SUPPORTING INFORMATION

Thermodynamic, Raman Spectroscopic and UV-Visible Optical Characterization of the Deltic, Squaric and Croconic Cyclic Oxocarbon Acids

Francisco Colmenero and Rafael Escribano*

Instituto de Estructura de la Materia (CSIC). C/ Serrano, 113. 28006 – Madrid, Spain.

*E-mail: francisco.colmenero@iem.cfmac.csic.es

Table S.1. Calculated isobaric heat capacity function, C_P, of deltic acid. Temperature and heat capacity values are given in K and $J \cdot K^{-1} \cdot mol^{-1}$ units, respectively.

T	C_P	T	C_P	T	C_P
10	0.4298	350	99.9177	690	145.8089
20	2.7947	360	101.7846	700	146.7145
30	7.5390	370	103.6155	710	147.6009
40	13.3213	380	105.4106	720	148.4684
50	19.0360	390	107.1701	730	149.3176
60	24.2933	400	108.8944	740	150.1488
70	29.0358	410	110.5837	750	150.9625
80	33.3091	420	112.2385	760	151.7590
90	37.1822	430	113.8592	770	152.5388
100	40.7238	440	115.4463	780	153.3022
110	43.9964	450	117.0003	790	154.0496
120	47.0547	460	118.5217	800	154.7815
130	49.9449	470	120.0111	810	155.4980
140	52.7046	480	121.4689	820	156.1997
150	55.3638	490	122.8959	830	156.8869
160	57.9456	500	124.2925	840	157.5598
170	60.4669	510	125.6592	850	158.2189
180	62.9397	520	126.9968	860	158.8644
190	65.3723	530	128.3058	870	159.4966
200	67.7701	540	129.5867	880	160.1160
210	70.1360	550	130.8401	890	160.7227
220	72.4717	560	132.0665	900	161.3170
230	74.7778	570	133.2667	910	161.8994
240	77.0540	580	134.4410	920	162.4699
250	79.2997	590	135.5901	930	163.0290
260	81.5142	600	136.7145	940	163.5768
270	83.6967	610	137.8148	950	164.1136
280	85.8462	620	138.8914	960	164.6398
290	87.9619	630	139.9449	970	165.1555
300	90.0433	640	140.9758	980	165.6609
310	92.0896	650	141.9847	990	166.1564
320	94.1005	660	142.9719	1000	166.6421
330	96.0755	670	143.9380	-	-
340	98.0147	680	144.8835	-	-

Table S.2. Calculated entropy function, S, of deltic acid. Temperature and entropy values are given in K and $J \cdot K^{-1} \cdot mol^{-1}$ units, respectively.

T	S	T	S	T	S
10	0.1335	350	113.4833	690	196.9842
20	1.0125	360	116.3245	700	199.0885
30	2.9830	370	119.1385	710	201.1760
40	5.9338	380	121.9257	720	203.2463
50	9.5279	390	124.6863	730	205.3003
60	13.4677	400	127.4215	740	207.3375
70	17.5776	410	130.1311	750	209.3584
80	21.7394	420	132.8161	760	211.3632
90	25.8876	430	135.4761	770	213.3519
100	29.9925	440	138.1116	780	215.3253
110	34.0286	450	140.7239	790	217.2828
120	37.9891	460	143.3122	800	219.2252
130	41.8709	470	145.8771	810	221.1524
140	45.6737	480	148.4191	820	223.0650
150	49.4005	490	150.9380	830	224.9622
160	53.0564	500	153.4353	840	226.8453
170	56.6454	510	155.9099	850	228.7139
180	60.1720	520	158.3630	860	230.5682
190	63.6410	530	160.7946	870	232.4085
200	67.0549	540	163.2049	880	234.2349
210	70.4182	550	165.5943	890	236.0476
220	73.7356	560	167.9629	900	237.8465
230	77.0079	570	170.3110	910	239.6324
240	80.2386	580	172.6389	920	241.4050
250	83.4299	590	174.9471	930	243.1643
260	86.5835	600	177.2351	940	244.9108
270	89.7010	610	179.5042	950	246.6447
280	92.7836	620	181.7539	960	248.3661
290	95.8332	630	183.9845	970	250.0748
300	98.8500	640	186.1967	980	251.7713
310	101.8364	650	188.3902	990	253.4558
320	104.7914	660	190.5655	1000	255.1280
330	107.7178	670	192.7226	-	-
340	110.6148	680	194.8621	-	-

Table S.3. Calculated enthalpy function, ΔH ($\Delta H=H_T-H_{298}$), of deltic acid. Temperature and enthalpy values are given in K and $J \cdot K^{-1} \cdot mol^{-1}$ units, respectively.

T	H_T-H_{298}	T	H_T-H_{298}	T	H_T-H_{298}
10	-1512.0840	350	14.0545	690	69.0276
20	-755.3423	360	16.4655	700	70.1311
30	-501.8920	370	18.7964	710	71.2160
40	-373.8200	380	21.0523	720	72.2829
50	-295.8141	390	23.2375	730	73.3325
60	-242.8935	400	25.3576	740	74.3648
70	-204.3764	410	27.4160	750	75.3808
80	-174.9307	420	29.4160	760	76.3805
90	-151.5729	430	31.3606	770	77.3647
100	-132.5176	440	33.2540	780	78.3331
110	-116.6177	450	35.0976	790	79.2868
120	-103.1045	460	36.8947	800	80.2261
130	-91.4420	470	38.6475	810	81.1510
140	-81.2440	480	40.3575	820	82.0620
150	-72.2256	490	42.0278	830	82.9594
160	-64.1702	500	43.6592	840	83.8435
170	-56.9121	510	45.2535	850	84.7144
180	-50.3224	520	46.8126	860	85.5730
190	-44.2968	530	48.3378	870	86.4190
200	-38.7533	540	49.8307	880	87.2532
210	-33.6239	550	51.2925	890	88.0751
220	-28.8545	560	52.7237	900	88.8858
230	-24.3992	570	54.1262	910	89.6847
240	-20.2186	580	55.5011	920	90.4728
250	-16.2828	590	56.8487	930	91.2500
260	-12.5644	600	58.1706	940	92.0165
270	-9.0392	610	59.4670	950	92.7727
280	-5.6891	620	60.7395	960	93.5187
290	-2.4961	630	61.9884	970	94.2545
300	0.5540	640	63.2145	980	94.9805
310	3.4743	650	64.4188	990	95.6969
320	6.2746	660	65.6013	1000	96.4041
330	8.9666	670	66.7636	-	-
340	11.5570	680	67.9055	-	-

Table S.4. Calculated free-energy function, ΔG (ΔG = G_T-H_{298}), of deltic acid. Temperature and free-energy values are given in K and $J \cdot K^{-1} \cdot mol^{-1}$ units, respectively.

T	G_T-H_{298}	T	G_T-H_{298}	T	G_T-H_{298}
10	-0.04293	350	-95.64074	690	-177.15869
20	-0.50806	360	-98.43229	700	-179.20582
30	-1.56588	370	-101.19632	710	-181.23657
40	-3.12597	380	-103.93303	720	-183.25114
50	-5.07935	390	-106.64273	730	-185.24989
60	-7.34294	400	-109.32579	740	-187.23300
70	-9.85313	410	-111.98262	750	-189.20070
80	-12.55892	420	-114.61352	760	-191.15327
90	-15.41856	430	-117.21881	770	-193.09091
100	-18.39674	440	-119.79894	780	-195.01386
110	-21.46552	450	-122.35419	790	-196.92232
120	-24.60150	460	-124.88505	800	-198.81658
130	-27.78522	470	-127.39181	810	-200.69678
140	-31.00151	480	-129.87484	820	-202.56312
150	-34.23742	490	-132.33455	830	-204.41587
160	-37.48267	500	-134.77125	840	-206.25520
170	-40.72905	510	-137.18541	850	-208.08133
180	-43.97001	520	-139.57722	860	-209.89437
190	-47.20005	530	-141.94721	870	-211.69460
200	-50.41509	540	-144.29560	880	-213.48219
210	-53.61167	550	-146.62284	890	-215.25731
220	-56.78710	560	-148.92914	900	-217.02010
230	-59.93941	570	-151.21499	910	-218.77081
240	-63.06686	580	-153.48061	920	-220.50955
250	-66.16831	590	-155.72635	930	-222.23651
260	-69.24272	600	-157.95252	940	-223.95185
270	-72.28951	610	-160.15952	950	-225.65573
280	-75.30820	620	-162.34756	960	-227.34830
290	-78.29847	630	-164.51696	970	-229.02975
300	-81.26025	640	-166.66804	980	-230.70021
310	-84.19327	650	-168.80108	990	-232.35982
320	-87.09770	660	-170.91641	1000	-234.00873
330	-89.97367	670	-173.01426	-	-
340	-92.82128	680	-175.09493	-	-

Table S.5. Calculated isobaric heat capacity function, C_P, of squaric acid. Temperature and heat capacity values are given in K and $J \cdot K^{-1} \cdot mol^{-1}$ units, respectively.

T	C_P	T	C_P	T	C_P
10	0.4322	130	60.3728	250	97.9938
20	2.7995	140	63.9503	260	100.8014
30	7.7353	150	67.3973	270	103.5717
40	14.1503	160	70.7390	280	106.3053
50	20.9253	170	73.9939	290	109.0023
60	27.4389	180	77.1758	300	111.6625
70	33.4521	190	80.2947	310	114.2858
80	38.9241	200	83.3581	320	116.8719
90	43.9009	210	86.3716	330	119.4205
100	48.4591	220	89.3392	340	121.9310
110	52.6787	230	92.2641	350	124.4032
120	56.6306	240	95.1484	-	-

Table S.6. Calculated entropy function, S, of squaric acid. Temperature and entropy values are given in K and $J \cdot K^{-1} \cdot mol^{-1}$ units, respectively.

T	S	T	S	T	S
10	0.2084	130	47.9569	250	98.9013
20	1.0786	140	52.5638	260	102.7996
30	3.0714	150	57.0936	270	106.6574
40	6.1630	160	61.5486	280	110.4723
50	10.0441	170	65.9364	290	114.2503
60	14.4406	180	70.2574	300	117.9903
70	19.1317	190	74.5121	310	121.6945
80	23.9585	200	78.7103	320	125.3646
90	28.8384	210	82.8487	330	128.9994
100	33.7023	220	86.9355	340	132.6021
110	38.5196	230	90.9731	350	136.1725
120	43.2737	240	94.9597	-	-

Table S.7. Calculated enthalpy function, ΔH ($\Delta H=H_T-H_{298}$), of squaric acid. Temperature and enthalpy values are given in K and $J\cdot K^{-1}\cdot mol^{-1}$ units, respectively.

T	H_T-H_{298}	T	H_T-H_{298}	T	H_T-H_{298}
10	-1840.4692	130	-112.5545	250	-20.1561
20	-919.5410	140	-100.0731	260	-15.5586
30	-611.3338	150	-89.0211	270	-11.1962
40	-455.7746	160	-79.1396	280	-7.0489
50	-361.1173	170	-70.2276	290	-3.0945
60	-296.8948	180	-62.1263	300	0.6880
70	-250.1256	190	-54.7127	310	4.3089
80	-214.3311	200	-47.8861	320	7.7864
90	-185.9121	210	-41.5649	330	11.1307
100	-162.6992	220	-35.6824	340	14.3534
110	-143.3078	230	-30.1814	350	17.4622
120	-126.8105	240	-25.0202	-	-

Table S.8. Calculated free-energy function, ΔG ($\Delta G = G_T-H_{298}$), of squaric acid. Temperature and free-energy values are given in K and $J\cdot K^{-1}\cdot mol^{-1}$ units, respectively.

T	G_T-H_{298}	T	G_T-H_{298}	T	G_T-H_{298}
10	-1840.6776	130	-160.5114	250	-119.0574
20	-920.6196	140	-152.6369	260	-118.3581
30	-614.4056	150	-146.1147	270	-117.8536
40	-461.9376	160	-140.6912	280	-117.5212
50	-371.1614	170	-136.1640	290	-117.3447
60	-311.3354	180	-132.3837	300	-117.3039
70	-269.2573	190	-129.2273	310	-117.3856
80	-238.2896	200	-126.5964	320	-117.5767
90	-214.7451	210	-124.4136	330	-117.8688
100	-196.3967	220	-122.6179	340	-118.2487
110	-181.8273	230	-121.1545	350	-118.7103
120	-170.0842	240	-119.9799		

Table S.9. Calculated isobaric heat capacity function, C_P, of croconic acid. Temperature and heat capacity values are given in K and $J \cdot K^{-1} \cdot mol^{-1}$ units, respectively.

T	C_P	T	C_P	T	C_P
10	0.3338	350	148.8575	690	219.2149
20	3.2531	360	151.7138	700	220.5717
30	9.0761	370	154.5187	710	221.8969
40	16.4312	380	157.2724	720	223.1913
50	23.9444	390	159.9748	730	224.4557
60	31.0121	400	162.6262	740	225.6908
70	37.5248	410	165.2266	750	226.8973
80	43.5557	420	167.7763	760	228.0760
90	49.2116	430	170.2753	770	229.2275
100	54.5816	440	172.7240	780	230.3525
110	59.7263	450	175.1226	790	231.4517
120	64.6835	460	177.4716	800	232.5257
130	69.4751	470	179.7714	810	233.5752
140	74.1143	480	182.0223	820	234.6008
150	78.6102	490	184.2250	830	235.6031
160	82.9702	500	186.3800	840	236.5827
170	87.2017	510	188.4878	850	237.5402
180	91.3125	520	190.5492	860	238.4762
190	95.3104	530	192.5648	870	239.3911
200	99.2036	540	194.5354	880	240.2857
210	102.9999	550	196.4615	890	241.1603
220	106.7066	560	198.3441	900	242.0154
230	110.3307	570	200.1839	910	242.8517
240	113.8781	580	201.9816	920	243.6696
250	117.3542	590	203.7381	930	244.4695
260	120.7634	600	205.4541	940	245.2519
270	124.1095	610	207.1306	950	246.0173
280	127.3954	620	208.7683	960	246.7660
290	130.6235	630	210.3680	970	247.4986
300	133.7958	640	211.9306	980	248.2155
310	136.9137	650	213.4569	990	248.9170
320	139.9781	660	214.9476	1000	249.6035
330	142.9899	670	216.4037	-	-
340	145.9496	680	217.8259	-	-

Table S.10. Calculated entropy function, S, of croconic acid. Temperature and entropy values are given in K and $J \cdot K^{-1} \cdot mol^{-1}$ units, respectively.

T	S	T	S	T	S
10	0.0680	350	159.1271	690	284.2706
20	1.0146	360	163.3604	700	287.4346
30	3.3529	370	167.5553	710	290.5727
40	6.9530	380	171.7128	720	293.6856
50	11.4335	390	175.8334	730	296.7727
60	16.4347	400	179.9168	740	299.8350
70	21.7092	410	183.9646	750	302.8726
80	27.1184	420	187.9770	760	305.8858
90	32.5772	430	191.9542	770	308.8746
100	38.0442	440	195.8970	780	311.8397
110	43.4886	450	199.8056	790	314.7813
120	48.9000	460	203.6805	800	317.6994
130	54.2674	470	207.5220	810	320.5945
140	59.5866	480	211.3300	820	323.4668
150	64.8542	490	215.1062	830	326.3166
160	70.0664	500	218.8500	840	329.1439
170	75.2245	510	222.5614	850	331.9495
180	80.3254	520	226.2414	860	334.7334
190	85.3705	530	229.8904	870	337.4957
200	90.3585	540	233.5083	880	340.2366
210	95.2907	550	237.0956	890	342.9566
220	100.1682	560	240.6525	900	345.6560
230	104.9918	570	244.1794	910	348.3348
240	109.7631	580	247.6766	920	350.9934
250	114.4818	590	251.1444	930	353.6322
260	119.1520	600	254.5830	940	356.2510
270	123.7719	610	257.9927	950	358.8503
280	128.3453	620	261.3741	960	361.4303
290	132.8719	630	264.7274	970	363.9914
300	137.3541	640	268.0528	980	366.5335
310	141.7922	650	271.3501	990	369.0571
320	146.1873	660	274.6206	1000	371.5621
330	150.5412	670	277.8641	-	-
340	154.8540	680	281.0806	-	-

Table S.11. Calculated enthalpy function, ΔH ($\Delta H=H_T-H_{298}$), of croconic acid. Temperature and enthalpy values are given in K and $J \cdot K^{-1} \cdot mol^{-1}$ units, respectively.

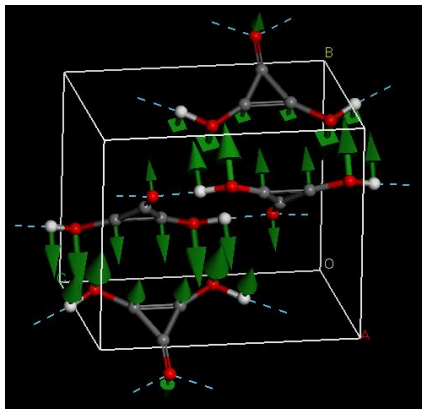
T	H_T-H_{298}	T	H_T-H_{298}	T	H_T-H_{298}
10	-2167.5740	350	20.9107	690	103.4243
20	-1083.0228	360	24.5048	700	105.0881
30	-720.0273	370	27.9809	710	106.7241
40	-536.8485	380	31.3471	720	108.3327
50	-425.4361	390	34.6106	730	109.9147
60	-349.9430	400	37.7778	740	111.4710
70	-295.0476	410	40.8547	750	113.0021
80	-253.0952	420	43.8464	760	114.5085
90	-219.8169	430	46.7580	770	115.9908
100	-192.6443	440	49.5931	780	117.4500
110	-169.9319	450	52.3558	790	118.8859
120	-150.5868	460	55.0503	800	120.2998
130	-133.8431	470	57.6799	810	121.6919
140	-119.1537	480	60.2467	820	123.0624
150	-106.1173	490	62.7545	830	124.4124
160	-94.4361	500	65.2054	840	125.7420
170	-83.8751	510	67.6023	850	127.0517
180	-74.2558	520	69.9469	860	128.3418
190	-65.4357	530	72.2417	870	129.6129
200	-57.3011	540	74.4882	880	130.8654
210	-49.7574	550	76.6884	890	132.0999
220	-42.7295	560	78.8442	900	133.3165
230	-36.1534	570	80.9568	910	134.5155
240	-29.9755	580	83.0278	920	135.6975
250	-24.1519	590	85.0589	930	136.8630
260	-18.6436	600	87.0512	940	138.0118
270	-13.4183	610	89.0063	950	139.1446
280	-8.4474	620	90.9247	960	140.2619
290	-3.7078	630	92.8079	970	141.3638
300	0.8236	640	94.6571	980	142.4503
310	5.1630	650	96.4732	990	143.5222
320	9.3284	660	98.2569	1000	144.5797
330	13.3335	670	100.0093	-	-
340	17.1902	680	101.7315	-	-

Table S.12. Calculated free-energy function, ΔG ($\Delta G = G_T - H_{298}$), of croconic acid. Temperature and free-energy values are given in K and $J \cdot K^{-1} \cdot mol^{-1}$ units, respectively.

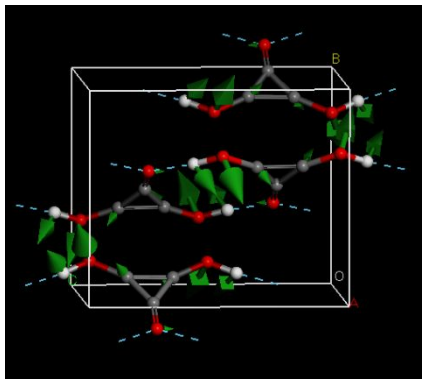
T	G_T-H_{298}	T	G_T-H_{298}	T	G_T-H_{298}
10	-2167.6654	350	-94.9930	690	-95.2994
20	-1083.9731	360	-94.2700	700	-95.6720
30	-722.9784	370	-93.6342	710	-96.0527
40	-542.8005	380	-93.0770	720	-96.4413
50	-435.0460	390	-92.5936	730	-96.8371
60	-363.5555	400	-92.1771	740	-97.2398
70	-312.8182	410	-91.8221	750	-97.6488
80	-275.0606	420	-91.5242	760	-98.0642
90	-245.9644	430	-91.2794	770	-98.4851
100	-222.9310	440	-91.0836	780	-98.9116
110	-204.3070	450	-90.9324	790	-99.3428
120	-188.9860	460	-90.8240	800	-99.7790
130	-176.2039	470	-90.7546	810	-100.2196
140	-165.4132	480	-90.7212	820	-100.6644
150	-156.2125	490	-90.7217	830	-101.1130
160	-148.3035	500	-90.7540	840	-101.5654
170	-141.4541	510	-90.8153	850	-102.0209
180	-135.4878	520	-90.9043	860	-102.4800
190	-130.2624	530	-91.0192	870	-102.9417
200	-125.6645	540	-91.1584	880	-103.4061
210	-121.6033	550	-91.3197	890	-103.8734
220	-118.0056	560	-91.5024	900	-104.3429
230	-114.8088	570	-91.7045	910	-104.8148
240	-111.9619	580	-91.9254	920	-105.2885
250	-109.4218	590	-92.1638	930	-105.7644
260	-107.1532	600	-92.4183	940	-106.2418
270	-105.1241	610	-92.6883	950	-106.7208
280	-103.3080	620	-92.9724	960	-107.2014
290	-101.6836	630	-93.2702	970	-107.6833
300	-100.2295	640	-93.5809	980	-108.1664
310	-98.9291	650	-93.9035	990	-108.6507
320	-97.7673	660	-94.2372	1000	-109.1357
330	-96.7322	670	-94.5814	-	-
340	-95.8104	680	-94.9358	-	-

Figure S.1. The atomic motions associated to some active Raman normal modes of deltic acid.

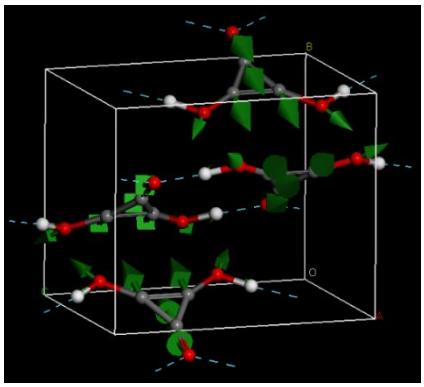
- Mode ν=86.1 cm^{-1} $-$ $T(C=C)+T(OH)+\delta^{oop}(C-C=O)-$ $C=C$ bond and hydroxyl ion (OH^-) translations and out of plane $C-C=O$ bending vibrations.



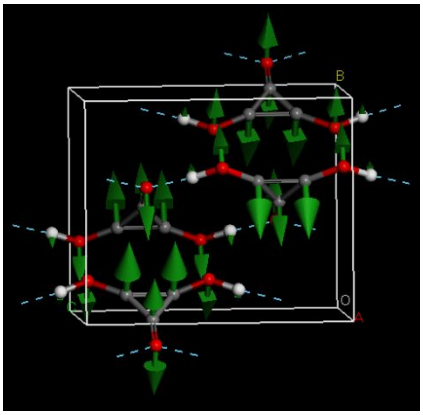
- Mode ν=127.4 cm^{-1} $-$ $R(C=C)+T(OH)-$ $C=C$ bond rotation and hydroxyl ion (OH^-) translations.



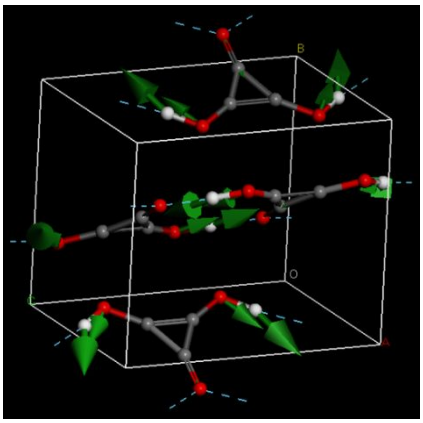
- Mode ν=169.3 cm^{-1} $-$ $T(C_3)+\nu(C=O)+\delta(C-H-O)-C_3$ carbon squeleton translation, $C=O$ stretching and $C-H-O$ bending vibrations.



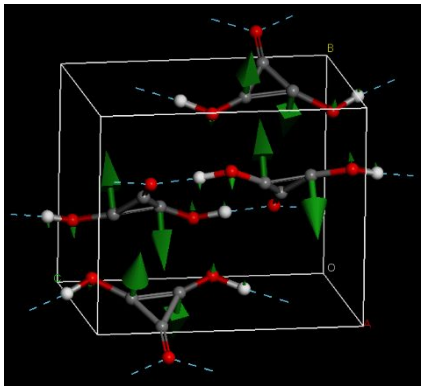
- Mode ν=268.1 cm^{-1} – $T(C_3) + \delta^{oop}(C-C=O) + \delta^{oop}(C-O-H) - C_3$ carbon squeleton translation and out of plane $C-C=O$ and $C-H-O$ bending vibrations.



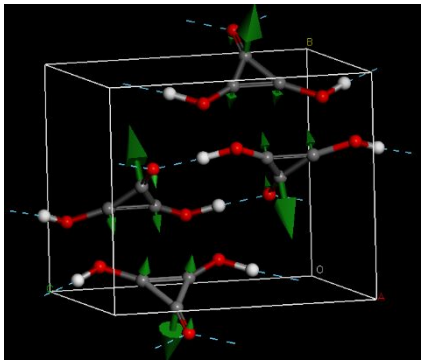
- Mode ν=326.3 cm^{-1} – $T(OH)$ – Hydroxyl ion (OH^-) translations.



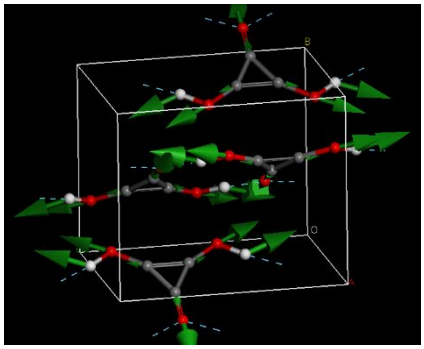
- Mode ν=622.0 cm^{-1} – $Ro(C=C) - C=C$ bond rotation.



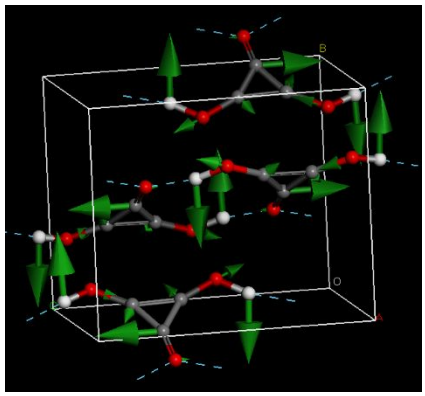
- Mode ν=627.5 cm^{-1} – $Pr\,(C_3) + \delta^{oop}(C-C=O)$ – C_3 carbon squeleton plane rotation and out of plane $C-C=O$ bending vibrations.



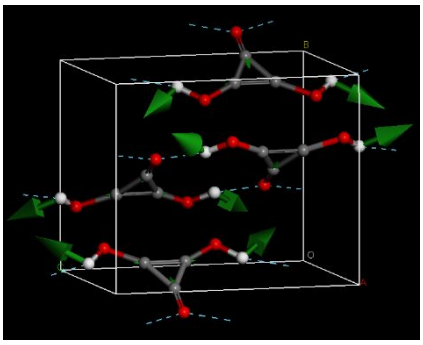
- Mode ν=796.5 cm^{-1} – $Di(C_3) + \nu(C=O) + T(OH)$ – C_3 carbon squeleton dilatation, C=O stretching and hydroxyl ion translations.



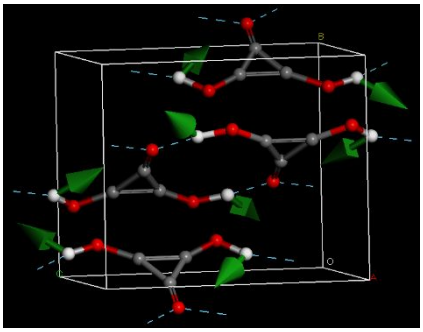
- Mode ν=952.2 cm^{-1} – $Ro\,(C_3) + \delta^{oop}(C-O-H)$ – C_3 carbon squeleton rotation and out of plane $C-O-H$ bending vibrations.



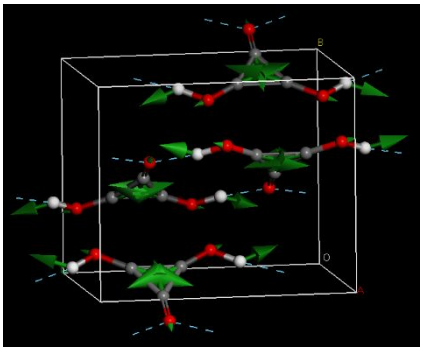
- Mode ν=1370.6 $cm^{-1} - \delta(C-O-H)$ – C-O-H bending vibrations.



- Mode ν=1472.6 $cm^{-1} - \delta(C-O-H)$ – C-O-H bending vibrations.



- Mode ν=1930.2 $cm^{-1} - Co(C_3) + \nu(C-O) + \delta(C-O-H)$ – C_3 carbon squeleton contraction, $C-O$ and $C-O-H$ bending vibrations.



- Mode ν=2537.5 $cm^{-1} - \nu(OH)$ – OH bond stretching vibrations.

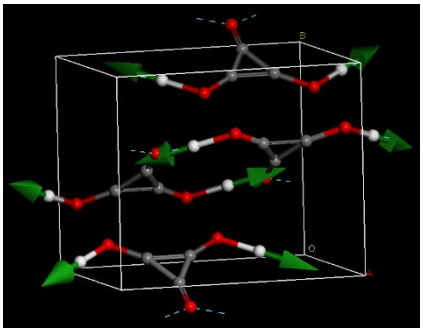
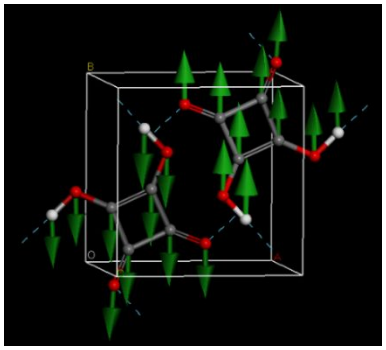


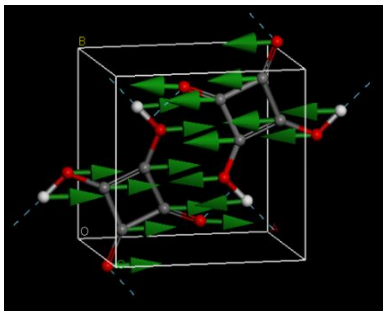
Figure S.2. The atomic motions associated to some active Raman normal modes of squaric acid.

Note: In most cases the vibrational motions performed by the two C-O-H fragments in a squaric acid molecule in a given vibrational mode are very similar. However, sometimes, these fragments behave differently. In these cases, to avoid confusions, the atoms in these fragments will be differentiated using prime symbols. As an example, the vibrational normal mode with wavenumber 151.8 cm^{-1} (see below) was assigned to $\delta^{oop}(C-O'-H')+T(OH)$ because the motion in one fragment is an out of plane bending vibration and in the other one the motion may be better described as a translation of the corresponding hydroxyl OH^- ion.

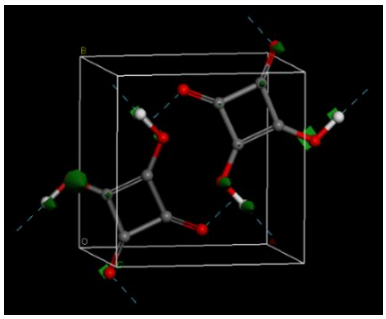
- Mode ν=76.4 cm^{-1} – $T^b(H_2C_4O_4)$ – Squaric acid molecule translations along b axis.



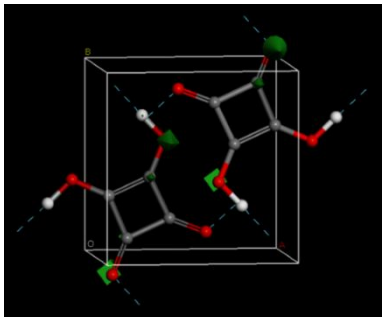
- Mode ν=99.2 cm^{-1} – $T^a(H_2C_4O_4)$ – Squaric acid molecule translations along a axis.



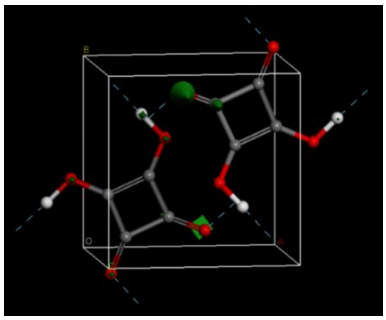
- Mode ν=151.8 cm^{-1} – $\delta^{oop}(C-O'-H')+T(OH^-)$ – $C-O'-H'$ out of plane bending vibrations plus hydroxyl OH^- ion translations.



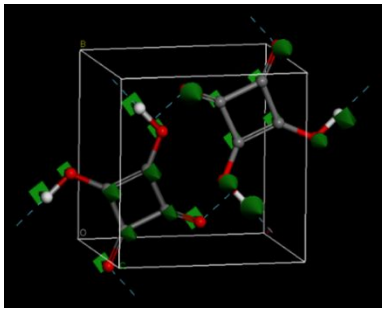
- Mode ν=162.8 cm^{-1} $-$ $\delta^{oop}(C-O-H)+\delta^{oop}(C-C=O)-C-O-H$ and $C-C=O$ out of plane bending vibrations.



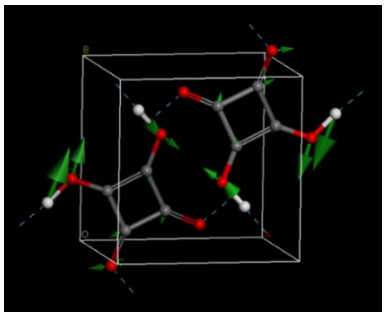
- Mode ν=171.5 cm^{-1} $-$ $\delta^{oop}(C-C=O)$ $-$ $C-C=O$ out of plane bending vibrations.



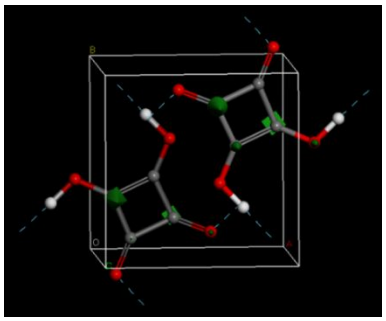
- Mode ν=260.1 cm^{-1} $-$ $T(C_4)+R(C=O)+R(C-O)+T(OH^-)$ $-$ C_4 carbon squeleton translations plus $C=O$ and $C-O$ bond rotations and hydroxyl OH^- ion translations.



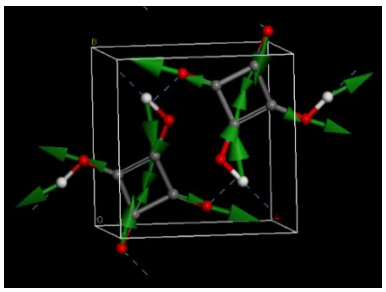
- Mode ν=272.2 cm^{-1} $-T(OH^-)+\nu(O'-H')+\delta(C-O'-H')$ – Hydroxyl OH^- ion translations plus $O'-H'$ bond stretching and $C-O'-H'$ bending vibrations.



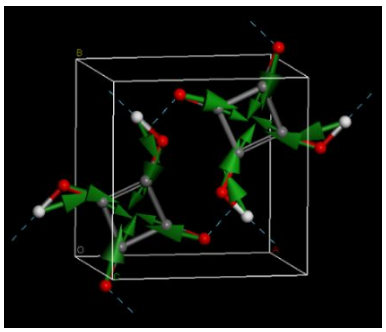
- Mode ν=613.2 cm^{-1} $-$ $Pr(C_4)$ $-$ C_4 carbon squeleton plane rotation.



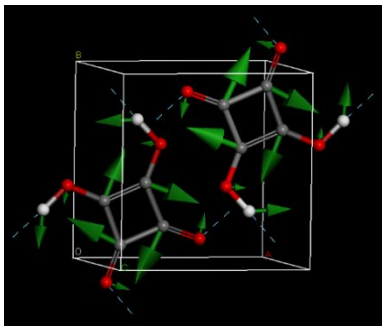
- Mode ν=620.1 cm^{-1} $-$ $Rh(C_4)$ $+\nu(C=O)$ $+\nu(C-O)$ $+\delta(C-O-H)$ $-$ Square to rhombus C_4 carbon squeleton deformation, $C=O$ and $C-O$ bond stretching and $C-O-H$ bending.



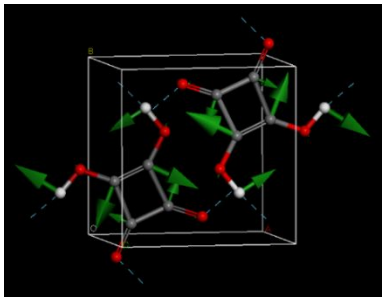
- Mode ν=721.1 cm^{-1} $-$ $Co(C_4)$ $+\nu(C=O)$ $+\nu(C-O)$ $+\delta(C-O-H)$ $-$ C_4 carbon squeleton contraction, $C=O$ and $C-O$ bond stretching and $C-O-H$ bending vibrations.



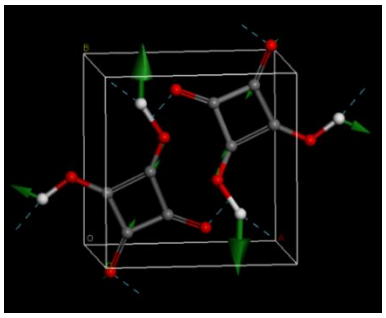
- Mode ν=851.6 cm^{-1} $-Ro(C_4)$ $+\nu(C=O)$ $+\nu(C-O)$ $+\delta(C-O-H)$ $-$ C_4 carbon squeleton rotation, $C=O$ and $C-O$ bond stretching and $C-O-H$ bending vibrations.



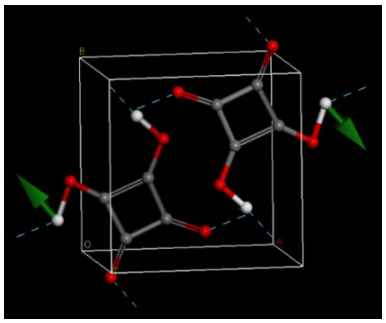
- Mode ν=1140.8 cm^{-1} $-Tp(C_4) + \delta(C-O-H)$ – Square to trapezium C_4 carbon squeleton deformation and $C-O-H$ bending vibrations.



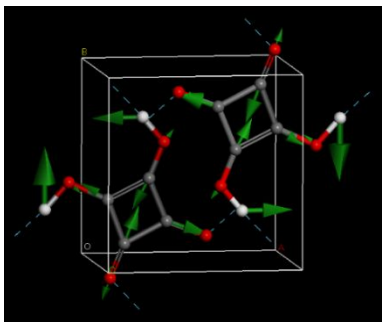
- Mode ν=1331.2 cm^{-1} $-\delta(C-O-H)$ – C-O-H bending vibrations.



- Mode ν=1551.0 cm^{-1} $-\delta(C-O-H)$ – C-O-H bending vibrations.



- Mode ν=1569.9 cm^{-1} $-Rh(C_4) + \nu(C=O) + \nu(C-O) + \delta(C-O-H)$ – Square to rhombus C_4 carbon squeleton deformation, $C=O$ and $C-O$ bond stretching and $C-O-H$ bending.



- Mode ν=1783.8 cm^{-1} $-Co(C_4)$ $+\nu(C=O)$ $+\nu(C-O)$ $+\nu(O-H)-C_4$ carbon squeleton contraction, $C=O$ and $C-O$ bond stretching and $O-H$ bond stretching vibrations.

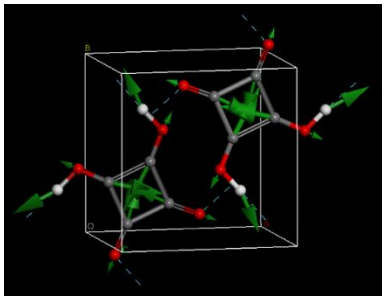
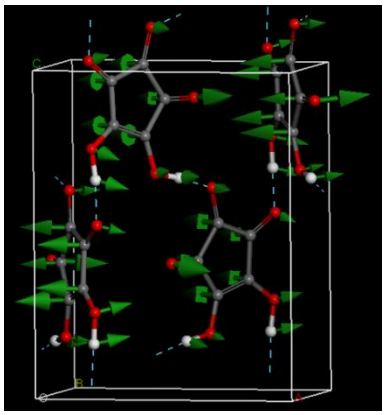
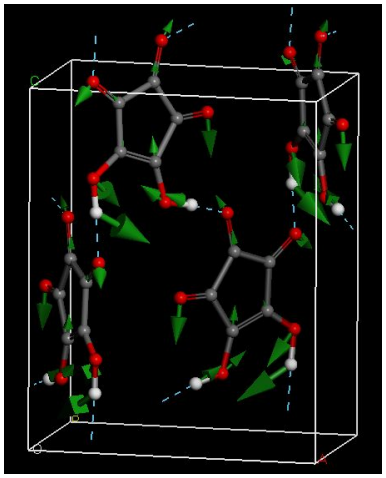


Figure S.3. The atomic motions associated to some active Raman normal modes of croconic acid.

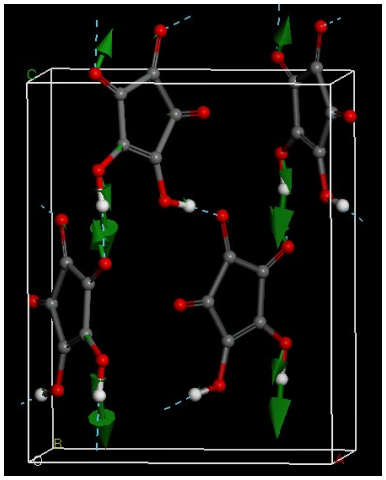
- Mode ν=242.7 cm^{-1} $-\ T(C_5) + \delta^{oop}(C-C=O) + T(OH^-) -$ C_5 carbon squeleton translations, out of plane $C-C=O$ bending vibrations and hydroxyl (OH^-) translations.



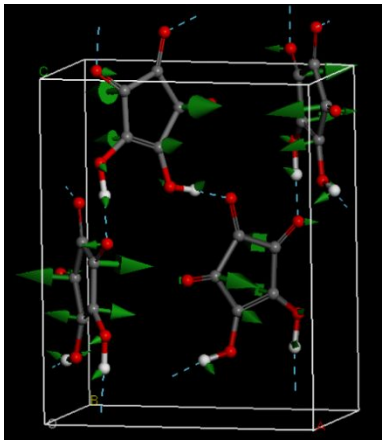
- Mode ν=382.6 cm^{-1} $-\ \delta(C-C=O) + T(OH^-) - C-C=O$ bending vibrations and hydroxyl (OH^-) translations.



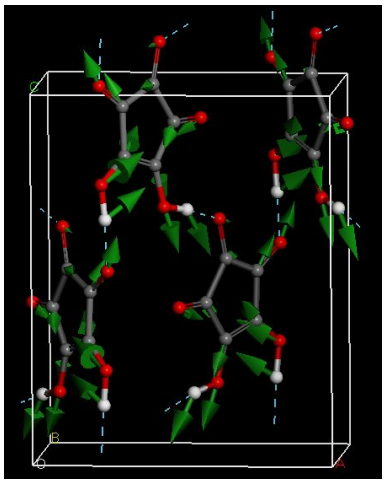
- Mode ν=407.3 cm^{-1} $-\ \delta(C-C=O) + T(OH^-) - C-C=O$ bending and hydroxyl OH^- translations.



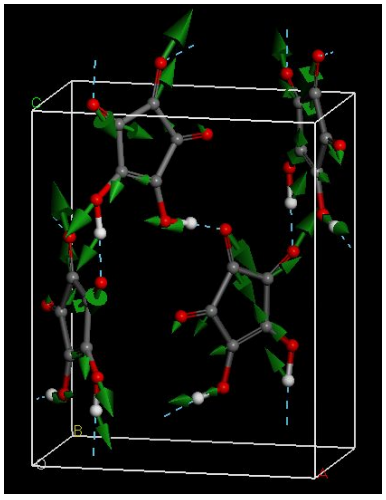
- Mode ν=506.4 cm^{-1} $-$ $Pr(C_5) + \delta^{oop}(C-C=O) + \delta^{oop}(C-O-H) - C_5$ carbon squeleton plane rotation plus out of plane $C-C=O$ and $C-O-H$ bending vibrations.



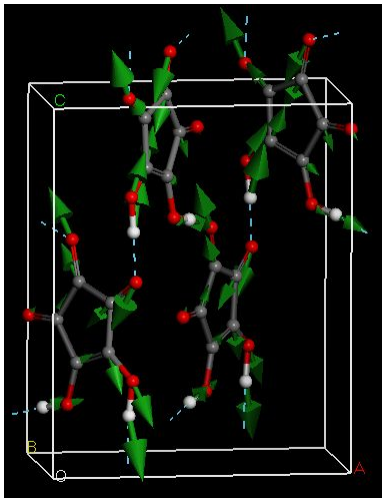
- Mode ν=522.0 cm^{-1} $-Def(C_5) + \nu(C_2-C_3) + \delta^{oop}(C-C=O) + T(OH^-) - C_5$ carbon squeleton deformation, C_2-C_3 stretching, out of plane $C-C=O$ bending and hydroxyl OH^- translations.



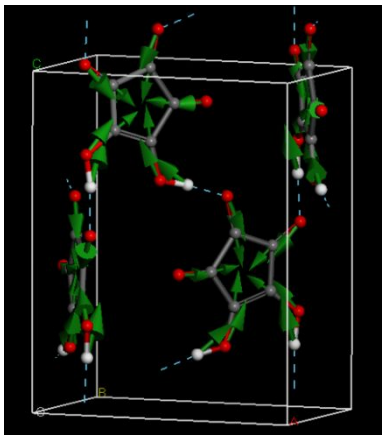
- Mode ν=547.3 cm^{-1} $-$ $El(C_5) + T(C=O) + T(OH) - C_5$ carbon squeleton elongation and $C=O$ and hydroxyl translations.



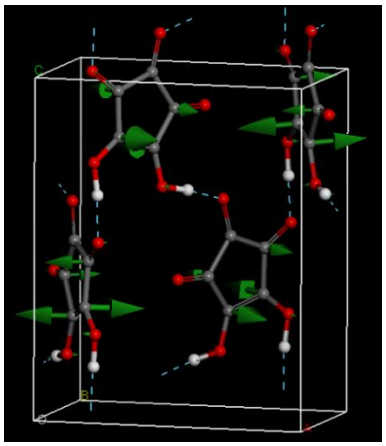
- Mode ν=561.3 cm^{-1} $-$ $Wi(C_5)$ $+T(C=O)$ $+T(OH)-C_5$ carbon squeleton widening and $C=O$ and hydroxyl translations.



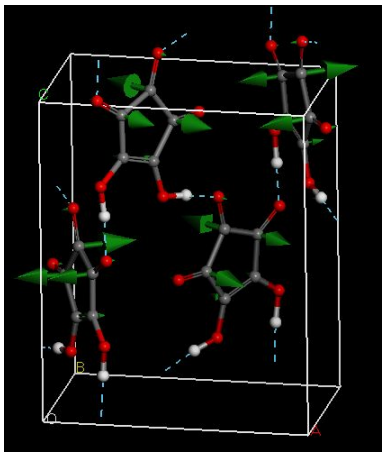
- Mode ν=630.6 cm^{-1} $-$ $Co(C_5)$ $+\nu(C=O)$ $+\nu(C-O)$ $+\delta(C-O-H)-C_5$ carbon squeleton contraction, $C=O$ and $C-O$ stretching and $C-O-H$ bending vibration.



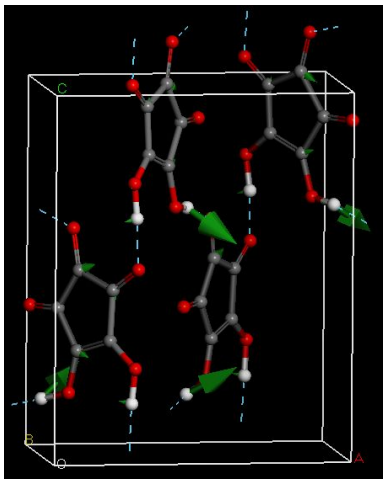
- Mode ν=733.6 cm^{-1} $-$ $Be(C_5)-C_5$ carbon squeleton bending vibration.



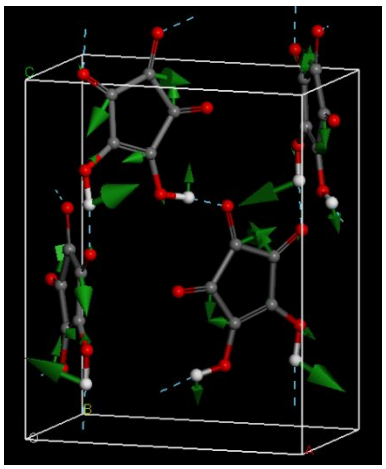
- Mode ν=783.0 cm^{-1} – $Be(C_5) - C_5$ carbon squeleton bending vibration.



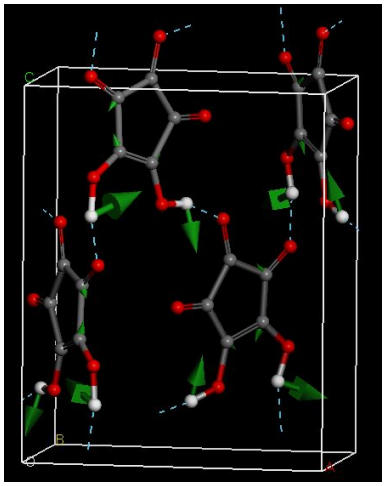
- Mode ν=1062.7 cm^{-1} – $\delta^{oop}(C - O - H)$ – Out of plane $C - O - H$ bending vibrations.



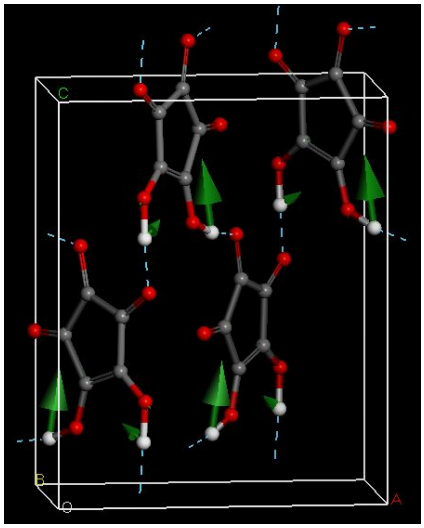
- Mode ν=1165.2 cm^{-1} – $El(C_2 - C_3) + Sh(C_3 - C_4) + El(C_4 - C_5) + \delta(C - O - H)$ – Elongation of $C_2 - C_3$ and $C_4 - C_5$ pentagon sides, $C_3 - C_4$ side shortening and $C - O - H$ bending vibrations.



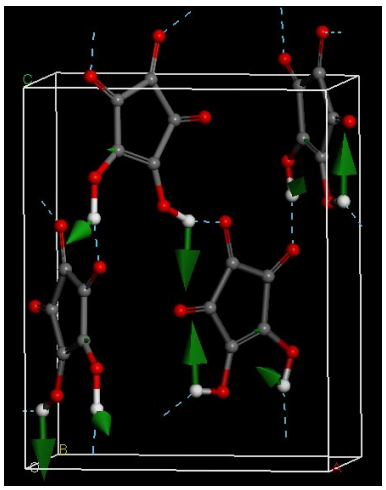
- Mode ν=1244.7 cm^{-1} $-$ $Sh(C_5 - C_1) + \delta(C-O-H)$ $-C_5-C_1$ side shortening and $C-O-H$ bending vibrations.



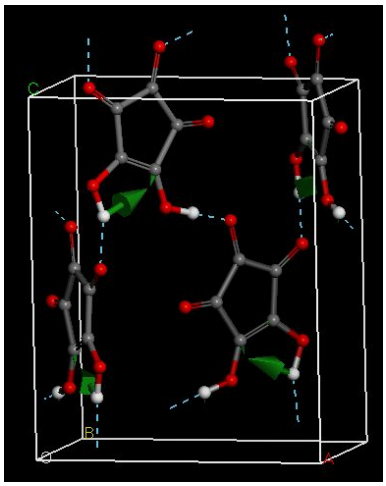
- Mode ν=1310.0 cm^{-1} $-\delta(C-O-H)$ $-$ C-O-H bending vibrations.



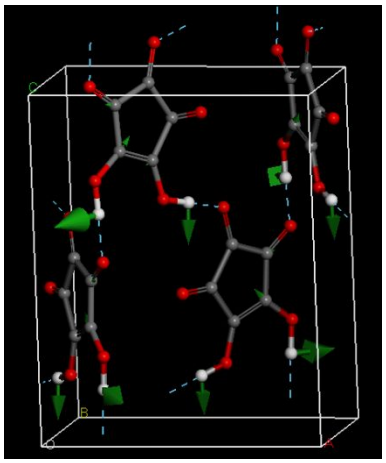
- Mode ν=1377.7 cm^{-1} $-\delta(C-O-H)$ $-$ C-O-H bending vibrations.



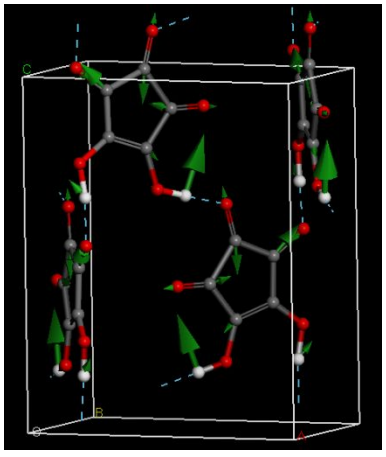
- Mode ν=1397.0 $cm^{-1} - \delta(C - O - H)$ – C-O-H bending vibrations.



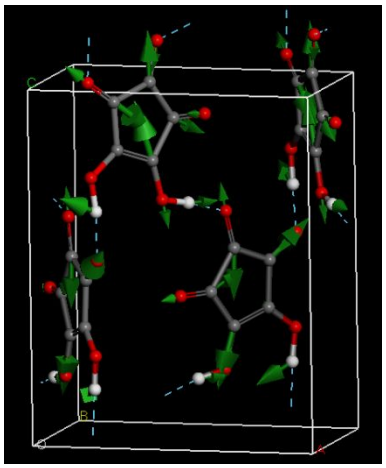
- Mode ν=1517.0 $cm^{-1} - \delta(C - O - H)$ – C-O-H bending vibrations.



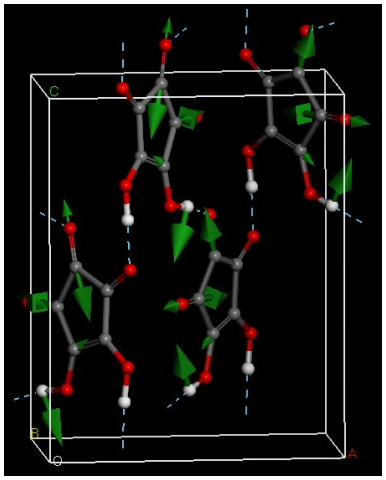
- Mode ν=1552.2 $cm^{-1} - Sh(C_3 - C_4) + Ro(C_4 - C_5) + \nu(C = O) + \delta(C - O - H) - C_3 - C_4$ pentagon side shortening, $C_4 - C_5$ side rotation, $C = O$ stretching and $C - O - H$ bending vibrations.



- Mode ν=1563.8 cm^{-1} $-$ El(C_3-C_4) +Ap$(C_2\cdots C_5)$ +ν$(C=O)$ +δ$(C-O-H)$ $-$ C_3-C_4 pentagon side elongation, $C_2\cdots C_5$ approach, $C=O$ stretching and $C-O-H$ bending vibrations.



- Mode ν=1632.1 cm^{-1} $-$ Ro(C_3-C_4) +ν$(C=O)$ +δ$(C-O-H)$ $-$ C_3-C_4 pentagon side rotation, $C=O$ stretching and $C-O-H$ bending vibrations.



- Mode ν=1693.9 cm^{-1} $-$ Co(C_5) +ν$(C=O)$ +ν$(C-O)$ +δ$(C-O-H)$ $-$ C_5 carbon squeleton contraction, $C=O$ and $C-O$ stretching and $C-O-H$ bending vibration.

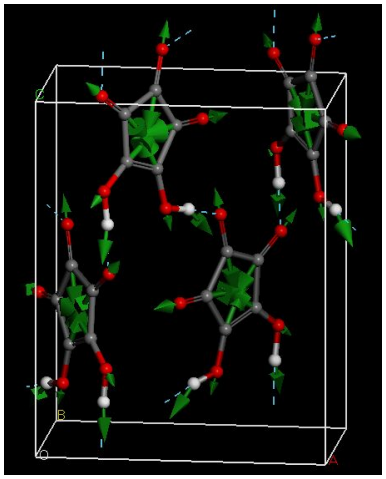


Table S.13. Calculated absorption (α), reflectivity (R), conductivity (σ), dielectric (ε), refractive index (n and k) and loss (ξ) functions of the deltic acid as a function of wavelength in the range from 150 to 300 nm.

λ (nm)	α (cm^{-1})	R	$Re(\sigma)$ (fs^{-1})	$Im(\sigma)$ (fs^{-1})	$Re(\varepsilon)$	$Im(\varepsilon)$	n	k	ξ
300.98	0.00	0.08	0.00	-1.09	3.19	0.00	1.79	0.00	0.00
290.63	0.00	0.08	0.00	-1.16	3.24	0.00	1.80	0.00	0.00
280.96	0.00	0.08	0.00	-1.23	3.30	0.00	1.82	0.00	0.00
271.92	0.00	0.09	0.00	-1.31	3.37	0.00	1.84	0.00	0.00
263.44	0.00	0.09	0.00	-1.39	3.45	0.00	1.86	0.00	0.00
255.47	0.00	0.09	0.00	-1.49	3.53	0.00	1.88	0.00	0.00
247.97	0.00	0.10	0.00	-1.59	3.63	0.00	1.91	0.00	0.00
240.90	0.00	0.10	0.00	-1.71	3.75	0.00	1.94	0.00	0.00
234.22	0.06	0.11	0.00	-1.85	3.89	0.00	1.97	0.00	0.00
227.90	4.84	0.11	0.00	-2.01	4.06	0.00	2.01	0.00	0.00
221.92	28.67	0.12	0.00	-2.21	4.27	0.00	2.07	0.00	0.00
214.86	49.56	0.13	0.00	-2.52	4.61	0.00	2.15	0.00	0.00
209.53	93.97	0.15	0.00	-2.87	5.01	0.00	2.24	0.00	0.00
204.46	270.55	0.16	0.01	-3.37	5.60	0.01	2.37	0.00	0.00
200.22	632.76	0.19	0.02	-4.12	6.51	0.03	2.55	0.01	0.00
199.63	973.80	0.20	0.04	-4.29	6.71	0.05	2.59	0.01	0.00
198.46	3015.22	0.21	0.12	-4.69	7.21	0.16	2.68	0.03	0.00
197.30	8911.29	0.22	0.37	-5.16	7.79	0.49	2.79	0.09	0.01
196.15	20240.00	0.24	0.88	-5.58	8.30	1.15	2.89	0.20	0.02
195.02	34811.15	0.25	1.54	-5.79	8.54	2.00	2.94	0.34	0.03
193.90	48142.58	0.25	2.13	-5.81	8.51	2.76	2.95	0.47	0.03
192.80	58622.01	0.26	2.59	-5.75	8.39	3.34	2.95	0.57	0.04
191.70	68412.80	0.26	3.03	-5.69	8.28	3.87	2.95	0.66	0.05
190.62	79452.04	0.27	3.50	-5.57	8.08	4.45	2.94	0.76	0.05
190.08	84543.44	0.27	3.71	-5.45	7.91	4.70	2.93	0.80	0.06
189.55	88144.23	0.27	3.84	-5.32	7.73	4.85	2.90	0.84	0.06
189.02	89642.61	0.27	3.87	-5.23	7.59	4.88	2.88	0.85	0.06
188.49	89347.27	0.27	3.85	-5.21	7.55	4.84	2.87	0.84	0.06
187.97	88546.04	0.27	3.83	-5.30	7.65	4.81	2.89	0.83	0.06
187.45	88883.17	0.27	3.90	-5.48	7.86	4.87	2.92	0.83	0.06
186.93	91561.56	0.28	4.09	-5.72	8.14	5.10	2.98	0.86	0.06
186.41	97073.18	0.29	4.42	-5.97	8.43	5.50	3.04	0.90	0.05
185.90	105487.92	0.30	4.91	-6.19	8.67	6.09	3.10	0.98	0.05
185.39	116755.34	0.32	5.53	-6.32	8.82	6.84	3.16	1.08	0.05
184.88	130666.32	0.33	6.27	-6.33	8.80	7.74	3.20	1.21	0.06
184.38	146637.65	0.34	7.09	-6.17	8.59	8.73	3.23	1.35	0.06
183.88	163659.40	0.36	7.91	-5.82	8.14	9.71	3.23	1.50	0.06
183.38	180534.22	0.37	8.65	-5.30	7.48	10.59	3.20	1.66	0.06
182.88	196281.84	0.38	9.25	-4.65	6.67	11.29	3.15	1.79	0.07
182.39	210475.70	0.39	9.70	-3.92	5.77	11.80	3.07	1.92	0.07
181.90	223316.37	0.40	10.02	-3.16	4.83	12.16	2.99	2.03	0.07
181.41	235367.91	0.41	10.24	-2.37	3.87	12.40	2.90	2.13	0.07
180.93	247095.54	0.42	10.40	-1.56	2.88	12.55	2.81	2.24	0.08
180.44	258507.57	0.44	10.46	-0.71	1.85	12.59	2.70	2.33	0.08
179.96	269126.97	0.45	10.40	0.19	0.78	12.48	2.58	2.42	0.08

179.48	278214.13	0.46	10.15	1.09	-0.30	12.16	2.43	2.50	0.08
179.01	285001.09	0.47	9.72	1.95	-1.33	11.61	2.27	2.55	0.09
178.54	288823.52	0.48	9.09	2.72	-2.24	10.83	2.10	2.58	0.09
178.07	289221.40	0.49	8.31	3.33	-2.95	9.87	1.92	2.58	0.09
177.60	286080.98	0.50	7.44	3.75	-3.44	8.82	1.74	2.54	0.10
177.13	279757.56	0.51	6.57	3.96	-3.68	7.76	1.57	2.48	0.11
176.67	271060.20	0.51	5.77	4.00	-3.71	6.81	1.42	2.39	0.11
176.21	261078.63	0.51	5.11	3.90	-3.59	6.01	1.31	2.30	0.12
175.75	250957.02	0.50	4.59	3.73	-3.37	5.38	1.22	2.21	0.13
175.29	241741.01	0.49	4.22	3.53	-3.13	4.93	1.16	2.12	0.14
174.84	234279.90	0.48	3.97	3.36	-2.92	4.63	1.13	2.05	0.15
174.39	229043.24	0.48	3.79	3.24	-2.77	4.41	1.10	2.00	0.16
173.94	225855.52	0.47	3.65	3.18	-2.69	4.24	1.08	1.96	0.17
173.49	223812.13	0.48	3.49	3.19	-2.69	4.04	1.04	1.94	0.17
173.05	221591.72	0.48	3.26	3.22	-2.71	3.76	0.98	1.92	0.17
172.61	217990.34	0.49	2.96	3.23	-2.72	3.41	0.91	1.88	0.18
172.17	212330.62	0.51	2.63	3.19	-2.66	3.02	0.82	1.83	0.19
171.73	204585.68	0.51	2.29	3.08	-2.53	2.62	0.75	1.76	0.20
171.30	195278.29	0.51	2.00	2.91	-2.33	2.29	0.68	1.67	0.21
170.86	185282.78	0.51	1.78	2.71	-2.09	2.03	0.64	1.58	0.24
170.43	175603.50	0.49	1.64	2.51	-1.85	1.86	0.62	1.50	0.27
170.00	167128.84	0.47	1.56	2.32	-1.63	1.76	0.62	1.42	0.31
169.15	155272.64	0.42	1.48	2.05	-1.32	1.68	0.64	1.31	0.37
168.73	151272.18	0.41	1.45	1.97	-1.22	1.63	0.64	1.28	0.39
168.31	147542.82	0.40	1.39	1.91	-1.14	1.56	0.63	1.24	0.42
167.48	138258.24	0.39	1.22	1.78	-0.99	1.37	0.59	1.16	0.48
167.06	132364.92	0.38	1.13	1.70	-0.90	1.26	0.57	1.11	0.53
166.65	126188.46	0.37	1.06	1.61	-0.79	1.18	0.56	1.05	0.58
165.83	115934.51	0.33	0.98	1.45	-0.60	1.09	0.57	0.96	0.70
165.43	112412.76	0.32	0.96	1.40	-0.54	1.06	0.57	0.93	0.75
165.02	109192.07	0.31	0.92	1.36	-0.50	1.01	0.56	0.90	0.80
164.22	99671.43	0.31	0.76	1.29	-0.41	0.84	0.51	0.82	0.97
163.82	92305.37	0.30	0.67	1.23	-0.34	0.73	0.48	0.76	1.13
163.43	83514.72	0.29	0.58	1.15	-0.25	0.63	0.46	0.68	1.37
162.64	65169.60	0.22	0.47	0.97	-0.05	0.51	0.48	0.53	1.95
162.25	56943.71	0.19	0.43	0.89	0.04	0.46	0.50	0.46	2.14
161.86	49257.60	0.15	0.39	0.81	0.12	0.42	0.53	0.40	2.18
161.09	34303.75	0.09	0.31	0.66	0.29	0.33	0.60	0.28	1.72
160.71	27632.28	0.06	0.27	0.58	0.38	0.29	0.65	0.22	1.28
160.32	22407.22	0.04	0.24	0.49	0.47	0.26	0.71	0.18	0.89
159.94	18960.56	0.02	0.22	0.41	0.57	0.23	0.77	0.15	0.62
158.44	16767.61	0.01	0.24	0.11	0.88	0.25	0.95	0.13	0.30
156.97	15843.64	0.00	0.25	-0.08	1.08	0.26	1.05	0.12	0.21
155.53	14144.65	0.01	0.24	-0.25	1.26	0.25	1.13	0.11	0.15
154.11	11108.49	0.01	0.20	-0.41	1.42	0.20	1.20	0.09	0.10
152.72	8733.76	0.02	0.17	-0.62	1.63	0.17	1.28	0.07	0.06
151.35	10484.93	0.02	0.21	-0.83	1.83	0.22	1.36	0.08	0.06
150.00	14444.92	0.03	0.30	-0.95	1.95	0.30	1.40	0.11	0.08

Table S.14. Calculated absorption (α), reflectivity (R), conductivity (σ), dielectric (ε), refractive index (n and k) and loss (ξ) functions of the squaric acid as a function of wavelength in the range from 200 to 400 nm.

λ (nm)	α (cm^{-1})	R	$Re(\sigma)$ (fs^{-1})	$Im(\sigma)$ (fs^{-1})	$Re(\varepsilon)$	$Im(\varepsilon)$	n	k	ξ
401.20	0.00	0.15	0.00	-1.51	5.04	0.00	2.25	0.00	0.00
395.73	0.00	0.15	0.00	-1.56	5.12	0.00	2.26	0.00	0.00
390.40	0.00	0.15	0.00	-1.62	5.22	0.00	2.28	0.00	0.00
385.21	0.00	0.16	0.00	-1.68	5.31	0.00	2.31	0.00	0.00
380.15	0.00	0.16	0.00	-1.74	5.42	0.00	2.33	0.00	0.00
375.23	0.00	0.16	0.00	-1.81	5.54	0.00	2.35	0.00	0.00
370.43	0.00	0.17	0.00	-1.89	5.68	0.00	2.38	0.00	0.00
365.76	0.03	0.17	0.00	-1.98	5.83	0.00	2.41	0.00	0.00
361.20	2.07	0.18	0.00	-2.08	6.01	0.00	2.45	0.00	0.00
356.75	41.04	0.18	0.00	-2.19	6.22	0.00	2.49	0.00	0.00
352.42	338.77	0.19	0.01	-2.33	6.48	0.03	2.55	0.01	0.00
350.29	781.14	0.19	0.03	-2.41	6.64	0.07	2.58	0.01	0.00
348.18	1616.65	0.20	0.06	-2.50	6.80	0.15	2.61	0.03	0.00
346.10	2973.18	0.20	0.12	-2.57	6.94	0.27	2.64	0.05	0.01
344.05	4733.81	0.21	0.19	-2.64	7.05	0.43	2.66	0.08	0.01
342.02	6384.44	0.21	0.26	-2.67	7.10	0.58	2.67	0.11	0.01
340.01	7210.30	0.21	0.29	-2.69	7.11	0.65	2.67	0.12	0.01
338.03	6827.24	0.21	0.27	-2.73	7.15	0.62	2.68	0.12	0.01
336.07	5640.85	0.21	0.23	-2.80	7.27	0.51	2.70	0.09	0.01
334.13	4735.81	0.22	0.19	-2.92	7.51	0.43	2.74	0.08	0.01
332.22	5096.31	0.22	0.21	-3.07	7.81	0.47	2.80	0.08	0.01
330.32	6808.08	0.23	0.29	-3.23	8.11	0.64	2.85	0.11	0.01
328.45	9194.38	0.24	0.40	-3.37	8.38	0.88	2.90	0.15	0.01
326.60	11872.17	0.24	0.52	-3.50	8.62	1.14	2.94	0.19	0.02
324.77	15198.94	0.25	0.68	-3.61	8.81	1.47	2.98	0.25	0.02
322.96	19118.59	0.25	0.86	-3.68	8.93	1.86	3.00	0.31	0.02
321.17	22436.61	0.26	1.01	-3.72	8.97	2.17	3.02	0.36	0.03
319.40	24435.75	0.26	1.11	-3.76	9.02	2.36	3.03	0.39	0.03
317.65	26268.00	0.26	1.20	-3.84	9.14	2.55	3.05	0.42	0.03
315.92	29222.79	0.27	1.35	-3.93	9.29	2.85	3.08	0.46	0.03
314.21	32867.14	0.27	1.53	-4.01	9.40	3.21	3.11	0.52	0.03
312.51	36495.44	0.28	1.71	-4.07	9.48	3.57	3.13	0.57	0.03
310.84	40864.98	0.29	1.93	-4.12	9.53	4.00	3.15	0.64	0.04
309.18	46738.77	0.29	2.21	-4.11	9.47	4.57	3.16	0.72	0.04
307.54	52698.78	0.29	2.48	-4.01	9.22	5.09	3.14	0.81	0.05
305.92	55988.63	0.29	2.60	-3.85	8.86	5.31	3.10	0.86	0.05
304.31	55393.59	0.29	2.54	-3.76	8.63	5.15	3.06	0.84	0.05
302.72	52660.99	0.28	2.41	-3.81	8.69	4.87	3.05	0.80	0.05
301.15	50913.70	0.29	2.37	-4.00	9.03	4.76	3.10	0.77	0.05
299.59	52294.03	0.30	2.50	-4.27	9.53	4.99	3.18	0.78	0.04
298.05	57588.89	0.31	2.83	-4.53	10.00	5.63	3.28	0.86	0.04
296.53	66587.85	0.33	3.35	-4.68	10.26	6.62	3.35	0.99	0.04
295.02	77631.84	0.34	3.94	-4.66	10.17	7.76	3.39	1.15	0.05
293.52	87835.81	0.35	4.45	-4.47	9.75	8.71	3.38	1.29	0.05
292.04	95004.17	0.36	4.75	-4.21	9.20	9.25	3.34	1.39	0.05
290.58	99337.43	0.36	4.90	-4.00	8.76	9.51	3.29	1.44	0.06
289.13	102768.51	0.36	5.04	-3.90	8.51	9.73	3.27	1.49	0.06
287.69	106985.94	0.37	5.27	-3.86	8.41	10.11	3.28	1.54	0.06

286.27	113200.09	0.38	5.62	-3.86	8.36	10.74	3.32	1.62	0.06
284.87	123066.26	0.39	6.19	-3.79	8.20	11.77	3.36	1.75	0.06
283.47	137342.75	0.41	6.96	-3.52	7.65	13.17	3.38	1.95	0.06
282.09	153726.38	0.43	7.73	-2.95	6.56	14.55	3.36	2.17	0.06
280.73	168216.36	0.45	8.22	-2.16	5.04	15.39	3.26	2.36	0.06
279.37	178730.56	0.46	8.34	-1.32	3.46	15.55	3.11	2.50	0.06
278.03	186359.15	0.47	8.27	-0.57	2.05	15.34	2.96	2.59	0.06
276.71	193065.37	0.48	8.15	0.11	0.80	15.05	2.82	2.67	0.07
275.39	199264.74	0.49	8.00	0.74	-0.36	14.69	2.68	2.74	0.07
274.09	204509.89	0.50	7.76	1.34	-1.44	14.19	2.53	2.80	0.07
272.80	209287.61	0.51	7.50	1.89	-2.44	13.64	2.39	2.85	0.07
271.52	214565.16	0.53	7.24	2.44	-3.42	13.11	2.25	2.91	0.07
270.26	220013.97	0.55	6.90	3.03	-4.46	12.45	2.09	2.97	0.07
269.00	223986.74	0.57	6.39	3.60	-5.46	11.46	1.90	3.01	0.07
267.76	225108.94	0.59	5.67	4.06	-6.26	10.12	1.68	3.01	0.07
266.53	222926.48	0.61	4.83	4.35	-6.73	8.59	1.45	2.97	0.07
265.31	217303.58	0.63	3.97	4.42	-6.82	7.03	1.22	2.88	0.07
264.10	208346.54	0.65	3.18	4.28	-6.53	5.60	1.02	2.75	0.08
262.90	197274.90	0.66	2.58	3.97	-5.96	4.53	0.87	2.59	0.08
261.71	186733.03	0.65	2.27	3.62	-5.32	3.96	0.81	2.44	0.09
260.54	179265.36	0.63	2.16	3.34	-4.81	3.75	0.80	2.34	0.10
259.37	175208.09	0.62	2.11	3.19	-4.52	3.64	0.80	2.27	0.11
258.22	173042.01	0.62	2.01	3.13	-4.39	3.47	0.78	2.23	0.11
257.07	171256.63	0.63	1.86	3.10	-4.32	3.19	0.72	2.20	0.11
255.94	169073.81	0.65	1.66	3.08	-4.25	2.83	0.65	2.16	0.11
254.81	166271.58	0.67	1.43	3.03	-4.16	2.44	0.57	2.12	0.10
253.69	162742.56	0.70	1.19	2.97	-4.02	2.02	0.49	2.06	0.10
252.59	158166.16	0.73	0.94	2.87	-3.83	1.59	0.40	2.00	0.09
251.49	152252.53	0.77	0.70	2.72	-3.57	1.17	0.31	1.91	0.08
250.41	145209.87	0.81	0.50	2.55	-3.25	0.83	0.23	1.82	0.07
248.26	130263.53	0.87	0.26	2.17	-2.60	0.42	0.13	1.62	0.06
244.08	100031.91	0.96	0.03	1.53	-1.49	0.06	0.02	1.22	0.03
240.04	70991.33	0.98	0.01	1.08	-0.73	0.02	0.01	0.85	0.04
236.13	37594.41	0.97	0.00	0.76	-0.20	0.01	0.01	0.44	0.18
232.34	265.58	0.14	0.00	0.51	0.21	0.00	0.46	0.00	0.06
228.67	82.02	0.02	0.00	0.30	0.54	0.00	0.74	0.00	0.00
225.12	28.15	0.00	0.00	0.12	0.82	0.00	0.91	0.00	0.00
221.68	91.82	0.00	0.00	-0.05	1.07	0.00	1.04	0.00	0.00
218.34	316.55	0.00	0.01	-0.21	1.31	0.01	1.15	0.00	0.00
215.09	2382.27	0.01	0.04	-0.38	1.54	0.06	1.24	0.03	0.03
211.95	6055.80	0.02	0.12	-0.47	1.67	0.17	1.29	0.06	0.06
208.89	5289.59	0.02	0.11	-0.55	1.77	0.15	1.33	0.06	0.05
205.92	5349.32	0.03	0.11	-0.65	1.90	0.15	1.38	0.06	0.04
203.04	4255.04	0.03	0.09	-0.75	2.02	0.12	1.42	0.04	0.03
200.23	2921.18	0.04	0.06	-0.88	2.18	0.09	1.48	0.03	0.02

Table S.15. Calculated absorption (α), reflectivity (R), conductivity (σ), dielectric (ε), refractive index (n and k) and loss (ξ) functions of the croconic acid as a function of wavelength in the range from 210 to 450 nm.

λ (nm)	α (cm^{-1})	R	$Re(\sigma)$ (fs^{-1})	$Im(\sigma)$ (fs^{-1})	$Re(\varepsilon)$	$Im(\varepsilon)$	n	k	ξ
450.25	0.07	0.20	0.00	-1.92	6.78	0.00	2.60	0.00	0.00
439.24	7.06	0.21	0.00	-2.13	7.26	0.00	2.69	0.00	0.00
428.76	133.94	0.23	0.01	-2.41	7.89	0.02	2.81	0.00	0.00
418.76	833.38	0.25	0.04	-2.79	8.81	0.10	2.97	0.02	0.00
409.22	4355.66	0.27	0.21	-3.35	10.14	0.57	3.19	0.09	0.01
400.11	14820.08	0.30	0.76	-3.93	11.48	2.02	3.40	0.30	0.01
395.70	21521.44	0.31	1.12	-4.12	11.87	2.96	3.47	0.43	0.02
391.39	27450.72	0.32	1.45	-4.28	12.17	3.79	3.53	0.54	0.02
387.17	33213.64	0.33	1.79	-4.48	12.58	4.63	3.60	0.64	0.03
383.05	41142.97	0.35	2.28	-4.71	13.04	5.83	3.70	0.79	0.03
379.00	51697.00	0.36	2.93	-4.86	13.29	7.40	3.77	0.98	0.03
375.05	63398.19	0.38	3.64	-4.90	13.27	9.11	3.83	1.19	0.04
371.17	77578.85	0.40	4.52	-4.85	13.01	11.18	3.88	1.44	0.04
367.38	96793.80	0.43	5.65	-4.48	11.99	13.84	3.89	1.78	0.04
365.51	107607.58	0.44	6.22	-4.10	11.00	15.17	3.86	1.97	0.04
363.66	118145.00	0.45	6.70	-3.59	9.71	16.26	3.78	2.15	0.05
361.83	127588.21	0.46	7.04	-2.99	8.21	16.98	3.68	2.31	0.05
360.01	135421.81	0.47	7.20	-2.35	6.64	17.29	3.55	2.44	0.05
358.22	141543.97	0.47	7.22	-1.73	5.14	17.24	3.40	2.54	0.05
356.44	146215.94	0.48	7.12	-1.17	3.77	16.94	3.25	2.61	0.06
354.68	149864.28	0.48	6.97	-0.66	2.57	16.49	3.10	2.66	0.06
352.94	152806.85	0.48	6.78	-0.21	1.49	15.96	2.96	2.70	0.06
351.22	155053.22	0.49	6.55	0.21	0.52	15.34	2.82	2.72	0.07
349.51	156317.47	0.49	6.26	0.57	-0.33	14.59	2.67	2.73	0.07
347.81	156248.25	0.49	5.91	0.87	-1.01	13.72	2.53	2.72	0.07
346.14	154739.71	0.49	5.54	1.07	-1.47	12.79	2.39	2.68	0.08
344.48	152149.58	0.48	5.19	1.17	-1.70	11.92	2.27	2.62	0.08
342.84	149297.08	0.48	4.90	1.20	-1.75	11.21	2.19	2.56	0.09
341.21	147187.99	0.47	4.73	1.19	-1.72	10.76	2.14	2.51	0.09
339.60	146560.35	0.47	4.65	1.20	-1.72	10.53	2.12	2.49	0.09
338.00	147537.24	0.47	4.63	1.26	-1.83	10.44	2.09	2.49	0.09
336.42	149635.17	0.48	4.62	1.38	-2.09	10.37	2.06	2.52	0.09
334.85	152064.32	0.48	4.57	1.55	-2.47	10.20	2.00	2.55	0.09
333.29	154053.53	0.49	4.44	1.75	-2.89	9.88	1.92	2.57	0.09
331.76	155047.63	0.50	4.25	1.93	-3.28	9.40	1.83	2.57	0.09
330.23	154780.67	0.51	3.99	2.07	-3.57	8.80	1.72	2.56	0.10
328.72	153283.17	0.51	3.72	2.16	-3.73	8.16	1.62	2.52	0.10
327.22	150840.23	0.51	3.45	2.18	-3.76	7.54	1.53	2.47	0.11
325.74	147890.13	0.51	3.22	2.16	-3.69	7.01	1.45	2.41	0.11
324.27	144876.79	0.50	3.04	2.11	-3.56	6.58	1.40	2.35	0.12
322.81	142127.80	0.50	2.90	2.05	-3.41	6.25	1.36	2.29	0.12
321.37	139836.11	0.49	2.80	1.99	-3.26	6.01	1.34	2.25	0.13

319.94	138133.46	0.49	2.73	1.94	-3.14	5.83	1.32	2.21	0.13
318.52	137140.42	0.48	2.69	1.91	-3.06	5.71	1.31	2.18	0.14
317.11	136902.33	0.48	2.66	1.91	-3.04	5.62	1.29	2.17	0.14
315.72	137257.09	0.48	2.62	1.93	-3.07	5.52	1.27	2.17	0.14
314.34	137773.63	0.49	2.56	1.98	-3.15	5.37	1.24	2.17	0.14
312.97	137852.91	0.50	2.46	2.03	-3.24	5.14	1.19	2.16	0.14
311.61	136961.08	0.50	2.32	2.06	-3.28	4.82	1.13	2.13	0.14
310.27	134891.63	0.51	2.16	2.05	-3.24	4.48	1.07	2.09	0.15
308.93	131958.53	0.50	2.03	1.99	-3.11	4.18	1.02	2.04	0.15
307.61	129010.05	0.49	1.95	1.91	-2.92	3.99	1.01	1.98	0.16
306.30	127134.45	0.48	1.94	1.84	-2.76	3.96	1.02	1.95	0.17
305.00	127066.83	0.47	1.98	1.81	-2.68	4.02	1.04	1.94	0.17
303.71	128716.55	0.48	2.03	1.83	-2.71	4.11	1.05	1.95	0.17
302.43	131277.53	0.49	2.05	1.91	-2.85	4.14	1.04	1.99	0.16
301.16	133754.33	0.50	2.01	2.02	-3.05	4.04	1.00	2.01	0.16
299.91	135409.01	0.52	1.91	2.12	-3.24	3.82	0.94	2.03	0.15
298.66	135917.78	0.54	1.76	2.19	-3.37	3.51	0.86	2.03	0.15
297.42	135304.31	0.57	1.59	2.23	-3.43	3.16	0.78	2.01	0.15
296.20	133784.27	0.59	1.42	2.24	-3.42	2.81	0.71	1.98	0.14
294.98	131626.92	0.60	1.27	2.21	-3.36	2.49	0.64	1.94	0.14
293.78	129082.81	0.62	1.13	2.17	-3.25	2.22	0.58	1.90	0.14
292.58	126367.84	0.63	1.01	2.12	-3.13	1.98	0.54	1.85	0.14
291.39	123659.26	0.64	0.92	2.06	-3.00	1.78	0.49	1.80	0.15
290.22	121072.96	0.65	0.83	2.00	-2.88	1.61	0.46	1.76	0.15
287.89	116262.35	0.67	0.68	1.90	-2.65	1.31	0.39	1.67	0.15
283.35	104920.56	0.75	0.37	1.67	-2.15	0.71	0.24	1.49	0.14
278.95	89916.01	0.81	0.18	1.37	-1.55	0.34	0.13	1.25	0.13
274.68	74101.03	0.86	0.09	1.11	-1.03	0.16	0.08	1.02	0.15
270.55	56945.97	0.87	0.05	0.88	-0.59	0.09	0.06	0.77	0.25
266.53	37337.15	0.78	0.04	0.70	-0.24	0.08	0.08	0.50	1.20
262.63	12653.55	0.41	0.04	0.56	0.02	0.07	0.23	0.17	12.20
258.85	4121.32	0.11	0.03	0.43	0.26	0.05	0.51	0.05	0.78
255.17	3086.37	0.04	0.03	0.31	0.47	0.05	0.68	0.04	0.24
251.60	2145.92	0.01	0.03	0.21	0.65	0.04	0.81	0.03	0.10
244.74	1473.69	0.00	0.02	0.01	0.99	0.04	0.99	0.02	0.04
238.25	2550.42	0.00	0.04	-0.18	1.29	0.07	1.14	0.03	0.04
232.09	2464.56	0.01	0.05	-0.33	1.51	0.07	1.23	0.03	0.03
226.25	1809.68	0.02	0.04	-0.51	1.77	0.05	1.33	0.02	0.02
220.69	1159.47	0.03	0.02	-0.71	2.05	0.04	1.43	0.01	0.01
215.40	959.44	0.05	0.02	-0.97	2.39	0.03	1.55	0.01	0.01
210.35	652.85	0.07	0.02	-1.31	2.84	0.02	1.69	0.01	0.00

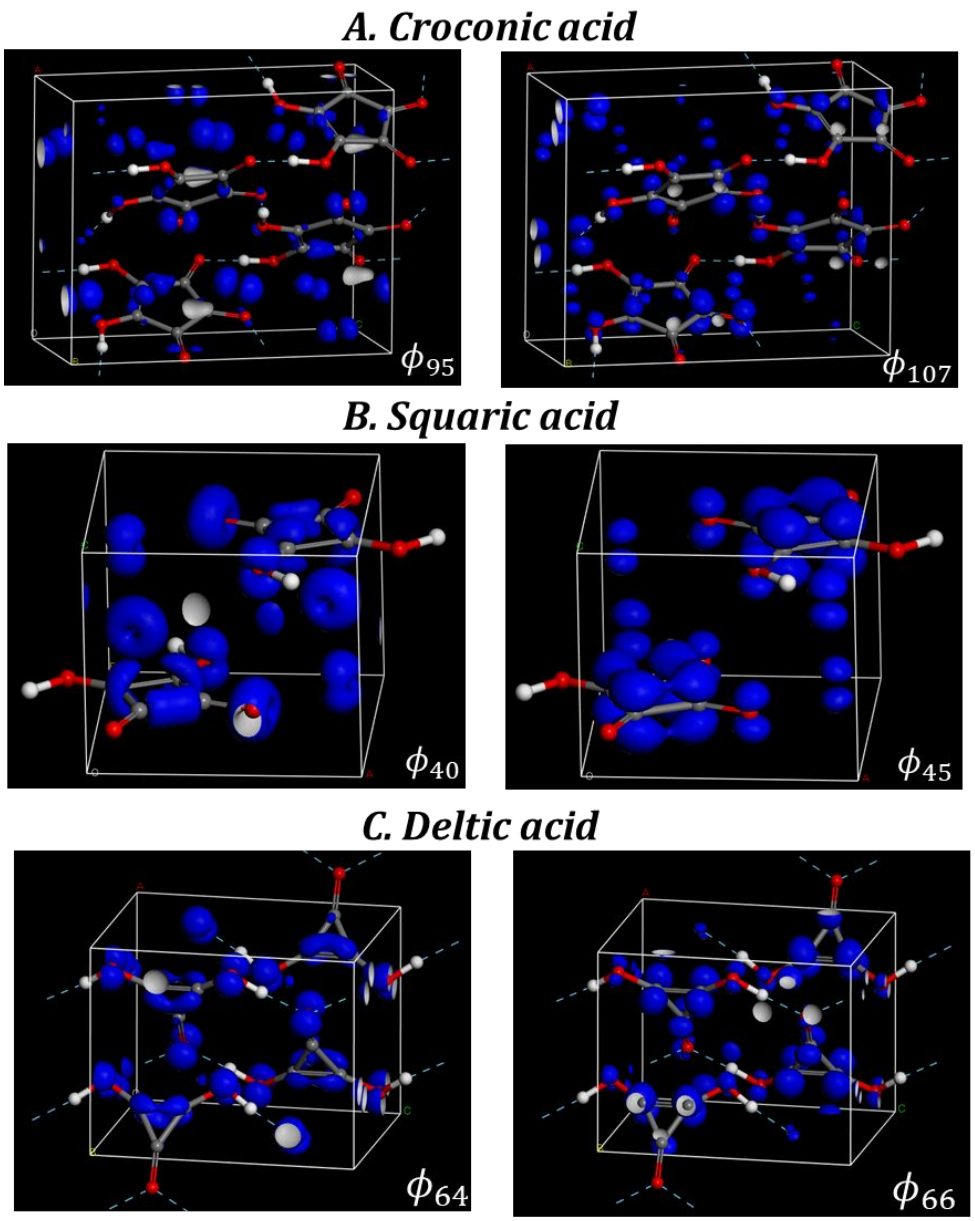


Figure S.4. Constant density plots of some band functions of croconic, squaric and deltic acids.