

Supplementary Materials

Glycerol Carbonate as Fuel Additive for Sustainable Future

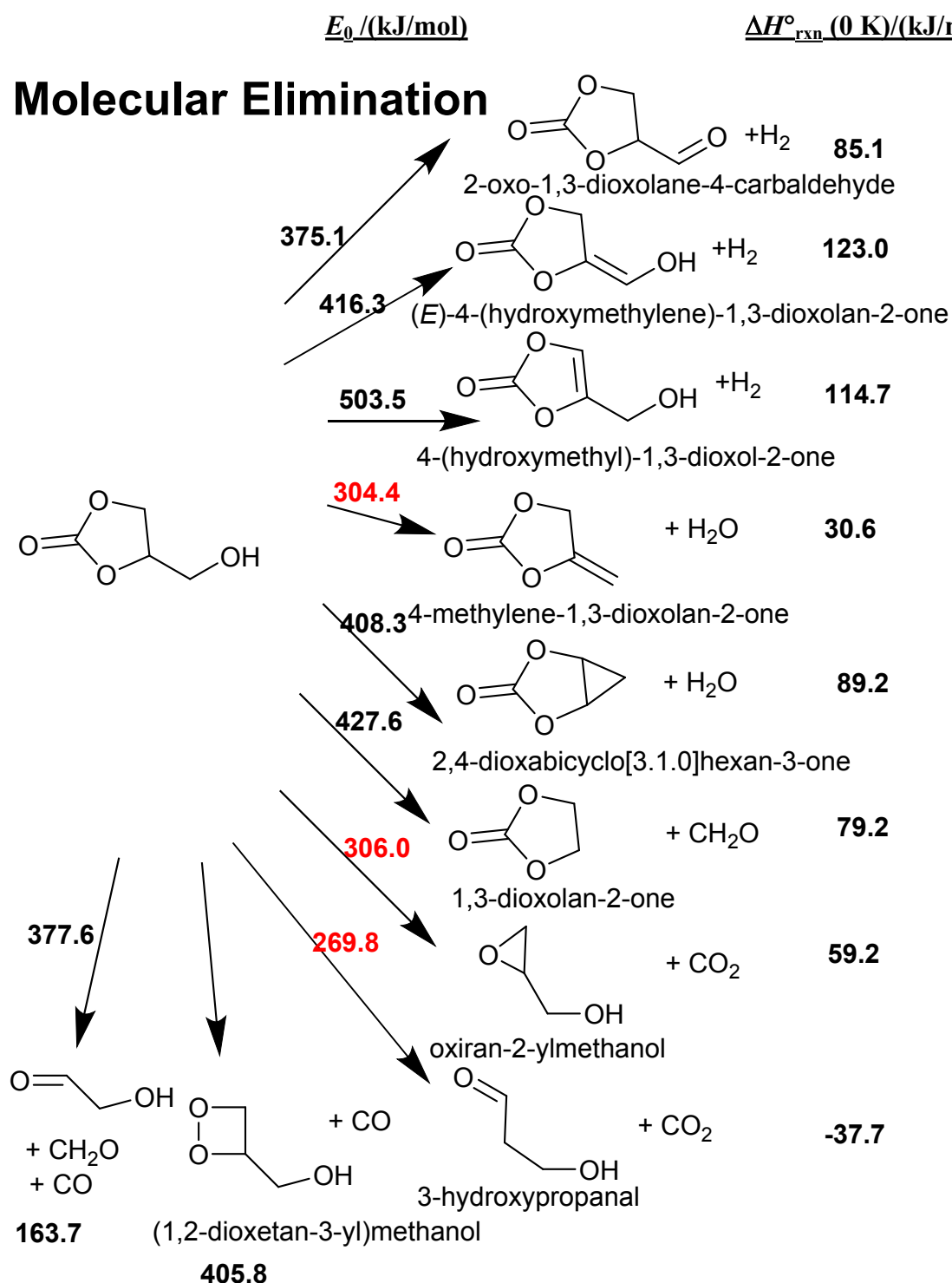
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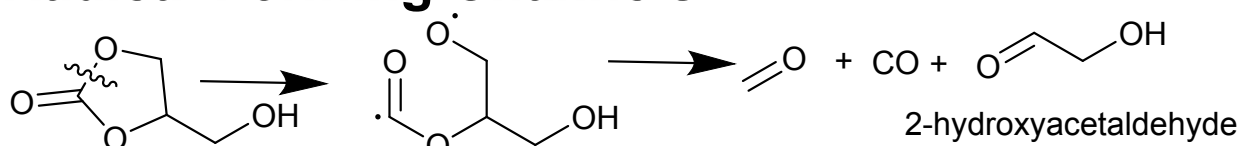
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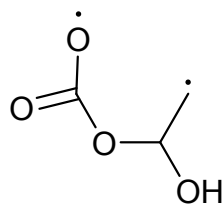
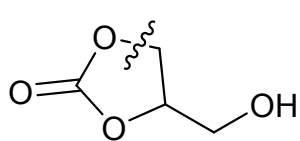
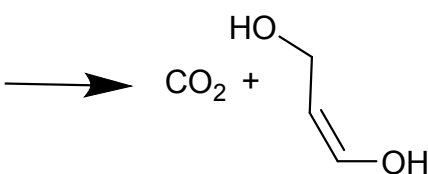
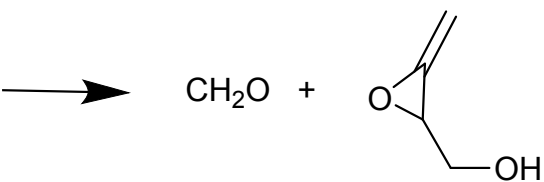
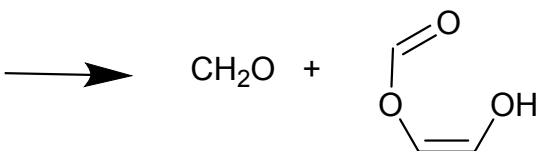
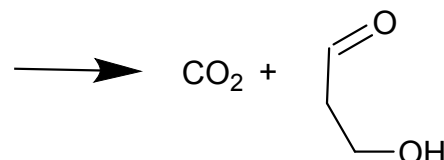
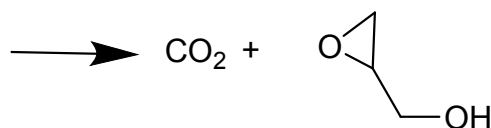
Figure 1S Reaction scheme showing various reaction pathways for the decomposition of glycerol carbonate. G4 zero-point corrected energies are provided for each channels. The barrier heights (E_0) for the major channels are identified with red color.



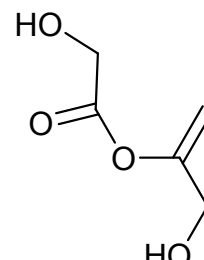
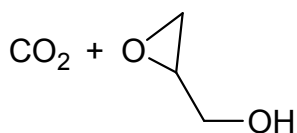
Radical Forming Channels



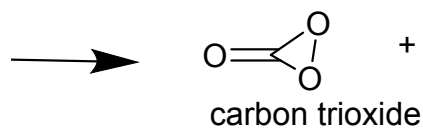
401.8



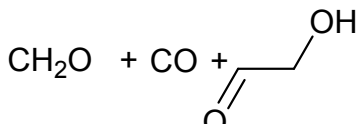
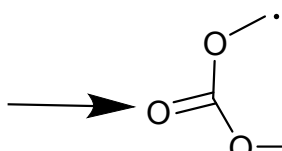
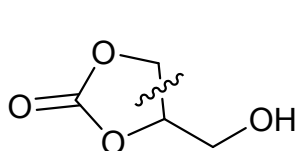
337.6



3-hydroxyprop-1-en-2-yl 2-hydroxyacetate



carbon trioxide



**Glycerol Carbonate
(GC)**

<i>T</i> /K	J·K⁻¹ mol⁻¹			kJ·mol⁻¹			log K_f
	<i>C_p</i> ^o	<i>S</i> ^o	$-[G^o-H^o(T_r)]/T$	<i>H-H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0	0	inf	-21.806	-677.735	-677.735	inf
100	59.335	267.729	440.947	-17.322	-688.296	-649.807	339.424
200	86.734	317.081	367.314	-10.047	-696.229	-608.138	158.829
298.15	118.608	357.528	357.528	0	-702.9	-563.346	98.696
300	119.232	358.263	357.53	0.22	-703.011	-562.569	97.952
400	151.734	397.094	362.605	13.796	-708.187	-514.928	67.243
500	179.504	434.039	373.231	30.404	-711.77	-466.168	48.7
600	201.953	468.826	386.296	49.518	-714.075	-416.813	36.287
700	220.04	501.364	400.436	70.649	-715.36	-367.152	27.397
800	234.807	531.742	414.973	93.416	-715.808	-317.373	20.722
900	247.043	560.127	429.541	117.527	-715.571	-267.574	15.53
1000	257.302	586.702	443.943	142.759	-714.767	-217.837	11.379
1100	265.981	611.643	458.067	168.934	-713.503	-168.201	7.987
1200	273.371	635.112	471.852	195.912	-711.861	-118.698	5.167
1300	279.7	657.25	485.27	223.573	-709.925	-69.345	2.786
1400	285.147	678.182	498.309	251.822	-707.754	-20.142	0.752
1500	289.856	698.02	510.967	280.578	-705.402	28.885	-1.006
1600	293.945	716.86	523.252	309.773	-702.914	77.761	-2.539
1700	297.511	734.79	535.172	339.35	-700.331	126.47	-3.886
1800	300.634	751.885	546.741	369.26	-697.681	175.033	-5.079
1900	303.379	768.215	557.971	399.464	-694.989	223.442	-6.143
2000	305.803	783.839	568.876	429.925	-692.278	271.709	-7.096
2100	307.951	798.812	579.472	460.615	-689.574	319.838	-7.956
2200	309.861	813.183	589.771	491.508	-686.882	367.845	-8.734
2300	311.566	826.995	599.786	522.581	-684.216	415.734	-9.442
2400	313.093	840.288	609.532	553.815	-681.591	463.497	-10.088
2500	314.464	853.098	619.02	585.194	-679.012	511.155	-10.68
2600	315.701	865.456	628.262	616.703	-676.489	558.711	-11.225
2700	316.818	877.392	637.269	648.33	-674.024	606.17	-11.727
2800	317.832	888.932	646.052	680.063	-671.626	653.542	-12.192
2900	318.753	900.102	654.621	711.893	-669.3	700.827	-12.623
3000	319.592	910.922	662.985	743.811	-667.043	748.038	-13.024
3100	320.359	921.414	671.153	775.809	-664.869	795.162	-13.398
3200	321.061	931.596	679.134	807.881	-662.771	842.234	-13.748
3300	321.706	941.486	686.935	840.02	-660.754	889.229	-14.075
3400	322.299	951.099	694.563	872.22	-658.822	936.174	-14.383
3500	322.846	960.449	702.027	904.478	-656.973	983.067	-14.671
3600	323.351	969.551	709.333	936.788	-655.21	1029.893	-14.943
3700	323.818	978.417	716.486	969.147	-653.531	1076.678	-15.2
3800	324.251	987.059	723.493	1001.55	-651.947	1123.422	-15.443
3900	324.653	995.487	730.36	1033.996	-650.446	1170.116	-15.672
4000	325.027	1003.711	737.091	1066.48	-649.036	1216.772	-15.889
4100	325.376	1011.741	743.692	1099.001	-647.72	1263.414	-16.096
4200	325.701	1019.586	750.168	1131.555	-646.493	1310.008	-16.292

4300	326.005	1027.253	756.523	1164.14	-645.36	1356.58	-16.479
4400	326.29	1034.751	762.762	1196.755	-644.318	1403.127	-16.657
4500	326.556	1042.087	768.888	1229.397	-643.367	1449.632	-16.827
4600	326.807	1049.267	774.905	1262.066	-642.514	1496.148	-16.989
4700	327.042	1056.298	780.818	1294.758	-641.758	1542.635	-17.144
4800	327.263	1063.186	786.629	1327.474	-641.089	1589.101	-17.293
4900	327.471	1069.936	792.342	1360.21	-640.525	1635.572	-17.435
5000	327.667	1076.554	797.96	1392.967	-640.047	1682.009	-17.572
5100	327.853	1083.044	803.487	1425.744	-639.671	1728.45	-17.703
5200	328.028	1089.412	808.924	1458.538	-639.385	1774.858	-17.829
5300	328.193	1095.662	814.276	1491.349	-639.201	1821.296	-17.95
5400	328.35	1101.798	819.543	1524.176	-639.116	1867.709	-18.067
5500	328.499	1107.824	824.73	1557.019	-639.118	1914.131	-18.179
5600	328.64	1113.745	829.838	1589.876	-639.219	1960.558	-18.287
5700	328.773	1119.563	834.87	1622.746	-639.417	2006.986	-18.392
5800	328.901	1125.282	839.828	1655.63	-639.713	2053.426	-18.493
5900	329.022	1130.905	844.714	1688.526	-640.098	2099.84	-18.591
6000	329.137	1136.436	849.53	1721.434	-640.585	2146.305	-18.685

Enthalpy Reference Temperature = $T_r = 298.15$ K

Standard State Pressure = $p^\circ = 0.1$ MPa

P1a

T/K	$\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$			$\text{kJ}\cdot\text{mol}^{-1}$			$\log K_f$
	C_p°	S°	$-[G^\circ - H^\circ(T_r)]/T$	$H - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0	0	inf	-17.545	-323.308	-323.308	inf
100	49.312	240.771	377.185	-13.641	-331.485	-307.727	160.74
200	68.542	280.864	319.605	-7.748	-337.563	-281.542	73.531
298.15	89.801	312.102	312.102	0	-343	-252.798	44.289
300	90.222	312.659	312.104	0.167	-343.094	-252.308	43.931
400	112.566	341.708	315.913	10.318	-347.701	-221.321	28.902
500	132.371	369.014	323.831	22.592	-351.233	-189.296	19.776
600	148.941	394.66	333.521	36.683	-353.823	-156.651	13.638
700	162.728	418.686	343.99	52.287	-355.607	-123.636	9.226
800	174.312	441.193	354.749	69.155	-356.697	-90.419	5.904
900	184.145	462.307	365.539	87.091	-357.194	-57.096	3.314
1000	192.553	482.155	376.219	105.937	-357.191	-23.75	1.241
1100	199.775	500.855	386.707	125.562	-356.774	9.578	-0.455
1200	206.001	518.511	396.962	145.859	-356.013	42.851	-1.865
1300	211.384	535.218	406.961	166.734	-354.981	76.049	-3.056
1400	216.051	551.058	416.693	188.112	-353.728	109.166	-4.073
1500	220.111	566.106	426.156	209.924	-352.304	142.175	-4.951
1600	223.653	580.427	435.354	232.117	-350.746	175.094	-5.716
1700	226.755	594.081	444.292	254.64	-349.093	207.905	-6.388
1800	229.48	607.121	452.979	277.455	-347.366	240.623	-6.983
1900	231.882	619.594	461.422	300.526	-345.588	273.24	-7.512
2000	234.008	631.543	469.632	323.822	-343.781	305.763	-7.986
2100	235.895	643.007	477.617	347.319	-341.965	338.193	-8.412
2200	237.577	654.02	485.386	370.994	-340.146	370.539	-8.798

2300	239.079	664.615	492.95	394.829	-338.334	402.807	-9.148
2400	240.427	674.819	500.317	418.805	-336.544	434.99	-9.467
2500	241.639	684.658	507.495	442.909	-334.78	467.101	-9.76
2600	242.732	694.157	514.492	467.129	-333.05	499.139	-10.028
2700	243.722	703.337	521.318	491.452	-331.358	531.113	-10.275
2800	244.619	712.217	527.978	515.87	-329.709	563.028	-10.503
2900	245.436	720.815	534.48	540.374	-328.11	594.884	-10.715
3000	246.18	729.149	540.831	564.955	-326.559	626.685	-10.912
3100	246.861	737.232	547.036	589.607	-325.067	658.429	-11.094
3200	247.484	745.08	553.103	614.325	-323.629	690.139	-11.265
3300	248.057	752.704	559.037	639.103	-322.25	721.792	-11.425
3400	248.584	760.117	564.842	663.935	-320.933	753.414	-11.575
3500	249.07	767.33	570.525	688.818	-319.679	785	-11.715
3600	249.519	774.353	576.09	713.748	-318.488	816.539	-11.848
3700	249.935	781.196	581.541	738.721	-317.361	848.055	-11.972
3800	250.32	787.866	586.883	763.734	-316.307	879.538	-12.09
3900	250.678	794.373	592.121	788.784	-315.317	910.988	-12.201
4000	251.011	800.724	597.257	813.868	-314.397	942.417	-12.307
4100	251.322	806.926	602.295	838.985	-313.55	973.837	-12.407
4200	251.611	812.985	607.24	864.132	-312.772	1005.226	-12.502
4300	251.882	818.909	612.094	889.307	-312.068	1036.596	-12.592
4400	252.136	824.703	616.86	914.508	-311.435	1067.956	-12.678
4500	252.373	830.372	621.542	939.734	-310.873	1099.286	-12.76
4600	252.596	835.921	626.142	964.982	-310.389	1130.631	-12.839
4700	252.806	841.356	630.664	990.252	-309.981	1161.955	-12.914
4800	253.003	846.68	635.109	1015.543	-309.64	1193.265	-12.985
4900	253.188	851.899	639.48	1040.852	-309.381	1224.583	-13.054
5000	253.364	857.016	643.78	1066.18	-309.188	1255.881	-13.12
5100	253.529	862.035	648.01	1091.525	-309.075	1287.183	-13.183
5200	253.685	866.959	652.174	1116.886	-309.029	1318.465	-13.244
5300	253.833	871.793	656.272	1142.262	-309.061	1349.773	-13.303
5400	253.973	876.539	660.307	1167.652	-309.167	1381.063	-13.359
5500	254.105	881.2	664.281	1193.056	-309.337	1412.363	-13.414
5600	254.231	885.78	668.196	1218.473	-309.58	1443.676	-13.466
5700	254.35	890.281	672.052	1243.902	-309.892	1474.989	-13.517
5800	254.464	894.705	675.853	1269.343	-310.274	1506.311	-13.566
5900	254.572	899.056	679.6	1294.794	-310.719	1537.615	-13.613
6000	254.674	903.336	683.293	1320.257	-311.233	1568.966	-13.659

Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$

Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$

P1b

$\text{J}\cdot\text{K}^{-1}\text{ mol}^{-1}$

$\text{kJ}\cdot\text{mol}^{-1}$

T/K	C_p°	S°	$-[G^\circ - H^\circ(T_r)]/T$	$H - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0	0	inf	-16.232	-225.095	-225.095	inf
100	44.196	235.844	361.412	-12.557	-233.501	-209.249	109.301
200	62.683	271.998	308.179	-7.236	-240.151	-182.357	47.627
298.15	85.471	301.133	301.133	0	-246.1	-152.627	26.74
300	85.931	301.663	301.135	0.159	-246.202	-152.117	26.486
400	110.247	329.758	304.801	9.983	-251.136	-119.976	15.667
500	131.346	356.7	312.508	22.096	-254.829	-86.734	9.061
600	148.555	382.224	322.021	36.121	-257.485	-52.851	4.601
700	162.583	406.212	332.353	51.701	-259.293	-18.59	1.387
800	174.215	428.705	343.007	68.558	-260.394	15.876	-1.037
900	184.018	449.806	353.713	86.483	-260.902	50.447	-2.928
1000	192.373	469.638	364.324	105.314	-260.914	85.045	-4.442
1100	199.546	488.318	374.755	124.919	-260.517	119.625	-5.681
1200	205.733	505.952	384.961	145.19	-259.782	154.153	-6.71
1300	211.089	522.636	394.915	166.038	-258.777	188.608	-7.578
1400	215.741	538.454	404.608	187.384	-257.556	222.984	-8.32
1500	219.794	553.48	414.036	209.166	-256.162	257.255	-8.958
1600	223.337	567.781	423.202	231.326	-254.637	291.438	-9.514
1700	226.443	581.416	432.111	253.819	-253.014	325.514	-10.002
1800	229.176	594.438	440.77	276.602	-251.319	359.499	-10.432
1900	231.588	606.895	449.188	299.643	-249.571	393.385	-10.815
2000	233.725	618.829	457.374	322.911	-247.792	427.179	-11.157
2100	235.625	630.28	465.337	346.38	-246.004	460.881	-11.464
2200	237.318	641.281	473.086	370.029	-244.211	494.5	-11.741
2300	238.833	651.864	480.63	393.838	-242.425	528.043	-11.992
2400	240.192	662.058	487.978	417.79	-240.659	561.501	-12.221
2500	241.416	671.888	495.139	441.872	-238.917	594.889	-12.43
2600	242.52	681.378	502.121	466.07	-237.209	628.205	-12.621
2700	243.52	690.55	508.931	490.372	-235.538	661.457	-12.797
2800	244.427	699.423	515.577	514.77	-233.909	694.651	-12.959
2900	245.253	708.015	522.065	539.255	-232.329	727.786	-13.109
3000	246.006	716.342	528.403	563.819	-230.795	760.868	-13.248
3100	246.695	724.42	534.596	588.454	-229.32	793.893	-13.377
3200	247.327	732.263	540.652	613.156	-227.898	826.884	-13.497
3300	247.907	739.882	546.574	637.918	-226.535	859.819	-13.61
3400	248.441	747.291	552.369	662.736	-225.232	892.723	-13.715
3500	248.933	754.5	558.042	687.605	-223.992	925.593	-13.814
3600	249.388	761.519	563.597	712.521	-222.815	958.414	-13.906
3700	249.81	768.358	569.039	737.481	-221.701	991.214	-13.993
3800	250.201	775.025	574.372	762.482	-220.659	1023.981	-14.076
3900	250.564	781.529	579.601	787.52	-219.681	1056.715	-14.153
4000	250.902	787.877	584.729	812.594	-218.771	1089.429	-14.226
4100	251.217	794.076	589.759	837.7	-217.935	1122.134	-14.296
4200	251.511	800.134	594.696	862.837	-217.167	1154.808	-14.362
4300	251.786	806.055	599.543	888.002	-216.473	1187.463	-14.425
4400	252.043	811.847	604.303	913.193	-215.85	1220.109	-14.485
4500	252.284	817.513	608.978	938.41	-215.297	1252.724	-14.541

4600	252.51	823.061	613.572	963.649	-214.822	1285.356	-14.596
4700	252.723	828.494	618.087	988.911	-214.422	1317.966	-14.648
4800	252.923	833.817	622.526	1014.194	-214.089	1350.562	-14.697
4900	253.112	839.034	626.892	1039.495	-213.838	1383.166	-14.745
5000	253.29	844.149	631.186	1064.816	-213.652	1415.751	-14.79
5100	253.458	849.166	635.411	1090.153	-213.547	1448.34	-14.834
5200	253.616	854.09	639.569	1115.507	-213.508	1480.908	-14.876
5300	253.766	858.922	643.662	1140.876	-213.547	1513.503	-14.916
5400	253.908	863.667	647.693	1166.26	-213.659	1546.081	-14.955
5500	254.043	868.327	651.662	1191.657	-213.836	1578.668	-14.993
5600	254.171	872.906	655.572	1217.068	-214.085	1611.269	-15.029
5700	254.292	877.405	659.424	1242.491	-214.403	1643.869	-15.064
5800	254.407	881.829	663.221	1267.926	-214.791	1676.478	-15.098
5900	254.517	886.179	666.963	1293.373	-215.24	1709.07	-15.131
6000	254.622	890.457	670.653	1318.83	-215.76	1741.709	-15.163

Enthalpy Reference Temperature = $T_r = 298.15$ K

Standard State Pressure = $p^\circ = 0.1$ MPa

P2

T/K	$J \cdot K^{-1} \cdot mol^{-1}$			$kJ \cdot mol^{-1}$			$\log K_f$
	C_p°	S°	$-[G^\circ - H^\circ(T_r)]/T$	$H - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0	0	inf	-18.277	-404.714	-404.714	inf
100	49.333	255.316	397.079	-14.176	-411.208	-390.215	203.828
200	70.666	295.431	336.77	-8.268	-416.358	-367.168	95.894
298.15	98.054	328.7	328.7	0	-420.6	-342.018	59.92
300	98.571	329.309	328.702	0.182	-420.669	-341.597	59.477
400	124.626	361.334	332.892	11.377	-423.835	-314.731	41.1
500	145.972	391.526	341.633	24.947	-426.003	-287.186	30.002
600	162.905	419.697	352.324	40.423	-427.437	-259.278	22.572
700	176.423	445.861	363.841	57.414	-428.296	-231.175	17.25
800	187.394	470.16	375.631	75.623	-428.681	-202.987	13.254
900	196.439	492.771	387.405	94.829	-428.672	-174.769	10.143
1000	203.985	513.87	399.008	114.861	-428.333	-146.576	7.656
1100	210.336	533.618	410.358	135.586	-427.726	-118.426	5.624
1200	215.72	552.157	421.41	156.896	-426.899	-90.343	3.933
1300	220.31	569.61	432.145	178.704	-425.904	-62.337	2.505
1400	224.244	586.084	442.558	200.937	-424.779	-34.405	1.284
1500	227.632	601.674	452.65	223.535	-423.556	-6.569	0.229
1600	230.564	616.46	462.431	246.448	-422.265	21.191	-0.692
1700	233.113	630.517	471.908	269.635	-420.932	48.864	-1.501
1800	235.34	643.905	481.094	293.06	-419.576	76.461	-2.219
1900	237.292	656.683	490.002	316.694	-418.212	103.981	-2.859
2000	239.011	668.899	498.644	340.51	-416.854	131.428	-3.433
2100	240.532	680.598	507.032	364.489	-415.522	158.806	-3.95
2200	241.882	691.819	515.178	388.611	-414.218	186.128	-4.419
2300	243.085	702.599	523.094	412.861	-412.949	213.393	-4.846
2400	244.16	712.967	530.791	437.224	-411.728	240.595	-5.236
2500	245.125	722.954	538.279	461.689	-410.555	267.75	-5.594

2600	245.994	732.585	545.568	486.246	-409.438	294.86	-5.924
2700	246.778	741.884	552.668	510.885	-408.379	321.927	-6.228
2800	247.489	750.872	559.587	535.599	-407.382	348.958	-6.51
2900	248.134	759.568	566.334	560.38	-406.452	375.951	-6.772
3000	248.721	767.99	572.916	585.224	-405.584	402.92	-7.015
3100	249.258	776.155	579.341	610.123	-404.791	429.848	-7.243
3200	249.748	784.076	585.616	635.074	-404.065	456.767	-7.456
3300	250.199	791.768	591.747	660.071	-403.41	483.655	-7.656
3400	250.612	799.244	597.74	685.112	-402.829	510.53	-7.843
3500	250.994	806.514	603.602	710.193	-402.321	537.393	-8.02
3600	251.346	813.59	609.337	735.31	-401.886	564.23	-8.187
3700	251.671	820.481	614.951	760.461	-401.524	591.062	-8.344
3800	251.973	827.197	620.448	785.643	-401.241	617.886	-8.493
3900	252.253	833.745	625.834	810.855	-401.031	644.697	-8.635
4000	252.514	840.135	631.112	836.093	-400.896	671.503	-8.769
4100	252.756	846.373	636.286	861.357	-400.842	698.322	-8.897
4200	252.982	852.467	641.361	886.644	-400.862	725.128	-9.018
4300	253.194	858.422	646.34	911.953	-400.961	751.943	-9.134
4400	253.391	864.245	651.227	937.282	-401.137	778.756	-9.245
4500	253.577	869.942	656.024	962.631	-401.387	805.56	-9.351
4600	253.751	875.517	660.735	987.997	-401.721	832.396	-9.452
4700	253.914	880.976	665.363	1013.381	-402.135	859.233	-9.549
4800	254.067	886.323	669.911	1038.78	-402.622	886.075	-9.642
4900	254.212	891.564	674.381	1064.194	-403.196	912.939	-9.732
5000	254.348	896.701	678.776	1089.622	-403.842	939.795	-9.818
5100	254.477	901.739	683.099	1115.063	-404.573	966.681	-9.901
5200	254.598	906.682	687.351	1140.517	-405.38	993.557	-9.98
5300	254.713	911.532	691.536	1165.983	-406.27	1020.478	-10.057
5400	254.822	916.294	695.654	1191.459	-407.244	1047.397	-10.132
5500	254.925	920.971	699.708	1216.947	-408.292	1074.344	-10.203
5600	255.023	925.565	703.7	1242.444	-409.421	1101.313	-10.273
5700	255.115	930.08	707.632	1267.951	-410.631	1128.301	-10.34
5800	255.203	934.518	711.506	1293.467	-411.925	1155.323	-10.405
5900	255.287	938.881	715.323	1318.992	-413.293	1182.335	-10.468
6000	255.367	943.172	719.085	1344.524	-414.749	1209.412	-10.529

Table S2: NASA polynomials coefficients for the species involved in various pathways of glycerol carbonate decomposition.

```

THERMO
GC      H   6C   4O   4   0g   300.00  5000.00 1000.00  1
14.7974  0.02415      -9.54E-06  1.72E-09  -1.16E-13  2
-91450.8967 -51.55165 -1.57129  0.06316  -3.29E-05  3
-5.61E-09  7.90E-12  -86582.5811  34.61705  4

P1a     H   6C   3O   2   0g   300.00  5000.00 1000.00  1
9.62449  0.02012      -7.85E-06  1.40E-09  -9.44E-14  2
-45900.8237 -25.11901  0.83967  0.03697  -8.53E-06  3
-1.45E-08  8.36E-12  -43048.6018  22.21815  4

P1b     H   6C   3O   2   0g   300.00  5000.00 1000.00  1
9.71496  0.01992      -7.74E-06  1.38E-09  -9.27E-14  2
-34342.6934 -27.09723 -1.24334  0.04489  -1.92E-05  3
-8.74E-09  7.41E-12  -31041.8017  30.83064  4

P2      H   4C   4O   3   0g   300.00  5000.00 1000.00  1
12.7203  0.01773      -7.06E-06  1.28E-09  -8.69E-14  2
-56292.188 -40.6486  -2.28374  0.06108  -5.25E-05  3
2.04E-08  -2.17E-12  -52197.3278  36.49176  4
END

```

Table S3: Calculated MP2/cc-pVTZ scaled harmonic vibrational wavenumbers (scaling factor = 0.95) and rotational constants of the species involved in various pathways of glycerol carbonate decomposition. Imaginary wavenumber is denoted by *i*. Frequencies corresponding to the torsional modes are shown in bold.

Species	Rotational Constants /	Wavenumbers / cm ⁻¹
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	GHZ	
GC	4.1579 1.57017 1.37869	61.1, 120.1 , 186.2, 257.4, 275.9, 390.3 , 511.0, 597.6, 644.5, 691.2, 738.2, 833.0, 868.4, 910.4, 955.2, 1037.1, 1055.7, 1070.1, 1095.5, 1116.8, 1181.8, 1200.5, 1293.0, 1304.5, 1334.5, 1355.7, 1365.0, 1434.9, 1460.7, 1809.7, 2921.3, 2948.0, 2966.2, 2987.7, 3036.4, 3640.5
TS1a	3.17406 1.67965 1.60695	826.9i, 65.0, 97.2, 179.6 , 225.9, 279.4, 315.5, 382.3, 412.6, 466.8, 600.1, 646.7 , 721.1, 790.7, 818.6, 842.0, 934.7, 995.6, 1035.0, 1130.2, 1179.2, 1203.0, 1217.6, 1262.5, 1299.7, 1366.3, 1398.3, 1408.6, 1450.8, 2085.7, 2267.3, 2867.8, 2893.2, 2906.7, 3029.4, 3221.9
TS1b	4.659 1.28894 1.13437	820.3i, 62.5, 94.1, 129.4 , 204.0, 249.3, 358.7, 431.7, 463.8, 517.0 , 591.9, 639.0, 707.2, 799.4, 844.9, 869.3, 946.4, 969.4, 1054.3, 1081.5, 1149.2, 1178.0, 1212.4, 1224.1, 1295.7, 1352.3, 1359.6, 1431.1, 1455.3, 1931.9, 2914.2, 2987.5, 2995.2, 3061.4, 3178.5, 3615.2
TS2	4.93387 1.31756 1.13236	-, 92.3, 107.6 , 172.3, 304.7, 359.9, 421.5, 449.2 , 510.1, 587.1, 682.2, 735.8, 754.5, 788.8, 851.2, 871.6, 931.7, 970.1, 1005.9, 1056.9, 1081.1, 1131.9, 1155.5, 1174.6, 1303.8, 1341.5, 1380.1, 1420.6, 1456.0, 1760.6, 1797.8, 2938.3, 2983.2, 3004.7, 3086.7, 3528.6
P1a	8.63383 4.21656 3.16593	132.3, 174.3, 243.5, 380.0, 494.0, 607.5, 739.6, 826.4, 914.1, 924.5, 1045.5, 1063.6, 1165.6, 1195.9, 1317.2, 1333.2, 1356.3, 1358.4, 1378.1, 1445.7, 1674.0, 2827.1, 2910.8, 2914.9, 2961.3, 2994.7, 3628.4 ,
P1b	10.35052 4.18933 3.85259	155.8, 247.7, 338.2, 454.2, 597.5, 741.6, 820.8, 887.6, 938.3, 996.5, 1059.4, 1082.2, 1110.6, 1117.0, 1173.0, 1230.5, 1306.2, 1362.7, 1384.2, 1445.7, 1460.9, 2897.1, 2980.1, 3004.1, 3018.0, 3105.7, 3604.8
P2	6.55922 2.39031 1.77149	63.0, 162.9, 308.9, 458.8, 522.5, 610.0, 696.4, 704.1, 730.6, 808.8, 841.0, 866.0, 958.2, 994.4, 1064.5, 1085.6, 1167.0, 1261.4, 1316.0, 1370.5, 1454.0, 1664.8, 1827.4, 2957.4, 3011.9, 3056.2, 3156.2
CO ₂	11.55316	623.0, 623.0, 1265.4, 2304.7
H ₂ O	801.1297 441.8747 284.793	1569.5, 3662.6, 3776.9

Table S4 Calculated MP2/cc-pVTZ geometries in cartesian coordinates of the stationary points for the decomposition pathway of glycerol carbonates

Species	Cartesian coordinates / Å			
CO ₂	C	0.949700328	-0.043668	0.012432
	O	2.119071291	-0.043668	0.012432

	O	-0.219670618	-0.043668	0.012432
H₂O	O	0.126692761	-1.656858743	-0.085703
	H	1.084461305	-1.606815663	-0.085703
	H	-0.145844066	-0.737321594	-0.085703
GC	C	0.411970597	-1.239645469	-0.056557934
	C	1.933233715	-1.252889009	0.032743088
	H	0.020551651	-1.927842219	-0.798491434
	H	-0.042099842	-1.421044632	0.914981952
	H	2.394287517	-1.637858793	-0.877907172
	O	0.108341256	0.096793182	-0.47048639
	O	2.254606678	0.141010455	0.145677405
	C	1.18016261	0.890706613	-0.236635629
	O	1.193032137	2.077264347	-0.34729281
	C	2.482846874	-1.966654115	1.248517837
	H	2.205305128	-3.019111928	1.20058487
	H	3.573125398	-1.903631169	1.237328118
	O	1.941123174	-1.452206803	2.446391976
	H	2.223515107	-0.53289246	2.506149122
P1a	C	0.067901469	0.527093552	-1.148000854
	C	-1.248070241	-0.193212311	-1.108513749
	H	0.457477848	0.771253079	-2.151238307
	H	-1.996744581	0.467298426	-1.554585588
	H	-1.176317743	-1.064948473	-1.765072151
	O	0.698275656	0.846686059	-0.15686271
	C	-1.657971674	-0.585605881	0.300331011
	H	-2.604732622	-1.119968369	0.273298981
	H	-0.906630524	-1.257475707	0.72382162
	O	-1.856746436	0.546299935	1.126427981
	H	-0.985185151	0.947114691	1.221255765
P1b	C	0.244409959	1.188988485	-0.082548967
	C	0.836098517	0.208944154	0.822783116
	H	-0.505831194	1.871840152	0.291581722
	H	0.813532011	1.50753185	-0.94409756
	H	0.509049118	0.196227686	1.856674598
	O	-0.1726368	-0.194345255	-0.118617251
	C	2.193807772	-0.381793856	0.549743194
	H	2.963808439	0.229029636	1.019157005
	H	2.238086273	-1.380581345	0.995373342
	O	2.474035296	-0.425438994	-0.832942877
	H	1.68019261	-0.795202513	-1.240178322
	P2	C	0.064121276	1.349589812
C		-0.587560764	-0.004970487	-0.085610384
H		-0.129578858	1.911441358	-0.98993685

	H	-0.21474403	1.944051809	0.787651972
	O	1.458789576	1.046366505	-0.006841167
	O	0.423472143	-0.936466821	-0.020615564
	C	1.637351407	-0.294172753	0.025851506
	O	2.685435218	-0.85190016	0.086023351
	C	-1.870852197	-0.33678602	-0.140623739
	H	-2.176330345	-1.370084169	-0.136422491
	H	-2.615934425	0.440388928	-0.190161235
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TS1a	C	-0.226114396	0.669670691	-1.234271709
	C	-0.861728311	-0.554310714	-0.863453787
	H	0.24085132	0.668789819	-2.224852922
	H	-1.35388638	0.948976087	-1.475813779
	H	-1.034448186	-1.305809572	-1.630469238
	O	0.354789223	1.350416183	-0.263250665
	O	1.004211227	-1.072971766	0.079402061
	C	1.492367377	-0.064357395	0.53735927
	O	2.266012569	0.526828631	1.196893369
	C	-1.647523145	-0.692158695	0.382615808
	H	-2.687757595	-0.854516662	0.069769414
	H	-1.326738686	-1.635848376	0.842609562
	O	-1.586318157	0.393098539	1.253585694
	H	-0.839200861	0.956772232	0.946712922
<hr/>				
TS1b	C	0.285334148	1.342686698	-0.026937686
	C	0.68269607	0.16803702	0.705153154
	H	-0.185505039	2.210304139	0.396537197
	H	0.690453726	1.416001791	-1.024520244
	H	0.328698032	0.111321826	1.732326098
	O	-1.843733844	1.017541647	0.114279034
	O	-0.157942523	-0.536635331	-0.23004436
	C	-1.794370047	-0.203780771	-0.057309617
	O	-2.447115645	-1.18823501	-0.180949334
	C	2.096496874	-0.349433304	0.534285499
	H	2.792958547	0.272929178	1.093240204
	H	2.116547943	-1.359811101	0.951378105
	O	2.500901301	-0.327829659	-0.814258976
	H	1.857196457	-0.867046125	-1.290550075
<hr/>				
TS2	C	0.127108248	1.44008657	-0.16997587
	C	-0.637624843	0.157929484	-0.252187266
	H	0.318369809	1.896561211	-1.140548348
	H	-0.31174077	2.173239815	0.50260206
	H	-2.011665627	-0.141644229	-1.036056113
	O	1.401520951	1.018866608	0.365241586
	O	0.393709848	-0.82543951	-0.401707494
	C	1.5487648	-0.305429014	0.098594917

O	2.554743781	-0.926269197	0.272304109
C	-1.653132194	-0.190021704	0.697328122
H	-1.603200012	-1.152296854	1.190376687
H	-2.101691636	0.605303595	1.283899941
O	-2.885428923	-0.524512752	-0.435907443
H	-3.566685431	0.168955978	-0.391428887
