(d,p) geometries, and combined with B3LYP/6-31+G(d,p) free energy corrections to obtain BMK/6-311+G(d,p)//B3LYP/6-31+G(d,p) free energies. Transition-state structures were all characterized by a single imaginary vibrational frequency, and intrinsic reaction coordinate (IRC) calculations were performed to confirm they connected to the appropriate energy minima. gCP-D3 corrections were applied to B3LYP/6-31G(d) energies using the gCP-D3 Webservice.[5] CYLView[6] was used to generate all the 3D-molecular structure figures.



Relative Transition State Energies for the Cyclisation Modes Depicted in Scheme 5 (R^1=Me, R^2=OH).

Method	Relative Energy (kcal/mol)			
	E-exo	*Z-endo*	*Z-exo*	*E-endo*
B3LYP-gCP-D3/6-31G(d)	5.9	3.8	0	0.3
B3LYP/6-31+G(d,p)	4.8	2.8	0	1.0
BMK/6-311+G(d,p)//B3LYP/6-31+G(d,p)	3.9	2.2	0.4	0
MO6-2X/6-31+G(d,p)	4.4	3.3	0	0.1

B3LYP/6-31+G(d,p) Optimized Transition State Structures:

(i) Transition State 22→26

```
Sum of electronic and zero-point Energies=          -1149.319273
Sum of electronic and thermal Energies=             -1149.295179
Sum of electronic and thermal Enthalpies=           -1149.294235
Sum of electronic and thermal Free Energies=        -1149.374095


H                     1.41206  -3.32429   0.43168
C                     1.98693  -2.41523   0.26718
C                     1.87663  -0.28427  -1.19514
C                    -0.31092   0.80414   0.39418
C                     0.9432    1.16292  -0.17109
C                     3.12632  -2.19009   0.9874
C                     1.49091  -1.54901  -0.73855
H                     2.87381   0.11836  -1.0562
H                     1.72212   1.29032   0.57867
C                     1.04801   2.14585  -1.34642
C                     1.15718  -0.04221  -2.51865
H                     1.79907  -0.30338  -3.36606
C                     0.61223   1.39221  -2.62104
H                     0.99714   1.9083   -3.50473
```

H	-0.47575	1.35418	-2.7217
C	-1.63313	0.78347	-0.02439
O	-0.25423	0.27143	1.6762
C	-1.50674	-0.05374	2.06223
C	-2.39856	0.24923	1.03531
C	-1.67415	-0.62045	3.41865
H	-2.73004	-0.80536	3.61238
H	-1.27423	0.0697	4.17039
H	-1.11814	-1.56154	3.50717
C	-3.86678	0.03521	1.07454
O	-4.44421	0.442	-0.06592
C	-5.88236	0.26862	-0.1475
H	-6.37173	0.84018	0.64312
H	-6.13532	-0.78843	-0.04875
H	-6.15859	0.64557	-1.13036
O	-4.4593	-0.44677	2.01984
C	3.66634	-3.10494	2.02114
H	4.6817	-3.42274	1.74502
H	3.04262	-3.98853	2.16947
H	3.7773	-2.57358	2.97662
C	0.25917	-1.932	-1.519
O	0.06851	-1.00441	-2.49572
H	-2.02293	1.10474	-0.97807
O	-0.46899	-2.87041	-1.3211
H	3.70273	-1.28489	0.79336
C	0.28399	3.45436	-1.10266
H	0.64252	3.94276	-0.19274
H	-0.79192	3.2932	-1.0145
H	0.45232	4.13325	-1.94644
O	2.45863	2.41365	-1.41595
H	2.61789	3.17504	-1.99096

(ii) Transition State 23→26'

Sum of electronic and zero-point Energies=	-1149.321722
Sum of electronic and thermal Energies=	-1149.297570
Sum of electronic and thermal Enthalpies=	-1149.296626
Sum of electronic and thermal Free Energies=	-1149.377228

H	-0.09855	-3.06347	1.52804
C	-0.65915	-2.7638	0.64489
C	-2.38498	-0.97226	-0.04427
C	-1.33854	0.34828	-1.20046
C	-0.4836	-3.4346	-0.53244
C	-1.54655	-1.67276	0.8235
C	-2.51424	1.33531	-1.21995
C	-3.17878	0.02848	0.78755
H	-4.21359	-0.30313	0.91406
C	-3.08648	1.44964	0.20256
H	-4.06011	1.94716	0.17783
H	-2.42756	2.04604	0.83892
C	0.42758	-4.59025	-0.71921
H	1.1267	-4.40025	-1.54461
H	-0.15257	-5.47281	-1.02469
H	0.99125	-4.8309	0.18424
C	-1.62016	-0.98967	2.16674
O	-2.55729	-0.01142	2.09711
O	-0.96535	-1.23981	3.14667

H	-1.06356	-3.1294	-1.4044
C	-2.10347	2.68579	-1.82438
H	-1.71629	2.55246	-2.83787
H	-1.3477	3.18475	-1.21381
H	-2.98046	3.34082	-1.87525
O	-3.46616	0.67367	-2.06908
H	-4.1878	1.28059	-2.28563
H	-2.84885	-1.41707	-0.91815
C	-0.05058	0.66067	-0.70751
O	0.0909	1.51163	0.37354
C	1.206	0.19752	-1.07237
C	2.13899	0.79958	-0.19834
C	1.40753	1.59379	0.68318
H	1.43026	-0.4693	-1.89246
C	3.61487	0.64524	-0.1974
O	4.35934	1.20295	0.58373
O	4.01342	-0.18928	-1.17164
C	5.44542	-0.40001	-1.2774
H	5.94783	0.54934	-1.47067
H	5.57127	-1.08465	-2.11405
H	5.82749	-0.83602	-0.35266
C	1.77859	2.4518	1.82837
H	2.86266	2.48465	1.92924
H	1.33905	2.05427	2.75184
H	1.38579	3.46525	1.68888
H	-1.28839	-0.26383	-2.09863

(iii) Transition State 24→27

Sum of electronic and zero-point Energies=	-1149.325446
Sum of electronic and thermal Energies=	-1149.301359
Sum of electronic and thermal Enthalpies=	-1149.300415
Sum of electronic and thermal Free Energies=	-1149.380003

H	-0.7435	3.46637	0.22692
C	-0.74703	2.50419	0.73522
C	-2.21454	0.40628	0.9024
C	0.15598	-0.86978	-0.30698
C	-1.21112	-0.80756	-0.60392
C	0.30751	2.14128	1.51854
C	-1.89584	1.69277	0.51308
H	-1.77364	-0.14781	1.72199
C	-2.24977	-1.90157	-0.40022
C	-3.60562	0.07578	0.40529
H	-4.32536	0.06053	1.23025
C	-3.64181	-1.23196	-0.41467
H	-4.3796	-1.93459	-0.01797
H	-3.94827	-0.98557	-1.43593
C	1.21793	-0.11101	-0.81431
O	0.67124	-1.77554	0.60554
C	2.00837	-1.6259	0.64435
C	2.39698	-0.59976	-0.22289
C	2.76422	-2.54227	1.52542
H	2.24751	-2.66362	2.48212
H	3.77699	-2.16898	1.6739
H	2.82861	-3.53426	1.05902
C	3.79317	-0.15608	-0.4636
O	3.83622	0.82964	-1.3725

C	5.158	1.32524	-1.71405
H	5.76129	0.51595	-2.12879
H	5.64606	1.72956	-0.82561
H	4.98638	2.10327	-2.45527
O	4.762	-0.63011	0.09581
C	1.51025	2.98042	1.76518
H	2.42718	2.41961	1.54255
H	1.57041	3.23868	2.83149
H	1.50262	3.90258	1.1802
C	-3.00607	2.17376	-0.38322
O	-3.95545	1.19697	-0.44443
H	1.14314	0.6698	-1.55799
O	-3.07231	3.22031	-0.97333
H	0.2634	1.19135	2.05117
H	-1.42053	-0.1653	-1.45523
C	-2.10897	-2.94945	-1.52243
H	-1.14618	-3.46067	-1.44957
H	-2.19979	-2.49666	-2.51378
H	-2.90849	-3.6925	-1.42405
O	-1.9987	-2.47879	0.8811
H	-2.49595	-3.30422	0.966

(iv) Transition State 25→27'-Ts

Sum of electronic and zero-point Energies=	-1149.326691
Sum of electronic and thermal Energies=	-1149.302596
Sum of electronic and thermal Enthalpies=	-1149.301652
Sum of electronic and thermal Free Energies=	-1149.381667

H	0.1813	0.06738	-4.74052
C	0.09802	0.60212	-3.79664
C	-1.59922	0.90392	-1.88603
C	0.16989	-0.79663	-0.24909
C	-1.18641	-0.7643	-0.61367
C	1.13993	1.35058	-3.34093
C	-1.15799	0.49197	-3.1325
H	-1.1106	1.6329	-1.25139
C	-2.30639	-0.34748	0.32896
C	-3.09995	0.70634	-1.81955
H	-3.62641	1.65568	-1.96586
C	-3.54371	-0.00429	-0.52825
H	-4.22608	0.61834	0.05707
H	-4.09197	-0.90983	-0.80431
C	0.95976	-0.17096	0.7144
O	0.97588	-1.68993	-0.95556
C	2.21182	-1.65382	-0.43187
C	2.25256	-0.71626	0.6072
C	3.21964	-2.57283	-1.0053
H	2.99435	-3.60482	-0.70656
H	4.21228	-2.31385	-0.63881
H	3.1894	-2.53787	-2.09906
C	3.44982	-0.3897	1.42322
O	3.16112	0.52056	2.36413
C	4.25781	0.90961	3.23183
H	5.06334	1.34826	2.6404
H	4.63081	0.03797	3.77231
H	3.83231	1.6409	3.91626
O	4.5452	-0.88721	1.24965
C	2.44928	1.48845	-4.03045

H	3.26872	1.19555	-3.35975
H	2.63485	2.54211	-4.27961
H	2.50507	0.8931	-4.9442
C	-2.30688	-0.22974	-3.78787
O	-3.39461	-0.12541	-2.97068
H	0.61958	0.57783	1.41285
O	-2.30217	-0.81859	-4.83671
H	1.01707	1.91852	-2.41825
H	-1.46994	-1.55586	-1.30325
C	-2.5983	-1.49217	1.31839
H	-1.73457	-1.67027	1.96299
H	-2.85277	-2.42011	0.79857
H	-3.45492	-1.21847	1.94473
O	-1.83533	0.8159	1.02031
H	-2.45105	1.03846	1.73294

Relative Transition State Energies for the Cyclisation Modes Depicted in Scheme 5 (R^1=OH, R^2=Me).

Method	Relative Energy (kcal/mol)			
	E-exo	*Z-endo*	*Z-exo*	*E-endo*
B3LYP-gCP-D3/6-31G(d)	0	2.9	4.6	6.1
B3LYP/6-31+G(d,p)	0	1.8	1.8	3.7
BMK/6-311+G(d,p)//B3LYP/6-31+G(d,p)	0	2.3	3.4	5.6
MO6-2X/6-31+G(d,p)	0	2.0	5.3	7.3

B3LYP/6-31+G(d,p) Optimized Transition State Structures:

(i) Transition State 22→26

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Sum of electronic and zero-point Energies=          -1149.327918
Sum of electronic and thermal Energies=             -1149.304057
Sum of electronic and thermal Enthalpies=           -1149.303113
Sum of electronic and thermal Free Energies=        -1149.381778
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H	0.48286	-3.01021	-1.31893
C	1.06977	-2.29754	-0.74319
C	2.52616	-0.21597	-1.13308
C	0.22174	0.80691	0.48612
C	1.24127	1.30726	-0.33982
C	1.08963	-2.36769	0.61881
C	1.74521	-1.30568	-1.49825
H	3.14574	-0.18952	-0.24361
H	2.05007	1.76467	0.2268
H	1.71086	-1.66387	1.17257
C	1.01382	1.96026	-1.69142
C	2.93258	0.50712	-2.40887
H	4.0145	0.49727	-2.57155
C	2.37014	1.93303	-2.42788
H	3.06857	2.60549	-1.91616
H	2.27654	2.28964	-3.45815
C	-1.07236	0.32177	0.29633
O	0.47349	0.83358	1.86151
C	-0.63873	0.43542	2.50549
C	-1.62548	0.10164	1.5732
C	-0.61051	0.45733	3.98558
H	0.31983	0.01851	4.35964
H	-1.47381	-0.07559	4.38267
H	-0.64792	1.49511	4.34136
C	-2.9901	-0.38522	1.90219

O	-3.71983	-0.56219	0.79291
C	-5.08159	-1.02566	0.98979
H	-5.63357	-0.30764	1.59867
H	-5.07625	-1.9993	1.48291
H	-5.504	-1.09636	-0.01054
O	-3.38001	-0.59528	3.03446
C	0.51062	3.4054	-1.49141
H	1.21305	4.00365	-0.90376
H	-0.46052	3.4026	-0.99135
H	0.39701	3.88628	-2.46867
C	0.3382	-3.35888	1.42807
H	1.02689	-3.9322	2.06303
H	-0.24136	-4.04968	0.81237
H	-0.34177	-2.84192	2.12175
C	1.59626	-1.28687	-2.99595
O	2.33228	-0.25358	-3.48176
O	0.96833	-2.05387	-3.67771
H	-1.55259	0.18279	-0.66037
O	0.02831	1.16687	-2.35153
H	-0.11335	1.49212	-3.25227

(ii) Transition State 23→26'

Sum of electronic and zero-point Energies=	-1149.324020
Sum of electronic and thermal Energies=	-1149.299946
Sum of electronic and thermal Enthalpies=	-1149.299002
Sum of electronic and thermal Free Energies=	-1149.378869

H	-2.13738	1.5166	0.40379
C	-1.35758	0.92162	-0.06736
C	0.41079	1.14686	-1.91183
C	1.97677	1.26786	0.60992
C	2.13619	1.53776	-0.76593
C	-1.08557	-0.33454	0.39202
C	-0.68598	1.53949	-1.15333
H	0.68022	0.10962	-2.07775
H	2.68106	0.73547	-1.25928
H	-0.34646	-0.94135	-0.13021
C	2.41732	2.90245	-1.38354
C	0.63236	2.19611	-2.98943
H	0.43941	1.80593	-3.99387
C	2.03767	2.7929	-2.87589
H	2.74786	2.13336	-3.38894
H	2.08519	3.7662	-3.37412
C	2.23677	0.10225	1.33251
O	1.54284	2.23512	1.49499
C	1.56576	1.71995	2.73858
C	1.99049	0.38955	2.68977
C	1.16621	2.61684	3.84457
H	1.17152	2.07279	4.78802
H	0.17036	3.03229	3.65281
H	1.86045	3.46354	3.90767
C	2.15853	-0.51112	3.85659
O	2.59409	-1.72244	3.47215
C	2.8233	-2.68269	4.53664
H	1.89506	-2.86645	5.08046
H	3.58158	-2.30208	5.22305
H	3.16878	-3.58505	4.03584

O	1.9281	-0.1907	5.00556
C	-1.77193	-0.97478	1.54414
H	-2.26503	-1.90176	1.22157
H	-2.51413	-0.31887	2.00375
H	-1.0405	-1.27675	2.30598
C	-1.11795	2.89675	-1.64436
O	-0.35999	3.21419	-2.72813
O	-2.00009	3.58542	-1.20464
H	2.60755	-0.83069	0.93053
C	3.91052	3.24752	-1.1974
H	4.5659	2.49454	-1.6454
H	4.11889	4.2066	-1.68293
H	4.14615	3.34258	-0.13505
O	1.59148	3.83648	-0.70104
H	1.61927	4.69311	-1.15046

(iii) Transition State 24→27

Sum of electronic and zero-point Energies=	-1149.323839
Sum of electronic and thermal Energies=	-1149.299740
Sum of electronic and thermal Enthalpies=	-1149.298796
Sum of electronic and thermal Free Energies=	-1149.378853

H	-1.95956	-3.94974	0.76568
C	-1.16203	-3.28674	0.43655
C	-0.78133	-1.4857	-1.37713
C	0.03477	-3.28721	1.08654
C	-1.46501	-2.49485	-0.70859
H	0.8381	-2.64894	0.7162
C	-2.32474	0.76874	-1.23972
C	-1.5523	-1.14892	-2.6406
H	-1.00473	-1.43839	-3.54368
C	-1.93075	0.33264	-2.66531
H	-1.06394	0.91401	-2.99669
H	-2.74136	0.51759	-3.37765
C	0.35452	-4.13443	2.26508
H	1.2006	-4.79587	2.03345
H	-0.4947	-4.74253	2.58319
H	0.68539	-3.51261	3.10768
C	-2.76105	-2.72388	-1.45049
O	-2.74226	-1.96723	-2.58049
O	-3.64911	-3.47592	-1.14995
H	0.29107	-1.3455	-1.32846
C	-0.02241	0.89314	-0.0095
C	-1.26537	0.27712	-0.25422
C	0.7668	0.93518	1.13376
O	0.63724	1.57194	-1.02242
C	1.80399	2.04583	-0.52691
C	1.92454	1.67523	0.81272
C	2.66052	2.83075	-1.44247
H	2.13327	3.73488	-1.77017
H	2.8968	2.24682	-2.33937
H	3.58088	3.11455	-0.93351
C	3.05934	2.02314	1.70594
O	2.86961	1.52963	2.93873
C	3.90942	1.82429	3.90871
H	4.00786	2.90424	4.03059
H	4.85943	1.40301	3.57548

H	3.57621	1.35635	4.83299
O	4.02723	2.66848	1.35629
H	0.51936	0.51035	2.09634
H	-1.69595	-0.16594	0.6399
C	-2.52966	2.2923	-1.1284
H	-1.63746	2.84554	-1.43067
H	-2.79788	2.56585	-0.1051
H	-3.35521	2.5857	-1.78451
O	-3.49469	0.08527	-0.78309
H	-4.20546	0.15182	-1.43673

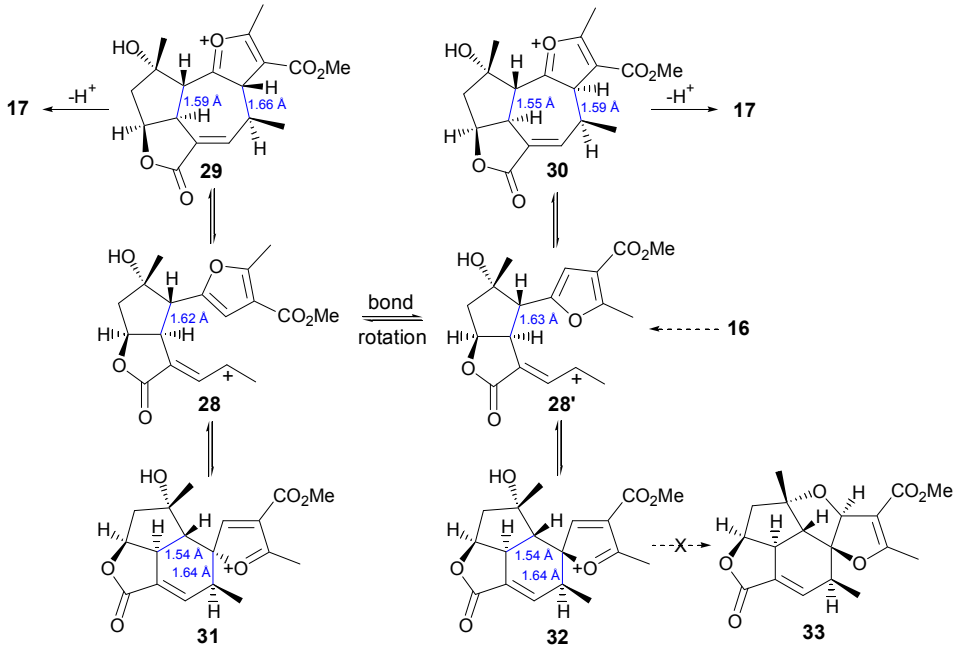
(iv) Transition State 25→27'

Sum of electronic and zero-point Energies= -1149.320685
Sum of electronic and thermal Energies= -1149.296585
Sum of electronic and thermal Enthalpies= -1149.295641
Sum of electronic and thermal Free Energies= -1149.375821

H	-4.78581	0.18958	1.68649
C	-3.93544	0.49406	1.07995
C	-2.60812	2.65954	0.57845
C	-3.28526	-0.4243	0.31238
C	-3.60191	1.87574	1.15982
H	-2.43627	-0.10269	-0.2919
C	-1.07312	3.60114	2.62422
C	-2.87271	4.10874	0.96263
H	-3.13645	4.72325	0.09601
C	-1.68917	4.70255	1.73338
H	-0.94143	5.06508	1.01956
H	-2.01066	5.56508	2.32594
C	-3.65264	-1.86056	0.22331
H	-3.88576	-2.12577	-0.81714
H	-4.50719	-2.11232	0.85446
H	-2.79926	-2.49132	0.50729
C	-4.45586	2.7853	2.01005
O	-4.03351	4.06395	1.82176
O	-5.38827	2.47383	2.70173
H	-2.12437	2.40825	-0.35655
C	0.21894	2.2153	0.84878
C	-0.8452	2.36404	1.76276
C	1.91799	2.25625	-0.63429
C	1.51579	0.93417	-0.42896
H	-1.1521	1.43591	2.23766
C	0.20808	4.06332	3.34429
H	0.97429	4.41	2.64725
H	0.61799	3.24945	3.94713
H	-0.04182	4.89149	4.01495
O	-2.01799	3.12741	3.58736
H	-2.35434	3.86112	4.1219
O	0.49456	0.9091	0.44836
C	1.08853	3.0621	0.17022
C	3.01943	2.69672	-1.52868
O	3.68521	1.9414	-2.20836
O	3.1725	4.02811	-1.48403
C	4.22818	4.57631	-2.3173
H	4.03378	4.34201	-3.36528
H	4.19731	5.65025	-2.14435
H	5.19112	4.15887	-2.01838
C	2.00217	-0.36285	-0.94956

H	2.428	-0.95853	-0.13272
H	1.17465	-0.93901	-1.37785
H	2.76755	-0.19358	-1.70597
H	1.13947	4.13814	0.24176

Geometries for structures relating to Scheme 6.



B3LYP/6-31+G(d,p) Optimized Structures:

(i) 28

Sum of electronic and zero-point Energies=	-1149.333985
Sum of electronic and thermal Energies=	-1149.309868
Sum of electronic and thermal Enthalpies=	-1149.308924
Sum of electronic and thermal Free Energies=	-1149.388767

H	-1.33429	-3.63086	-0.3102
C	-0.67012	-2.81592	-0.59179
C	-0.47245	-0.81232	-2.20388
C	0.0528	0.54615	-0.06209
C	-0.84063	0.4243	-1.21796
C	0.45782	-2.5384	0.16765
C	-1.03059	-2.05439	-1.69334
H	0.60826	-0.78108	-2.35322
C	-0.94641	1.58735	-2.26048
C	-1.29284	-0.51141	-3.48531
H	-0.73099	-0.72825	-4.39549
C	-1.78006	0.9427	-3.39104
H	-1.65645	1.48891	-4.32953
H	-2.84667	0.94656	-3.14411
C	-0.19003	0.46959	1.29504
O	1.39175	0.795	-0.25932
C	1.99221	0.91702	0.95767
C	1.04832	0.7203	1.95356
C	3.43743	1.24125	0.96244
H	3.99787	0.52946	0.34648
H	3.81474	1.22721	1.98446
H	3.59989	2.238	0.53457
C	1.30306	0.78208	3.41187

O	0.17595	0.55479	4.10976
C	0.29872	0.61973	5.5537
H	0.62754	1.61595	5.85479
H	1.01755	-0.12375	5.90289
H	-0.69886	0.4079	5.934
O	2.38924	1.00309	3.91121
C	0.82965	-3.25304	1.40388
H	1.74319	-3.83894	1.21259
H	0.04769	-3.92145	1.76753
H	1.11185	-2.53779	2.18764
C	-2.28292	-2.36351	-2.47539
O	-2.41471	-1.43654	-3.45183
H	-1.14679	0.29922	1.76832
O	-3.04984	-3.26899	-2.2706
H	1.16744	-1.80329	-0.20461
H	-1.8473	0.25865	-0.82158
C	-1.55633	2.85937	-1.67708
H	-0.915	3.27072	-0.89308
H	-2.55068	2.67343	-1.25969
H	-1.6657	3.6166	-2.46168
O	0.39031	1.80394	-2.71533
H	0.4164	2.58068	-3.29141

(ii) Transition State 28→29

Sum of electronic and zero-point Energies=	-1149.323467
Sum of electronic and thermal Energies=	-1149.300883
Sum of electronic and thermal Enthalpies=	-1149.299939
Sum of electronic and thermal Free Energies=	-1149.374335

H	-1.45494	-3.14363	0.27376
C	-0.79798	-2.42559	-0.2147
C	-0.53289	-0.81969	-2.14029
C	0.08764	0.62059	-0.17041
C	-0.81376	0.53439	-1.32316
C	0.37529	-1.95937	0.49155
C	-1.14582	-1.95196	-1.43634
H	0.53773	-0.88287	-2.34112
C	-0.84391	1.58501	-2.46706
C	-1.38478	-0.63124	-3.41715
H	-0.87673	-1.00479	-4.30847
C	-1.74901	0.86292	-3.5038
H	-1.59333	1.2751	-4.50396
H	-2.80793	0.9891	-3.25624
C	-0.04226	0.00956	1.10869
O	1.28264	1.19942	-0.26508
C	1.9255	1.14046	0.97895
C	1.12963	0.46434	1.85353
C	3.23454	1.82384	1.05583
H	3.94972	1.36114	0.36601
H	3.61931	1.75607	2.07324
H	3.13273	2.87594	0.76777
C	1.39345	0.30136	3.30404
O	0.32497	-0.22162	3.93171
C	0.4452	-0.37185	5.3721
H	0.6123	0.60312	5.83274
H	1.27639	-1.03765	5.6107
H	-0.50345	-0.79726	5.69377

O	2.42973	0.61999	3.85077
C	0.76329	-2.67243	1.75612
H	1.64065	-2.23689	2.23341
H	1.0259	-3.70062	1.4678
H	-0.05787	-2.73028	2.47411
C	-2.42353	-2.3021	-2.14656
O	-2.55725	-1.46249	-3.21497
O	-3.23172	-3.13696	-1.83816
H	-1.82997	0.4558	-0.92751
C	-1.35817	2.95805	-2.04141
H	-0.67201	3.42697	-1.33058
H	-2.35123	2.89125	-1.58649
H	-1.44204	3.61457	-2.91446
O	0.49777	1.65123	-2.95604
H	0.56681	2.34433	-3.62742
H	1.21558	-1.66611	-0.13534
H	-0.99619	-0.20916	1.5701

(iii) 29

Sum of electronic and zero-point Energies=	-1149.327819
Sum of electronic and thermal Energies=	-1149.305231
Sum of electronic and thermal Enthalpies=	-1149.304287
Sum of electronic and thermal Free Energies=	-1149.378541

H	-1.52828	-3.0812	0.36354
C	-0.89396	-2.35355	-0.14011
C	-0.5656	-0.83595	-2.10583
C	0.11389	0.60761	-0.21322
C	-0.79398	0.55191	-1.36067
C	0.30181	-1.81483	0.59813
C	-1.22716	-1.93707	-1.36994
H	0.49838	-0.96814	-2.31051
C	-0.78221	1.57178	-2.52523
C	-1.39834	-0.66099	-3.39884
H	-0.88335	-1.07467	-4.26863
C	-1.70927	0.84218	-3.53974
H	-1.5394	1.21437	-4.55339
H	-2.76349	1.0137	-3.29888
C	0.06684	-0.23052	1.01816
O	1.16911	1.35722	-0.21663
C	1.868	1.23814	1.03688
C	1.2074	0.35611	1.8074
C	3.0492	2.11457	1.16311
H	3.80294	1.84563	0.41414
H	3.47985	1.99271	2.15732
H	2.77393	3.16205	0.99972
C	1.51695	0.13381	3.24729
O	0.43548	-0.31003	3.9045
C	0.59489	-0.50517	5.33732
H	0.85966	0.44135	5.81106
H	1.37559	-1.24367	5.52703
H	-0.37386	-0.85866	5.68444
O	2.59375	0.37279	3.75264
C	0.64394	-2.67155	1.82103
H	1.58652	-2.37337	2.28313
H	0.75691	-3.70801	1.48829
H	-0.14697	-2.63845	2.57418

C	-2.4877	-2.28634	-2.10223
O	-2.59261	-1.45105	-3.18866
O	-3.32197	-3.09981	-1.81077
H	-1.81063	0.50786	-0.95497
C	-1.25304	2.97554	-2.15259
H	-0.55504	3.44978	-1.4569
H	-2.25018	2.95762	-1.70156
H	-1.31249	3.60245	-3.04891
O	0.56682	1.57487	-3.0025
H	0.65567	2.20782	-3.72879
H	1.17005	-1.79722	-0.07122
H	-0.89805	-0.19164	1.53139

(iv) Transition State 28→31

Sum of electronic and zero-point Energies= -1149.319394
Sum of electronic and thermal Energies= -1149.296723
Sum of electronic and thermal Enthalpies= -1149.295779
Sum of electronic and thermal Free Energies= -1149.371141

H	-1.6811	3.24226	-0.12064
C	-1.58161	2.28589	0.3885
C	-2.3225	-0.04769	0.68945
C	0.18576	0.02936	0.22922
C	-1.13732	-0.50642	-0.2262
C	-0.33563	1.92264	1.02955
C	-2.56881	1.35854	0.33213
H	-2.09284	-0.26082	1.7362
C	-1.43322	-2.01736	-0.43504
C	-3.53786	-0.82503	0.15498
H	-4.2078	-1.17457	0.94184
C	-2.96709	-1.97023	-0.71229
H	-3.43082	-2.93488	-0.48816
H	-3.16216	-1.75159	-1.76705
C	1.2963	0.2867	-0.62037
O	0.73353	-0.54644	1.40486
C	2.05422	-0.56902	1.30864
C	2.45972	-0.05351	0.05406
C	2.82903	-1.08897	2.45366
H	2.16326	-1.38678	3.2642
H	3.5465	-0.33722	2.79931
H	3.43319	-1.94314	2.12781
C	3.87326	0.06851	-0.38809
O	3.9579	0.59832	-1.61268
C	5.29943	0.75602	-2.15262
H	5.78581	-0.21813	-2.2232
H	5.88236	1.41593	-1.5082
H	5.1574	1.19525	-3.1378
O	4.81124	-0.27892	0.30123
C	0.81733	2.88248	1.01059
H	1.75053	2.4288	1.35265
H	0.58441	3.68897	1.72023
H	0.9711	3.33652	0.0286
C	-3.82348	1.41941	-0.48689
O	-4.28809	0.14102	-0.6349
O	-4.33815	2.38425	-0.98692
H	-1.28954	-0.04236	-1.20833
C	-0.63161	-2.67988	-1.55314

H	0.43388	-2.70499	-1.30631
H	-0.76338	-2.15785	-2.5063
H	-0.96517	-3.7133	-1.69802
O	-1.17016	-2.63641	0.82868
H	-1.39997	-3.57529	0.78246
H	-0.45333	1.38699	1.96924
H	1.23199	0.70292	-1.61762

(v) 31

Sum of electronic and zero-point Energies=	-1149.327362
Sum of electronic and thermal Energies=	-1149.304702
Sum of electronic and thermal Enthalpies=	-1149.303758
Sum of electronic and thermal Free Energies=	-1149.379325

H	-2.4129	3.22892	-0.45432
C	-2.16212	2.31323	0.07488
C	-2.52326	-0.00319	0.70994
C	-0.14261	0.65635	0.33542
C	-1.26128	-0.30613	-0.12418
C	-0.76661	2.14057	0.64093
C	-3.02442	1.29346	0.19466
H	-2.30687	-0.03965	1.78118
C	-1.21713	-1.84898	-0.21395
C	-3.54875	-1.05253	0.26389
H	-4.13629	-1.4622	1.08719
C	-2.73354	-2.135	-0.48669
H	-2.99466	-3.14986	-0.17216
H	-2.94577	-2.06402	-1.55834
C	1.05953	0.6267	-0.52403
O	0.40861	0.19517	1.63243
C	1.67043	-0.07105	1.52086
C	2.13795	0.18765	0.18024
C	2.39831	-0.57235	2.69766
H	1.7589	-0.57041	3.58011
H	3.30693	0.01806	2.85434
H	2.7487	-1.59088	2.48583
C	3.54548	-0.01321	-0.27199
O	3.69074	0.30262	-1.55816
C	5.02968	0.15237	-2.11388
H	5.3479	-0.88769	-2.02954
H	5.72423	0.80063	-1.57772
H	4.9365	0.45215	-3.15529
O	4.41636	-0.41557	0.47193
C	0.17728	3.28842	0.262
H	1.16565	3.18131	0.71791
H	-0.24529	4.23059	0.62185
H	0.29986	3.37682	-0.82239
C	-4.29452	1.03415	-0.55211
O	-4.47416	-0.33405	-0.59528
O	-5.02572	1.80925	-1.10617
H	-1.47107	0.03029	-1.14699
C	-0.31175	-2.43402	-1.29886
H	0.74399	-2.27274	-1.06375
H	-0.52764	-2.00043	-2.28076
H	-0.47005	-3.51497	-1.37948
O	-0.82589	-2.31933	1.08414
H	-0.94418	-3.27898	1.12623

H	-0.85674	2.11381	1.73369
H	1.05621	0.90475	-1.57127

(vi) 28'

```
 Sum of electronic and zero-point Energies=          -1149.333564
 Sum of electronic and thermal Energies=             -1149.309364
 Sum of electronic and thermal Enthalpies=           -1149.308419
 Sum of electronic and thermal Free Energies=        -1149.388648


 H                  -4.06956   1.49399   1.33571
 C                  -3.31648   0.7552    1.06857
 C                  -2.20415  -0.38229  -0.96034
 C                   0.04754   0.62641  -0.09753
 C                  -0.86384   0.50333  -1.24089
 C                  -2.48765   0.21592   2.03717
 C                  -3.20463   0.41211  -0.27379
 H                  -1.88183  -1.30545  -0.4798
 C                  -0.34894  -0.21162  -2.53014
 C                  -2.77583  -0.57662  -2.38637
 H                  -3.27459  -1.54096  -2.5037
 C                  -1.63179  -0.34204  -3.38373
 H                  -1.53878  -1.15628  -4.10675
 H                  -1.82696   0.57763  -3.94395
 C                   0.82863  -0.24104   0.63329
 O                   0.26929   1.91548   0.36008
 C                   1.19578   1.86882   1.35086
 C                   1.5653    0.5476    1.5629
 C                   1.61229   3.16045   1.94637
 H                   2.13847   3.76854   1.2004
 H                   2.27891   2.9793    2.78895
 H                   0.73976   3.73499   2.27613
 C                   2.55216   0.08003   2.56431
 O                   2.72037  -1.25211   2.49621
 C                   3.68307  -1.81817   3.42073
 H                   3.37224  -1.62676   4.44953
 H                   4.66772  -1.37975   3.2489
 H                   3.68943  -2.88548   3.20726
 O                   3.13005   0.80697   3.34979
 C                  -2.44554   0.64914   3.44492
 H                  -2.62576  -0.20934   4.10837
 H                  -3.15026   1.45011   3.67301
 H                  -1.42292   0.97922   3.68929
 C                  -4.12696   0.99062  -1.3179
 O                  -3.80047   0.45024  -2.51695
 H                   0.89692  -1.30937   0.49399
 O                  -4.99901   1.80025  -1.1359
 H                  -1.8228   -0.59897   1.75747
 H                  -1.17756   1.51177  -1.52752
 C                   0.78891   0.53764  -3.21741
 H                   1.67      0.57694  -2.57161
 H                   0.49467   1.55861  -3.47837
 H                   1.06613   0.02687  -4.14657
 O                   0.07094  -1.50687  -2.08208
 H                   0.51932  -1.97323  -2.80133
```

(vii) Transition State 28'→30

```
 Sum of electronic and zero-point Energies=          -1149.311691
 Sum of electronic and thermal Energies=             -1149.289165
 Sum of electronic and thermal Enthalpies=           -1149.288220
 Sum of electronic and thermal Free Energies=        -1149.363135
```

H	-0.86577	2.63098	-2.11132
C	-0.85715	2.1486	-1.13445
C	-2.09652	0.72057	0.49837
C	-0.09522	-0.63904	-0.14307
C	-1.55664	-0.64918	-0.01342
C	0.43821	2.0551	-0.44002
C	-2.00948	1.66825	-0.6297
C	-2.29718	-1.65983	0.92711
C	-3.5995	0.44749	0.68526
H	-4.04408	1.02907	1.49514
C	-3.74249	-1.07718	0.87443
H	-4.2866	-1.33093	1.78825
H	-4.30008	-1.4967	0.03143
C	0.89107	0.23513	0.39756
O	0.4588	-1.44387	-1.03859
C	1.86017	-1.27331	-1.01708
C	2.15781	-0.29098	-0.12837
C	2.62636	-2.17539	-1.902
H	2.40959	-3.2222	-1.66171
H	3.69199	-1.98498	-1.77477
H	2.34978	-2.01191	-2.95003
C	3.52726	0.11082	0.27447
O	3.48727	1.03122	1.25655
C	4.77502	1.45897	1.77865
H	5.37161	1.90604	0.98165
H	5.30566	0.60296	2.19846
H	4.54049	2.1893	2.55059
O	4.54469	-0.34311	-0.20656
C	1.63676	2.48696	-1.24028
H	1.46027	3.53038	-1.53794
H	1.75554	1.90638	-2.15934
H	2.55876	2.46301	-0.66216
C	-3.35856	1.6972	-1.28956
O	-4.20691	0.90928	-0.55439
O	-3.67948	2.26307	-2.30004
C	-2.19672	-3.11939	0.49919
H	-1.1655	-3.47704	0.56437
H	-2.55754	-3.26295	-0.52361
H	-2.81332	-3.743	1.15624
O	-1.70059	-1.44509	2.20968
H	-2.0882	-2.05004	2.85811
H	-1.95069	-0.84712	-1.02034
H	-1.59628	1.00741	1.42521
H	0.80926	0.5822	1.42002
H	0.4081	2.46286	0.56805

(viii) 30

Sum of electronic and zero-point Energies=	-1149.327649
Sum of electronic and thermal Energies=	-1149.305074
Sum of electronic and thermal Enthalpies=	-1149.304130
Sum of electronic and thermal Free Energies=	-1149.378549

H	-0.83845	3.34463	-0.93937
C	-0.71654	2.39689	-0.41553
C	-1.92399	0.54791	0.84284
C	0.00157	-0.6854	-0.04689

C	-1.46745	-0.61063	-0.07186
C	0.66567	1.79009	-0.54759
C	-1.80279	1.87382	0.16523
C	-2.38941	-1.8003	0.30667
C	-3.44152	0.32999	1.03216
H	-3.74042	0.39836	2.07967
C	-3.75221	-1.05584	0.425
H	-4.46026	-1.6329	1.0258
H	-4.1958	-0.92178	-0.56767
C	0.91303	0.447	0.2696
O	0.65765	-1.75143	-0.3405
C	2.08424	-1.5012	-0.24467
C	2.2598	-0.21692	0.112
C	2.92655	-2.6782	-0.52854
H	2.69332	-3.49444	0.16426
H	3.97443	-2.39572	-0.42362
H	2.74971	-3.03978	-1.54795
C	3.59057	0.39466	0.38261
O	3.45598	1.61606	0.9214
C	4.69421	2.30181	1.26488
H	5.30018	2.44012	0.36828
H	5.24732	1.71483	1.99954
H	4.38236	3.25732	1.68135
O	4.64664	-0.15612	0.15435
C	1.01491	1.62084	-2.04207
H	0.9005	2.57784	-2.55805
H	0.35373	0.90291	-2.54043
H	2.04923	1.29417	-2.17798
C	-3.19302	2.40116	-0.04183
O	-4.08418	1.42237	0.33766
O	-3.53517	3.44708	-0.52308
C	-2.41181	-2.9712	-0.67135
H	-1.44159	-3.47301	-0.70522
H	-2.67893	-2.64436	-1.68127
H	-3.16217	-3.7048	-0.35734
O	-1.90491	-2.19844	1.59717
H	-2.42956	-2.93925	1.93262
H	-1.70559	-0.32992	-1.11381
H	-1.41409	0.49139	1.80761
H	0.73953	0.70137	1.3289
H	1.38871	2.489	-0.11295

(ix) Transition State 28'→32

Sum of electronic and zero-point Energies=	-1149.321596
Sum of electronic and thermal Energies=	-1149.298856
Sum of electronic and thermal Enthalpies=	-1149.297912
Sum of electronic and thermal Free Energies=	-1149.373227

H	-1.61185	3.33411	-1.35258
C	-1.66504	2.48192	-0.6776
C	-2.49456	0.2104	-0.21548
C	0.04587	0.21698	-0.17825
C	-1.16788	-0.37466	-0.81774
C	-0.60793	2.25684	0.28294
C	-2.63275	1.54377	-0.81785
H	-2.4752	0.15597	0.87526
C	-1.45049	-1.89944	-0.80037

C	-3.59959	-0.64803	-0.85101
H	-4.43546	-0.84531	-0.17789
C	-2.9065	-1.93387	-1.35584
H	-3.4246	-2.84067	-1.03223
H	-2.90117	-1.93306	-2.45034
O	1.11052	0.47181	-1.07801
C	0.65519	-0.14403	1.04997
C	2.03308	-0.02335	0.90712
C	2.26679	0.35825	-0.43245
C	0.5953	3.14156	0.28264
H	1.43238	2.71929	0.84499
H	0.32411	4.07499	0.79764
H	0.91968	3.40168	-0.72773
C	-3.66855	1.45624	-1.89928
O	-4.12124	0.16453	-1.94131
O	-4.03426	2.32147	-2.64945
H	-1.12429	-0.08036	-1.87264
C	-0.46606	-2.74695	-1.60093
H	0.53305	-2.70486	-1.15712
H	-0.40589	-2.41317	-2.64127
H	-0.78526	-3.79507	-1.60986
O	-1.43186	-2.25795	0.59002
H	-1.60101	-3.20573	0.68677
H	-0.93883	1.91866	1.26116
C	3.51326	0.62687	-1.18068
H	4.15315	1.31549	-0.62152
H	3.28905	1.02246	-2.17208
H	4.08972	-0.30125	-1.27611
C	3.10397	-0.25219	1.91234
O	4.28557	-0.13627	1.65412
O	2.59558	-0.59253	3.10082
C	3.55817	-0.85566	4.15851
H	4.15303	0.03909	4.34901
H	4.21143	-1.67959	3.86692
H	2.95838	-1.11969	5.02696
H	0.12301	-0.44868	1.94042

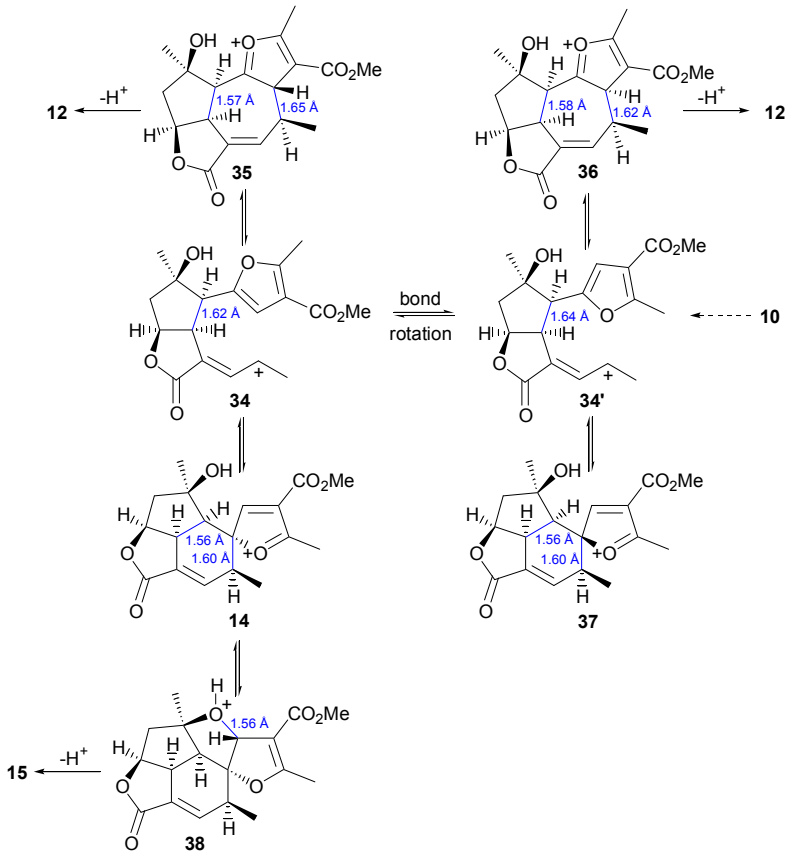
(x) 32

Sum of electronic and zero-point Energies=	-1149.330534
Sum of electronic and thermal Energies=	-1149.308020
Sum of electronic and thermal Enthalpies=	-1149.307076
Sum of electronic and thermal Free Energies=	-1149.381631

H	-1.77967	3.40636	-1.39652
C	-1.7847	2.50172	-0.79438
C	-2.51525	0.2745	-0.20132
C	-0.05223	0.68203	-0.09129
C	-1.14529	-0.20429	-0.72679
C	-0.61906	2.20331	0.13175
C	-2.74779	1.57273	-0.87699
H	-2.54732	0.2923	0.89186
C	-1.23933	-1.73751	-0.64711
C	-3.51798	-0.70865	-0.81302
H	-4.3398	-0.96669	-0.14278
C	-2.67929	-1.94307	-1.23288
H	-3.11077	-2.88183	-0.87389
H	-2.63922	-1.99952	-2.32527

O	1.0827	0.75145	-1.03985
C	0.60028	0.15281	1.12493
C	1.93673	-0.00926	0.90897
C	2.18128	0.37621	-0.45429
C	0.48328	3.26438	0.08566
H	1.31146	3.03813	0.76409
H	0.06217	4.22219	0.40344
H	0.87918	3.39299	-0.9251
C	-3.80282	1.36104	-1.91701
O	-4.09875	0.01038	-1.93473
O	-4.28805	2.14694	-2.68409
H	-1.10825	0.04395	-1.7933
C	-0.17098	-2.52366	-1.40473
H	0.81237	-2.40019	-0.94081
H	-0.11247	-2.20973	-2.45137
H	-0.40666	-3.59353	-1.39624
O	-1.20167	-2.0427	0.75837
H	-1.30946	-2.99497	0.89339
H	-1.01378	2.15817	1.15486
C	3.4363	0.39294	-1.22544
H	4.16809	1.03091	-0.71584
H	3.26404	0.73789	-2.24492
H	3.88159	-0.60869	-1.21855
C	2.99487	-0.49668	1.84107
O	4.15179	-0.62955	1.49617
O	2.49956	-0.74929	3.05078
C	3.44553	-1.23056	4.04885
H	4.22263	-0.48183	4.20949
H	3.8927	-2.16633	3.71049
H	2.85244	-1.38033	4.94824
H	0.0716	-0.05449	2.04609

Geometries for structures relating to Scheme 7.



B3LYP/6-31+G(d,p) Optimized Structures:

(i) 34

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 Sum of electronic and zero-point Energies=          -1149.337158
 Sum of electronic and thermal Energies=             -1149.313476
 Sum of electronic and thermal Enthalpies=           -1149.312532
 Sum of electronic and thermal Free Energies=        -1149.390350

 H                     0.59767  -3.00269  -1.72215
 C                     1.07858  -2.27771  -1.06819
 C                     2.47273  -0.10819  -1.07448
 C                     0.41204   0.53433   0.47809
 C                     1.47937   0.99856  -0.42525
 C                     0.87627  -2.33472   0.30798
 C                     1.82826  -1.28615  -1.66481
 H                     3.20124  -0.37555  -0.30293
 H                     2.13758   1.63346   0.17552
 H                     1.49943  -1.71736   0.95042
 C                     1.04974   1.81122  -1.67704
 C                     3.09744   0.61808  -2.30878
 H                     4.18381   0.70379  -2.2567
 C                     2.38587   1.97104  -2.42905
 H                     2.98722   2.75226  -1.95116
 H                     2.25218   2.25563  -3.47681
 C                    -0.85617   0.0034    0.32683
 O                     0.63052   0.77252   1.82058
 C                    -0.49332   0.42901   2.51414
 C                    -1.44117  -0.05061   1.62759
 C                    -0.46902   0.64717   3.97913
 H                     0.36453   0.10399   4.43877
 H                    -1.40995   0.31336   4.41531
```

H	-0.32547	1.71145	4.20002
C	-2.80518	-0.50701	1.9857
O	-3.48699	-0.89906	0.89496
C	-4.85141	-1.33617	1.12247
H	-5.43541	-0.52238	1.55596
H	-4.863	-2.19406	1.79726
H	-5.23131	-1.60689	0.1391
O	-3.24707	-0.52785	3.11814
C	0.35084	3.13032	-1.35774
H	0.98376	3.77614	-0.74131
H	-0.59096	2.95276	-0.83267
H	0.12751	3.67034	-2.28389
C	0.00297	-3.31464	0.98342
H	0.63969	-4.03929	1.51621
H	-0.65025	-3.85329	0.29522
H	-0.59081	-2.82604	1.76626
C	2.04224	-1.27643	-3.15205
O	2.80701	-0.20689	-3.46482
O	1.63321	-2.08671	-3.94281
H	-1.32984	-0.24347	-0.61061
O	0.17739	0.91751	-2.38861
H	-0.04058	1.28344	-3.2583

(ii) Transition State 34→35

Sum of electronic and zero-point Energies=	-1149.331777
Sum of electronic and thermal Energies=	-1149.309372
Sum of electronic and thermal Enthalpies=	-1149.308427
Sum of electronic and thermal Free Energies=	-1149.382270

H	3.4171	1.28461	-0.92884
C	2.91255	2.09541	-0.40538
C	1.14738	2.64054	1.36698
C	3.21481	4.1007	1.97236
C	2.00393	3.41825	2.45898
C	3.42641	3.43324	-0.54415
C	1.90608	1.76962	0.43716
H	0.53282	3.37088	0.83076
H	1.35547	4.19585	2.87391
C	2.21016	2.33871	3.57256
C	0.29998	1.61859	2.1946
H	-0.77506	1.78552	2.11051
C	0.80493	1.70416	3.64106
H	0.1404	2.3471	4.22874
H	0.81361	0.72015	4.11917
C	4.40371	3.68638	1.32939
O	3.23522	5.43646	2.11159
C	4.47096	5.92993	1.68836
C	5.22568	4.88611	1.24085
C	4.67222	7.38794	1.83731
H	5.67667	7.64938	1.50509
H	4.54198	7.68654	2.88351
H	3.93696	7.94132	1.24184
C	6.63537	4.97538	0.78851
O	7.13417	3.75596	0.51995
C	8.52877	3.71627	0.11435
H	9.15597	4.13207	0.90455
H	8.66704	4.29003	-0.80371

H	8.74916	2.66236	-0.04414
O	7.25628	6.01431	0.68802
C	4.49158	3.69931	-1.56597
H	4.00966	3.5951	-2.54971
H	5.30865	2.97687	-1.51582
H	4.8865	4.71401	-1.50766
C	1.47938	0.34663	0.63579
O	0.55618	0.31221	1.63096
O	1.86784	-0.62398	0.04057
H	4.7904	2.67985	1.38791
H	2.70883	4.24253	-0.42348
C	2.70877	2.90403	4.90025
H	2.03663	3.67737	5.28474
H	2.76138	2.10787	5.65038
H	3.71108	3.32804	4.79171
O	3.1579	1.42243	3.01021
H	3.23171	0.63521	3.5689

(iii) 35

Sum of electronic and zero-point Energies=	-1149.336378
Sum of electronic and thermal Energies=	-1149.313819
Sum of electronic and thermal Enthalpies=	-1149.312875
Sum of electronic and thermal Free Energies=	-1149.387120

H	3.51506	-1.46465	0.96905
C	3.81703	-0.44351	1.19835
C	3.01009	1.9811	1.357
C	4.61726	1.63518	3.34268
C	3.47154	2.37933	2.80063
C	5.18089	-0.23285	1.78007
C	2.89956	0.5188	1.05499
H	3.65048	2.48895	0.62798
H	3.75555	3.43656	2.79958
C	2.15178	2.26948	3.66807
C	1.52225	2.46344	1.27652
H	1.37509	3.26486	0.55029
C	1.12193	2.88788	2.69703
H	1.15466	3.97943	2.78205
H	0.10077	2.57358	2.93365
C	4.9731	0.203	3.36062
O	5.57152	2.34449	3.8754
C	6.58512	1.48883	4.42684
C	6.2333	0.21407	4.17975
C	7.68101	2.19619	5.11955
H	8.36997	1.46149	5.53704
H	7.28796	2.83511	5.9177
H	8.22764	2.83477	4.41606
C	6.94702	-0.96278	4.74848
O	6.15161	-2.04127	4.76979
C	6.72196	-3.24322	5.35778
H	6.9837	-3.05506	6.40019
H	7.61233	-3.54179	4.80198
H	5.93906	-3.99493	5.28083
O	8.0841	-0.92339	5.17106
C	6.07354	-1.46838	1.63617
H	6.14288	-1.71256	0.57143
H	5.65568	-2.33132	2.15926

H	7.08795	-1.28845	1.99816
C	1.49157	0.21095	0.65935
O	0.74329	1.34364	0.81393
O	1.03277	-0.83767	0.29124
H	4.17233	-0.4293	3.75185
H	5.68183	0.61439	1.29622
O	1.94422	0.8662	3.83872
H	1.05414	0.70038	4.18151
C	2.2412	2.98111	5.01609
H	1.26845	2.94352	5.5178
H	2.96989	2.49581	5.67194
H	2.5138	4.03451	4.90025

(iv) Transition State 34→14

Sum of electronic and zero-point Energies=	-1149.331060
Sum of electronic and thermal Energies=	-1149.308549
Sum of electronic and thermal Enthalpies=	-1149.307605
Sum of electronic and thermal Free Energies=	-1149.382241

C	0.86035	-2.31671	-1.00807
C	2.38261	-0.36748	-1.36547
C	0.51747	0.10498	0.4424
C	1.515	0.67401	-0.5332
C	0.91	-2.07004	0.40309
C	1.59123	-1.52506	-1.82721
H	3.25146	-0.66294	-0.76839
H	2.21844	1.25686	0.06933
C	0.94341	1.6227	-1.63249
C	2.77113	0.35411	-2.68619
H	3.84715	0.39429	-2.86283
C	2.13042	1.74414	-2.61066
H	2.86195	2.45771	-2.21436
H	1.82588	2.10562	-3.59747
C	-0.88643	-0.02474	0.37279
O	-0.12464	0.87542	-2.23944
O	0.81843	0.40055	1.78776
C	-0.31472	0.40164	2.5028
C	-1.40557	0.13957	1.66085
C	-0.21395	0.6723	3.95368
H	0.80207	0.49351	4.31024
H	-0.94035	0.07242	4.50546
H	-0.47303	1.72187	4.14579
C	-2.81887	0.05175	2.1103
O	-3.63511	-0.25558	1.0955
C	-5.0492	-0.35353	1.41702
H	-5.40748	0.60109	1.80571
H	-5.20778	-1.13768	2.15917
H	-5.53648	-0.60072	0.4761
O	-3.16365	0.23924	3.26039
C	0.43836	2.96408	-1.10573
H	1.22976	3.51447	-0.58727
H	-0.40166	2.82223	-0.41957
H	0.08773	3.58801	-1.93456
C	0.05839	-2.82399	1.36575
H	0.601	-3.74317	1.63267
H	-0.9108	-3.10532	0.94905
H	-0.08748	-2.2837	2.30647

C	1.52764	-1.52385	-3.31985
O	2.21049	-0.43406	-3.76664
H	-0.39741	1.30039	-3.06527
O	0.97459	-2.31643	-4.03656
H	1.87247	-1.75805	0.8037
H	-1.43595	-0.2274	-0.5341
H	0.1631	-3.04249	-1.4207

(v) 14

Sum of electronic and zero-point Energies=	-1149.344556
Sum of electronic and thermal Energies=	-1149.322120
Sum of electronic and thermal Enthalpies=	-1149.321175
Sum of electronic and thermal Free Energies=	-1149.395627

H	0.85684	-3.15741	-1.29913
C	1.3604	-2.26176	-0.94438
C	2.53361	-0.12702	-1.24729
C	0.65083	-0.39515	0.51784
C	1.52363	0.61468	-0.32001
C	1.28623	-1.86572	0.51208
C	1.94918	-1.39395	-1.77075
H	3.47765	-0.30422	-0.72078
H	2.08448	1.19512	0.41818
H	2.29795	-1.71561	0.91225
C	0.78457	1.62572	-1.25379
C	2.72038	0.73644	-2.51917
H	3.76291	0.98065	-2.73171
C	1.8707	1.9913	-2.29179
H	2.51331	2.77986	-1.88329
H	1.44015	2.37503	-3.22182
C	-0.80931	-0.46603	0.26329
O	0.68478	0.0938	1.9219
C	-0.5261	0.25677	2.37131
C	-1.50054	-0.07641	1.37411
C	-0.70761	0.7185	3.7592
H	0.25312	0.84603	4.25795
H	-1.34084	0.00737	4.30183
H	-1.27432	1.65719	3.75789
C	-2.97446	-0.02645	1.59665
O	-3.64314	-0.44964	0.52546
C	-5.09587	-0.45163	0.62867
H	-5.45301	0.5623	0.81479
H	-5.40587	-1.1113	1.44048
H	-5.44494	-0.82142	-0.33288
O	-3.46174	0.35825	2.64085
C	0.20609	2.84992	-0.54123
H	0.9806	3.397	0.00524
H	-0.58455	2.56587	0.15929
H	-0.23408	3.53896	-1.26999
C	0.55635	-2.8837	1.39229
H	1.13756	-3.80983	1.41167
H	-0.43865	-3.12812	1.00811
H	0.46029	-2.54419	2.42734
C	1.88234	-1.3311	-3.25788
O	2.25644	-0.06612	-3.63251
O	1.51682	-2.17113	-4.03679
H	-1.23026	-0.85026	-0.65342

O	-0.26491	0.87076	-1.88542
H	-0.65701	1.38666	-2.60464

(iv) Transition State 14→38

Sum of electronic and zero-point Energies= -1149.335474
Sum of electronic and thermal Energies= -1149.313996
Sum of electronic and thermal Enthalpies= -1149.313052
Sum of electronic and thermal Free Energies= -1149.385589

H	0.78278	-3.41803	-0.88745
C	1.29802	-2.47523	-0.71902
C	2.36476	-0.38638	-1.5171
C	0.84676	-0.44405	0.58052
C	1.65192	0.44395	-0.41338
C	1.41222	-1.90643	0.6804
C	1.71408	-1.7158	-1.73627
H	3.42616	-0.50605	-1.27506
H	2.38649	1.00606	0.16925
C	0.71353	1.43361	-1.1594
C	2.15543	0.32932	-2.87787
H	3.08944	0.62684	-3.35787
C	1.25615	1.54686	-2.59914
H	1.8526	2.4624	-2.66799
H	0.4529	1.6308	-3.33636
C	-0.63599	-0.41239	0.25419
O	-0.56545	0.66592	-1.19411
O	0.91095	0.18637	1.90368
C	-0.32258	0.48317	2.31947
C	-1.29373	0.17396	1.37894
C	-0.44186	1.05622	3.67972
H	0.19771	1.94202	3.7641
H	-0.07703	0.32889	4.41437
H	-1.47789	1.30798	3.90089
C	-2.75224	0.36524	1.52121
O	-3.36056	0.16766	0.32951
C	-4.81235	0.26808	0.33035
H	-5.11526	1.27402	0.6251
H	-5.23209	-0.46159	1.02433
H	-5.11327	0.05042	-0.69262
O	-3.32467	0.676	2.54438
C	0.47924	2.78076	-0.48447
H	1.42636	3.32075	-0.4003
H	0.0603	2.67485	0.51878
H	-0.19731	3.40213	-1.08216
C	0.72604	-2.77495	1.7412
H	1.22045	-3.7494	1.78123
H	-0.32993	-2.95319	1.51234
H	0.79757	-2.32934	2.73597
C	1.35743	-1.86074	-3.17469
O	1.53726	-0.63124	-3.76408
O	0.91204	-2.81107	-3.75954
H	2.47009	-1.7926	0.95615
H	-1.08988	-1.20892	-0.32261
H	-1.35659	1.23312	-1.24457

(vii) 38

```
Sum of electronic and zero-point Energies=          -1149.336345
Sum of electronic and thermal Energies=             -1149.314906
Sum of electronic and thermal Enthalpies=           -1149.313962
Sum of electronic and thermal Free Energies=        -1149.385585

H                     1.0558   -3.48696  -0.89597
C                     1.46698  -2.49656  -0.71485
C                     2.34493  -0.31149  -1.50913
C                     0.89658  -0.51581   0.63286
C                     1.59287   0.44228  -0.38002
C                     1.53308  -1.93874   0.6911
C                     1.8186   -1.69725  -1.72562
H                     3.42053  -0.33312  -1.30266
H                     2.27559   1.08868   0.17746
C                     0.52338   1.30875  -1.09497
C                     2.02682   0.37863  -2.86188
H                     2.89334   0.85977  -3.31819
C                     0.90249   1.3997   -2.58291
H                     1.25306   2.41554  -2.78802
H                     0.04281   1.22487  -3.23626
C                    -0.60262  -0.51373   0.28555
O                    -0.69461   0.36258  -0.98758
O                     0.95465   0.0738    1.96979
C                    -0.28992   0.38736   2.38815
C                    -1.2506    0.11502   1.45482
C                    -0.39564   0.96882   3.74796
H                     0.27829   1.82664   3.84376
H                    -0.07827   0.22518   4.48805
H                    -1.42286   1.26469   3.95945
C                    -2.66601   0.49022   1.49114
O                    -3.14576   0.52793   0.19819
C                    -4.56113   0.84599   0.05195
H                    -4.75576   1.85017   0.43081
H                    -5.15653   0.11884   0.60494
H                    -4.76299   0.78106  -1.01575
O                    -3.33295   0.78157   2.45619
C                     0.16442   2.64336  -0.46095
H                     1.04097   3.29647  -0.50598
H                    -0.13347   2.54818   0.58432
H                    -0.63797   3.13982  -1.01729
C                     0.88443  -2.86073   1.73152
H                     1.41408  -3.81716   1.74737
H                    -0.16486  -3.07403   1.49982
H                     0.93986  -2.43443   2.73529
C                     1.52969  -1.89377  -3.17165
O                     1.61534  -0.65896  -3.77649
O                     1.20867  -2.88993  -3.76082
H                     2.5834   -1.78292   0.97747
H                    -1.02125  -1.45099  -0.07819
H                    -1.58745   0.79069  -0.96277
```

(viii) 34'

```
Sum of electronic and zero-point Energies=          -1149.330611
Sum of electronic and thermal Energies=             -1149.306818
Sum of electronic and thermal Enthalpies=           -1149.305874
Sum of electronic and thermal Free Energies=        -1149.384120
```

C	1.72131	-0.03474	-1.75789
C	-0.04751	0.6887	0.1162
C	0.99084	1.10892	-0.84491
C	0.8184	-0.99453	-2.38547
H	2.47077	-0.51033	-1.11923
H	1.80976	1.50176	-0.23453
C	0.6418	2.19038	-1.90593
C	2.31887	0.75574	-2.96098
H	3.39341	0.60917	-3.08318
C	1.92249	2.22233	-2.7651
H	2.72045	2.75346	-2.23375
H	1.77526	2.72626	-3.72467
O	-0.43527	1.62239	-2.66013
O	-1.36673	0.56782	-0.27645
C	-2.12674	0.3388	0.82299
C	-1.30652	0.28245	1.94319
C	-3.59175	0.23944	0.61868
H	-3.99684	1.21788	0.33242
H	-4.07294	-0.083	1.54158
H	-3.8251	-0.45659	-0.19372
C	-1.75904	0.05662	3.3363
O	-0.72949	0.12347	4.19757
C	-1.05938	-0.06263	5.59781
H	-1.49125	-1.05314	5.75221
H	-1.77066	0.70095	5.9174
H	-0.11458	0.03827	6.12864
O	-2.91141	-0.1654	3.65491
C	0.25387	3.54008	-1.30486
H	1.04886	3.93676	-0.66557
H	-0.6627	3.45118	-0.71669
H	0.07474	4.26782	-2.10328
C	-0.85176	-3.10979	0.27745
H	-0.3548	-3.82139	0.94753
H	-1.55555	-3.62391	-0.37964
H	-1.42557	-2.43907	0.94616
C	0.78357	-0.74232	-3.8675
O	1.69303	0.2164	-4.15379
H	-0.61668	2.16389	-3.44198
O	0.10454	-1.31689	-4.67806
C	0.1211	-2.27976	-0.44955
H	0.95972	-1.89166	0.12321
C	0.04048	-1.97906	-1.80125
H	-0.68256	-2.48706	-2.43653
C	0.01922	0.51281	1.48316
H	0.90739	0.57121	2.09704

(ix) Transition State 34'→36

Sum of electronic and zero-point Energies=	-1149.317763
Sum of electronic and thermal Energies=	-1149.295420
Sum of electronic and thermal Enthalpies=	-1149.294475
Sum of electronic and thermal Free Energies=	-1149.368137

H	-0.16093	-2.83894	-1.08188
C	0.53157	-2.06115	-0.76587
C	1.9853	-0.11902	-1.42596
C	0.0401	0.69259	0.07004
C	1.10899	1.11576	-0.8648

C	0.76548	-1.84955	0.65142
C	1.169	-1.3182	-1.69898
H	2.80919	-0.30307	-0.73113
H	1.81321	1.72322	-0.28413
C	0.71546	1.91041	-2.14795
C	2.46362	0.33489	-2.83357
H	3.53973	0.21643	-2.9769
C	1.99559	1.78161	-3.00082
H	2.7724	2.45717	-2.62308
H	1.82339	2.03702	-4.05053
C	0.11545	0.03167	1.32619
O	-0.34089	1.15689	-2.75142
O	-1.23162	0.79084	-0.28935
C	-2.0589	0.35234	0.75291
C	-1.27199	-0.07806	1.77541
C	-3.51211	0.48186	0.51371
H	-3.77109	1.52211	0.28765
H	-4.05575	0.15135	1.39846
H	-3.81238	-0.12696	-0.34681
C	-1.75999	-0.50186	3.10955
O	-0.73767	-0.66208	3.97195
C	-1.10732	-1.0113	5.33347
H	-1.64698	-1.95985	5.34308
H	-1.73649	-0.22734	5.758
H	-0.16544	-1.08942	5.87315
O	-2.93006	-0.65901	3.39144
C	0.28948	3.35383	-1.87984
H	1.072	3.91533	-1.35923
H	-0.62657	3.38412	-1.28443
H	0.08877	3.86476	-2.82711
C	0.1696	-2.82793	1.61982
H	0.68144	-3.78736	1.4535
H	-0.89551	-2.99341	1.43814
H	0.32859	-2.54151	2.65921
C	1.05002	-1.49832	-3.18031
O	1.8194	-0.54828	-3.78265
H	-0.46743	1.44312	-3.66704
O	0.41709	-2.33081	-3.77341
H	0.94331	0.15537	2.01234
H	1.78097	-1.53927	0.88776

(x) 36

Sum of electronic and zero-point Energies=	-1149.324986
Sum of electronic and thermal Energies=	-1149.302575
Sum of electronic and thermal Enthalpies=	-1149.301631
Sum of electronic and thermal Free Energies=	-1149.375399

H	0.00884	-2.88623	-0.81791
C	0.61049	-2.0091	-0.58894
C	1.98442	-0.06484	-1.40856
C	0.03996	0.7174	0.01491
C	1.10934	1.15936	-0.91747
C	0.82286	-1.6043	0.85393
C	1.18	-1.31645	-1.58142
H	2.84398	-0.2051	-0.7463
H	1.76202	1.82652	-0.33351
C	0.66731	1.90228	-2.22185

C	2.4104	0.29437	-2.86172
H	3.48535	0.19068	-3.02528
C	1.91252	1.71886	-3.11315
H	2.69203	2.43059	-2.81561
H	1.69549	1.89873	-4.17038
C	0.12384	-0.19061	1.20335
O	-0.42482	1.12834	-2.73181
O	-1.1713	1.09873	-0.17562
C	-2.0516	0.55319	0.82788
C	-1.31371	-0.19046	1.66699
C	-3.46207	0.96613	0.69192
H	-3.55462	2.05707	0.72223
H	-4.04411	0.52063	1.49922
H	-3.86387	0.62	-0.26715
C	-1.85883	-0.73905	2.94222
O	-0.91343	-0.77249	3.89277
C	-1.34452	-1.23147	5.20494
H	-1.72227	-2.25284	5.13463
H	-2.12681	-0.574	5.58708
H	-0.45403	-1.18293	5.82839
O	-3.01901	-1.05524	3.09647
C	0.26635	3.36366	-2.01897
H	1.0747	3.94362	-1.56145
H	-0.62706	3.44328	-1.39486
H	0.03702	3.8213	-2.9865
C	0.44024	-2.7204	1.82899
H	1.02597	-3.61002	1.57799
H	-0.61719	-2.98944	1.74528
H	0.6565	-2.45155	2.86351
C	1.05132	-1.60826	-3.0396
O	1.76196	-0.66139	-3.72848
H	-0.54261	1.30249	-3.67608
O	0.44426	-2.49688	-3.57501
H	0.76459	0.27942	1.96504
H	1.89231	-1.39825	0.98239

(xi) Transition State 34'→37

Sum of electronic and zero-point Energies=	-1149.323267
Sum of electronic and thermal Energies=	-1149.300575
Sum of electronic and thermal Enthalpies=	-1149.299631
Sum of electronic and thermal Free Energies=	-1149.374753

C	2.24413	-1.03999	-0.88776
C	4.35859	-1.37383	0.38196
C	2.52207	-0.01316	1.70923
C	3.98484	-0.35294	1.5476
C	1.50123	-1.39997	0.28272
C	3.59784	-1.09035	-0.84535
H	4.2187	-2.39589	0.74837
H	4.27239	-0.84508	2.48224
C	4.99551	0.82105	1.33028
C	5.82718	-1.06197	-0.01224
H	6.48523	-1.93186	0.02225
C	6.2787	0.06358	0.92468
H	6.75355	-0.37446	1.81053
H	7.01614	0.71826	0.45024
O	4.49497	1.55424	0.20678

C	0.77719	0.75076	2.95959
C	0.99897	1.61465	1.87004
C	5.16889	1.72752	2.54803
H	5.49421	1.16308	3.42791
H	4.23419	2.24341	2.78448
H	5.92632	2.49141	2.34408
C	0.02844	-1.18084	0.34349
H	-0.43092	-1.71924	-0.49786
H	-0.23546	-0.12561	0.20189
H	-0.42006	-1.54661	1.26706
C	4.53339	-0.62435	-1.91361
O	5.79387	-0.62964	-1.39647
H	5.19165	2.12548	-0.14691
O	4.26471	-0.29697	-3.03951
H	1.89148	-2.22629	0.87063
H	1.73817	-0.61878	-1.75396
O	2.03267	1.18117	1.15082
C	-0.29592	0.92234	3.97087
C	1.74751	-0.24608	2.86799
H	1.88285	-1.07125	3.55545
O	-0.28089	-0.0674	4.87297
O	-1.07724	1.85254	3.95836
C	-1.28331	0.00942	5.92301
H	-1.10805	-0.86511	6.54619
H	-1.15167	0.93036	6.4933
H	-2.28234	-0.01433	5.48469
C	0.32281	2.855	1.42921
H	0.59447	3.67643	2.10439
H	0.62592	3.11569	0.41407
H	-0.76193	2.74934	1.50501

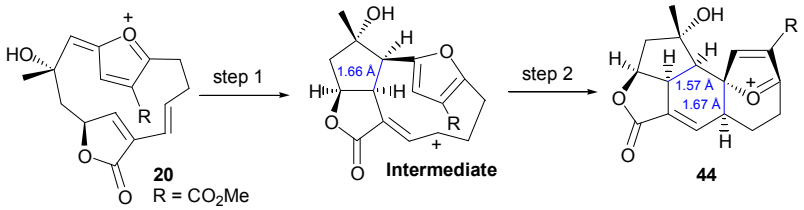
(xii) 37

Sum of electronic and zero-point Energies=	-1149.336574
Sum of electronic and thermal Energies=	-1149.313997
Sum of electronic and thermal Enthalpies=	-1149.313053
Sum of electronic and thermal Free Energies=	-1149.387874

H	-1.935	-1.8146	-2.03237
C	-1.29798	-2.2658	-1.27671
C	0.75665	-3.34741	-0.49349
C	-0.32003	-1.40638	0.86049
C	1.00456	-2.20971	0.54625
C	-1.60757	-2.08897	0.1893
C	-0.15063	-2.87886	-1.57619
H	0.37858	-4.24746	0.00374
H	1.30704	-2.67476	1.49054
H	-1.65142	-3.0732	0.67656
C	2.27406	-1.45786	0.00903
C	2.09999	-3.59081	-1.22651
H	2.43762	-4.62828	-1.19019
C	3.09888	-2.63127	-0.57004
H	3.61535	-3.15785	0.24128
H	3.86732	-2.28814	-1.2703
C	-0.53514	0.1914	2.55372
C	-0.4226	0.83798	1.26704
C	3.03614	-0.66197	1.0716
H	3.31424	-1.28821	1.92579

H	2.4454	0.18339	1.43551
H	3.95703	-0.25324	0.64359
C	-2.92377	-1.35219	0.45467
H	-3.73845	-1.91578	-0.00824
H	-2.93068	-0.35284	0.00934
H	-3.15133	-1.2665	1.52069
C	0.5646	-2.93199	-2.88047
O	1.86665	-3.28485	-2.62218
O	0.15701	-2.67868	-3.98259
O	1.84005	-0.59873	-1.05039
H	2.57353	-0.44102	-1.66114
O	-0.28799	-0.02998	0.31866
C	-0.48469	-1.14457	2.31019
H	-0.55655	-1.92846	3.05543
C	-0.69161	0.91591	3.84863
O	-0.72143	2.12759	3.91553
O	-0.78862	0.0671	4.8711
C	-0.94766	0.66231	6.1919
H	-1.86601	1.25049	6.22123
H	-0.99986	-0.18195	6.87572
H	-0.08934	1.29785	6.41424
C	-0.44901	2.26885	0.9194
H	-1.38244	2.7164	1.2806
H	0.34537	2.78898	1.4677
H	-0.33632	2.40758	-0.15559

Geometries for structures relating to Figure 5.



B3LYP/6-31+G(d,p) Optimized Structures:

(i) 20

Sum of electronic and zero-point Energies=	-1148.115457
Sum of electronic and thermal Energies=	-1148.093380
Sum of electronic and thermal Enthalpies=	-1148.092436
Sum of electronic and thermal Free Energies=	-1148.165995

C	0.62386000	-2.21063600	-0.61874600
C	-1.71917000	-1.70209000	-1.56533700
C	-0.09193700	1.16960400	-0.60239100
C	-1.32016500	1.17760500	-1.18445100
C	1.46310900	-1.91850700	-1.63483200
C	-0.82311400	-2.08205200	-0.62817000
C	-1.53546000	-2.07035500	0.69144300
O	-1.08301300	-2.28686600	1.78821000
O	-2.83257100	-1.69000800	0.47884100
C	-3.04220100	-1.40185700	-0.91674200
H	-3.82844500	-2.07851600	-1.27656800
C	-3.55368700	0.03871700	-1.11154800
H	-3.70396000	0.19003300	-2.18663300
H	-4.53883000	0.11676400	-0.63758700
C	-2.70932400	1.26120500	-0.59308600
C	2.90266400	-1.59000700	-1.40262000

H	3.56190800	-2.01517200	-2.16556800
H	3.23258200	-1.94111500	-0.42212000
C	0.46460500	1.22272000	0.70648200
O	0.97528400	0.89476500	-1.48208600
C	3.16872300	-0.00118300	-1.47266400
H	3.18074000	0.30895400	-2.52042300
H	4.12964600	0.19925700	-0.99846300
C	2.07690500	0.69272000	-0.77368300
C	1.81820300	0.95111900	0.59899700
H	-0.07389100	1.42222600	1.62104400
H	-1.31201300	1.14624600	-2.27248600
C	-2.78436800	1.43731900	0.92528700
H	-3.83341400	1.53332700	1.22186900
H	-2.27135200	2.35447400	1.22704600
H	-2.38534300	0.57819100	1.46787900
O	-3.21112200	2.43316100	-1.25510200
H	-4.12112400	2.60292900	-0.96860200
H	-1.56118800	-1.60306400	-2.63382000
H	1.07081900	-1.73748500	-2.63514800
H	1.03624100	-2.40710600	0.37001600
C	2.83164000	0.83269400	1.68628200
O	3.95306300	0.40799500	1.49020700
O	2.33653300	1.23446000	2.85483800
C	3.22890400	1.14458500	4.00199300
H	4.11102200	1.76309900	3.83019600
H	3.52394600	0.10572400	4.15693600
H	2.64529600	1.51612700	4.84130800

(ii) Transition State 20→Intermediate

Sum of electronic and zero-point Energies= -1148.103994
Sum of electronic and thermal Energies= -1148.083043
Sum of electronic and thermal Enthalpies= -1148.082099
Sum of electronic and thermal Free Energies= -1148.153161

C	0.83290900	-2.10292900	-0.06337700
C	-1.31990000	-1.14834400	-1.09471400
C	0.18331300	1.09893300	-0.26327000
C	-1.09646600	0.78394300	-0.82474400
C	1.73259200	-1.82008100	-1.06768400
C	-0.55282600	-1.87445900	-0.15701000
C	-1.45223800	-2.17589000	1.01231900
O	-1.13715500	-2.66879200	2.06456300
O	-2.70990500	-1.77306300	0.69340900
C	-2.77898400	-1.26383000	-0.66456700
H	-3.32553400	-2.00391200	-1.25851000
C	-3.45599500	0.09627700	-0.70586300
H	-3.72037600	0.31590000	-1.74685200
H	-4.38146100	0.10272700	-0.12550800
C	-2.47183500	1.18949500	-0.23394600
C	3.16192500	-1.53364500	-0.83383200
H	3.80169700	-2.04693200	-1.56001800
H	3.46837800	-1.80933800	0.17740400
C	0.73115300	1.43565400	0.96156800
O	1.23253800	0.78502800	-1.12653400
C	3.47332000	0.04408400	-1.05613500
H	3.52483800	0.23342500	-2.13080400
H	4.43514600	0.25022100	-0.58691600

C	2.39343000	0.83535200	-0.43994400
C	2.13946300	1.29027100	0.84731900
H	0.20568000	1.72758600	1.85684900
H	-1.10062600	0.97041200	-1.89850300
C	-2.51979100	1.41357100	1.27960500
H	-3.55198900	1.62487900	1.56968300
H	-1.91046200	2.27415100	1.57314000
H	-2.18973300	0.53886300	1.84454200
O	-2.85726200	2.37734000	-0.92819100
H	-2.50999200	3.15989100	-0.47608600
H	-1.07207000	-1.17407100	-2.15215400
H	1.36005300	-1.66739000	-2.07956000
H	1.19369900	-2.41720100	0.91497900
C	3.17319300	1.46360200	1.89954700
O	4.33080700	1.11652600	1.75716300
O	2.66414300	2.02487700	3.00039400
C	3.58941900	2.23856100	4.10017600
H	2.99532000	2.70570700	4.88287400
H	3.99620500	1.28249100	4.43393100
H	4.40036100	2.89414000	3.77874100

(iii) Intermediate

Sum of electronic and zero-point Energies=	-1148.105054
Sum of electronic and thermal Energies=	-1148.083716
Sum of electronic and thermal Enthalpies=	-1148.082772
Sum of electronic and thermal Free Energies=	-1148.155165

C	0.39832500	-2.44535400	-0.50689400
C	-1.59209700	-1.10937500	-1.49498600
C	-0.06313500	0.82597400	-0.55238900
C	-1.38330100	0.49928700	-1.13594100
C	1.38006400	-2.07380200	-1.43393800
C	-0.92592400	-2.07038300	-0.60865500
C	-1.93433300	-2.54222800	0.40797300
O	-1.71134300	-3.21252100	1.38331300
O	-3.14850900	-2.08029600	0.03863100
C	-3.10172500	-1.34299200	-1.21891000
H	-3.58052300	-1.97558300	-1.97042600
C	-3.75748200	0.01844800	-1.07023700
H	-4.00574300	0.39532500	-2.06905500
H	-4.68434800	-0.03888200	-0.49362600
C	-2.70278200	0.97031700	-0.44757300
C	2.80294500	-1.90763700	-1.11246400
H	3.43172700	-2.44310200	-1.83504500
H	3.03482800	-2.24621400	-0.10088600
C	0.48573400	1.32314300	0.59306200
O	0.97280800	0.37093300	-1.36790700
C	3.21818700	-0.34953200	-1.27105900
H	3.35748200	-0.14395300	-2.33567500
H	4.15867600	-0.20739400	-0.73802700
C	2.14934400	0.49643600	-0.69940700
C	1.90810600	1.11415300	0.50584700
H	-0.02073000	1.77349400	1.43004600
H	-1.41570100	0.94809600	-2.13515400
C	-2.73584100	0.94289700	1.08586600
H	-3.76030300	1.12647600	1.42698300
H	-2.10286700	1.72718200	1.50315300

H	-2.43305100	-0.01847800	1.50684900
O	-2.87351000	2.30613100	-0.91986500
H	-3.55091300	2.75979600	-0.39899900
H	-1.30756700	-1.22467700	-2.54348500
H	1.07026600	-1.83664100	-2.44996200
H	0.68796200	-2.97454200	0.40099000
C	2.95008100	1.41023500	1.51833600
O	4.10608100	1.04071100	1.41390500
O	2.45672200	2.10936700	2.54629500
C	3.39639500	2.45541800	3.59705600
H	3.80259700	1.54768300	4.04681600
H	2.81576900	3.02415100	4.32056800
H	4.20763100	3.05792800	3.18487600

(iv) Transition State Intermediate→44

Sum of electronic and zero-point Energies= -1148.070996
Sum of electronic and thermal Energies= -1148.050972
Sum of electronic and thermal Enthalpies= -1148.050027
Sum of electronic and thermal Free Energies= -1148.118980

C	0.22587000	-2.28406200	-0.18034000
C	-1.68160800	-1.32174300	-1.45573400
C	0.16167600	0.35357200	-0.78684300
C	-1.24907200	0.20020100	-1.28738200
C	1.06072100	-1.44738600	-1.03794300
C	-1.10112400	-2.21116300	-0.41754300
C	-2.19679900	-2.70978100	0.46495000
O	-2.11301000	-3.44072300	1.41778000
O	-3.36026100	-2.12346000	0.05395800
C	-3.20348200	-1.37875800	-1.18655400
H	-3.75839700	-1.93136200	-1.94751300
C	-3.66258100	0.07116600	-1.06722000
H	-3.92265900	0.43099400	-2.06928900
H	-4.54858900	0.17134700	-0.43474700
C	-2.45228400	0.90237100	-0.55834800
C	2.55615200	-1.30145900	-0.87525500
H	3.00847900	-2.10464200	-1.47169800
H	2.86528600	-1.42395800	0.16503900
C	0.64562900	0.75184000	0.51129600
O	1.12531500	0.86391400	-1.70667100
C	3.26866900	0.05423200	-1.46044200
H	3.33249600	0.00058900	-2.54784000
H	4.24474900	0.17300500	-0.99476400
C	2.24497900	0.99740900	-0.99496000
C	1.93522100	1.21680400	0.37644500
H	0.13780100	0.56893900	1.44628900
H	-1.24682700	0.64464800	-2.28833600
C	-2.43001700	0.95675300	0.97520200
H	-3.40356500	1.30924700	1.33157800
H	-1.68012000	1.66560100	1.33382000
H	-2.26857500	-0.02093000	1.43882400
O	-2.44831000	2.22984800	-1.08501600
H	-3.13586800	2.76009300	-0.65738200
H	-1.42866600	-1.64683700	-2.47012800
H	0.62843700	-2.81987400	0.67615300
C	2.94584900	1.52716600	1.42712700
O	4.13651000	1.56522200	1.19095500

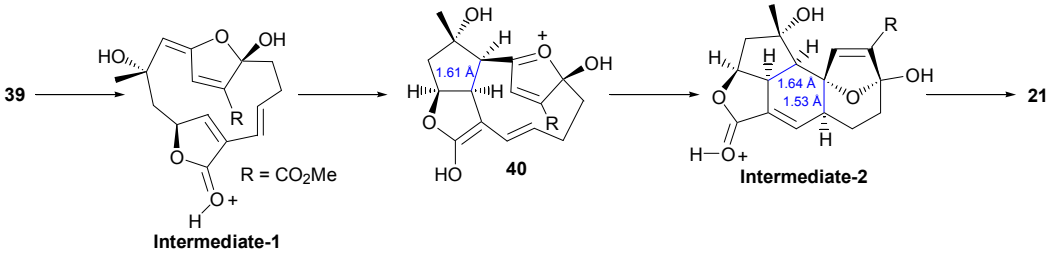
O	2.36893200	1.73619700	2.60960900
C	3.25991700	2.06474000	3.71434500
H	3.95187300	1.23929500	3.88832700
H	2.60413600	2.21509500	4.56899000
H	3.81518400	2.97376000	3.47856400
H	0.76793100	-1.47791100	-2.08730000

(ii) 44

Sum of electronic and zero-point Energies= -1148.074228
Sum of electronic and thermal Energies= -1148.053934
Sum of electronic and thermal Enthalpies= -1148.052989
Sum of electronic and thermal Free Energies= -1148.122838

C	0.13692900	-2.30855100	-0.18657800
C	-1.71538000	-1.34324600	-1.49883500
C	0.25264000	0.12447400	-0.81171000
C	-1.19789900	0.12276400	-1.30871200
C	0.96549800	-1.36828100	-1.02175000
C	-1.17732900	-2.25037200	-0.44196000
C	-2.31010800	-2.76040100	0.38532200
O	-2.28147600	-3.53171100	1.30830900
O	-3.44322700	-2.11166700	-0.02679300
C	-3.23806200	-1.32908500	-1.23732100
H	-3.82130700	-1.82031200	-2.01849000
C	-3.60983200	0.14370900	-1.07607500
H	-3.85129500	0.54235200	-2.06815600
H	-4.48541100	0.28280400	-0.43645600
C	-2.34684600	0.88711000	-0.55467200
C	2.49384500	-1.35273700	-0.80798800
H	2.92301500	-2.19590400	-1.35732000
H	2.75719600	-1.45221400	0.24727800
C	0.68937300	0.65345300	0.51275100
O	1.20187700	0.82947900	-1.73031400
C	3.31693900	-0.04179000	-1.38229600
H	3.42543700	-0.12286600	-2.46418000
H	4.26767700	0.05327000	-0.86232200
C	2.27997900	0.90045400	-0.98100200
C	1.93322600	1.18833600	0.39340300
H	0.17842500	0.45879400	1.44436700
H	-1.15767400	0.60722900	-2.29037300
C	-2.33213800	0.90413800	0.98146700
H	-3.29434500	1.28399500	1.34033700
H	-1.56313500	1.58026600	1.36271300
H	-2.20853400	-0.08889700	1.42359800
O	-2.26106000	2.22691700	-1.04527300
H	-2.93483000	2.77930100	-0.62367100
H	-1.47364700	-1.70370200	-2.50450700
H	0.55843600	-2.89157000	0.62792800
C	2.91238100	1.59661600	1.44285900
O	4.10643200	1.62699700	1.22477800
O	2.30471500	1.89101200	2.58778000
C	3.16428500	2.31158500	3.68841400
H	3.85757400	1.50795300	3.94066400
H	2.48407000	2.51847100	4.51139000
H	3.71691400	3.20625100	3.39827000
H	0.77667200	-1.55442600	-2.08487500

Geometries for structures relating to Figure 6.



B3LYP/6-31+G(d,p) Optimized Structures:

(i) Intermediate-1

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Sum of electronic and zero-point Energies=          -1224.518018
Sum of electronic and thermal Energies=             -1224.494457
Sum of electronic and thermal Enthalpies=           -1224.493513
Sum of electronic and thermal Free Energies=        -1224.569514

C                 -0.19756300   -1.92682300   -1.40089900
C                 -2.36177000   -0.55546900   -1.49526400
C                  0.00015700    1.31878000   -0.19105300
C                 -1.31197100    1.66639500   -0.21978000
C                  0.52347900   -1.19575700   -2.26948500
C                 -1.58714900   -1.61256000   -1.09092300
H                  0.28319100   -2.67076000   -0.77092300
C                 -2.34434000   -2.20069700   -0.03001100
O                 -3.45221200   -1.57680900    0.27551100
C                 -3.57310800   -0.41977700   -0.64776900
H                 -4.50595700   -0.60969600   -1.19178300
C                 -3.69191700    0.91364400    0.10732100
H                 -4.01595600    1.64419700   -0.64310100
H                 -4.51029800    0.82730500    0.83166300
C                 -2.41990900    1.51213000    0.80344600
C                  2.01607800   -1.17756000   -2.35453500
H                  2.34413200   -1.58664400   -3.31951500
H                  2.45264700   -1.81428400   -1.57835900
C                  0.85054500    0.66402300    0.80014100
O                  0.77169100    1.59169500   -1.29357300
C                  2.59297200    0.25858000   -2.27040000
H                  2.34302500    0.82136100   -3.17590800
H                  3.68105500    0.18621800   -2.21551400
C                  2.15991800    1.14942200   -1.09600000
C                  2.09112500    0.53317700    0.29403800
H                  0.54452800    0.35745600    1.78818100
O                  2.99974600    2.26299800   -1.15111900
C                  3.26730900   -0.10219400    0.93916200
O                  4.24426400   -0.48065300    0.32276800
O                  3.10733600   -0.22693400    2.26834700
C                  4.20882300   -0.84189300    2.98268200
H                  5.12182600   -0.26382200    2.82915100
H                  4.36075200   -1.86437200    2.63108700
H                  3.91195300   -0.82900400    4.02985400
H                  2.73523900    2.91379600   -0.48357600
H                  0.01498900   -0.46624000   -2.89845900
H                 -2.15887800    0.11249200   -2.32058600
H                 -1.60715400    2.25750200   -1.08482700
C                 -2.06475600    0.75615400    2.08974000
H                 -2.95218100    0.66928200    2.72619700
H                 -1.30670000    1.30775100    2.64970200
```

H	-1.69652500	-0.25650700	1.90348300
O	-2.77175000	2.86687100	1.13872300
H	-3.43050100	2.87307700	1.84926200
O	-2.00360600	-3.26895900	0.62914000
H	-2.66257800	-3.51689500	1.30376400

(ii) Transition State Intermediate-1→40

Sum of electronic and zero-point Energies=	-1224.514573
Sum of electronic and thermal Energies=	-1224.491816
Sum of electronic and thermal Enthalpies=	-1224.490871
Sum of electronic and thermal Free Energies=	-1224.564958

C	-0.60617300	-2.09409800	-0.84688100
C	-2.40556600	-0.30504900	-1.14894100
C	0.08445400	1.08981000	-0.40108400
C	-1.25372500	1.46271600	-0.47559500
C	0.18658200	-1.66543900	-1.84758400
C	-1.91398900	-1.50865000	-0.60546200
C	-2.80129100	-1.82926900	0.42706300
O	-3.80607100	-0.98165900	0.59989300
C	-3.68628300	0.05468100	-0.44675800
H	-4.56836800	-0.08390700	-1.08082600
C	-3.64086300	1.45689000	0.15108800
H	-3.90263900	2.15461300	-0.65270000
H	-4.39622000	1.56855100	0.93593200
C	-2.21564200	1.83930100	0.65170300
C	1.66367200	-1.88127200	-1.95715100
H	1.89475100	-2.54991400	-2.79671800
H	2.04772000	-2.37161900	-1.05617900
C	0.90683800	0.56631500	0.68246500
O	0.83639200	1.19053200	-1.51321100
C	2.42979000	-0.55994400	-2.23188200
H	2.20136100	-0.19043800	-3.23683700
H	3.50196000	-0.76458800	-2.18780100
C	2.19948700	0.62759100	-1.28470900
C	2.13976800	0.31148800	0.20100200
H	0.58407900	0.41820000	1.70076400
O	3.12403500	1.59398900	-1.63753300
C	3.29795700	-0.26639100	0.93243200
O	4.25514500	-0.76255800	0.37276500
O	3.13822000	-0.18486800	2.26204000
C	4.21785200	-0.72974800	3.06499400
H	5.15007100	-0.21073300	2.83520800
H	4.33222300	-1.79632100	2.86266900
H	3.91932200	-0.55670100	4.09709800
H	3.02793200	2.38257000	-1.08188500
H	-1.47179800	2.02005300	-1.38545700
C	-1.91585300	1.24954200	2.03623400
H	-2.74179400	1.47635700	2.71871400
H	-1.01208700	1.70017300	2.45145400
H	-1.79773000	0.16256300	2.02031800
O	-2.13032300	3.27055400	0.71661300
H	-2.70682700	3.60411700	1.42014100
H	-2.22111200	0.01424200	-2.16579900
H	-0.23715200	-1.00720800	-2.60446900
H	-0.22781800	-2.78566600	-0.09716600
O	-2.72035200	-2.86993000	1.22192100

H	-3.47746200	-2.91651700	1.83142800

(iii) 40

Sum of electronic and zero-point Energies= -1224.528537
Sum of electronic and thermal Energies= -1224.505857
Sum of electronic and thermal Enthalpies= -1224.504913
Sum of electronic and thermal Free Energies= -1224.578709

C	-0.60436900	-2.04327100	-0.81210800
C	-2.27433700	-0.14292300	-1.15073500
C	0.10714000	0.81978000	-0.59188700
C	-1.34924000	1.09478900	-0.68955600
C	0.22169300	-1.53760200	-1.77818500
C	-1.89269100	-1.47550900	-0.59267900
C	-2.84957800	-1.82002200	0.32753000
O	-3.85497000	-0.94689100	0.47140700
C	-3.66089500	0.13476200	-0.51884500
H	-4.49268200	0.03425000	-1.21758700
C	-3.58568300	1.50040200	0.14621100
H	-3.87352300	2.25705000	-0.59243800
H	-4.26725900	1.58857300	0.99714500
C	-2.09810600	1.74376700	0.52763000
C	1.69665000	-1.76854700	-1.91628800
H	1.89715000	-2.48981400	-2.71952200
H	2.10059100	-2.21703600	-1.00127000
C	0.92969100	0.32911900	0.49801600
O	0.86159200	1.23456300	-1.58406400
C	2.48378700	-0.47571500	-2.28201200
H	2.24047600	-0.14943300	-3.29792800
H	3.55467200	-0.69244800	-2.24605100
C	2.29041500	0.74095600	-1.36486000
C	2.22266400	0.36415900	0.10297900
H	0.56121000	-0.01840900	1.44991200
O	3.14306000	1.72986900	-1.75437000
C	3.41982200	-0.08943500	0.85572700
O	4.49087400	-0.30312000	0.32326100
O	3.15788900	-0.23493700	2.16220900
C	4.26955300	-0.67574400	2.98752400
H	5.09182400	0.03794700	2.91290000
H	4.60689300	-1.66134900	2.66188500
H	3.87356900	-0.71179600	4.00036300
H	3.14225200	2.47109300	-1.12948900
H	-1.43577700	1.83776500	-1.48899600
C	-1.78048500	1.20421800	1.92805100
H	-2.49606800	1.62260900	2.64413700
H	-0.78158100	1.50726000	2.24872900
H	-1.86624900	0.11598000	1.99186000
O	-1.75253100	3.12681100	0.45524100
H	-2.12150500	3.60309700	1.21263700
H	-2.30785300	-0.12322300	-2.24311500
H	-0.21883000	-0.89713200	-2.53836900
H	-0.24342600	-2.80318800	-0.12000700
O	-2.87138100	-2.89609900	1.09701400
H	-3.68444700	-2.92517800	1.62799300

(iv) Transition State 40→Intermediate-2

```
 Sum of electronic and zero-point Energies=          -1224.525760
 Sum of electronic and thermal Energies=             -1224.503936
 Sum of electronic and thermal Enthalpies=           -1224.502992
 Sum of electronic and thermal Free Energies=        -1224.575254

 C                 -0.95069000   -1.72883100    1.22539000
 C                 -2.41089300   -0.88737200   -0.63401000
 C                  0.13597300   -0.29394500   -0.83537500
 C                 -1.28001300    0.01656200   -1.27572500
 C                 -0.04383600   -2.14089900    0.23753200
 C                 -2.16327500   -1.17828100    0.81360800
 C                 -3.13673900   -0.50956900    1.54500300
 O                 -4.00872900    0.17316800    0.82328400
 C                 -3.69914000   -0.03654400   -0.62581700
 H                 -4.58471500   -0.53788100   -1.01613300
 C                 -3.36649000    1.26625100   -1.33324900
 H                 -3.59746100    1.13465000   -2.39653800
 H                 -3.96021800    2.10891700   -0.96733600
 C                 -1.82976600    1.48907500   -1.20230000
 C                  1.36703100   -2.60419900    0.51710200
 H                  1.35461400   -3.67879500    0.73880600
 H                  1.74831400   -2.11299100    1.41936000
 C                  1.00090500    0.42056600    0.11822800
 O                  0.92041000   -0.79106500   -1.80971700
 C                  2.34761500   -2.37855100   -0.66549000
 H                  2.13497800   -3.06885000   -1.48790200
 H                  3.37149800   -2.55764800   -0.32860300
 C                  2.29729400   -0.96173000   -1.24491200
 C                  2.27929600    0.09422000   -0.14526300
 H                  0.65377100    1.02401800    0.94271300
 O                  3.20591000   -0.84677200   -2.25881500
 C                  3.48661500    0.44833800    0.64142300
 O                  4.51147300   -0.20322300    0.61178000
 O                  3.29297300    1.54903600    1.38691200
 C                  4.41811200    1.96549000    2.20360600
 H                  5.28589700    2.15956000    1.57081300
 H                  4.66117100    1.18781800    2.93016300
 H                  4.08708500    2.87518300    2.70100700
 H                  3.23564800    0.06071000   -2.59774000
 C                 -1.49699800    2.32259600    0.04300000
 H                 -2.10703000    3.23261200    0.04162800
 H                 -0.44956600    2.62836000    0.04013400
 H                 -1.71042200    1.79729600    0.97876200
 O                 -1.29917900    2.12951600   -2.36096200
 H                 -1.48862300    3.07814200   -2.33663900
 H                 -0.65871700   -1.68724100    2.27398000
 H                 -1.27292200   -0.20615300   -2.34755000
 H                 -2.52392100   -1.79465300   -1.23440500
 H                 -0.47961800   -2.52822600   -0.68084900
 O                 -3.25345100   -0.47769700    2.85307900
 H                 -4.02417100    0.04903100    3.12801800
```

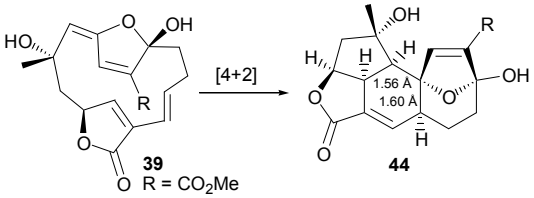
(v) Intermediate-2

```
 Sum of electronic and zero-point Energies=          -1224.533279
 Sum of electronic and thermal Energies=             -1224.511487
 Sum of electronic and thermal Enthalpies=           -1224.510543
```

Sum of electronic and thermal Free Energies= -1224.582931

C	-1.13167700	-1.76571800	1.17197500
C	-2.43061600	-0.86570400	-0.74573500
C	0.12825400	-0.52518000	-0.64872100
C	-1.22516900	0.01522500	-1.19873200
C	-0.07828600	-1.94165300	0.14632300
C	-2.29414600	-1.24046200	0.70539400
C	-3.39408100	-0.66633800	1.39845300
O	-4.16993000	0.06148300	0.65683100
C	-3.69065600	0.01648500	-0.79264600
H	-4.55209600	-0.39972500	-1.31287200
C	-3.24311500	1.37506500	-1.29505300
H	-3.38038200	1.37127900	-2.38279600
H	-3.83903900	2.19976000	-0.89359700
C	-1.71093700	1.50143200	-1.01135700
C	1.27174700	-2.52609300	0.59793700
H	1.13428200	-3.57698600	0.87300700
H	1.61367200	-2.00924000	1.50120900
C	1.05285300	0.35006300	0.18017900
O	0.95063000	-0.89449300	-1.74550400
C	2.34980400	-2.42256400	-0.50813000
H	2.18577800	-3.17500900	-1.28645600
H	3.34528000	-2.57912600	-0.08569600
C	2.29665100	-1.05336700	-1.19863200
C	2.31620600	0.07396800	-0.15957600
H	0.74922700	0.97992700	1.00289900
O	3.21108500	-1.01328700	-2.22354600
C	3.55170800	0.52713100	0.52592900
O	4.56955800	-0.13371900	0.57155700
O	3.39636700	1.73449200	1.10241900
C	4.55143700	2.24310500	1.81464200
H	5.40108300	2.33091700	1.13494300
H	4.81149100	1.57418600	2.63753700
H	4.24980300	3.22054600	2.18724400
H	3.15480200	-0.16196500	-2.68273900
C	-1.47700900	2.19958000	0.33937000
H	-2.10000500	3.09911200	0.39534900
H	-0.43836000	2.51268800	0.44312900
H	-1.73719500	1.57519000	1.20008800
O	-1.06957000	2.23870800	-2.04719400
H	-1.16362400	3.18953500	-1.89529400
H	-0.95595800	-1.94712300	2.23097600
H	-1.12480000	-0.08498900	-2.28393600
H	-2.52715600	-1.75519100	-1.37656500
H	-0.48787800	-2.57324500	-0.65550500
O	-3.63710900	-0.78661600	2.67016800
H	-4.43292200	-0.29208600	2.94272300

Geometries for structures relating to Figure 7.



B3LYP/6-31+G(d,p) Optimized Structures:

(i) 39

```
 Sum of electronic and zero-point Energies=          -1224.183602
 Sum of electronic and thermal Energies=             -1224.160282
 Sum of electronic and thermal Enthalpies=           -1224.159338
 Sum of electronic and thermal Free Energies=        -1224.234915

 C                 -0.23787000   -1.90392600   -1.38304700
 C                 -2.52013700   -0.76252500   -1.48877400
 C                 -0.08685500    1.33957300   -0.14724000
 C                 -1.38507600    1.70232700   -0.19004100
 C                  0.45162300   -1.15317800   -2.25896700
 C                 -1.62985700   -1.65894400   -1.02509300
 H                  0.27783500   -2.62985600   -0.75748500
 C                 -2.19247400   -2.22437700    0.23506200
 O                 -1.73247100   -3.07277600    0.96415600
 O                 -3.37963100   -1.58808600    0.50400800
 C                 -3.64055600   -0.59471400   -0.51070800
 H                 -4.61917700   -0.83943700   -0.94489100
 C                 -3.74935500    0.82352300    0.09068200
 H                 -4.06166400    1.48932400   -0.72299800
 H                 -4.57437100    0.80552000    0.81465100
 C                 -2.52418200    1.50559900    0.78797500
 C                  1.94670700   -1.11831700   -2.36494000
 H                  2.27425800   -1.49423500   -3.34450300
 H                  2.39073600   -1.77992600   -1.61338500
 C                  0.73501100    0.63597700    0.82731700
 O                  0.71883600    1.63034400   -1.23863700
 C                  2.52874400    0.31074100   -2.22957400
 H                  2.27965400    0.90485700   -3.11581400
 H                  3.61741100    0.24009700   -2.17341100
 C                  2.08016500    1.15937300   -1.02990800
 C                  1.98189600    0.49390200    0.33508700
 H                  0.39832600    0.28201600    1.78913300
 O                  2.94610100    2.27137900   -1.02086300
 C                  3.11860400   -0.19577500    0.97528700
 O                  4.14699100   -0.50643700    0.40128600
 O                  2.87958700   -0.46470800    2.27883300
 C                  3.91853100   -1.18574500    2.97084800
 H                  4.85123900   -0.61728200    2.95379800
 H                  4.08091300   -2.15983600    2.50349100
 H                  3.55554700   -1.30388100    3.99111500
 H                  2.63599900    2.89945800   -0.35200000
 H                 -0.07911500   -0.41654800   -2.86115200
 H                 -2.42861700   -0.14423500   -2.37355100
 H                 -1.67655600    2.25942100   -1.07827000
 C                 -2.17033700    0.83442900    2.11968000
 H                 -3.06604200    0.78098700    2.74852600
 H                 -1.42204100    1.42996300    2.64880000
 H                 -1.81201400   -0.18915600    2.00210200
 O                 -2.94872700    2.86706800    1.06523400
 H                 -3.68333900    2.83838500    1.69557800
```

(ii) Transition State 39→44

```
 Sum of electronic and zero-point Energies=          -1224.155868
 Sum of electronic and thermal Energies=             -1224.133691
```

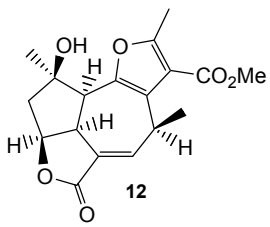
```
Sum of electronic and thermal Enthalpies=          -1224.132747
Sum of electronic and thermal Free Energies=       -1224.205420

C                 -1.12430400    1.78529700    1.48722200
C                 -1.34018300    2.50251700   -0.90320800
C                  1.16358300    1.15472500   -0.55650900
C                  0.48306300    1.99281600   -1.46979000
C                 -0.85316800    0.48495300    1.15676100
C                 -1.43221500    2.73542800    0.48603400
C                 -1.48280600    4.18245400    0.71984000
O                 -1.51004200    4.80260200    1.76213000
O                 -1.47758500    4.82312400   -0.50671000
C                 -1.48270200    3.85772700   -1.58212400
H                 -2.43789600    3.96662600   -2.10800500
C                 -0.29992700    4.06880500   -2.52421800
H                 -0.52783800    3.57898800   -3.47857100
H                 -0.13766800    5.13314100   -2.72434700
C                  0.96045200    3.38106300   -1.94062900
C                 -0.20713800   -0.55343900    2.02240900
H                 -0.97037500   -1.15656100    2.53491500
H                  0.37442800   -0.06979100    2.81732600
C                  2.02883000    1.43020900    0.55934200
O                  1.15762400   -0.19493800   -0.78602800
C                  0.68893600   -1.53528700    1.22137500
H                  0.07634200   -2.15117900    0.55377100
H                  1.20243900   -2.20014300    1.92057300
C                  1.78195700   -0.88830900    0.36080100
C                  2.49114500    0.25745900    1.06685500
H                  2.26338800    2.41344400    0.93627500
O                  2.57633000   -1.90876700   -0.14253900
H                  3.29387200   -1.52297000   -0.66654700
H                  0.18987000    1.41177200   -2.34489700
C                  1.66398900    4.25653900   -0.89632600
H                  1.81421400    5.26138500   -1.30694700
H                  2.64536100    3.84237600   -0.65509100
H                  1.08325500    4.37460600    0.02093800
O                  1.88774600    3.09393400   -3.00876500
H                  2.23681500    3.93023800   -3.34839200
H                 -1.81189500    1.63882900   -1.36287700
H                 -1.13374100    0.14345800    0.16444700
H                 -0.96257100    2.15361700    2.49927000
C                  3.36142100    0.07018000    2.23241900
O                  3.55860600   -0.99694000    2.79040400
O                  3.92923900    1.23617500    2.63307200
C                  4.78494000    1.14857000    3.78836200
H                  5.61752600    0.46782400    3.59535100
H                  5.14671400    2.16248900    3.95632200
H                  4.22296300    0.79082200    4.65452300
```

(iii) 44

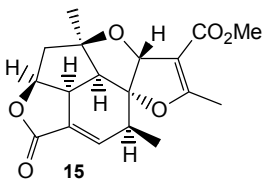
```
Sum of electronic and zero-point Energies=          -1224.198360
Sum of electronic and thermal Energies=             -1224.176879
Sum of electronic and thermal Enthalpies=           -1224.175935
Sum of electronic and thermal Free Energies=        -1224.247897

C                 -1.19125900   -1.68428600    1.24174900
C                 -2.49384800   -0.78993200   -0.63848300
```

C	0.06444300	-0.48230700	-0.59052500
C	-1.28781500	0.06568200	-1.13539300
C	-0.13808800	-1.86709600	0.18510800
C	-2.33964400	-1.14701000	0.80536800
C	-3.46379900	-0.56989000	1.57869200
O	-3.72481100	-0.66829300	2.75474000
O	-4.20119600	0.21295400	0.72460300
C	-3.75113000	0.10575500	-0.65856100
H	-4.59186000	-0.31896900	-1.21172100
C	-3.28389600	1.43684300	-1.24388000
H	-3.41677800	1.39634400	-2.33122800
H	-3.86109500	2.28548800	-0.86432400
C	-1.75745200	1.55408800	-0.96176700
C	1.21232900	-2.45268800	0.64029700
H	1.07209200	-3.50251000	0.92035100
H	1.55337000	-1.93598600	1.54459600
C	0.98284700	0.40028300	0.23659300
O	0.90962400	-0.82242700	-1.70537000
C	2.29686100	-2.35083700	-0.46033200
H	2.13207600	-3.10115700	-1.24124700
H	3.29346400	-2.50798000	-0.03863600
C	2.23518800	-0.98033400	-1.14920700
C	2.25143000	0.14411400	-0.10508500
H	0.66994600	1.01746600	1.06476700
O	3.16555500	-0.92378700	-2.17348000
C	3.46952200	0.61525000	0.58319100
O	4.53257500	0.02344300	0.58494200
O	3.26471100	1.78581100	1.23462800
C	4.39490100	2.29449400	1.97060100
H	5.24093200	2.46243300	1.30021400
H	4.69052900	1.58973500	2.75166000
H	4.05571800	3.23346700	2.40691100
H	3.03271800	-0.09687500	-2.66029000
C	-1.52221900	2.25562300	0.38659800
H	-2.13910500	3.16075600	0.43185600
H	-0.48082500	2.56106600	0.49320600
H	-1.80365600	1.63864600	1.24379700
O	-1.09753000	2.29741300	-1.99761600
H	-1.26499400	3.24063400	-1.86619800
H	-1.00371200	-1.88586700	2.29409300
H	-1.20390700	-0.05206500	-2.22077100
H	-2.60967000	-1.68310300	-1.26276600
H	-0.53867200	-2.52630100	-0.59882400

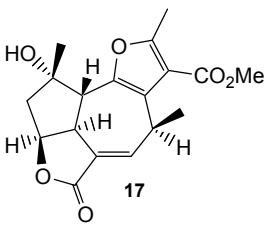
Relative Energies for the Potential Cyclisation Products Depicted in Scheme 2.



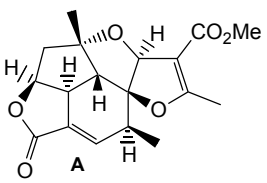
12



15



17



A
(not observed)

Method[a]	Relative Energy (kcal/mol)			
	12	**15**	**17**	**A**
B3LYP-gCP-D3/6-31G*	0.2	0	4.8	27.4
BMK/6-311+G**//B3LYP/6-31+G**	0	1.3	3.8	28.2
MO6-2X/6-31+G**	0	1.6	3.6	27.9

B3LYP/6-31+G(d,p) Optimized Structures:

(i) 12

```
 Sum of electronic and zero-point Energies=          -1149.014035
 Sum of electronic and thermal Energies=             -1148.991729
 Sum of electronic and thermal Enthalpies=           -1148.990785
 Sum of electronic and thermal Free Energies=        -1149.065014


 H                  -1.29345   2.99509  -0.40688
 C                  -0.988     2.02657  -0.01077
 C                  -2.00629  -0.0599    1.16448
 C                   0.22941  -0.83799   0.26597
 C                  -1.20347  -1.18329   0.48383
 C                   0.45628   1.70068  -0.27008
 C                  -1.97975   1.30101   0.51976
 H                  -1.72081   0.02216   2.21976
 H                  -1.20131  -2.03977   1.1722
 C                  -2.09357  -1.63242  -0.71507
 C                  -3.49291  -0.47774   1.00131
 H                  -3.94664  -0.83018   1.93038
 C                  -3.51408  -1.57289  -0.09067
 H                  -3.75621  -2.53916   0.36622
 H                  -4.28424  -1.36639  -0.84065
 C                   0.9416    0.30983   0.06787
 O                   1.10048  -1.90165   0.45144
 C                   2.37151  -1.44297   0.37097
 C                   2.34283  -0.08488   0.14287
 C                   3.44536  -2.46167   0.54739
 H                   4.13064  -2.17691   1.35049
 H                   4.04544  -2.56668  -0.36208
 H                   2.99268  -3.42659   0.78694
 C                   3.50493   0.80856   0.06828
 O                   4.68346   0.13112   0.10202
 C                   5.87002   0.94548   0.05603
 H                   5.89801   1.63035   0.90688
 H                   5.90101   1.52449  -0.87
 H                   6.70288   0.24371   0.09853
 O                   3.45667   2.02561  -0.00646
 C                   0.73298   2.0041   -1.77211
 H                   0.45124   3.03548  -2.00776
 H                   0.15087   1.32745  -2.40383
 H                   1.79472   1.88774  -1.99658
 C                  -3.3883    1.76524   0.375
 O                  -4.22706   0.70911   0.62838
 O                  -3.81315   2.84903   0.04953
 O                  -1.94246  -0.63642  -1.7365
 H                  -2.54849  -0.8386   -2.46218
 C                  -1.72861  -3.00931  -1.27156
 H                  -2.42458  -3.29698  -2.06923
 H                  -0.71811  -2.99344  -1.68963
 H                  -1.77272  -3.78084  -0.49568
 H                   1.068     2.41288   0.29966
```

(ii) 15

```
 Sum of electronic and zero-point Energies=          -1148.940925
 Sum of electronic and thermal Energies=             -1148.919931
 Sum of electronic and thermal Enthalpies=           -1148.918987
```

```
Sum of electronic and thermal Free Energies=       -1148.990069

H                    -2.06855   1.62087  -2.22029
C                    -1.92988   1.50945  -1.14706
C                    -2.47985   0.42473   1.02189
C                    -0.06374   1.11601   0.41309
C                    -0.98517   0.39137   1.42169
C                    -0.78091   2.19885  -0.44539
C                    -2.6845    0.66411  -0.44183
H                    -3.02767   1.16929   1.61319
H                    -0.84101   0.82019   2.41696
C                    -0.5661   -1.1092    1.36264
C                    -3.06758  -0.99857   1.19831
H                    -3.78455  -1.06865   2.0194
C                    -1.86886  -1.94739   1.40746
H                    -1.96152  -2.45682   2.3723
H                    -1.84281  -2.71539   0.63023
C                     0.59311  -0.0403   -0.40243
O                     0.0096   -1.26477   0.05115
O                     1.02948   1.75959   1.1362
C                     2.20355   1.17403   0.77905
C                     2.06063   0.14978  -0.09721
C                     3.4124    1.76716   1.4141
H                     3.33785   1.68509   2.50538
H                     3.47735   2.83534   1.17476
H                     4.30651   1.25037   1.06677
C                     3.15045  -0.63379  -0.68032
O                     2.67652  -1.4898   -1.62002
C                     3.6638   -2.31317  -2.25493
H                     4.18515  -2.92911  -1.5171
H                     4.39844  -1.69938  -2.78387
H                     3.11231  -2.94041  -2.95614
O                     4.33617  -0.55381  -0.39987
C                     0.43068  -1.53837   2.44456
H                    -0.012    -1.43771   3.44274
H                     1.34503  -0.94056   2.4108
H                     0.70925  -2.58712   2.29594
C                     0.15347   2.93391  -1.41407
H                    -0.40365   3.7053   -1.95679
H                     0.58823   2.25483  -2.15599
H                     0.9696    3.42261  -0.87567
C                    -3.63924  -0.33976  -0.97392
O                    -3.82508  -1.29027  -0.0035
O                    -4.16383  -0.40157  -2.05741
H                    -1.17916   2.93989   0.26565
H                     0.38246   0.00141  -1.47458
```

(iii) 17

```
Sum of electronic and zero-point Energies=          -1149.008281
Sum of electronic and thermal Energies=             -1148.985911
Sum of electronic and thermal Enthalpies=           -1148.984966
Sum of electronic and thermal Free Energies=        -1149.059415

H                    -0.60048   3.32796  -0.48296
C                    -0.51849   2.29915  -0.13329
C                    -1.83421   0.31346   0.7368
C                     0.11734  -0.79328  -0.26841
```

C	-1.37191	-0.69107	-0.34075
C	0.87258	1.70865	-0.25804
C	-1.65006	1.72249	0.29263
C	-2.32742	-1.88587	-0.13019
C	-3.36052	0.12791	0.84755
H	-3.70246	0.04018	1.88106
C	-3.68517	-1.13257	0.01709
H	-4.44386	-1.76832	0.4842
H	-4.06372	-0.83119	-0.96582
C	1.05019	0.19856	-0.13753
O	0.71465	-2.02892	-0.2322
C	2.04995	-1.853	-0.07073
C	2.32501	-0.50439	0.00099
C	2.86818	-3.0924	0.00103
H	2.43247	-3.79392	0.72065
H	3.88899	-2.84723	0.29076
H	2.89712	-3.59289	-0.97492
C	3.68362	0.0095	0.24166
O	3.7009	1.33436	0.53753
C	5.00003	1.89893	0.79928
H	5.65489	1.76947	-0.06555
H	5.45592	1.4189	1.66832
H	4.82086	2.95623	0.99367
O	4.70598	-0.65689	0.20488
C	1.46371	2.19348	-1.61226
H	1.43958	3.2868	-1.67275
H	0.88542	1.79126	-2.45053
H	2.50062	1.87085	-1.7208
C	-3.00434	2.32523	0.11284
O	-3.95001	1.34596	0.31944
O	-3.30759	3.44728	-0.21668
C	-2.31967	-2.93086	-1.24368
H	-1.34718	-3.42715	-1.29099
H	-2.52942	-2.47312	-2.21608
H	-3.08969	-3.69164	-1.06403
O	-1.97112	-2.4789	1.13112
H	-2.52883	-3.25411	1.27984
H	-1.64476	-0.27547	-1.32067
H	-1.33402	0.08521	1.68023
H	1.48355	2.17388	0.52698

(iv) A

Sum of electronic and zero-point Energies=	-1148.967647
Sum of electronic and thermal Energies=	-1148.946607
Sum of electronic and thermal Enthalpies=	-1148.945662
Sum of electronic and thermal Free Energies=	-1149.016364

H	-2.92717	-2.82348	-0.48239
C	-2.3778	-1.90953	-0.69436
C	-1.97725	0.4234	-0.7568
C	-0.11657	-0.83773	0.02546
C	-1.10813	0.18074	0.50462
C	-0.84859	-1.95935	-0.87455
C	-2.9407	-0.68599	-0.70111
H	-1.36197	0.47623	-1.6559
C	-0.46558	1.53437	0.70183
C	-2.6927	1.71175	-0.46703

H	-3.02632	2.26748	-1.34729
C	-1.65935	2.51049	0.37923
H	-1.30414	3.38386	-0.17605
H	-2.10935	2.8708	1.30954
O	0.58316	-1.48986	1.12296
C	0.9511	0.12026	-0.62939
C	2.21292	-0.29576	0.07876
C	1.90484	-1.18074	1.06305
C	-0.2879	-3.37087	-0.66624
H	0.79389	-3.39864	-0.82461
H	-0.74919	-4.0582	-1.38275
H	-0.48988	-3.73847	0.34314
C	-4.17962	-0.09764	-0.09779
O	-3.9097	1.23823	0.20509
O	-5.229	-0.61347	0.1929
H	-1.72331	-0.14658	1.34568
C	0.1834	1.84938	2.04787
H	0.99886	1.15899	2.27161
H	-0.55409	1.79283	2.8559
H	0.59768	2.86272	2.03084
O	0.53722	1.50145	-0.36004
C	2.74617	-1.85996	2.08461
H	2.62628	-2.94605	2.00563
H	2.41216	-1.56927	3.08766
H	3.79209	-1.5858	1.95493
C	3.55683	0.18391	-0.24635
O	4.58188	-0.05039	0.3782
O	3.54538	0.94064	-1.37275
C	4.81458	1.48378	-1.77533
H	5.5237	0.68175	-1.9954
H	5.22604	2.11768	-0.98612
H	4.60662	2.07028	-2.67002
H	1.02643	0.04659	-1.71705
H	-0.63519	-1.67127	-1.9136

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