Supplementary information for

Geminal Diol of Dihydrolevoglucosenone as a Switchable Hydrotrope: A Continuum of Green Nanostructured Solvents

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- **Figure 3S_B:** ^{1}H NMR spectra showing the evolution of a 65 wt% Cyrene in H_2O mixture when decreasing the temperature from 298K to 258K.
- **Quantum Chemical and Density Functional Theory Calculations**

Materials, methods and instrumentation

Double distilled dihydrolevoglucosenone (Cyrene) was provided by the Circa company and used as is.

^{1}H and ^{13}C NMR experiments were recorded in the absence of a deuterated solvent. It was determined that a relaxation delay of 20s allowed for reliable quantification of the ^{1}H and ^{13}C NMR signals. To aid with the quantification the NMR tubes were filled to ~4 cm height in an as consistent manner as possible. Composition of the TM-H_2O mixture was determined from ^{1}H NMR data while the solubility data was recorded from ^{13}C NMR data as to avoid the higher complexity of the ^{1}H NMR data.

All Cyrene-H_2O mixtures were prepared to a total volume of 2 mL and stirred at 400 rpm for 30 minutes. This allows in all cases to obtain a homogeneous solution. Inhomogeneity of the Cyrene/water mixtures is commonly observed for samples rich in Cyrene but disappearing through continued stirring (30 min is ample) or gentle heating (e.g. in the hand). To determine the solubility, saturated solutions were prepared and stirred for 35 minutes at 400 rpm. This is followed by room temperature centrifugation at 3500 rpm. The supernatant was pipetted out, filtered over cotton if still cloudy, and added into an NMR tube to a liquid height of 4 cm.

The NMR spectra at the University of Wisconsin-Madison were taken using an Avance-400. No D spectra were taken by turning off the lock and shimming on ^{1}H using the topshim option 1h lockoff o1p=<value in ppm> selwid=0.5. A preliminary ^{1}H NMR spectrum without shimming is used to determine the chemical shift of a peak used in the shimming routine.

The NMR spectra at the University of York were taken on a Bruker AVIIIHD 500 MHz. The instrument runs Topspin 3.5. and uses a TBO triple resonance probe for HFX.

An exemplary calculation of maximal solubility for the particular case of aspirin is shown below in illustrative ^{13}C and ^{1}H NMR spectra

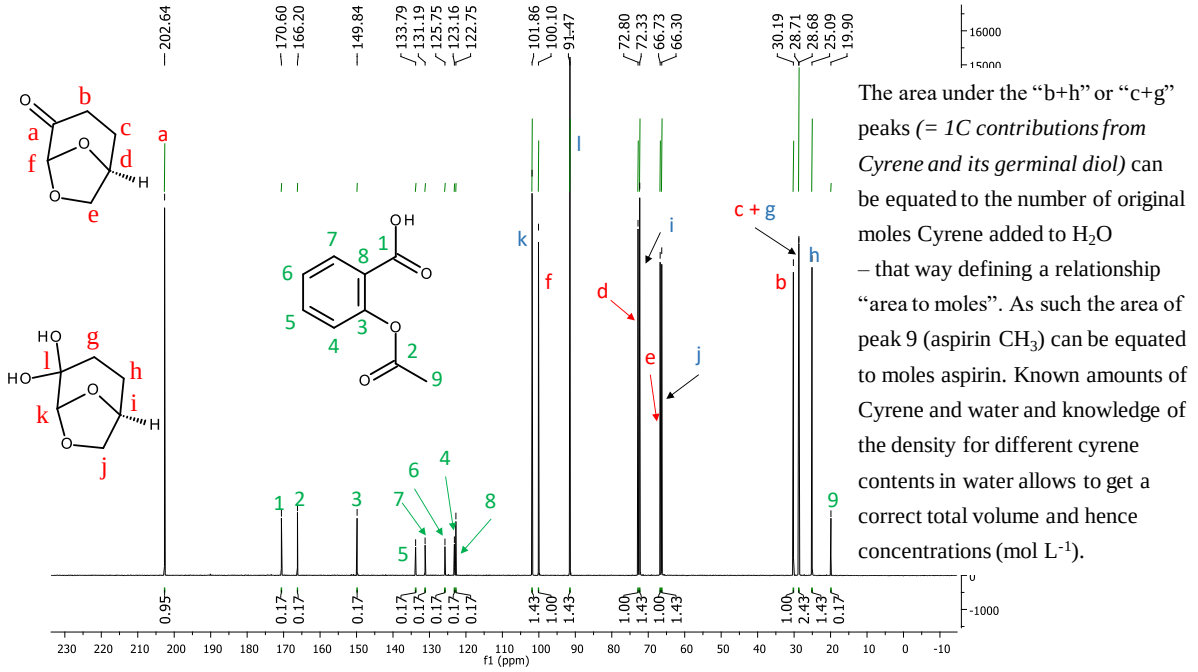


Figure 1S_A: ^{13}C NMR spectrum (with annotations) of the maximal dissolution of aspirin in a Cyrene/ Cyrene gem diol /H_2O mixture made by adding Cyrene in 70 wt% to H_2O.

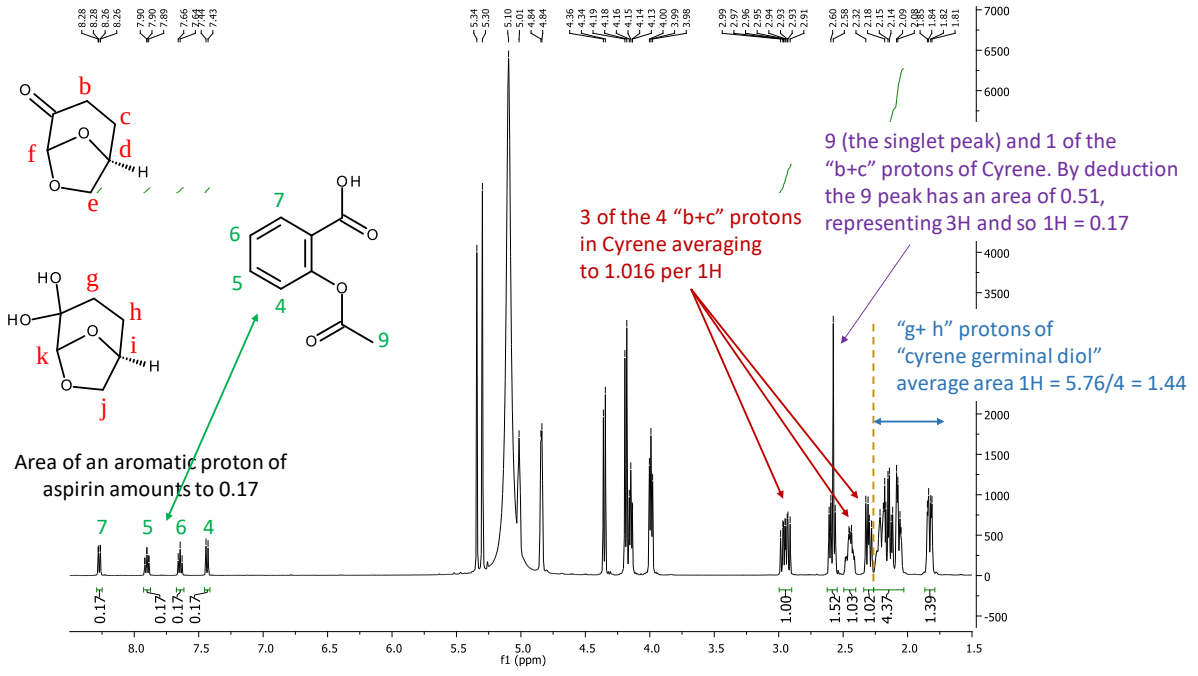


Figure 1S_B: ^{1}H NMR spectrum (with annotations) of the maximal dissolution of aspirin in a Cyrene/ Cyrene gem diol /H_2O mixture made by adding Cyrene in 70 wt% to H_2O.

Table 1S_A: Solubilities of aspirin, salicylic acid, ferulic acid and phthalic acid as a function of the wt% of Cyrene in H_2O. [293 K]

wt% Cyrene	Salicylic acid (mol L^{-1})	wt% Cyrene	Aspirin (mol L^{-1})	wt% Cyrene	Ferulic acid (mol L^{-1})	wt% Cyrene	Phthalic acid (mol L^{-1})	wt% Cyrene	Ibuprofen (mol L^{-1})
100.0	0.68	100.0	0.29	100.0	0.20	100.0	0.05	100.0	0.68
97.2	1.09	97.5	0.72	**94.9**	**0.50**	95.1	0.21	**97.1**	**0.99**
94.6	1.35	**95.0**	**0.93**	**90.1**	**0.58**	90.0	0.35	**95.0**	**1.02**
92.4	1.49	**89.7**	**0.92**	**85.0**	**0.59**	**84.9**	**0.41**	**92.5**	**1.02**
89.4	**1.65**	84.6	0.88	80.2	0.52	**79.8**	**0.44**	89.9	0.93
84.8	1.55	80.1	0.77	75.3	0.44	**75.3**	**0.42**	85.1	0.72
79.5	1.49	74.6	0.66	70.0	0.39	70.2	0.41	80.2	0.54
77.5	1.22	70.2	0.48	64.9	0.26	65.4	0.35	75.2	0.30
74.8	1.06	64.8	0.34	59.8	0.16	60.2	0.27	70.1	0.14
70.4	0.98	60.1	0.26	55.0	0.11	55.0	0.22	64.9	0.05
64.9	0.52	54.8	0.15	49.9	0.06	50.0	0.16		
59.9	0.32	49.9	0.11						
50.2	0.12	45.2	0.07						
39.8	0.05	29.9	0.04						
19.9	0.01	25.2	0.03						
10.3	0.01	9.9	0.02						
		8.9	0.02						

Table 1S_B: Experimental solubilities of mandelic acid and caffeine as a function of the wt% of Cyrene in H_2O. [293 K]

wt% Cyrene	Mandelic acid (mol L^{-1})	wt% Cyrene	Caffeine (mol L^{-1})
100.0	1.66	100.0	0.10
95.0	3.40	94.9	0.25
89.9	4.37	89.9	0.42
85.0	**4.92**	85.0	0.46
80.1	**4.71**	**80.2**	**0.52**
75.1	**4.73**	**75.1**	**0.51**
70.1	4.67	**70.0**	**0.52**
64.9	4.59	65.1	0.47
63.3	5.63	60.0	0.48
62.4	5.48	54.9	0.41
59.7	5.74	50.4	0.39
55.0	5.35	45.2	0.26
49.7	4.87	40.0	0.21
45.1	4.72	30.2	0.17
40.1	4.18	19.8	0.15
34.9	3.55	9.9	0.11
30.2	3.67		
27.5	2.89		
25.7	2.70		
22.6	2.44		
19.9	2.58		
17.6	1.92		
14.7	1.63		
10.6	1.50		
5.2	1.21		

Table 2S_A: Composition of the Cyrene/gem diol/water ternary mixture (mol geminal diol and mol H_2O both normalized to 1 mol Cyrene). [298 K]

wt% Cyrene in H_2O	mol geminal diol/ mol Cyrene	mol H_2O/ mol Cyrene
5.2	6.4	955.1
10.1	8.6	600.6
15.0	10.2	442.9
20.0	10.7	322.4
25.0	10.5	235.5
30.2	10.0	171.4
35.1	9.2	125.3
39.4	8.3	93.2
45.0	7.1	63.1
50.3	5.6	41.0
53.8	4.7	30.0
60.1	3.3	16.9
65.0	2.3	10.4
70.3	1.6	6.1
75.5	1.0	3.7
80.1	0.7	2.3
84.8	0.5	1.4
89.9	0.3	0.7
95.1	0.1	0.3
100.0	0.0	0.0

Table 2S_B: Concentration data of the different components in the ternary mixture and calculated Keq. [298 K]

wt% Cyrene in H_2O	M Cyrene ($mol\ L^{-1}$)	M gem diol ($mol\ L^{-1}$)	M H_2O ($mol\ L^{-1}$)	Keq (basic)	Keq (advanced)
5.2	0.02	0.39	53.01	0.43	0.008
10.1	0.03	0.78	50.73	0.45	0.009
15.0	0.06	1.17	48.44	0.41	0.009
20.0	0.09	1.58	46.01	0.38	0.009
25.0	0.12	2.01	43.50	0.38	0.010
30.2	0.18	2.45	40.79	0.34	0.009
35.1	0.23	2.89	38.05	0.33	0.010
39.5	0.30	3.26	35.57	0.30	0.010
45.0	0.42	3.72	32.27	0.28	0.011
50.3	0.61	4.10	28.99	0.23	0.011
53.8	0.80	4.28	26.79	0.20	0.011
60.1	1.26	4.51	22.79	0.16	0.011
65.0	1.87	4.45	19.77	0.12	0.010
70.3	2.64	4.26	16.47	0.10	0.011
75.5	3.62	3.84	13.40	0.08	0.012
80.1	4.59	3.35	10.65	0.07	0.014
84.9	5.69	2.73	7.96	0.06	0.018
89.9	7.00	1.89	5.21	0.05	0.024
95.1	8.35	1.00	2.44	0.05	0.058

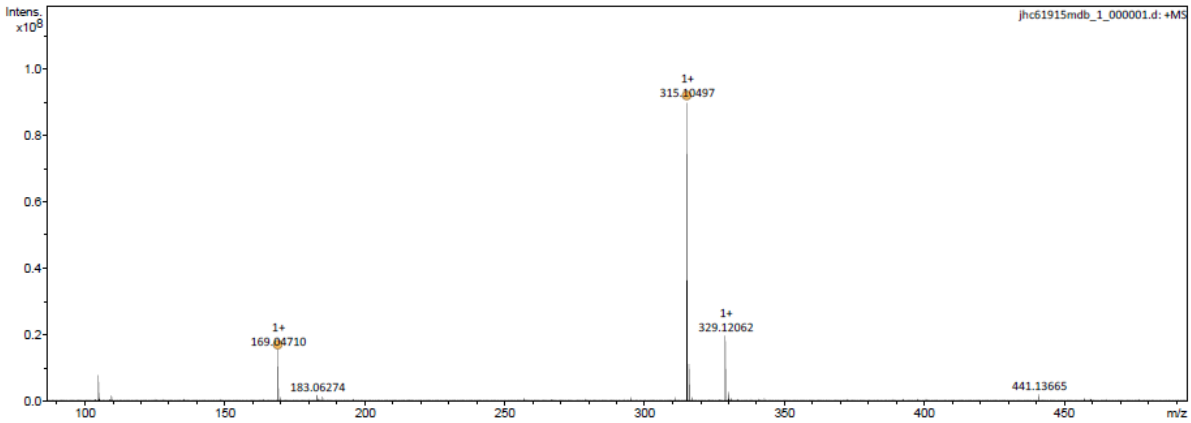
Table 3S: Data on relative solubility increases vis-à-vis water and ranges of maximum solubility.

Compound	MW	Solubility in water g L^{-1} / (mol L^{-1})	Maximum attainable solubility in TM-H_2O (mol L^{-1})	wt% Cyrene in H_2O range at which maximum dissolution is observed	Maximal increase in solubility vis-à-vis solubility in water (factor)	Log Kow
Aspirin (acetyl-salicylic acid)	180.159	4.6 (0.026)	0.93	89.7-95.0	36	1.19
Salicylic acid	138.122	2.24 (0.016)	1.65	89.4	102	2.26
Phthalic acid	166.132	6.25 (0.038)	0.41-0.44	75.2-84.9	11.6	0.73
Ferulic acid	194.186	5.97 (0.031)	0.50-0.59	85.0-94.9	19.0	1.51
Ibuprofen	206.285	0.021 (1.02 E-04)	0.99-1.02	92.5-97.1	10047	3.97
Caffeine	194.194	21.6 (0.11)	0.51-0.52	70.0-80.2	4.67	-0.07
Mandelic acid	152.149	181 (1.19)	5.74	59.7	4.13	0.62

Table 4S: Data on relative solubility increases vis-à-vis Cyrene and ranges of maximum solubility.

Compound	MW	Solubility in Cyrene (mol L^{-1})	Maximum attainable solubility in TM-H_2O (mol L^{-1})	wt% Cyrene in H_2O range at which maximum dissolution is observed	Maximal increase in solubility vis-à-vis solubility in Cyrene (factor)	Log Kow
Aspirin (acetyl-salicylic acid)	180.159	**0.29**	0.93	89.7-95.0	**3.15**	1.19
Salicylic acid	138.122	**0.68**	1.65	89.4	**2.41**	2.26
Phthalic acid	166.132	**0.049**	0.41-0.44	75.2-84.9	**8.94**	0.73
Ferulic acid	194.186	**0.20**	0.50-0.59	85.0-94.9	**2.99**	1.51
Ibuprofen	206.285	**0.69**	0.99-1.02	92.5-97.1	**1.49**	3.97
Caffeine	194.194	**0.097**	0.51-0.52	70.0-80.2	**5.33**	-0.07
Mandelic acid	152.149	**1.66**	**4.71-4.92**	**75.07-85.03**	**2.96**	0.62

Figure 2S: ESI(+) mass-spectrum of 80 wt% Cyrene in H_2O.



Meas. m/z	#	Ion Formula	m/z	err [ppm]	err [mDa]	mSigma	Mean err [ppm]
169.047103	1	C6H10NaO4	169.047129	0.2	0.0	7.1	0.1
315.104972	1	C12H20NaO8	315.105038	0.2	0.1	4.4	0.3

- $C_6H_{10}NaO_4$ is the sodium adduct of monomeric geminal diol
- $C_{12}H_{20}NaO_8$ is the sodium adduct of dimeric geminal diol

Figure 3S_A: ^{1}H NMR spectra showing the evolution of a 65 wt% Cyrene in H_2O mixture when increasing the temperature from 298K to 358K.

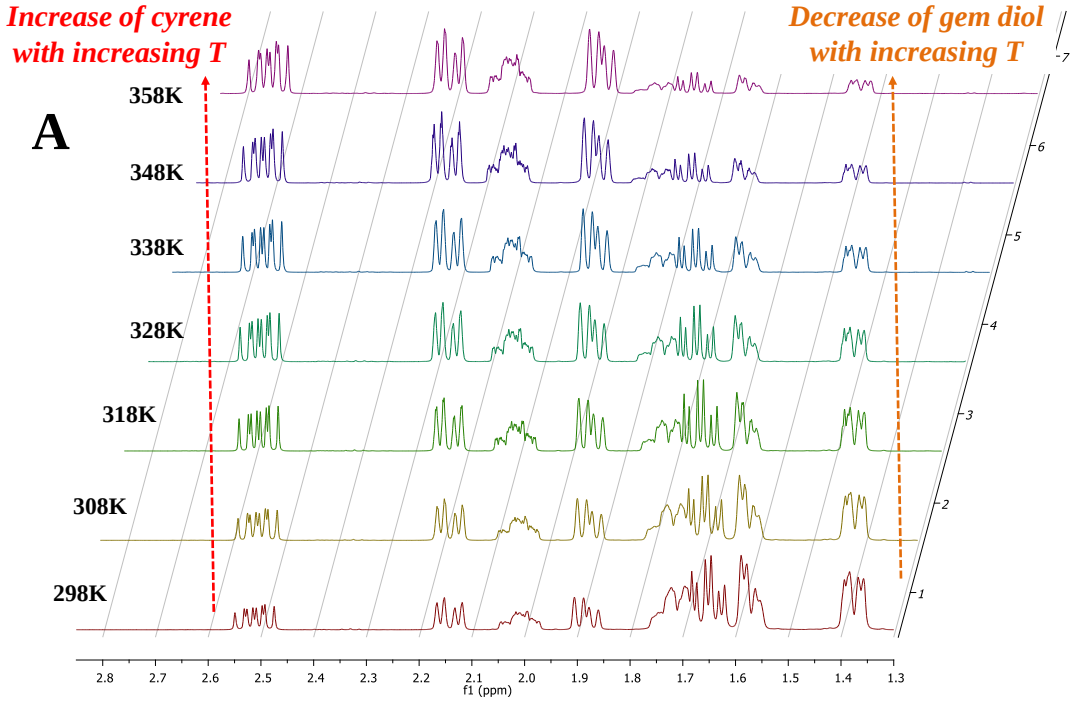
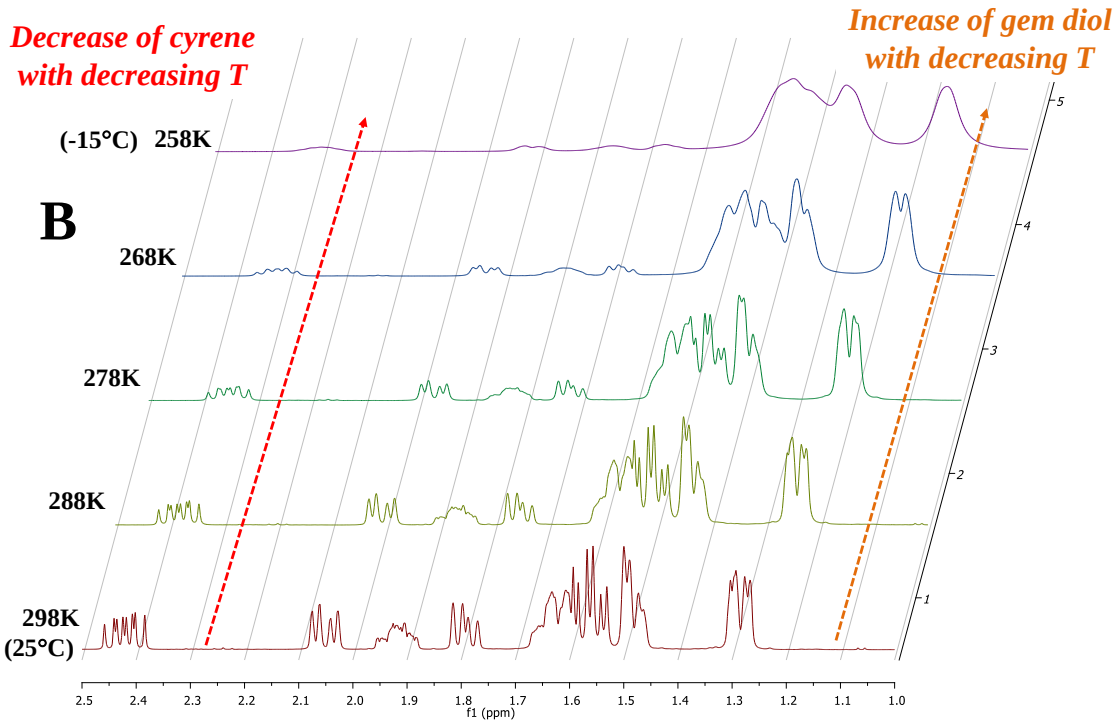


Figure 3S_B: ^{1}H NMR spectra showing the evolution of a 65 wt% Cyrene in H_2O mixture when decreasing the temperature from 298K to 258K.

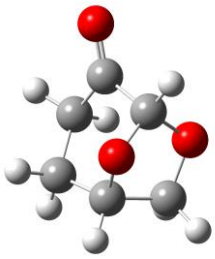


Quantum Chemical and Density Functional Theory Calculations

A series of quantum chemical molecular orbital and density functional theory (DFT) calculations were performed using the GAUSSIAN 16[i] suite of programmes to find minimum energy geometries of cyrene, its geminal diol and a number of different conformers of the cyrene dimer and trimer. Geometry optimizations and vibrational frequency calculations were performed at the mp2/cc-pVDZ level for Cyrene and at the M062x/cc-pVDZ level of theory for its geminal diol as well as for the $(Cyrene)_2$ and $(Cyrene)_3$ van der Waals dimers and trimer.

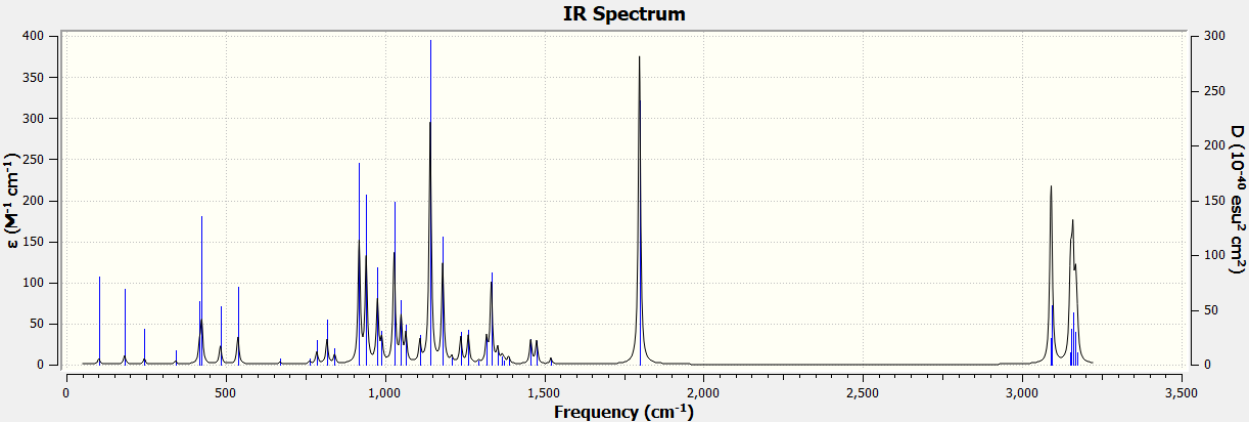
Vibrational frequency calculations allowed for the characterization of stationary points, as well as determination of thermal corrections to the electronic energy, enthalpy and Gibbs free energy at 298.15 K. The frequency calculations were also used to simulate infrared spectra of each species to aid comparison with the experimental FTIR spectra.

Cyrene (mp2/ccpVDZ)

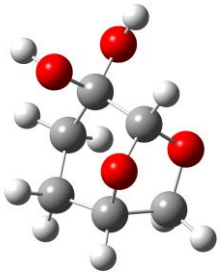


C	1.34803	-0.09717	-0.06354
O	2.5245	-0.36599	0.07548
C	0.2338	-1.06879	0.31218
C	0.82194	1.21168	-0.61004
C	-0.41957	1.67528	0.16807
C	-1.31501	0.49362	0.50346
O	-0.56934	-0.44894	1.29178
C	-1.67911	-0.35336	-0.71422
O	-0.59472	-1.28629	-0.81902
H	0.62421	-2.01034	0.68846
H	-2.18042	0.79236	1.08899
H	1.62019	1.9497	-0.59664
H	-0.97647	2.41854	-0.40424
H	-1.74725	0.23209	-1.63076
H	-2.60629	-0.90312	-0.56041
H	0.55634	1.02458	-1.65325
H	-0.11433	2.13842	1.1064

Electronic Energy (EE) =	-458.123930
Zero-point Energy Correction =	0.140120
Thermal Correction to Energy =	0.147052
Thermal Correction to Enthalpy =	0.147997
Thermal Correction to Free Energy =	0.108676
EE + Zero-point Energy =	-458.130862
EE + Thermal Energy Correction =	-458.123930
EE + Thermal Enthalpy Correction =	-458.122986
EE + Thermal Free Energy Correction =	-458.162307

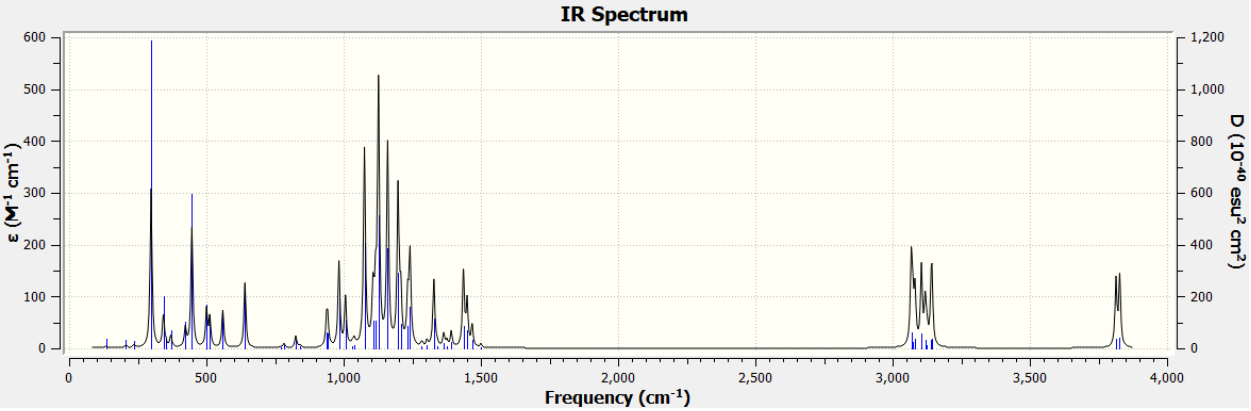


Geminal diol (m062x/cc-pVDZ)

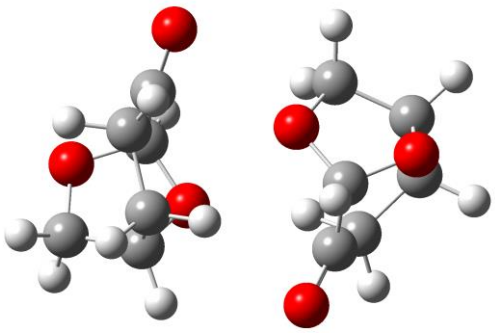


C	1.13349	-0.0324	-0.04468
O	1.81118	0.62094	0.99709
C	0.02536	-0.84963	0.64592
C	0.49036	0.93254	-1.03876
C	-0.73165	1.61906	-0.41646
C	-1.59924	0.59021	0.30834
O	-0.82738	0.00247	1.35622
C	-1.90671	-0.64781	-0.54652
O	-0.77203	-1.48557	-0.33332
H	0.45103	-1.59534	1.33361
H	-2.49037	1.04214	0.75948
H	1.24225	1.66596	-1.36898
H	-1.3163	2.14226	-1.1881
H	-2.00441	-0.41477	-1.61755
H	-2.81353	-1.16584	-0.20049
H	0.20308	0.34245	-1.92043
H	-0.40806	2.36061	0.32875
H	2.52611	1.12581	0.5836
O	2.00452	-0.85178	-0.77206
H	2.41028	-1.46356	-0.14027

Electronic Energy (EE) =	-535.376536
Zero-point Energy Correction =	0.168209
Thermal Correction to Energy =	0.176390
Thermal Correction to Enthalpy =	0.177335
Thermal Correction to Free Energy =	0.135866
EE + Zero-point Energy =	-535.208327
EE + Thermal Energy Correction =	-535.200146
EE + Thermal Enthalpy Correction =	-535.199202
EE + Thermal Free Energy Correction =	-535.240670



Cyrene dimer, Stucture 1 (m062x/cc-pVDZ)



C	-1.67707	1.46326	0.06954
C	-1.87887	0.49549	-1.10068
C	-1.90612	-1.33967	0.13949
C	-1.7221	-0.64714	1.48652
O	-1.2853	2.59206	-0.09409
C	-3.31208	-1.16015	-0.44277
O	-3.23344	0.08917	-1.12882
C	-2.05467	0.85629	1.4062
O	-1.12097	-0.66125	-0.85345
H	-1.58854	0.9495	-2.0575
H	-1.56403	-2.38061	0.17079
H	-0.67909	-0.79114	1.79378
H	-2.35447	-1.14101	2.24017
H	-4.09027	-1.1073	0.33314
H	-3.56292	-1.95507	-1.16081
H	-1.56852	1.43496	2.20081
H	-3.14507	1.00398	1.49811
O	1.10397	-2.39784	0.73494
H	2.21471	-2.19913	-1.60201
C	1.97399	-1.216	-1.17637
H	1.0274	-0.89114	-1.6396
C	1.61159	-1.39777	0.2854
C	3.08079	-0.17459	-1.41046
H	3.00897	0.2439	-2.42565
H	4.07141	-0.64255	-1.31395
H	1.72256	-0.39084	2.22636
C	1.85687	-0.16164	1.16148
O	3.14032	0.34257	0.9252
C	3.00146	0.93812	-0.36954
H	3.81113	1.66765	-0.48822
C	1.61196	1.59633	-0.26972
O	0.95537	0.84894	0.75624
H	1.04278	1.5261	-1.21019
H	1.65987	2.64835	0.04017

Electronic Energy (EE) =	-917.93336
Zero-point Energy Correction =	0.281906
Thermal Correction to Energy =	0.297252
Thermal Correction to Enthalpy =	0.298196

Thermal Correction to Free Energy =	0.238817
EE + Zero-point Energy =	-917.65145
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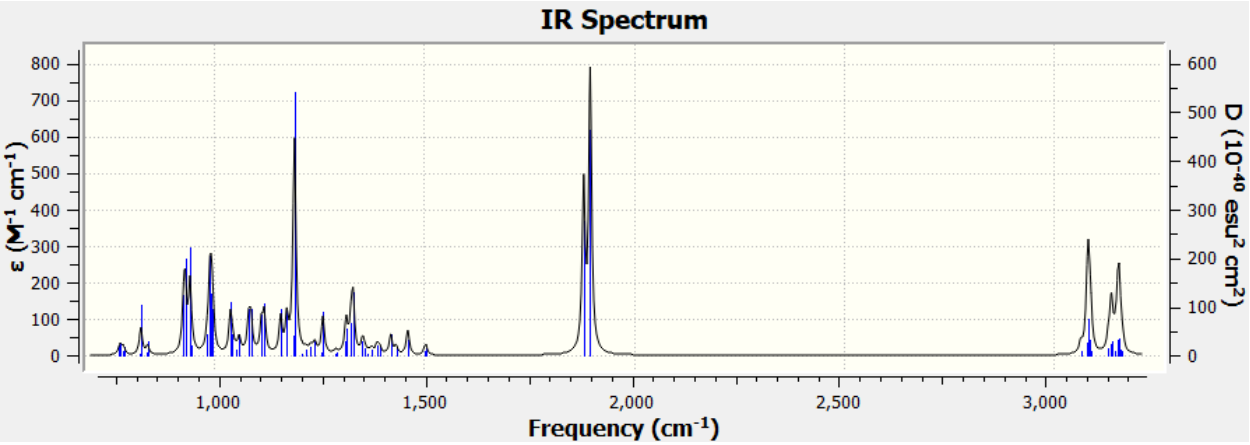
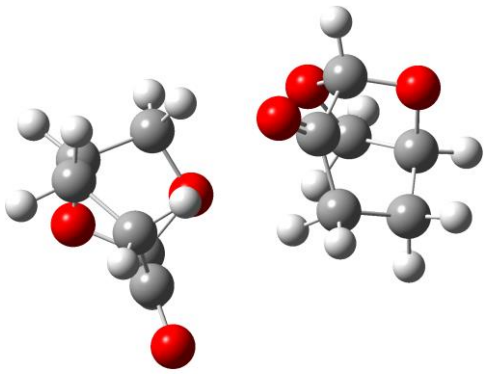
EE + Thermal Free Energy Correction =	-917.69454



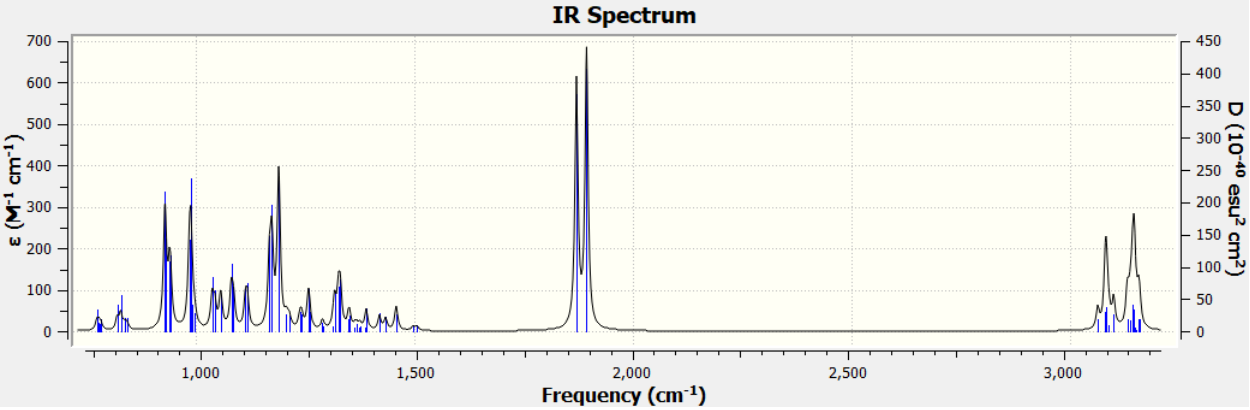
Cyrene dimer, Stucture 2 (m062x/cc-pVDZ)



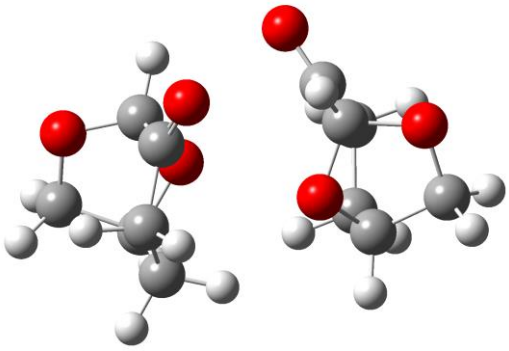
C	2.28787	-1.29259	0.3216
C	2.08417	-0.1231	1.29366
C	2.69979	1.43823	-0.13982
C	3.07344	0.50604	-1.28903
O	2.31892	-2.43782	0.69994
C	1.18449	1.58601	0.05871
O	0.86311	0.51915	0.96118
C	2.38616	-0.86284	-1.12985
O	3.09462	0.82417	1.09283
C	-1.47325	-0.27891	-1.26271
C	-2.41503	0.85765	-0.84424
C	-3.31599	-0.26206	0.82815
C	-2.67033	-1.61596	0.55418
O	-0.77858	-0.18644	-2.24967
C	-2.34613	0.77586	1.42956
O	-1.84731	1.47893	0.29034
C	-1.39656	-1.43774	-0.28784
O	-3.64475	0.33587	-0.43079
H	2.07267	-0.46253	2.33637
H	3.21918	2.40109	-0.21034
H	4.16659	0.38407	-1.27391
H	2.80023	0.96122	-2.25249
H	-2.54932	1.58498	-1.65344
H	0.62101	1.46585	-0.87705
H	0.91244	2.53968	0.53007
H	2.88722	-1.65693	-1.69796
H	1.34873	-0.804	-1.50607
H	-4.24573	-0.36094	1.40046
H	-3.40584	-2.22944	0.01399
H	-2.43659	-2.13003	1.4981
H	-1.50667	0.31572	1.97165
H	-2.86408	1.49253	2.08151
H	-1.1081	-2.34557	-0.83409
H	-0.55166	-1.17009	0.36839

Electronic Energy (EE) =	-917.93255 Hartree
Zero-point Energy Correction =	0.281418 Hartree
Thermal Correction to Energy =	0.297067 Hartree
Thermal Correction to Enthalpy =	0.298011 Hartree

Thermal Correction to Free Energy =	0.236413 Hartree
EE + Zero-point Energy =	-917.65113 Hartree
EE + Thermal Energy Correction =	-917.63548 Hartree
EE + Thermal Enthalpy Correction =	-917.63454 Hartree
EE + Thermal Free Energy Correction =	-917.69614 Hartree



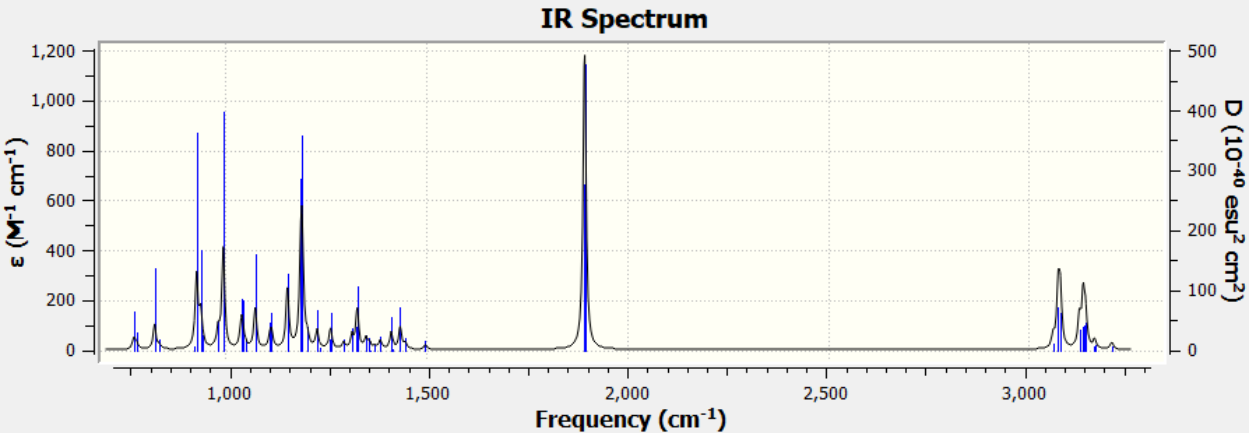
Cyrene dimer, Stucture 3 (m062x/cc-pVDZ)



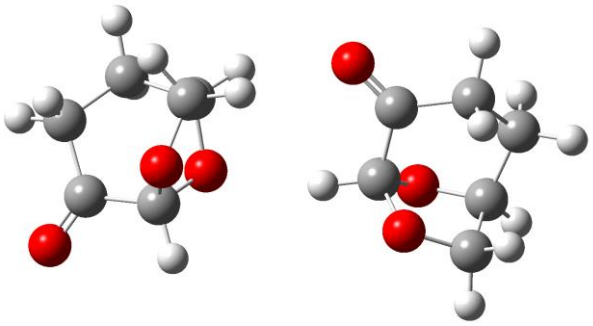
C	-1.42507	0.98089	0.95392
C	-1.84872	0.87649	-0.51632
C	-2.0956	-1.32728	-0.48109
C	-1.70284	-1.53994	0.97775
O	-0.85365	1.94507	1.39805
C	-3.49102	-0.71272	-0.64755
O	-3.25059	0.68865	-0.57032
C	-1.82468	-0.23041	1.77752
O	-1.27288	-0.29882	-1.04433
C	1.42534	0.98203	-0.95311
C	1.84896	0.87614	0.51711
C	2.09502	-1.32772	0.47974
C	1.70261	-1.53855	-0.97947
O	0.85325	1.94631	-1.39612
C	3.49062	-0.71391	0.6472
O	3.25073	0.68763	0.57114
C	1.82584	-0.22822	-1.77777
O	1.27262	-0.29949	1.04389
H	-1.53758	1.74991	-1.09814
H	-1.9516	-2.23488	-1.08164
H	-0.65847	-1.88023	1.00521
H	-2.32757	-2.32907	1.42369
H	1.53831	1.7492	1.09975
H	-4.18505	-1.01933	0.15007
H	-3.93061	-0.95382	-1.62682
H	-1.22119	-0.24241	2.69294
H	-2.87743	-0.0602	2.06339
H	1.95046	-2.23592	1.07923
H	0.65793	-1.87783	-1.00772
H	2.32689	-2.32767	-1.42604
H	4.1848	-1.0201	-0.15045
H	3.9298	-0.95609	1.62639
H	1.22375	-0.23921	-2.69412
H	2.87908	-0.05792	-2.0618

Electronic Energy (EE) =	-917.93138
Zero-point Energy Correction =	0.281254
Thermal Correction to Energy =	0.296859
Thermal Correction to Enthalpy =	0.297803

Thermal Correction to Free Energy =	0.237357
EE + Zero-point Energy =	-917.65012
EE + Thermal Energy Correction =	-917.63452
EE + Thermal Enthalpy Correction =	-917.63357
EE + Thermal Free Energy Correction =	-917.69402



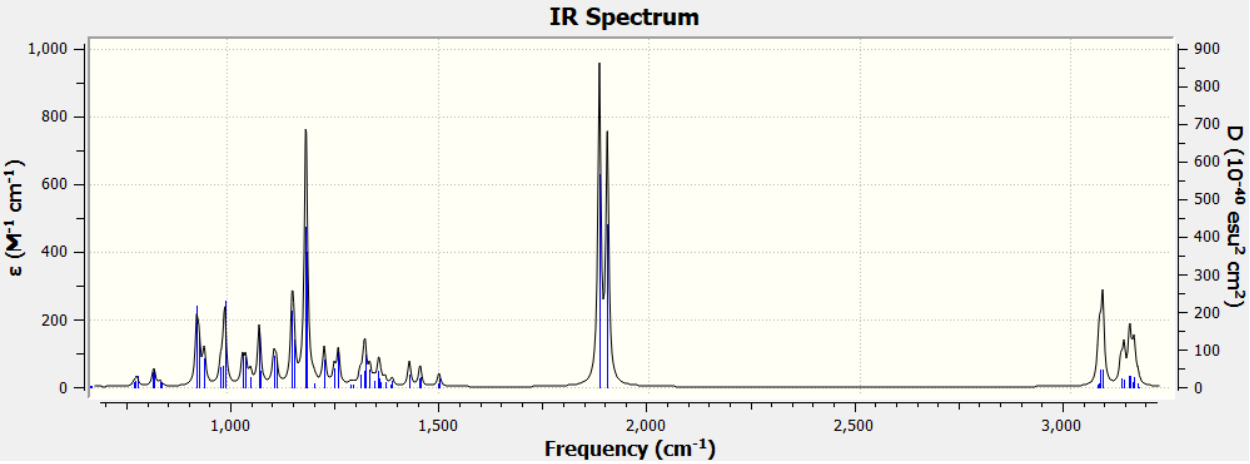
Cyrene dimer, Stucture 4 (m062x/cc-pVDZ)



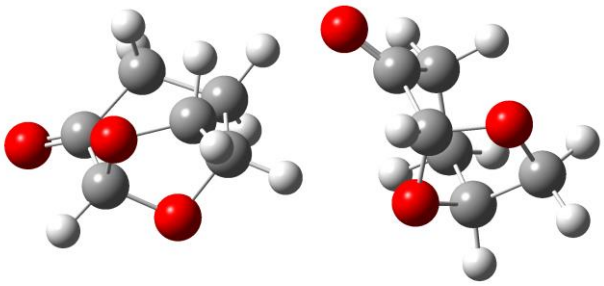
C	2.07135	1.04916	0.19893
C	1.78707	-0.41747	-0.1447
C	3.86962	-0.86287	-0.75253
C	4.43927	0.53153	-0.50134
O	1.2083	1.89457	0.24009
C	3.59468	-1.64401	0.53823
O	2.2823	-1.22705	0.90626
C	3.53955	1.31799	0.47143
O	2.5491	-0.73233	-1.28436
C	-3.83128	-0.91707	-0.10814
C	-2.43562	-0.9075	0.52786
C	-1.81133	0.99825	-0.42068
C	-3.1056	1.24575	-1.19052
O	-4.48434	-1.92238	-0.22805
C	-1.93568	1.2533	1.08396
O	-2.419	0.01017	1.59948
C	-4.27411	0.46356	-0.56094
O	-1.53761	-0.41213	-0.43769
H	0.72101	-0.60635	-0.32196
H	4.46826	-1.42334	-1.48021
H	4.48474	1.05286	-1.46882
H	5.46572	0.46321	-0.11098
H	-2.13209	-1.908	0.85794
H	4.30446	-1.39939	1.34318
H	3.5982	-2.73031	0.36681
H	3.71979	2.39942	0.43851
H	3.71913	0.97718	1.50537
H	-0.94803	1.50986	-0.8595
H	-2.94835	0.91094	-2.2265
H	-3.33027	2.32248	-1.2195
H	-2.64977	2.05623	1.32197
H	-0.95655	1.48232	1.52589
H	-5.13204	0.36073	-1.23663
H	-4.62166	0.9816	0.34919

Electronic Energy (EE) =	-917.92708
Zero-point Energy Correction =	0.28088
Thermal Correction to Energy =	0.296886
Thermal Correction to Enthalpy =	0.297831
Thermal Correction to Free Energy =	0.232485

EE + Zero-point Energy =	-917.6462
EE + Thermal Energy Correction =	-917.6302
EE + Thermal Enthalpy Correction =	-917.62925
EE + Thermal Free Energy Correction =	-917.6946



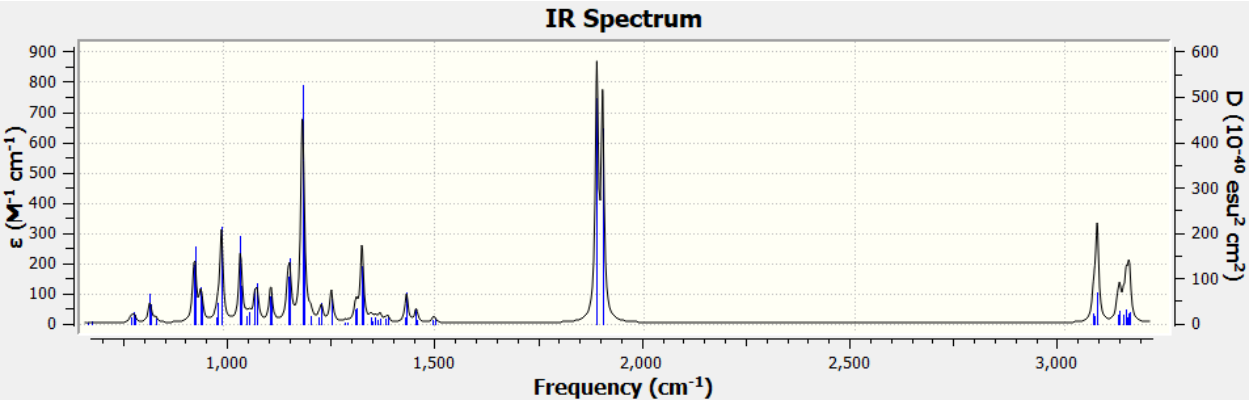
Cyrene dimer, Stucture 5 (m062x/cc-pVDZ)



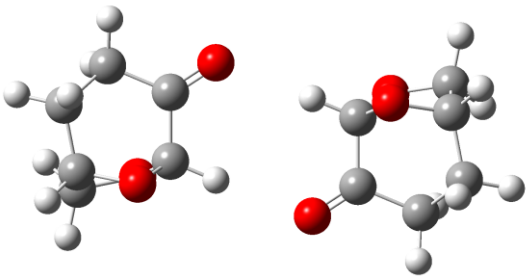
C	-3.88307	0.50041	-0.15857
C	-3.28133	-0.78715	-0.73351
C	-1.18539	-0.22755	-0.30073
C	-1.48342	1.13104	0.33163
O	-4.97771	0.90219	-0.46334
C	-1.54135	-1.40235	0.61879
O	-2.91952	-1.64486	0.32894
C	-2.94626	1.19593	0.81358
O	-2.08941	-0.43829	-1.39127
C	1.84507	0.02257	1.16767
C	2.58406	-1.02697	0.32845
C	3.02316	0.36241	-1.34016
C	2.38002	1.59972	-0.71732
O	1.00155	-0.27162	1.98013
C	4.36062	-0.01155	-0.69099
O	3.97525	-0.81589	0.42361
C	2.25281	1.43906	0.81157
O	2.23192	-0.78697	-1.01415
H	-3.97199	-1.28439	-1.42511
H	-0.16696	-0.29105	-0.70258
H	-1.31187	1.90508	-0.43281
H	-0.79661	1.31023	1.17179
H	2.31562	-2.05	0.61832
H	-1.41177	-1.16132	1.68282
H	-0.95496	-2.30107	0.37609
H	-3.29619	2.22281	0.97601
H	-3.04381	0.65203	1.76848
H	3.07234	0.43132	-2.43279
H	1.38148	1.72459	-1.16372
H	2.96501	2.49835	-0.96356
H	4.92317	0.86587	-0.33894
H	4.99252	-0.60506	-1.367
H	1.54302	2.14972	1.25266
H	3.23488	1.60287	1.28662

Electronic Energy (EE) =	-917.92667
Zero-point Energy Correction =	0.281
Thermal Correction to Energy =	0.296857
Thermal Correction to Enthalpy =	0.297801
Thermal Correction to Free Energy =	0.234374
EE + Zero-point Energy =	-917.64567

EE + Thermal Energy Correction =	-917.62981
EE + Thermal Enthalpy Correction =	-917.62887
EE + Thermal Free Energy Correction =	-917.6923



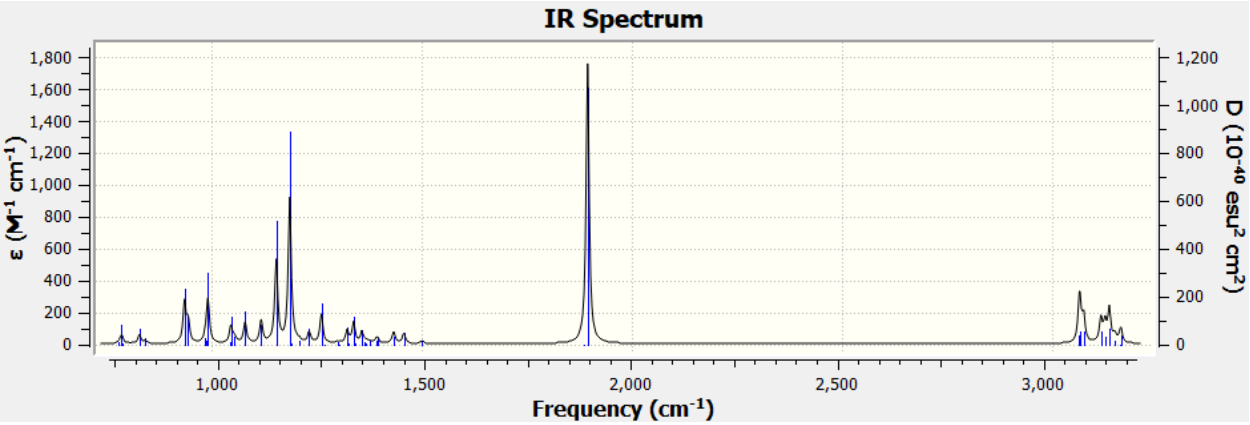
Cyrene dimer, Stucture 6 (m062x/cc-pVDZ)



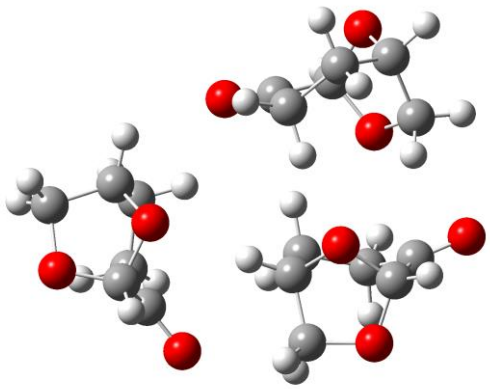
C	-1.1631	2.0217	-0.09134
C	-2.00632	0.74131	-0.09232
C	-3.84093	1.73869	0.64877
C	-3.25703	3.14561	0.75937
O	0.04392	2.01803	-0.06037
C	-4.10876	1.30958	-0.799
O	-2.85995	0.77236	-1.22351
C	-2.00632	3.28396	-0.12924
O	-2.84334	0.79341	1.03815
C	1.1631	-2.0217	-0.09134
C	2.00632	-0.74131	-0.09232
C	3.84093	-1.73869	0.64877
C	3.25703	-3.14561	0.75937
O	-0.04392	-2.01803	-0.06037
C	4.10876	-1.30958	-0.799
O	2.85995	-0.77236	-1.22351
C	2.00632	-3.28396	-0.12924
O	2.84334	-0.79341	1.03815
H	-1.39482	-0.16907	-0.08075
H	-4.70581	1.60277	1.30899
H	-2.98474	3.31181	1.8121
H	-4.01242	3.89828	0.48732
H	1.39482	0.16907	-0.08075
H	-4.39362	2.15304	-1.4467
H	-4.88161	0.52896	-0.85643
H	-1.3807	4.14158	0.14671
H	-2.30801	3.4112	-1.18286
H	4.70581	-1.60277	1.30899
H	2.98474	-3.31181	1.8121
H	4.01242	-3.89828	0.48732
H	4.39362	-2.15304	-1.4467
H	4.88161	-0.52896	-0.85643
H	1.3807	-4.14158	0.14671
H	2.30801	-3.4112	-1.18286

Electronic Energy (EE) =	-917.92488
Zero-point Energy Correction =	0.28102
Thermal Correction to Energy =	0.296958
Thermal Correction to Enthalpy =	0.297902
Thermal Correction to Free Energy =	0.234493
EE + Zero-point Energy =	-917.64386

EE + Thermal Energy Correction =	-917.62792
EE + Thermal Enthalpy Correction =	-917.62698
EE + Thermal Free Energy Correction =	-917.69039



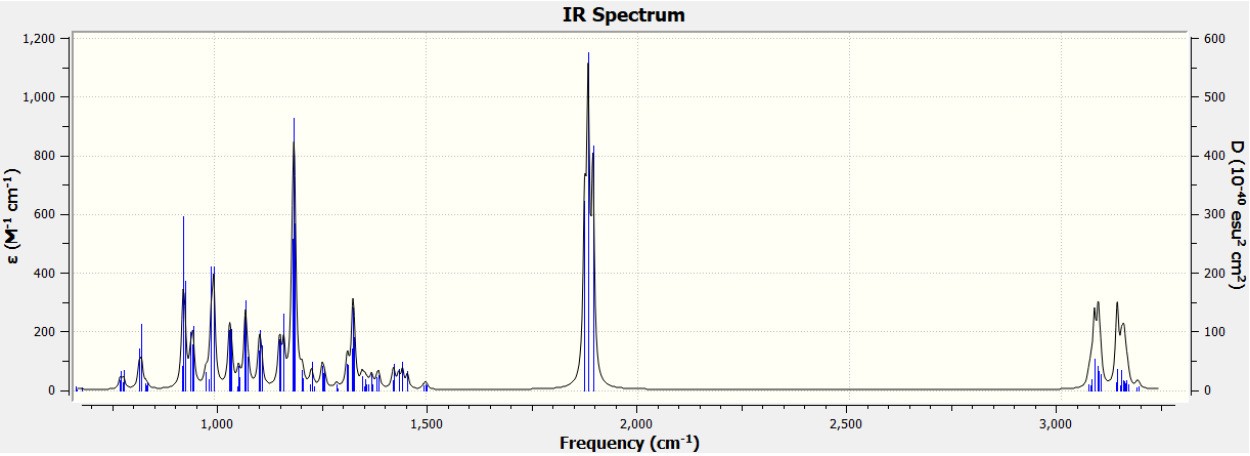
Cyrene trimer (m062x/cc-pVDZ)



C	2.51587	2.22208	0.58535
C	2.01208	2.511	-0.83355
C	-0.01057	1.66983	-0.49363
C	0.18853	1.30086	0.97352
O	3.69106	2.13627	0.84322
C	-0.17678	3.1748	-0.71293
O	1.17174	3.64235	-0.82347
C	1.38848	2.05268	1.58451
O	1.20754	1.41871	-1.21584
C	-3.26566	1.10742	0.2159
C	-3.33998	0.18511	-1.0082
C	-2.95983	-1.66706	0.15104
C	-2.88493	-1.0016	1.52169
O	-2.92984	2.26568	0.13379
C	-4.38451	-1.75411	-0.40236
O	-4.57818	-0.48609	-1.03327
C	-3.57443	0.37883	1.5067
O	-2.34814	-0.79819	-0.81888
H	2.84265	2.64281	-1.53909
H	-0.7901	1.06025	-0.95934
H	0.37121	0.21957	1.03362
H	-0.73232	1.52617	1.53269
H	-3.16697	0.73156	-1.94449
H	-0.6816	3.66842	0.12823
H	-0.72007	3.39753	-1.64208
H	1.78465	1.55362	2.47671
H	1.08263	3.0747	1.86736
H	-2.40626	-2.61033	0.13992
H	-1.82041	-0.89694	1.77515
H	-3.34026	-1.65268	2.28268
H	-5.1399	-1.89342	0.38513
H	-4.48685	-2.55125	-1.15272
H	-3.28546	1.00789	2.35813
H	-4.66992	0.25128	1.53413
O	-0.16595	-2.58431	0.97347
H	0.01197	-2.37687	-1.60665
C	0.90557	-1.97734	-1.11121
H	0.87631	-0.87726	-1.20541

C	0.83465	-2.2631	0.37259
C	2.22378	-2.49641	-1.71851
H	2.41925	-2.00314	-2.68203
H	2.15531	-3.57876	-1.90302
H	2.10724	-2.29553	2.15617
C	2.18177	-2.08218	1.08303
O	3.10827	-2.93949	0.4727
C	3.38768	-2.26117	-0.75803
H	4.32954	-2.66218	-1.14999
C	3.49923	-0.80567	-0.28653
O	2.63822	-0.76365	0.85733
H	3.13862	-0.0913	-1.03984
H	4.51733	-0.53828	0.02615

Electronic Energy (EE) =	-1376.907583
Zero-point Energy Correction =	0.422268
Thermal Correction to Energy =	0.446756
Thermal Correction to Enthalpy =	0.447701
Thermal Correction to Free Energy =	0.364489
EE + Zero-point Energy =	-1376.485315
EE + Thermal Energy Correction =	-1376.460827
EE + Thermal Enthalpy Correction =	-1376.459882
EE + Thermal Free Energy Correction =	-1376.543094



[i] Gaussian 16, Revision A.03,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone,
G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich,
J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian,
J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young,
F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone,
T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega,
G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda,
J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai,
T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta,
F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin,
V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand,
K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar,
J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi,
J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas,
J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.