

Supplementary Material

On the mechanism of the [4+2] cycloaddition of $^1\text{O}_2$ with 1,3-dienes: Identifying the putative biradical/dipolar intermediate by employing the *gem*-diphenylcyclopropylcarbinyl radical clock as a mechanistic probe

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This paper is dedicated to our mentor, Prof. Michael Orfanopoulos, on the occasion of his 67th birthday, and his outstanding contribution to singlet oxygen and fullerene chemistry

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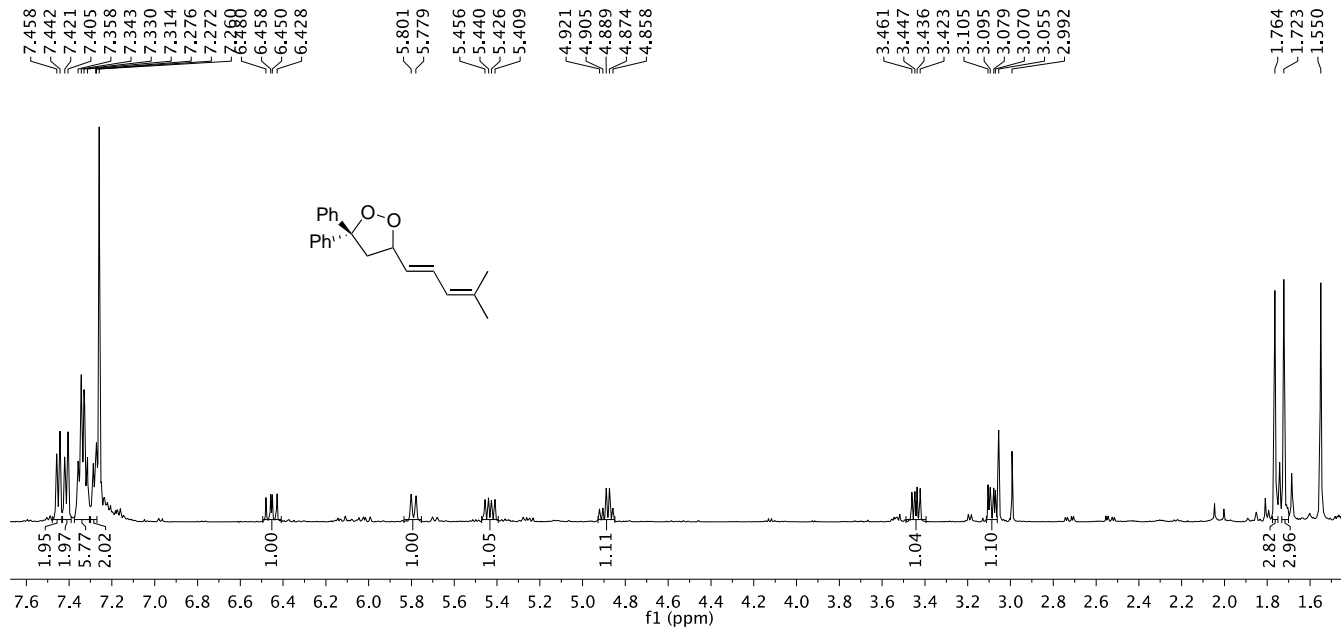
1. Copies of 1D and 2D NMR Spectra of (*E*)-13 and (*E,E*)-14

Figure S1. ¹H NMR (500 MHz) spectrum of (*E*)-13 recorded at 25 °C in CDCl₃.*

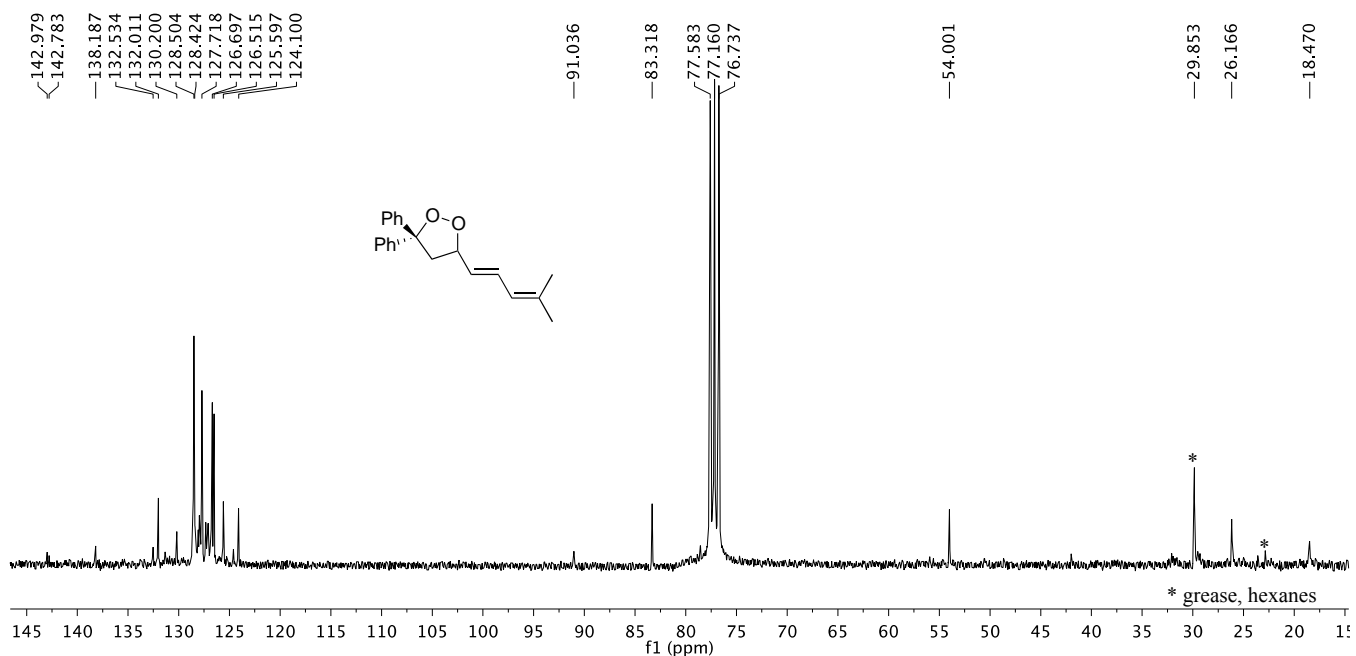


Figure S2. ¹³C NMR (75 MHz) spectrum of (*E*)-13 recorded at 25 °C in CDCl₃.

* The ¹H NMR spectra of this compound showed the presence of minor side-product(s), which could not be separated by flash column chromatography on silica gel (identical *R_f* values).

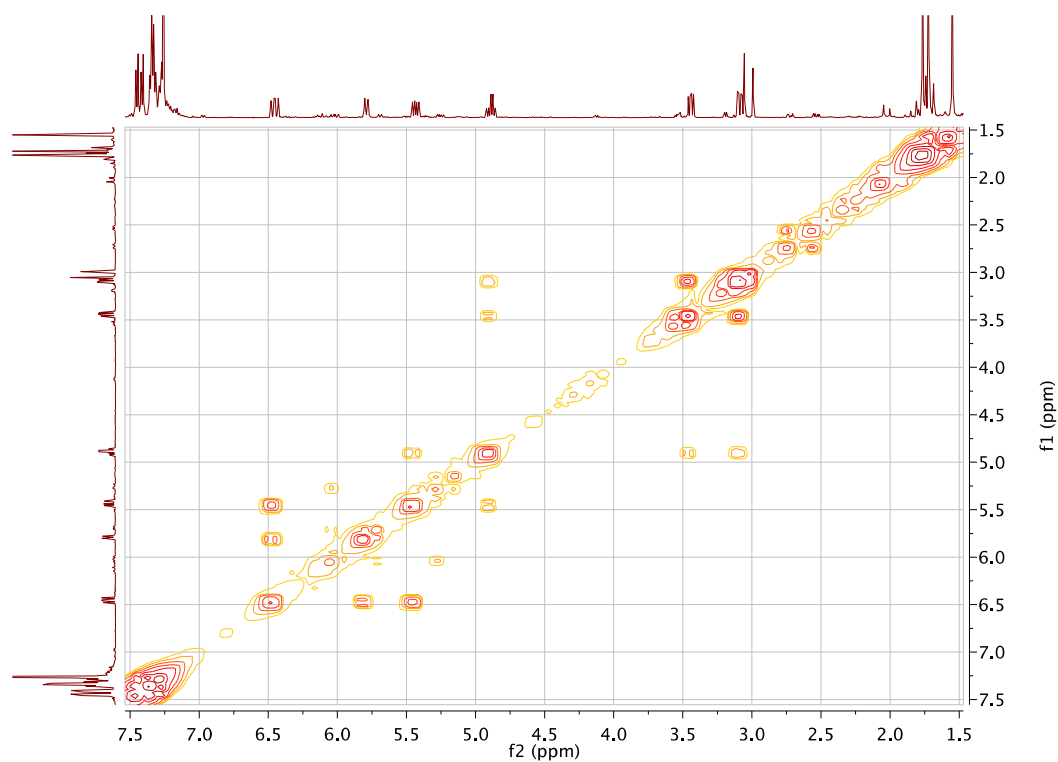


Figure S3. COSY (500 MHz) spectrum of (*E*)-**13** recorded at 25 °C in CDCl₃.

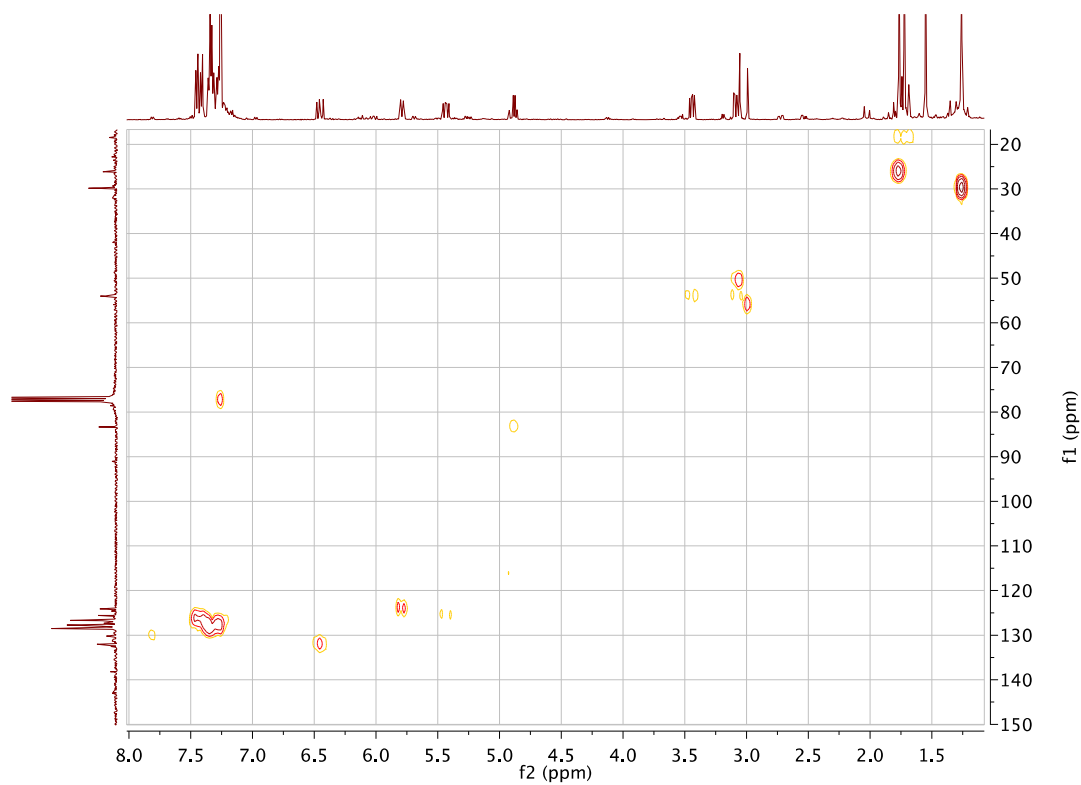


Figure S4. HMBC (500 MHz) spectrum of (*E*)-**13** recorded at 25 °C in CDCl₃.

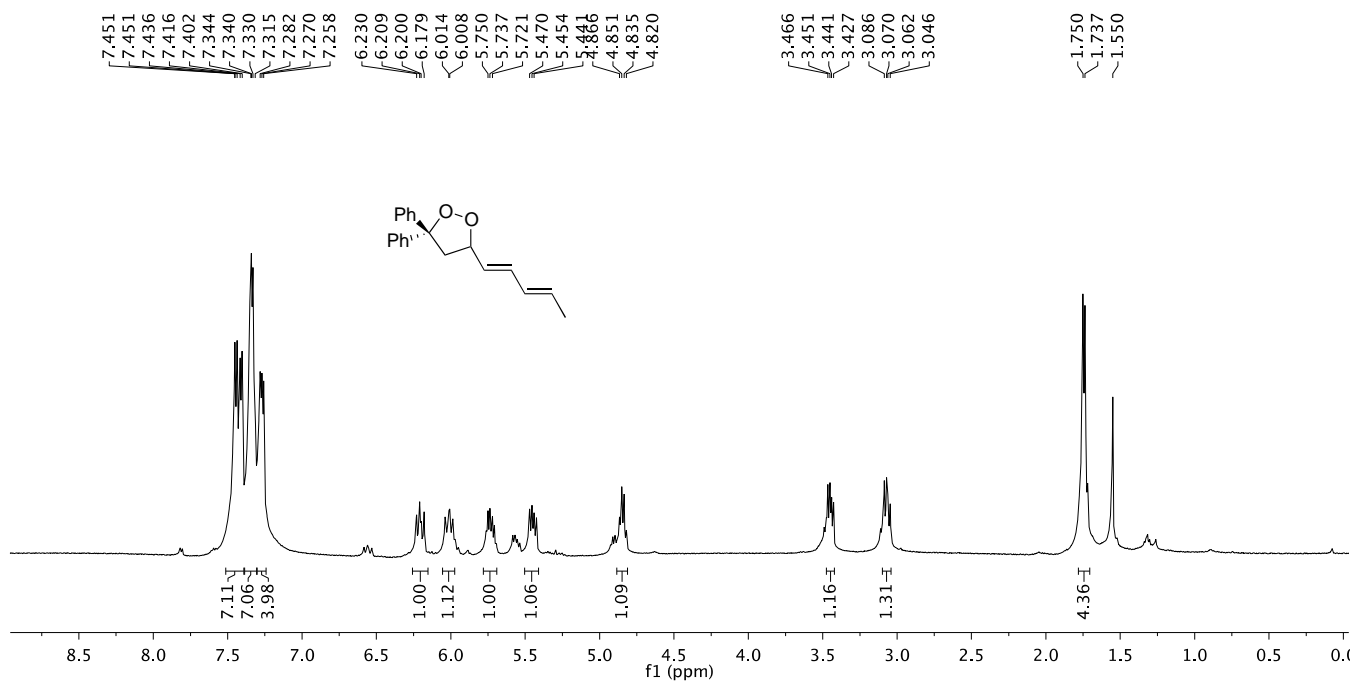


Figure S5. ¹H NMR (500 MHz) spectrum of *(E,E)*-14 recorded at 25 °C in CDCl₃. †

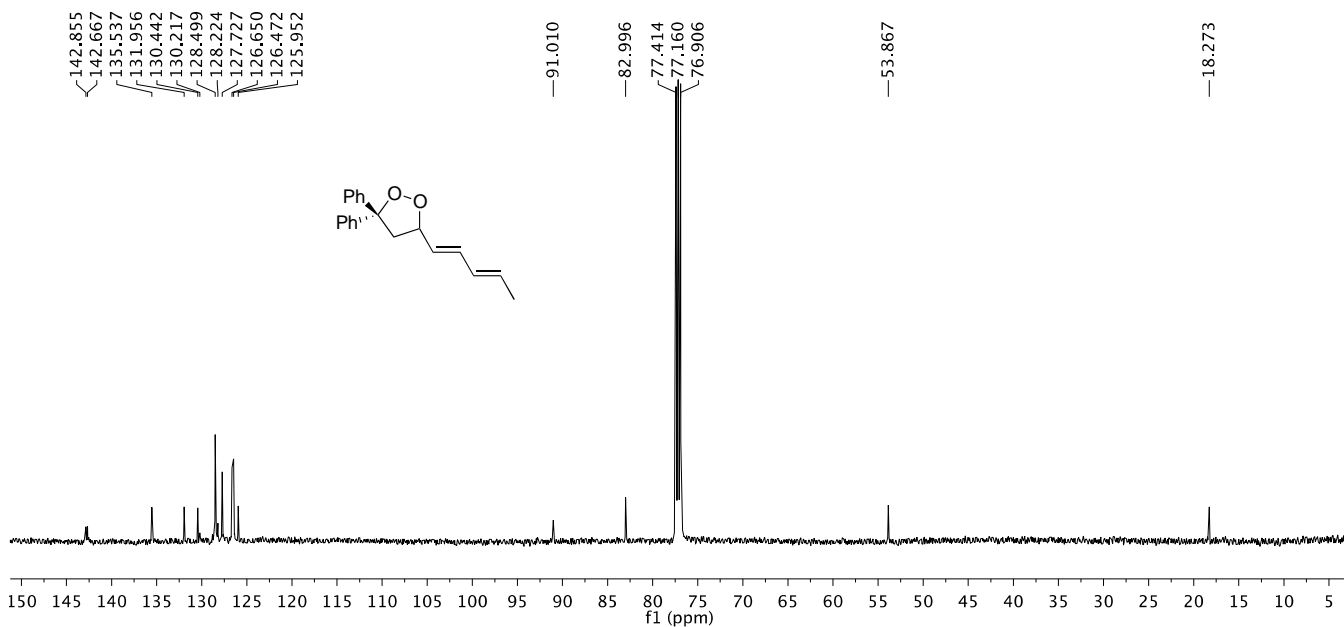


Figure S6. ¹³C NMR (125 MHz) spectrum of *(E,E)*-14 recorded at 25 °C in CDCl₃.

† The ¹H NMR spectra of this compound showed the presence of minor side-product(s), which could not be separated by flash column chromatography on silica gel (identical *R_f* values).

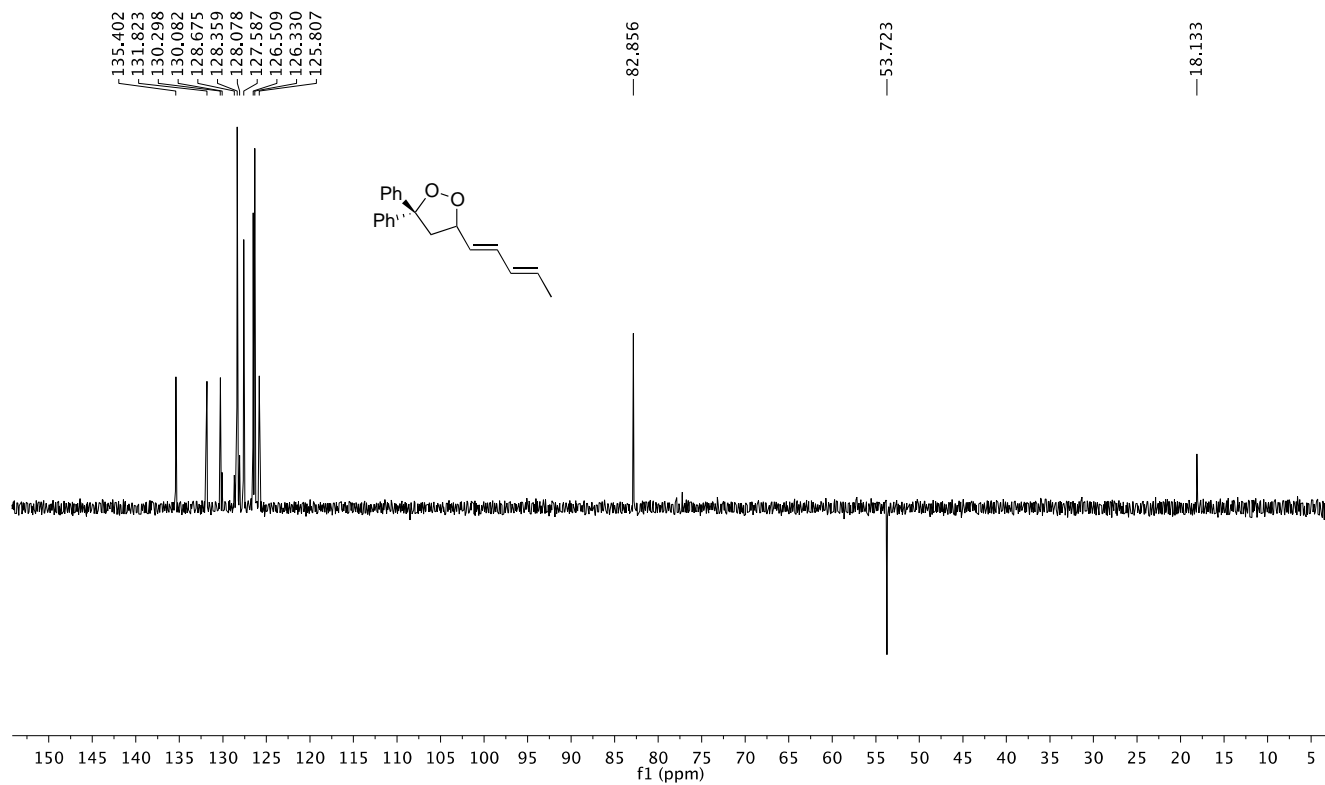


Figure S7. DEPT 135 (125 MHz) spectrum of (*E,E*)-**14** recorded at 25 °C in CDCl₃.

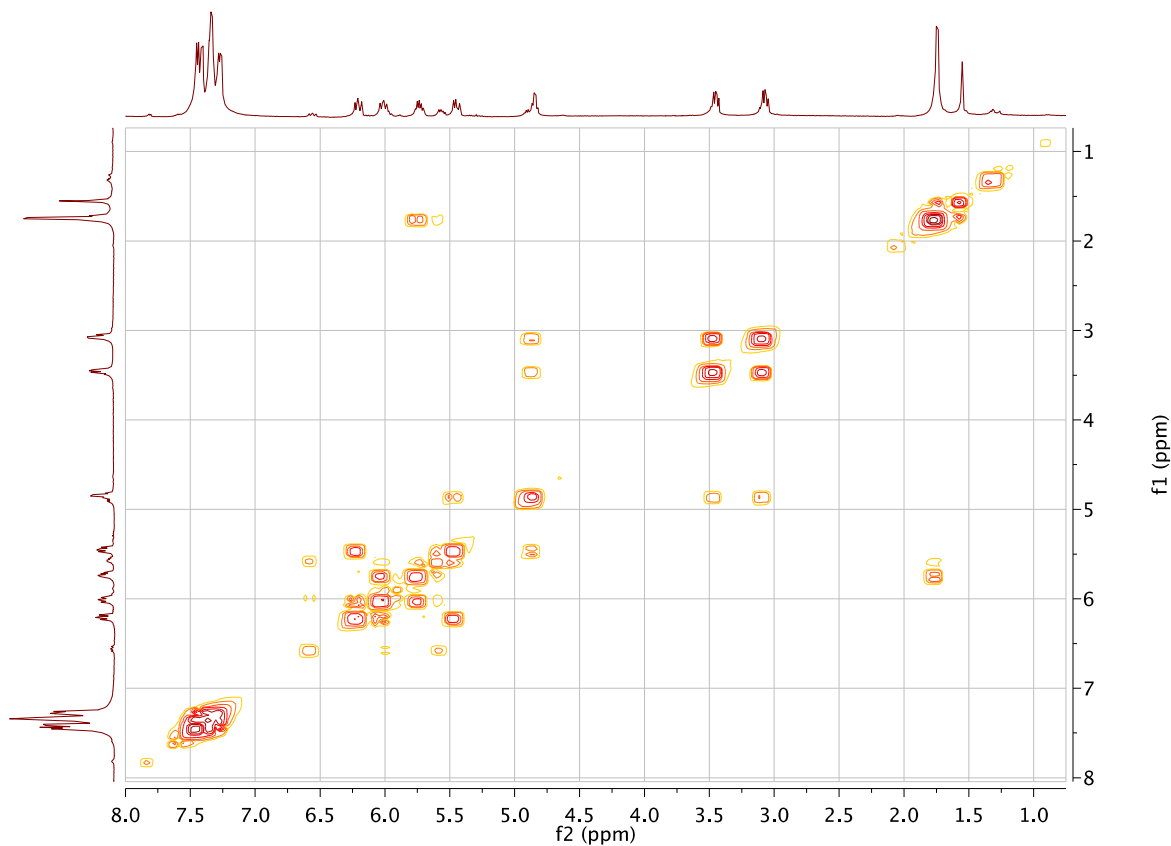


Figure S8. COSY (500 MHz) spectrum of (*E,E*)-**14** recorded at 25 °C in CDCl₃.

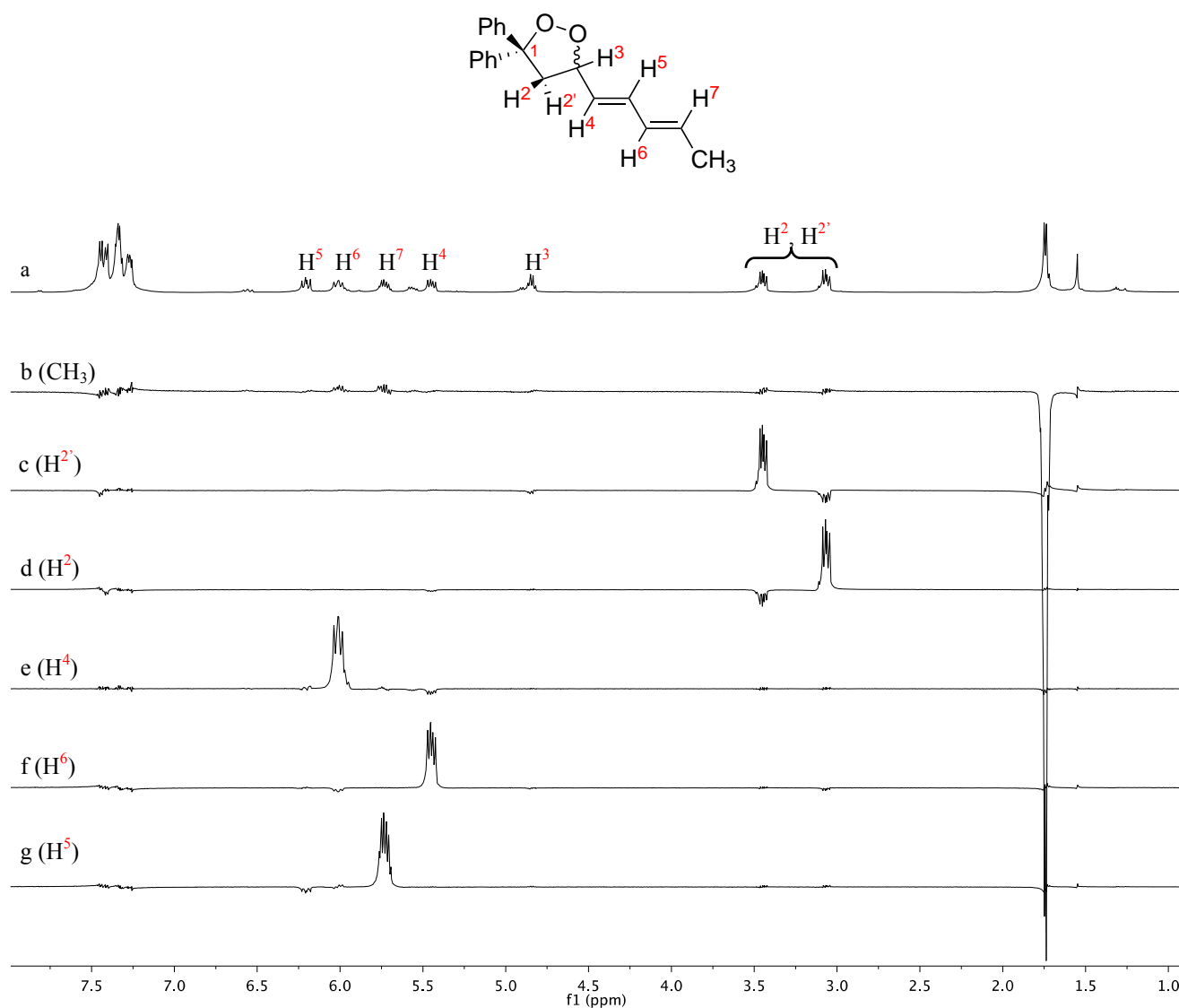


Figure S9. (a) ¹H NMR (500 MHz) spectrum of (*E,E*)-**14** recorded at 25 °C in CDCl₃. (b–g) Difference Nuclear Overhauser Effect (NOE; 500 MHz) spectra of (*E,E*)-**14** recorded at 25 °C in CDCl₃; the protons which were irradiated are depicted in parenthesis.

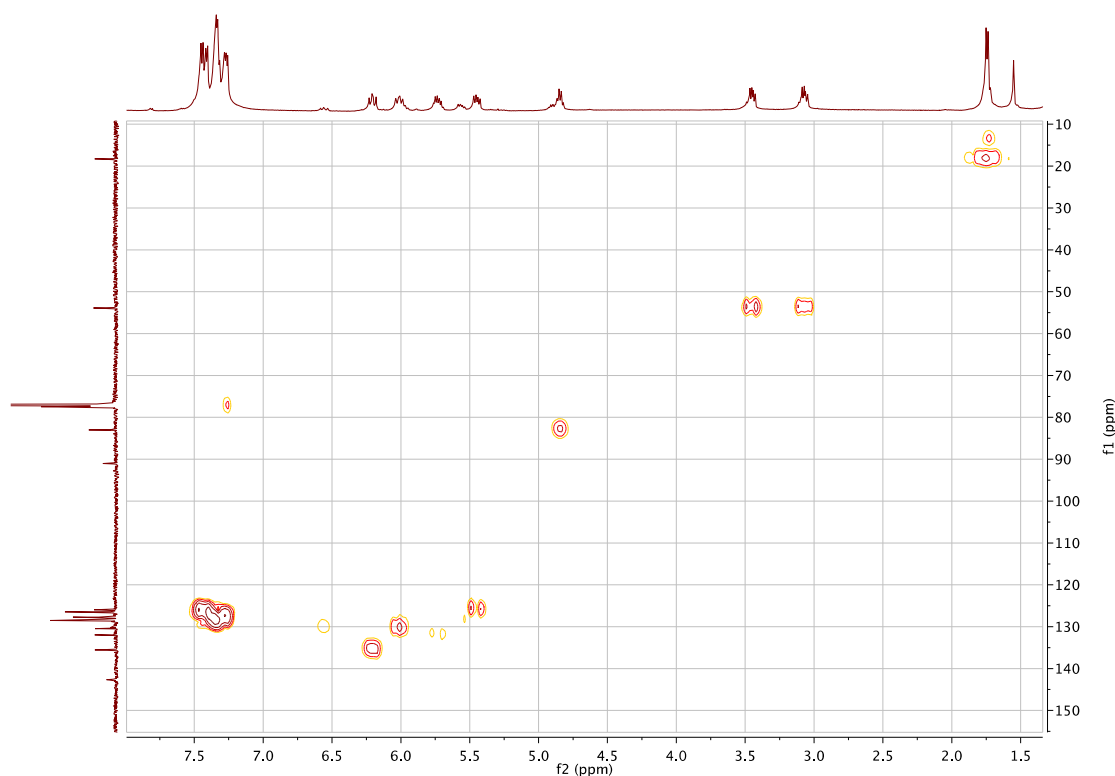


Figure S10. HMQC (500 MHz) spectrum of (*E,E*)-**14** recorded at 25 °C in CDCl₃.

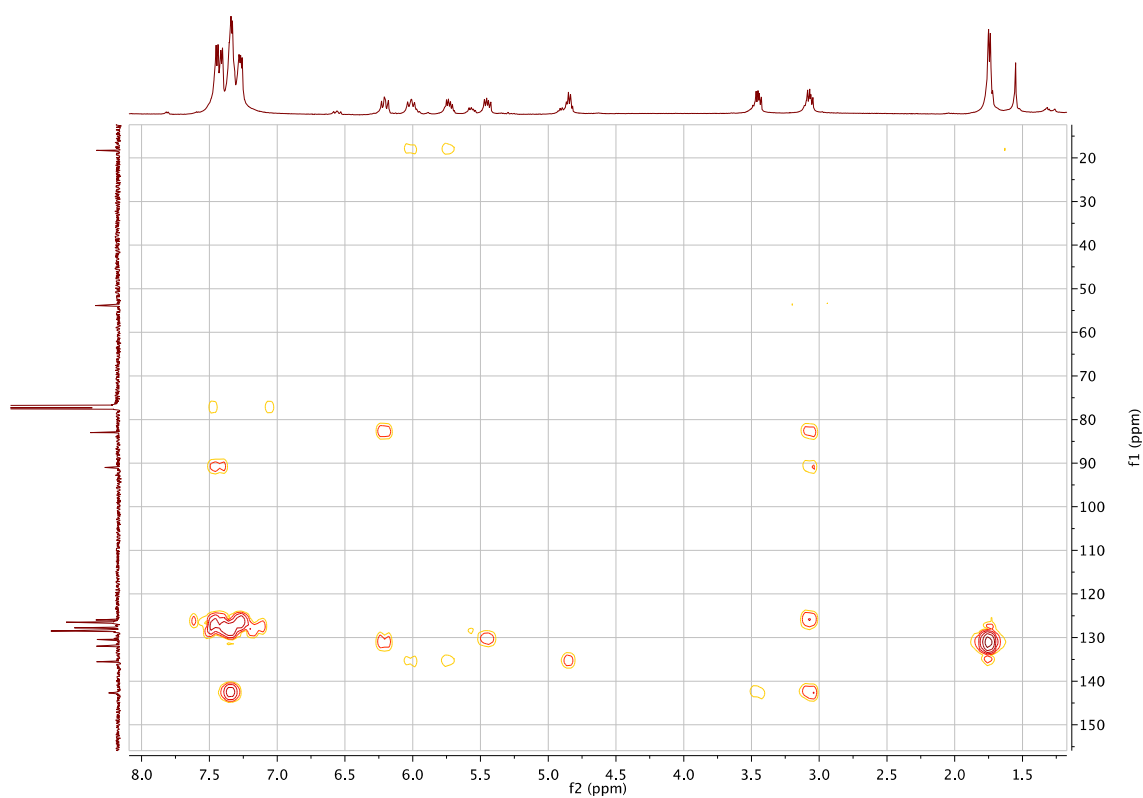


Figure S11. HMBC (500 MHz) spectrum of (*E,E*)-**14** recorded at 25 °C in CDCl₃.

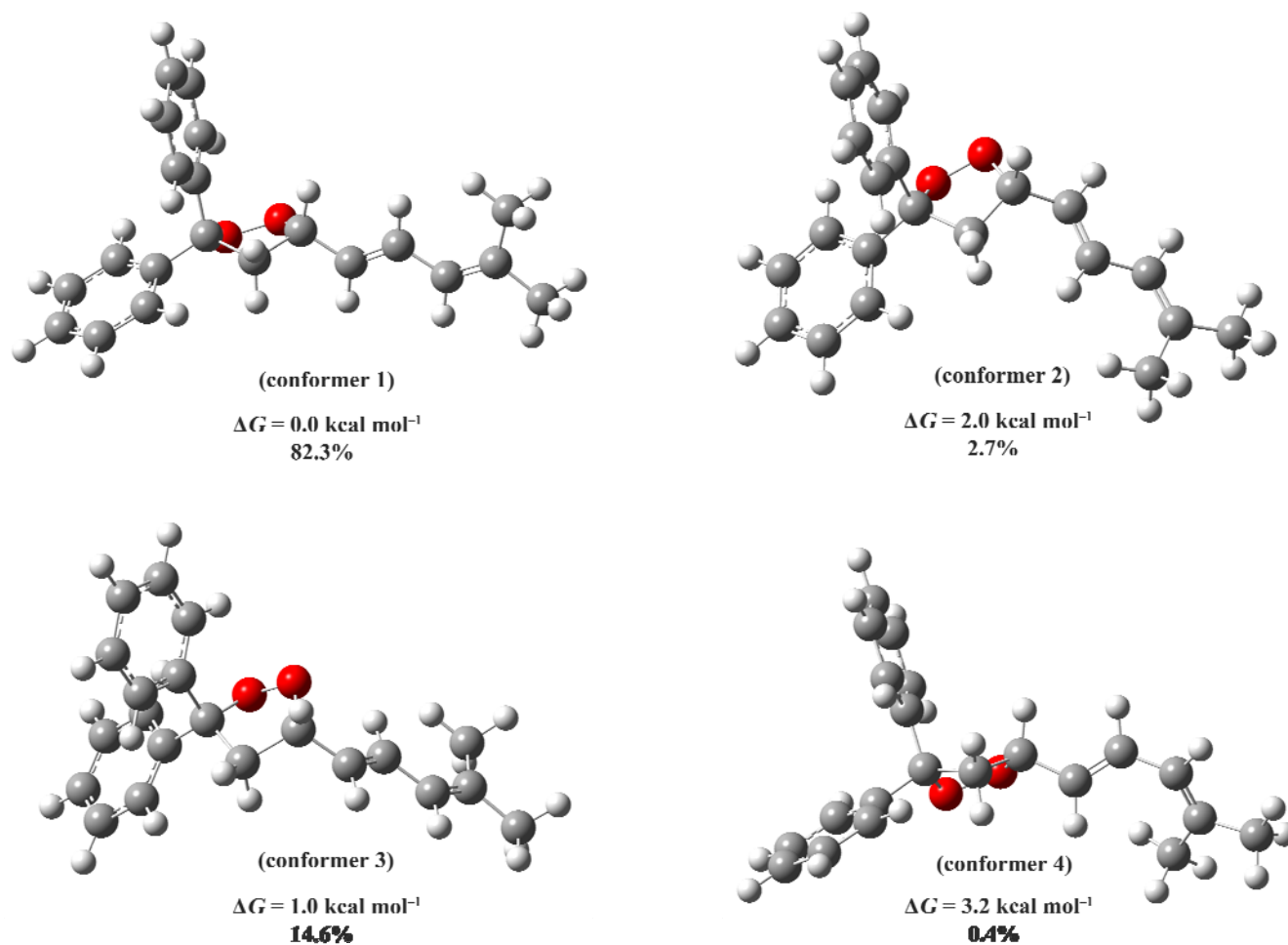
Optimized Geometries, Relative Free Energies (kcal mol^{-1}), and Boltzmann Populations (%) of the Four Low-Energy Conformers of (*E*)-13 and (*E,E*)-14

Figure S12. Optimized geometries, relative Gibbs free energies (ΔG in kcal mol^{-1}) and calculated Boltzmann populations (%) calculated thereof, for the four low-energy conformers of (*E*)-13 that are within 5 kcal mol^{-1} of the global minimum. Geometry optimizations and energy calculations were carried out at the M06-2X/6-31+G(d,p) level of theory using the IEFPCM solvation model for chloroform.

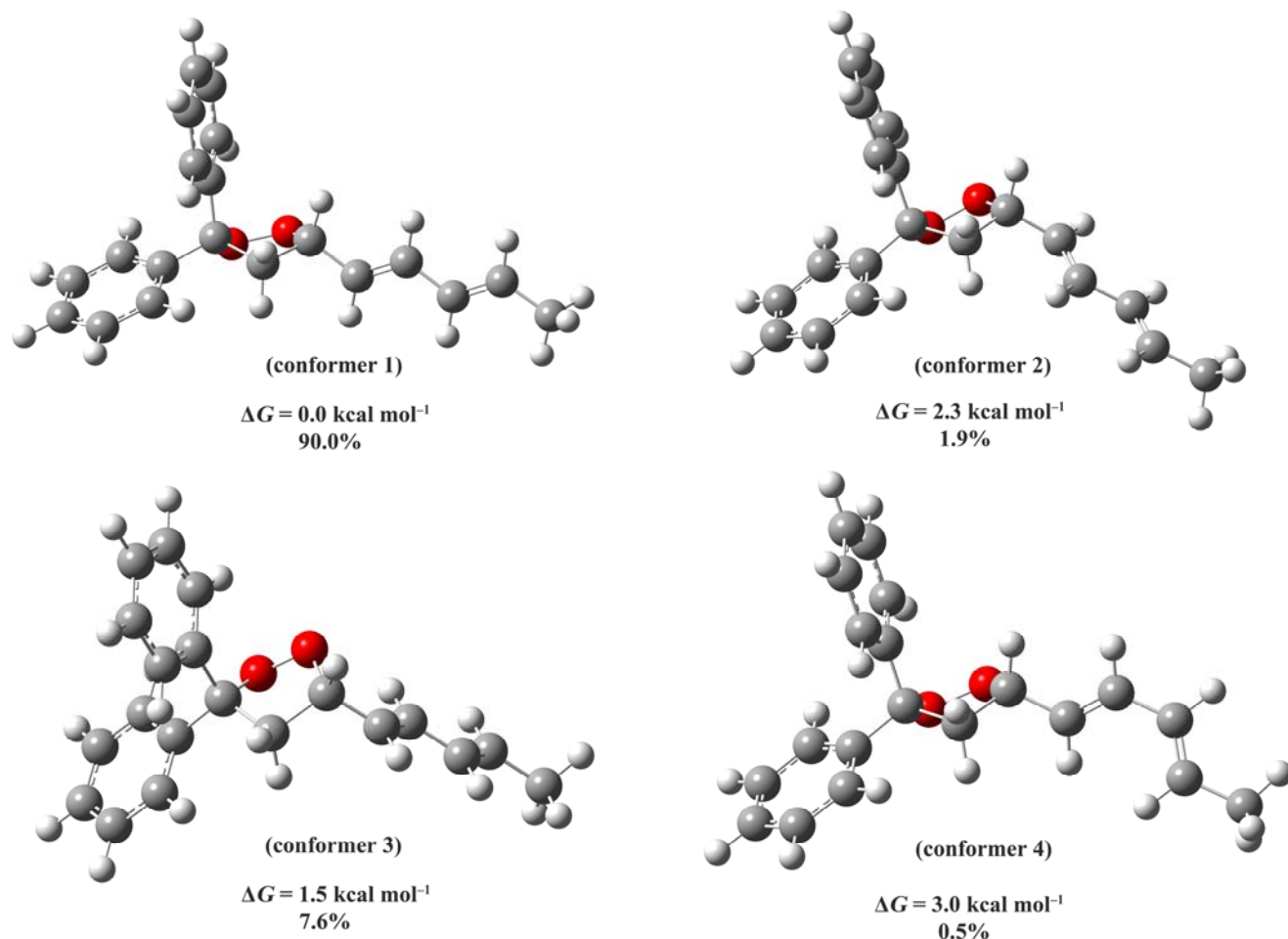
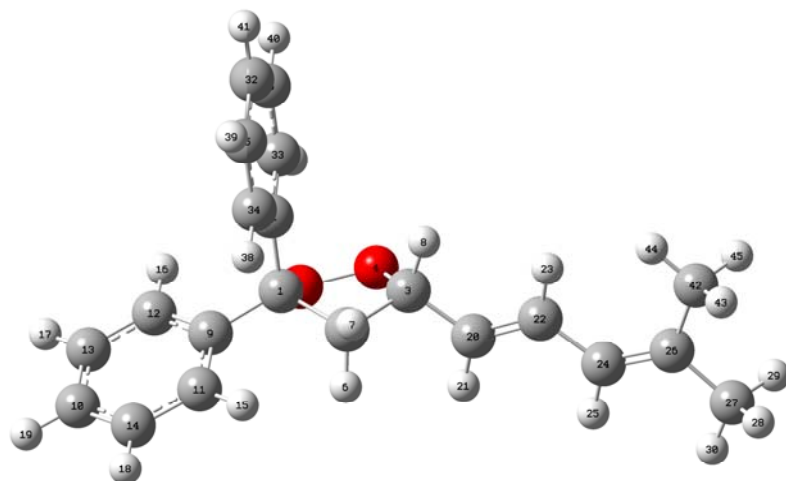


Figure S13. Optimized geometries, relative Gibbs free energies (ΔG , in kcal mol^{-1}) and Boltzmann populations (%) calculated thereof, for the four low-energy conformers of (*E,E*)-**14** that are within 5 kcal mol^{-1} of the global minimum. Geometry optimizations and energy calculations were carried out at the M06-2X/6-31+G(d,p) level of theory using the IEFPCM solvation model for chloroform.

2. Cartesian Coordinates (Å), Zero-Point Corrected Total Energies (a.u.), and Gibbs Free Energies (a.u.) of the Four Low-Energy Conformers of (*E*)-13 and (*E,E*)-14



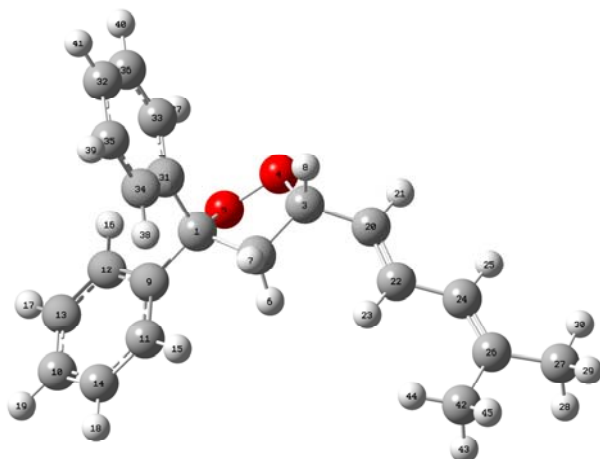
(*E*)-13 (Conformer 1)

Total energy after ZPVE correction: -963.071892 a.u.

Free Gibbs energy: -963.124618 a.u.

Atom label	Atom type	Cartesian coordinates (Å)		
		x	y	z
1	C	-1.264958	-0.23929	-0.222824
2	C	0.005702	-0.638548	0.529316
3	C	1.077212	0.010421	-0.345438
4	O	0.488182	0.045399	-1.671416
5	O	-0.857984	-0.461374	-1.577169
6	H	0.110939	-1.72798	0.518625
7	H	0.048868	-0.273591	1.557171
8	H	1.238657	1.053041	-0.040388
9	C	-2.472033	-1.13125	0.002948
10	C	-4.757519	-2.698064	0.396822
11	C	-2.589568	-1.930522	1.140319
12	C	-3.511154	-1.113002	-0.934135
13	C	-4.643327	-1.899236	-0.742788
14	C	-3.731897	-2.708247	1.338763
15	H	-1.795456	-1.950083	1.88208
16	H	-3.427175	-0.479206	-1.813514
17	H	-5.440648	-1.884881	-1.480315
18	H	-3.814838	-3.323868	2.229811

19	H	-5.643994	-3.306903	0.54918
20	C	2.373855	-0.72749	-0.399338
21	H	2.320299	-1.768891	-0.720544
22	C	3.548821	-0.170095	-0.071886
23	H	3.552955	0.876286	0.231322
24	C	4.813915	-0.89544	-0.096382
25	H	4.748336	-1.935509	-0.417805
26	C	6.027061	-0.412775	0.231378
27	C	7.249531	-1.286532	0.151824
28	H	7.73694	-1.357133	1.131567
29	H	7.986241	-0.855221	-0.536383
30	H	7.007048	-2.295729	-0.188408
31	C	-1.625569	1.228349	0.011719
32	C	-2.311597	3.902335	0.482342
33	C	-1.597659	2.154112	-1.031229
34	C	-2.001421	1.64817	1.291866
35	C	-2.34209	2.977408	1.527659
36	C	-1.940732	3.486819	-0.79459
37	H	-1.300668	1.82939	-2.023351
38	H	-2.042461	0.928455	2.107696
39	H	-2.635814	3.290631	2.525489
40	H	-1.914528	4.200655	-1.613168
41	H	-2.577853	4.939542	0.664213
42	C	6.297206	0.992654	0.695075
43	H	6.762754	0.976307	1.68746
44	H	5.404329	1.615457	0.748979
45	H	7.011809	1.478363	0.020429

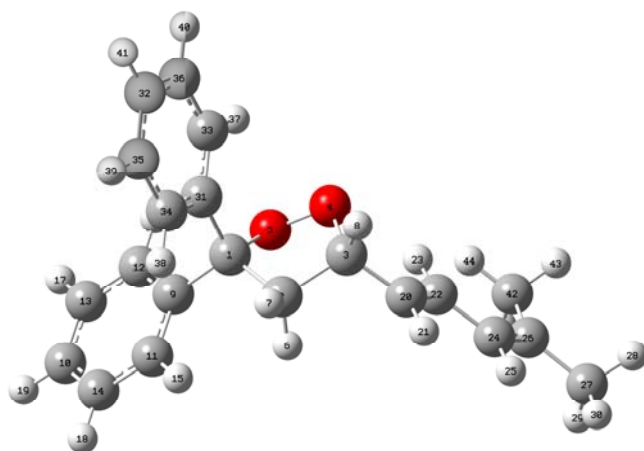
*(E)*-**13** (Conformer 2)

Total energy after ZPVE correction: -963.068399 a.u.

Free Gibbs energy: -963.121400 a.u.

Atom label	Atom type	Cartesian coordinates (Å)		
		x	y	z
1	C	1.051492	0.010845	-0.281007
2	C	-0.308114	-0.166007	0.401772
3	C	-0.892367	-1.335734	-0.390893
4	O	-0.140089	-1.363604	-1.63443
5	O	0.690036	-0.193524	-1.651205
6	H	-0.901923	0.738413	0.244507
7	H	-0.240165	-0.38241	1.469617
8	H	-0.648718	-2.287742	0.101665
9	C	1.642446	1.406666	-0.205695
10	C	2.829901	3.937894	-0.073537
11	C	1.30391	2.290145	0.819776
12	C	2.588312	1.793933	-1.161302
13	C	3.171841	3.056047	-1.100399
14	C	1.899435	3.550745	0.88791
15	H	0.57749	2.00156	1.575118
16	H	2.86382	1.101504	-1.952711
17	H	3.898116	3.350796	-1.852421
18	H	1.630637	4.229508	1.692185
19	H	3.289329	4.920784	-0.023202
20	C	-2.360789	-1.279278	-0.692624
21	H	-2.687566	-1.939999	-1.496243
22	C	-3.266526	-0.547009	-0.029001
23	H	-2.936323	0.096802	0.784087

24	C	-4.692195	-0.581065	-0.34187
25	H	-4.97127	-1.238939	-1.16576
26	C	-5.671591	0.106989	0.273216
27	C	-7.103559	-0.031692	-0.168544
28	H	-7.507733	0.940423	-0.475342
29	H	-7.729678	-0.386703	0.658795
30	H	-7.205831	-0.728131	-1.003781
31	C	2.074651	-1.026994	0.182701
32	C	3.991003	-2.869827	1.064122
33	C	2.661675	-1.915367	-0.718676
34	C	2.456048	-1.063883	1.527442
35	C	3.408115	-1.980005	1.967674
36	C	3.616501	-2.832979	-0.277556
37	H	2.362092	-1.890733	-1.761471
38	H	2.018964	-0.361583	2.235154
39	H	3.697645	-1.996544	3.014522
40	H	4.065651	-3.522357	-0.987033
41	H	4.733849	-3.58514	1.405093
42	C	-5.466374	1.054983	1.423527
43	H	-5.832744	2.053072	1.156396
44	H	-4.42557	1.147994	1.734111
45	H	-6.052543	0.725996	2.289571

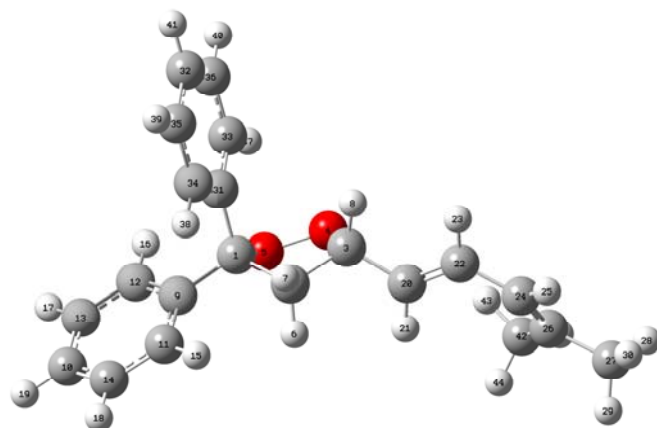
*(E)*-**13** (Conformer 3)

Total energy after ZPVE correction: -963.069762 a.u.

Free Gibbs energy: -963.122989 a.u.

Atom label	Atom type	Cartesian coordinates (Å)		
		x	y	z
1	C	-1.013492	0.012349	-0.142973
2	C	-0.119163	-0.232856	-1.364053
3	C	0.879526	-1.275822	-0.818907
4	O	0.660099	-1.300963	0.602624
5	O	-0.060661	-0.105687	0.921541
6	H	0.410335	0.688101	-1.621302
7	H	-0.663725	-0.595814	-2.237444
8	H	0.612326	-2.281996	-1.167008
9	C	-1.598106	1.409059	-0.032739
10	C	-2.764288	3.941055	0.222634
11	C	-1.809056	2.203937	-1.160039
12	C	-1.985237	1.885024	1.224791
13	C	-2.556447	3.147918	1.352468
14	C	-2.394553	3.464518	-1.032857
15	H	-1.522988	1.845663	-2.145574
16	H	-1.835949	1.2612	2.102358
17	H	-2.844551	3.512046	2.334447
18	H	-2.556444	4.073645	-1.917495
19	H	-3.214894	4.924302	0.321871
20	C	2.307418	-0.962202	-1.163487
21	H	2.552174	-1.027538	-2.225173
22	C	3.245025	-0.609138	-0.274947
23	H	2.959507	-0.559352	0.773086

24	C	4.61926	-0.29553	-0.655343
25	H	4.836744	-0.363348	-1.722321
26	C	5.623389	0.058824	0.167566
27	C	6.997209	0.350827	-0.373499
28	H	7.739726	-0.318746	0.077137
29	H	7.301822	1.373838	-0.121718
30	H	7.040211	0.234442	-1.458907
31	C	-2.119855	-1.035571	-0.006658
32	C	-4.208291	-2.886846	0.239451
33	C	-2.229307	-1.824016	1.139186
34	C	-3.066039	-1.176324	-1.026302
35	C	-4.104498	-2.096786	-0.906088
36	C	-3.269925	-2.745823	1.26011
37	H	-1.492767	-1.720146	1.929374
38	H	-3.002664	-0.552444	-1.916098
39	H	-4.834088	-2.194273	-1.70498
40	H	-3.343235	-3.357321	2.15509
41	H	-5.016819	-3.605797	0.335031
42	C	5.50043	0.199093	1.660571
43	H	6.202495	-0.478888	2.160204
44	H	4.499205	-0.010459	2.036941
45	H	5.774073	1.215937	1.965841

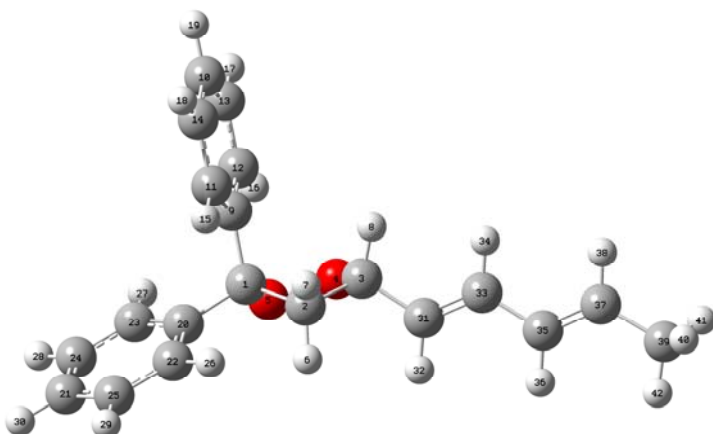
*(E)*-**13** (Conformer 4)

Total energy after ZPVE correction: -963.067142 a.u.

Free Gibbs energy: -963.119528 a.u.

Atom label	Atom type	Cartesian coordinates (Å)		
		x	y	z
1	C	1.09923	-0.182463	0.11359
2	C	-0.109401	-0.311248	-0.814947
3	C	-1.147688	0.511264	-0.05482
4	O	-0.751424	0.396931	1.336411
5	O	0.477648	-0.354853	1.391662
6	H	-0.418328	-1.359809	-0.871351
7	H	0.057304	0.079117	-1.820607
8	H	-1.067729	1.572909	-0.323913
9	C	2.136915	-1.284509	0.002524
10	C	4.116072	-3.256455	-0.164462
11	C	2.248704	-2.07366	-1.142322
12	C	3.029685	-1.481048	1.062145
13	C	4.007631	-2.467849	0.982807
14	C	3.239157	-3.054037	-1.227162
15	H	1.569474	-1.928268	-1.978131
16	H	2.953053	-0.856504	1.948814
17	H	4.689966	-2.618876	1.814358
18	H	3.319769	-3.660288	-2.12482
19	H	4.883309	-4.022579	-0.228856
20	C	-2.556385	0.035657	-0.204981
21	H	-2.732379	-1.011937	0.037916
22	C	-3.546363	0.826904	-0.639287
23	H	-3.290655	1.852562	-0.913784

24	C	-4.9495	0.444973	-0.842761
25	H	-5.430984	0.90461	-1.706177
26	C	-5.701378	-0.360897	-0.070989
27	C	-7.129578	-0.660633	-0.440742
28	H	-7.811765	-0.308297	0.341836
29	H	-7.281857	-1.743175	-0.527515
30	H	-7.413193	-0.194652	-1.387182
31	C	1.756992	1.193427	0.000496
32	C	2.990483	3.695352	-0.245396
33	C	1.767804	2.079386	1.077744
34	C	2.369517	1.565838	-1.200494
35	C	2.982524	2.809726	-1.324666
36	C	2.383946	3.326262	0.953212
37	H	1.287536	1.792412	2.007806
38	H	2.380682	0.87329	-2.040485
39	H	3.458022	3.086263	-2.261407
40	H	2.385829	4.010115	1.797415
41	H	3.469196	4.665739	-0.339994
42	C	-5.230953	-1.007077	1.204588
43	H	-4.363583	-0.49968	1.631524
44	H	-4.958209	-2.055787	1.032666
45	H	-6.039737	-1.007269	1.942841

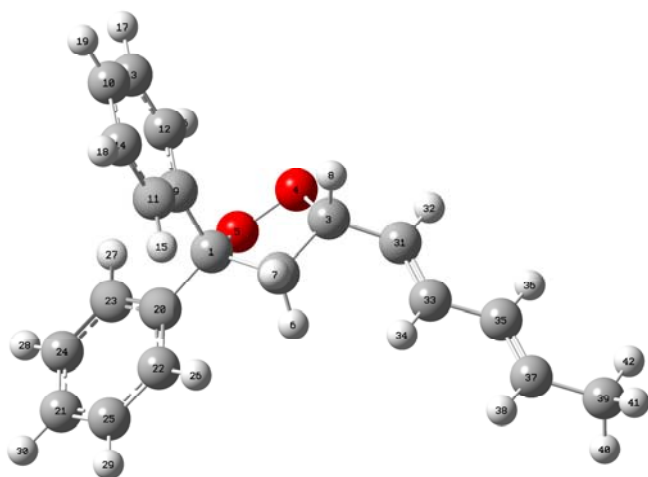
*(E,E)*-**14** (Conformer 1)

Total energy after ZPVE correction: -923.801146 a.u.

Free Gibbs energy: -923.851989 a.u.

Atom label	Atom type	Cartesian coordinates (Å)		
		x	y	z
1	C	-0.933244	-0.227447	-0.214853
2	C	0.333795	-0.611022	0.551267
3	C	1.401726	0.08536	-0.290395
4	O	0.838377	0.125869	-1.626739
5	O	-0.498064	-0.41179	-1.56617
6	H	0.468042	-1.696807	0.518166
7	H	0.349755	-0.268143	1.587442
8	H	1.526407	1.126341	0.036598
9	C	-1.332353	1.226052	0.043232
10	C	-2.088213	3.872726	0.557498
11	C	-1.736955	1.610181	1.32578
12	C	-1.310574	2.173461	-0.980174
13	C	-1.688572	3.492599	-0.721784
14	C	-2.112497	2.925912	1.583224
15	H	-1.773418	0.872754	2.125867
16	H	-0.991154	1.87622	-1.973977
17	H	-1.666974	4.223665	-1.525142
18	H	-2.428362	3.21161	2.582547
19	H	-2.381684	4.899429	0.756262
20	C	-2.122634	-1.15201	-0.02926
21	C	-4.376802	-2.780193	0.289319
22	C	-2.23571	-1.987179	1.082338
23	C	-3.150843	-1.128847	-0.978323

24	C	-4.267125	-1.945323	-0.824643
25	C	-3.362563	-2.795601	1.243369
26	H	-1.450609	-2.010958	1.833471
27	H	-3.070879	-0.467193	-1.837353
28	H	-5.05575	-1.926624	-1.571358
29	H	-3.442234	-3.439014	2.114863
30	H	-5.25115	-3.412683	0.412598
31	C	2.720983	-0.612688	-0.331484
32	H	2.706546	-1.648647	-0.673363
33	C	3.87027	-0.027209	0.030998
34	H	3.855003	1.014509	0.357823
35	C	5.167598	-0.695118	0.028169
36	H	5.188417	-1.734447	-0.303603
37	C	6.305342	-0.096435	0.406609
38	H	6.261418	0.943507	0.735081
39	C	7.652584	-0.749901	0.414116
40	H	8.084507	-0.743532	1.420791
41	H	8.351783	-0.2107	-0.234184
42	H	7.592544	-1.785822	0.070718

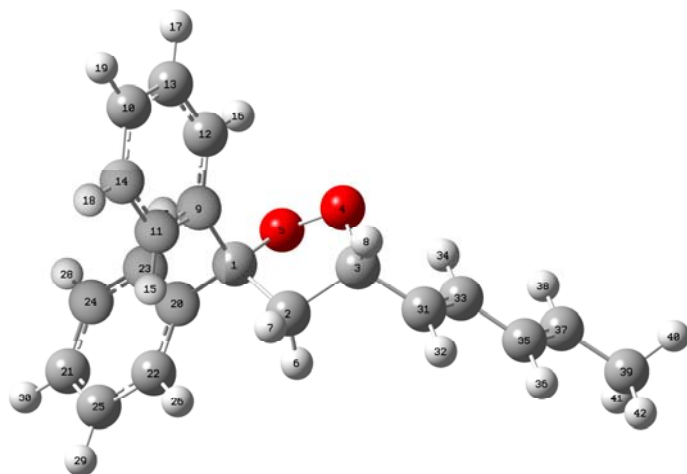
*(E,E)*-**14** (Conformer 2)

Total energy after ZPVE correction: -923.797575 a.u.

Free Gibbs energy: -923.848337 a.u.

Atom label	Atom type	Cartesian coordinates (Å)		
		x	y	z
1	C	0.756402	0.032656	-0.238178
2	C	-0.576956	-0.134228	0.497726
3	C	-1.232728	-1.251937	-0.315833
4	O	-0.5207	-1.267073	-1.582227
5	O	0.330405	-0.112999	-1.597373
6	H	-1.148956	0.792806	0.405715
7	H	-0.468885	-0.397799	1.551496
8	H	-1.014793	-2.230383	0.134809
9	C	1.771805	-1.046288	0.141527
10	C	3.678601	-2.965501	0.867285
11	C	2.206727	-1.146957	1.466568
12	C	2.301302	-1.908766	-0.818737
13	C	3.251228	-2.864592	-0.455226
14	C	3.15403	-2.101352	1.829414
15	H	1.815748	-0.465203	2.219862
16	H	1.960563	-1.834369	-1.846416
17	H	3.65492	-3.533441	-1.21019
18	H	3.485333	-2.167573	2.861817
19	H	4.417351	-3.710609	1.148048
20	C	1.387167	1.409391	-0.139498
21	C	2.647848	3.902478	0.032661
22	C	1.121936	2.259492	0.934617
23	C	2.296631	1.810369	-1.124208

24	C	2.916432	3.053967	-1.04299
25	C	1.754005	3.500879	1.022458
26	H	0.424559	1.959653	1.712633
27	H	2.515314	1.143386	-1.954262
28	H	3.613888	3.360005	-1.817431
29	H	1.542299	4.153511	1.864549
30	H	3.135749	4.870611	0.098618
31	C	-2.70653	-1.125085	-0.56763
32	H	-3.084077	-1.735458	-1.388568
33	C	-3.561496	-0.390165	0.155191
34	H	-3.19913	0.210586	0.990732
35	C	-4.999188	-0.3425	-0.097129
36	H	-5.372828	-0.937113	-0.932485
37	C	-5.855554	0.382712	0.634987
38	H	-5.46199	0.970449	1.466293
39	C	-7.333062	0.452498	0.399827
40	H	-7.649759	1.482648	0.203805
41	H	-7.886477	0.112987	1.282129
42	H	-7.628056	-0.166544	-0.45136

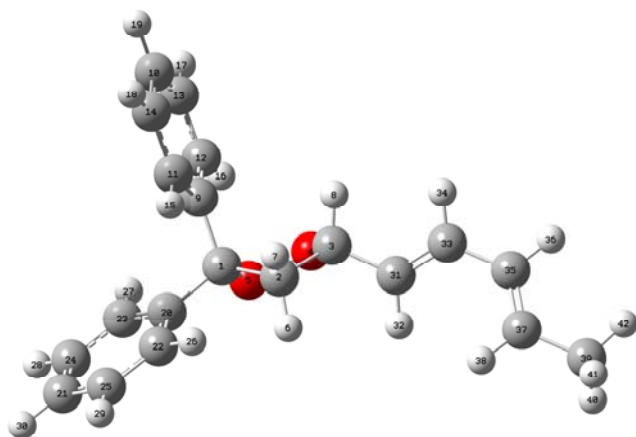
*(E,E)*-**14** (Conformer 3)

Total energy after ZPVE correction: -923.798972 a.u.

Free Gibbs energy: -923.849666 a.u.

Atom label	Atom type	Cartesian coordinates (Å)		
		x	y	z
1	C	0.720883	0.007158	0.107874
2	C	-0.213153	-0.238654	1.299639
3	C	-1.19647	-1.279695	0.721878
4	O	-0.910524	-1.32735	-0.686359
5	O	-0.191995	-0.127109	-0.989242
6	H	-0.749094	0.682548	1.542014
7	H	0.30371	-0.603198	2.189014
8	H	-0.95885	-2.284172	1.094813
9	C	1.842184	-1.03	0.016898
10	C	3.95897	-2.858317	-0.145811
11	C	2.752644	-1.155931	1.070382
12	C	2.001514	-1.821965	-1.120658
13	C	3.056173	-2.732294	-1.19994
14	C	3.805071	-2.064928	0.991731
15	H	2.650299	-0.529553	1.95479
16	H	1.292681	-1.729751	-1.937227
17	H	3.168437	-3.346596	-2.08895
18	H	4.506488	-2.150774	1.816753
19	H	4.778513	-3.568293	-0.209174
20	C	1.295887	1.408789	0.009916
21	C	2.448691	3.949487	-0.2187
22	C	1.473716	2.205689	1.141579
23	C	1.709522	1.887186	-1.238128

24	C	2.274024	3.154414	-1.352676
25	C	2.05253	3.470552	1.027865
26	H	1.166737	1.845533	2.120176
27	H	1.586216	1.262097	-2.118766
28	H	2.582805	3.520331	-2.327689
29	H	2.188469	4.081172	1.915832
30	H	2.893998	4.93613	-0.30757
31	C	-2.634872	-0.944033	0.995093
32	H	-2.927966	-0.98206	2.045739
33	C	-3.527811	-0.601334	0.059428
34	H	-3.213891	-0.571877	-0.98368
35	C	-4.917161	-0.260166	0.352492
36	H	-5.224769	-0.291813	1.399494
37	C	-5.809943	0.08089	-0.586717
38	H	-5.48447	0.107038	-1.62805
39	C	-7.240327	0.435024	-0.317011
40	H	-7.918693	-0.241246	-0.848633
41	H	-7.465787	1.4487	-0.665914
42	H	-7.467111	0.380237	0.751028

*(E,E)*-14 (Conformer 4)

Total energy after ZPVE correction: -923.796518 a.u.

Free Gibbs energy: -923.847114 a.u.

Atom label	Atom type	Cartesian coordinates (Å)		
		x	y	z
1	C	-0.815863	-0.17248	-0.217611
2	C	0.495274	-0.347816	0.550576
3	C	1.426055	0.553953	-0.25917
4	O	0.868718	0.540255	-1.597885
5	O	-0.34673	-0.23394	-1.568723
6	H	0.820382	-1.391054	0.486635
7	H	0.445051	-0.039818	1.596542
8	H	1.364397	1.588827	0.103248
9	C	-1.470736	1.177391	0.078236
10	C	-2.695922	3.627413	0.658628
11	C	-1.937227	1.447264	1.368821
12	C	-1.623284	2.139597	-0.920057
13	C	-2.234987	3.360468	-0.628629
14	C	-2.546143	2.665263	1.659167
15	H	-1.838031	0.694747	2.14932
16	H	-1.255621	1.931959	-1.919924
17	H	-2.347769	4.104295	-1.412426
18	H	-2.907815	2.862067	2.664402
19	H	-3.171355	4.577863	0.883068
20	C	-1.822268	-1.299488	-0.074655
21	C	-3.750566	-3.314344	0.160963
22	C	-1.795942	-2.174586	1.011323
23	C	-2.827595	-1.431655	-1.039189

24	C	-3.780681	-2.439295	-0.926864
25	C	-2.7608	-3.176722	1.130917
26	H	-1.027777	-2.079944	1.774369
27	H	-2.858094	-0.740643	-1.878009
28	H	-4.551553	-2.539474	-1.685546
29	H	-2.733265	-3.850361	1.982569
30	H	-4.49801	-4.097159	0.251925
31	C	2.848035	0.100223	-0.312408
32	H	3.018008	-0.898395	-0.717072
33	C	3.869836	0.861314	0.098763
34	H	3.655883	1.878456	0.430966
35	C	5.279267	0.445382	0.125408
36	H	6.018968	1.230014	-0.03774
37	C	5.702349	-0.803892	0.356919
38	H	4.963399	-1.575493	0.577993
39	C	7.139255	-1.228218	0.351195
40	H	7.313365	-1.998477	-0.408139
41	H	7.42455	-1.662651	1.315228
42	H	7.801039	-0.383913	0.141461

3. Full Citation for Gaussian 09 (Ref. 56 of Main Manuscript)

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