Supplementary Information

Mechanistic Insights into the Ring-opening of Biomass Derived Lactones

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Tables

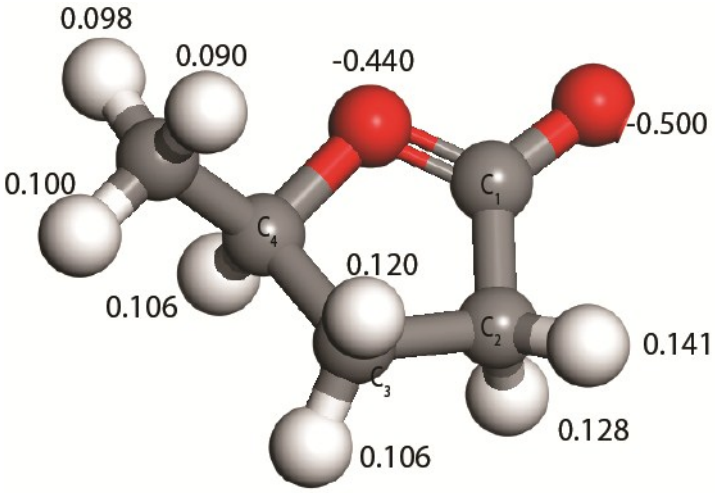
Table S1. Frequency analysis for the transition states.

GVL		**GCL**		**GBL**		**DVL**		**ECL**	
TS1a	TS1b	TS3a	TS3b	TS2a	TS2b	TS4a	TS4b	TS5a	TS5b
265.18ι	691.76ι	232.69ι	691.76ι	344.12ι	865.3ι	303.73ι	674.61ι	309.31ι	560.09ι
77.3	32.74	44.62	32.74	62.96	191.34ι (small intensity on water)	63.18	3.21	51.87	33.4
88.99	49.53	67.16	49.53	117.76	44.76	93.49	19.71	76.02	60.56
134.29	71.48	85.7	71.48	158.51	58.61	111.02	28.6	88.58	75.95
154.45	73.7	116.09	73.7	202.9	99.31	175.07	42.84	125.86	91.75
170.11	94.13	162.05	94.13	218.2	125.26	206.44	72.2	190.02	130.51
195.58	110.1	189.36	110.1	263.05	169.53	248.26	89.38	202.24	132.89
248.59	131.44	212.14	131.44	410.38	204.06	283.59	97.12	255.45	159.74
289.77	141.56	284.35	141.56	477.43	231.03	326.64	112.7	279.8	178.98
386.12	164.05	316.65	164.05	545.08	339.04	432.48	174.9	306.32	189.28
390.92	192.6	346.95	192.6	585.81	364.43	478.87	203.84	365.18	220.04
495.86	234.62	383.12	234.62	628.99	395.16	527.72	242.81	451.7	297.71
510.68	256.27	433.82	256.27	631.85	420.67	543.08	245.58	526.4	313.86
530.97	299.28	473.37	299.28	679.09	458.94	603.44	266.69	538.08	351.31
565.4	335.68	509.81	335.68	792.01	494.61	628.62	292.15	579.38	386.5
617.53	358.78	528.63	358.78	859	519.52	656.38	306.79	592.15	422.43
682.07	393.91	554.26	393.91	884.32	542.81	796.48	341.29	603.2	441.02
800.6	441.06	636.62	441.06	945.59	581.26	806.07	371.32	725.96	453.43
851.68	449.55	675.45	449.55	1.02E+03	602.83	861.82	385.06	750.65	483.63
895.45	530.42	692.46	530.42	1.05E+03	619.95	913.02	446.65	775.18	528.48
905.5	556.94	801.94	556.94	1.08E+03	713.74	942.95	481.56	798.52	555.45
961.59	587.21	856.55	587.21	1.13E+03	755.09	1.01E+03	536.66	878.3	588.66
1.01E+03	612.72	899.67	612.72	1.17E+03	858.06	1.01E+03	543.27	915.71	664.92
1.06E+03	643.1	936.72	643.1	1.20E+03	924.55	1.05E+03	545.99	958.75	687.3
1.10E+03	678.4	951.82	678.4	1.21E+03	931.98	1.11E+03	599.67	968.62	694.15

1.13E+03	709.1	1.00E+03	709.1	1.29E+03	968.73	1.14E+03	608.01	980.88	778.23
1.17E+03	774.49	1.04E+03	774.49	1.33E+03	1.05E+03	1.16E+03	653.72	1.03E+03	816.93
1.21E+03	857.73	1.07E+03	857.73	1.38E+03	1.07E+03	1.20E+03	676.07	1.08E+03	846.27
1.22E+03	877.17	1.10E+03	877.17	1.42E+03	1.17E+03	1.21E+03	719.36	1.09E+03	867.6
1.28E+03	889.87	1.11E+03	889.87	1.43E+03	1.21E+03	1.26E+03	802.36	1.13E+03	906.23
1.30E+03	939.53	1.14E+03	939.53	1.44E+03	1.23E+03	1.29E+03	836.38	1.15E+03	922.02
1.34E+03	960.47	1.19E+03	960.47	1.61E+03	1.26E+03	1.33E+03	852.07	1.18E+03	956.94
1.38E+03	983.66	1.20E+03	983.66	1.62E+03	1.28E+03	1.35E+03	911.69	1.23E+03	999.17
1.40E+03	1.05E+03	1.24E+03	1.05E+03	3.03E+03	1.36E+03	1.38E+03	929.95	1.25E+03	1.06E+03
1.40E+03	1.08E+03	1.27E+03	1.08E+03	3.05E+03	1.40E+03	1.42E+03	937.41	1.26E+03	1.09E+03
1.41E+03	1.12E+03	1.29E+03	1.12E+03	3.09E+03	1.40E+03	1.43E+03	1.06E+03	1.28E+03	1.11E+03
1.43E+03	1.15E+03	1.33E+03	1.15E+03	3.12E+03	1.46E+03	1.44E+03	1.07E+03	1.31E+03	1.12E+03
1.44E+03	1.22E+03	1.36E+03	1.22E+03	3.18E+03	1.54E+03	1.45E+03	1.10E+03	1.31E+03	1.16E+03
1.58E+03	1.23E+03	1.38E+03	1.23E+03	3.33E+03	1.57E+03	1.59E+03	1.13E+03	1.36E+03	1.20E+03
1.67E+03	1.24E+03	1.39E+03	1.24E+03	3.60E+03	1.58E+03	1.64E+03	1.20E+03	1.37E+03	1.21E+03
3.02E+03	1.27E+03	1.40E+03	1.27E+03	3.64E+03	1.69E+03	3.01E+03	1.21E+03	1.42E+03	1.26E+03
3.03E+03	1.30E+03	1.41E+03	1.30E+03	3.74E+03	3.02E+03	3.03E+03	1.24E+03	1.43E+03	1.28E+03
3.04E+03	1.32E+03	1.43E+03	1.32E+03		3.07E+03	3.04E+03	1.28E+03	1.44E+03	1.29E+03
3.08E+03	1.36E+03	1.45E+03	1.36E+03		3.10E+03	3.08E+03	1.29E+03	1.46E+03	1.31E+03
3.09E+03	1.37E+03	1.46E+03	1.37E+03		3.14E+03	3.09E+03	1.33E+03	1.47E+03	1.34E+03
3.12E+03	1.38E+03	1.59E+03	1.38E+03		3.14E+03	3.11E+03	1.37E+03	1.60E+03	1.36E+03
3.17E+03	1.40E+03	1.65E+03	1.40E+03		3.25E+03	3.20E+03	1.39E+03	1.65E+03	1.37E+03
3.23E+03	1.41E+03	3.00E+03	1.41E+03		3.66E+03	3.34E+03	1.40E+03	3.02E+03	1.41E+03
3.65E+03	1.44E+03	3.02E+03	1.44E+03		3.66E+03	3.58E+03	1.43E+03	3.04E+03	1.43E+03
3.66E+03	1.45E+03	3.03E+03	1.45E+03		3.66E+03	3.64E+03	1.43E+03	3.04E+03	1.44E+03
3.75E+03	1.46E+03	3.03E+03	1.46E+03		3.76E+03	3.74E+03	1.55E+03	3.05E+03	1.45E+03
	1.56E+03	3.04E+03	1.56E+03				1.58E+03	3.08E+03	1.54E+03
	1.58E+03	3.10E+03	1.58E+03				1.58E+03	3.08E+03	1.58E+03
	1.60E+03	3.10E+03	1.60E+03				1.63E+03	3.09E+03	1.61E+03
	1.68E+03	3.12E+03	1.68E+03				1.67E+03	3.10E+03	1.68E+03
	2.94E+03	3.14E+03	2.94E+03				3.01E+03	3.19E+03	3.00E+03
	3.02E+03	3.20E+03	3.02E+03				3.02E+03	3.32E+03	3.03E+03

	3.02E+03	3.61E+03	3.02E+03				3.05E+03	3.62E+03	3.03E+03
	3.03E+03	3.63E+03	3.03E+03				3.06E+03	3.65E+03	3.04E+03
	3.08E+03	3.73E+03	3.08E+03				3.08E+03	3.74E+03	3.08E+03
	3.09E+03		3.09E+03				3.13E+03		3.09E+03
	3.11E+03		3.11E+03				3.21E+03		3.11E+03
	3.12E+03		3.12E+03				3.23E+03		3.12E+03
	3.13E+03		3.13E+03				3.25E+03		3.14E+03
	3.18E+03		3.18E+03				3.61E+03		3.26E+03
	3.60E+03		3.60E+03				3.67E+03		3.64E+03
	3.67E+03		3.67E+03				3.69E+03		3.67E+03
	3.68E+03		3.68E+03				3.72E+03		3.69E+03
	3.78E+03		3.78E+03				3.78E+03		3.76E+03

Figures



C_1	0.530
C_2	-0.238
C_3	-0.16
C_4	0.13

Figure S1. Mulliken charge analysis for GVL.

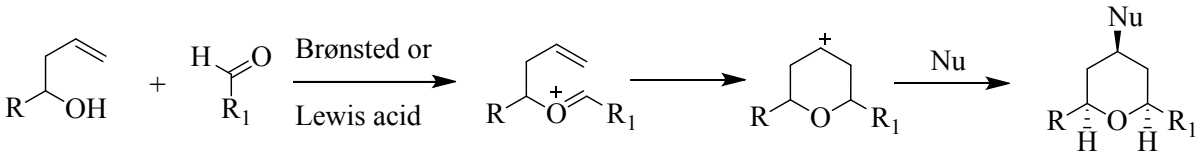


Figure S2. Formation of oxocarbenium ion during prins cyclization reaction.

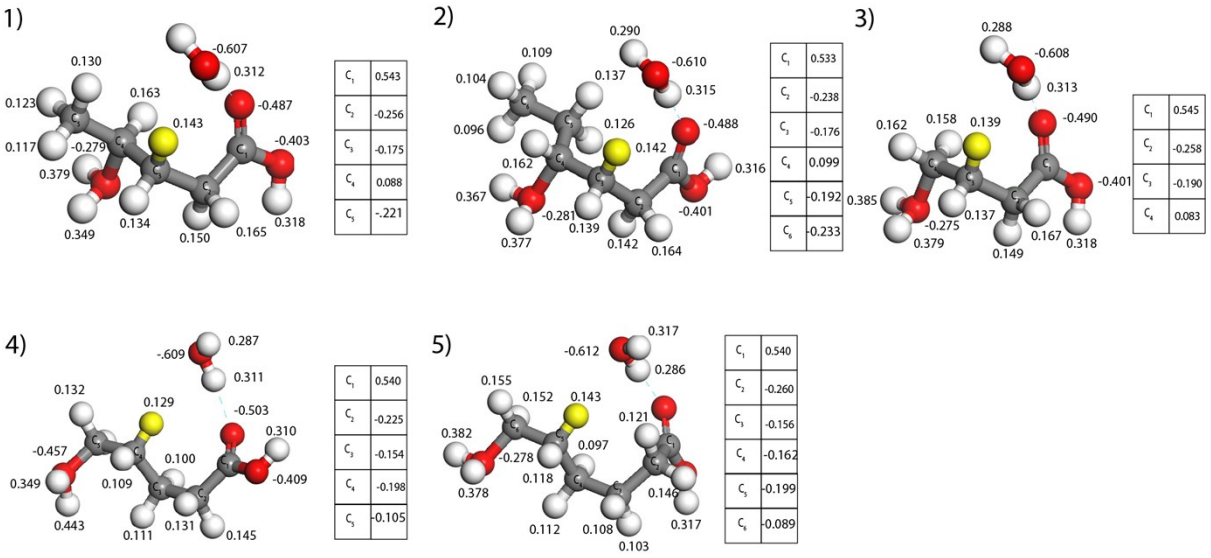


Figure S3. Charge analysis of carbenium ion formed in 1) GVL (1b), 2) GCL (2b), 3) GBL (3b), 4) DVL (4b) and 5) ECL (5b).

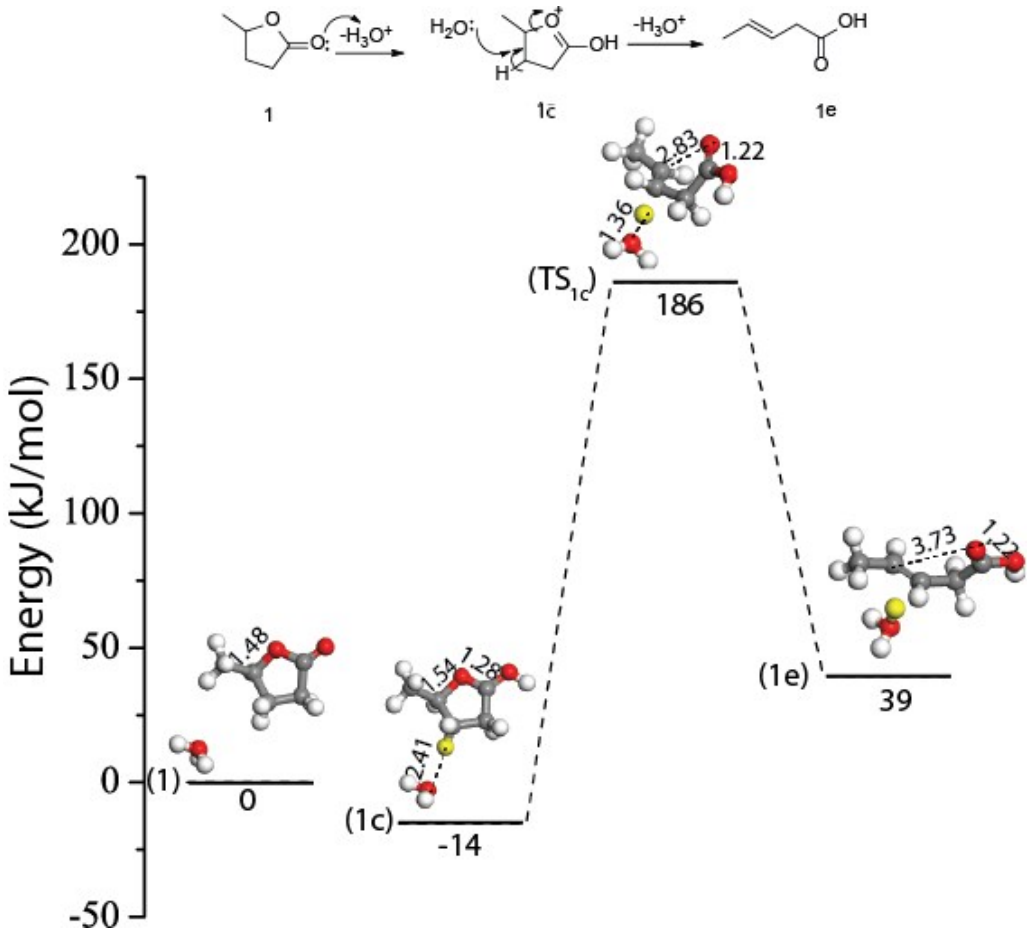


Figure S4. Activation barriers for the concerted mechanism of GVL ring-opening.

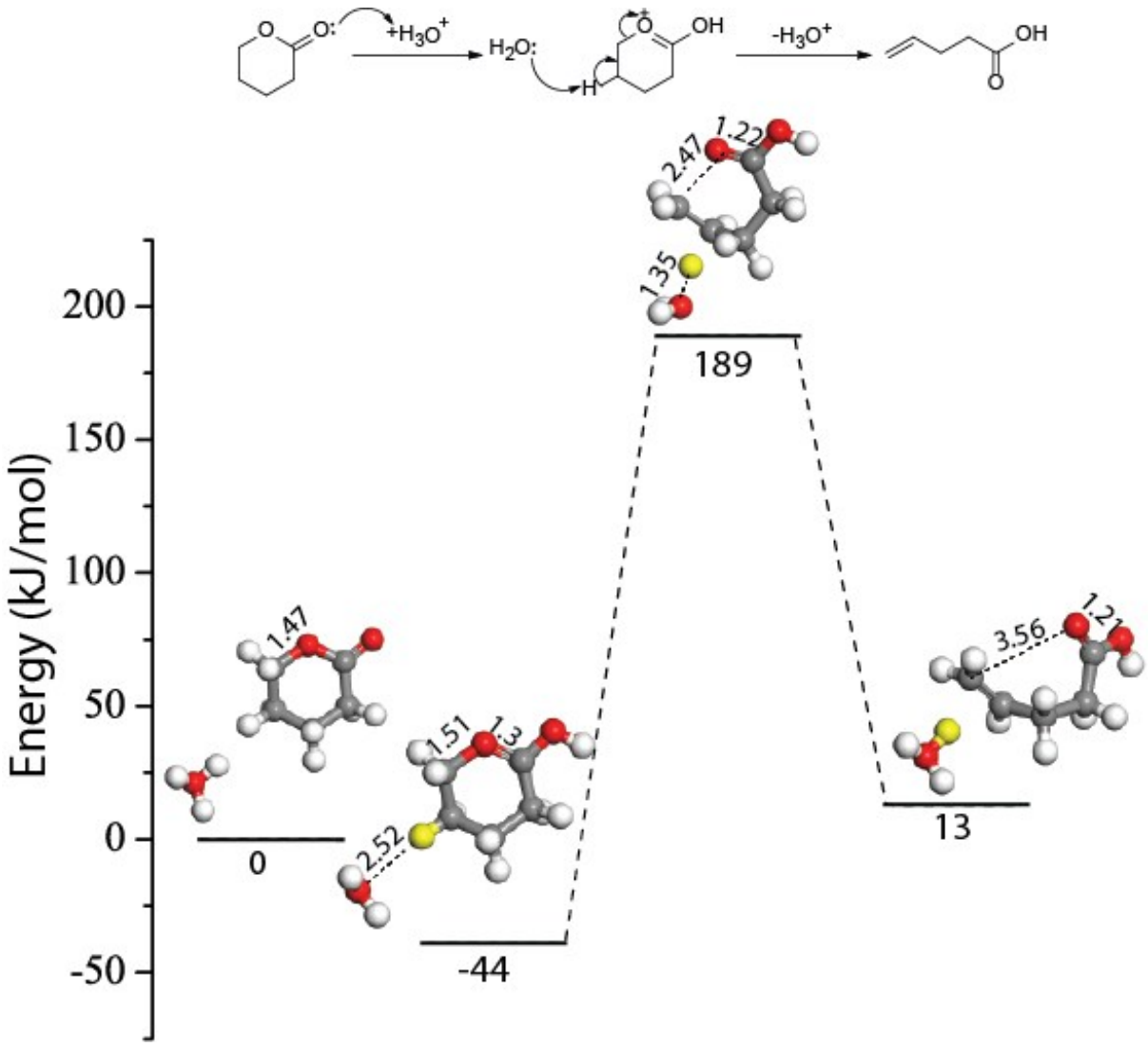


Figure S5. Activation barriers for the concerted mechanism of DVL ring-opening.

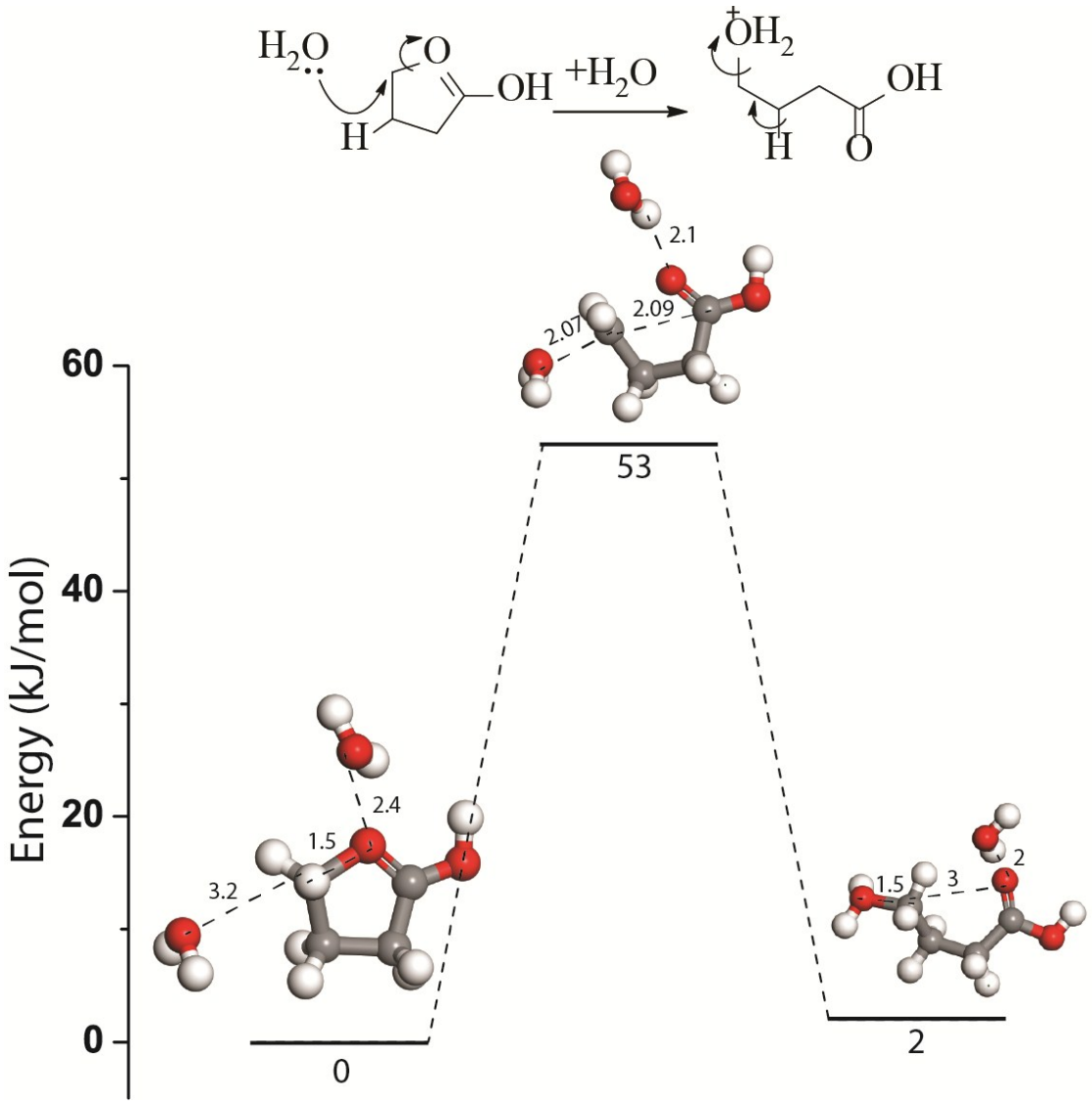


Fig S6. GBL ring-opening

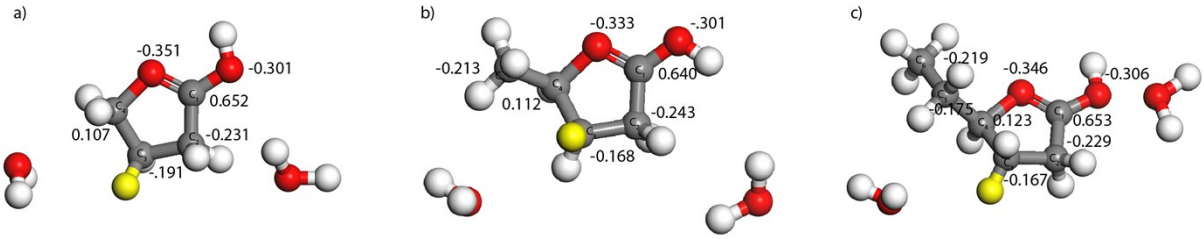


Figure S7. Charge analysis of the oxocarbenium ion a) GBL, b) GVL and c) GCL.

XYZ coordinates for 1

ATOM 1 C MOL 0.095 0.991 -0.479 1.00 0.00 C

ATOM 2 C MOL 0.723 -0.315 0.011 1.00 0.00 C

ATOM 3 C MOL 2.220 -0.038 -0.105 1.00 0.00 C

ATOM 4 C MOL 2.319 1.460 0.054 1.00 0.00 C

ATOM 5 C MOL -1.231 1.364 0.138 1.00 0.00 C

ATOM 6 O MOL 3.302 2.141 0.301 1.00 0.00 O

ATOM 7 O MOL 1.097 2.028 -0.130 1.00 0.00 O

ATOM 8 H MOL 0.030 1.003 -1.575 1.00 0.00 H

ATOM 9 H MOL 0.390 -1.170 -0.586 1.00 0.00 H

ATOM 10 H MOL 0.445 -0.491 1.058 1.00 0.00 H

ATOM 11 H MOL 2.612 -0.291 -1.101 1.00 0.00 H

ATOM 12 H MOL 2.846 -0.546 0.636 1.00 0.00 H

ATOM 13 H MOL -1.984 0.621 -0.153 1.00 0.00 H

ATOM 14 H MOL -1.571 2.345 -0.215 1.00 0.00 H

ATOM 15 H MOL -1.161 1.380 1.233 1.00 0.00 H

ATOM 16 H MOL -3.308 -2.168 0.435 1.00 0.00 H

ATOM 17 O MOL -2.371 -2.403 0.239 1.00 0.00 O1+

ATOM 18 H MOL -2.099 -3.088 0.894 1.00 0.00 H

ATOM 19 H MOL -2.352 -2.820 -0.654 1.00 0.00 H

ATOM 20 O MOL 4.492 -1.251 2.057 1.00 0.00 O

ATOM 21 H MOL 3.654 -0.735 2.115 1.00 0.00 H

ATOM 22 H MOL 5.174 -0.666 1.651 1.00 0.00 H

XYZ coordinates for 1a

ATOM	1	C	MOL	-0.227	0.322	-0.058	1.00	0.00	C
ATOM	2	C	MOL	0.397	-0.866	0.667	1.00	0.00	C
ATOM	3	C	MOL	1.890	-0.771	0.331	1.00	0.00	C
ATOM	4	C	MOL	2.045	0.669	0.036	1.00	0.00	C
ATOM	5	C	MOL	-1.354	1.034	0.630	1.00	0.00	C
ATOM	6	O	MOL	3.137	1.352	-0.055	1.00	0.00	O1+
ATOM	7	O	MOL	0.953	1.308	-0.168	1.00	0.00	O
ATOM	8	H	MOL	-0.455	0.101	-1.105	1.00	0.00	H
ATOM	9	H	MOL	-0.047	-1.806	0.330	1.00	0.00	H
ATOM	10	H	MOL	0.246	-0.772	1.748	1.00	0.00	H
ATOM	11	H	MOL	2.156	-1.317	-0.589	1.00	0.00	H
ATOM	12	H	MOL	2.575	-1.101	1.118	1.00	0.00	H
ATOM	13	H	MOL	-2.195	0.334	0.710	1.00	0.00	H
ATOM	14	H	MOL	-1.687	1.902	0.052	1.00	0.00	H
ATOM	15	H	MOL	-1.067	1.343	1.642	1.00	0.00	H
ATOM	16	H	MOL	3.921	0.793	0.133	1.00	0.00	H
ATOM	17	O	MOL	-3.126	-0.607	-1.931	1.00	0.00	O
ATOM	18	H	MOL	-3.646	-0.541	-1.112	1.00	0.00	H
ATOM	19	H	MOL	-3.518	-1.376	-2.379	1.00	0.00	H
ATOM	20	O	MOL	4.483	-1.731	2.449	1.00	0.00	O
ATOM	21	H	MOL	3.915	-1.144	1.920	1.00	0.00	H
ATOM	22	H	MOL	4.271	-2.614	2.101	1.00	0.00	H

XYZ coordinates for TS_{1a}

ATOM	1	C	MOL	-0.643	0.327	-0.329	1.00	0.00	C
ATOM	2	C	MOL	0.033	-0.790	0.388	1.00	0.00	C
ATOM	3	C	MOL	1.549	-0.616	0.369	1.00	0.00	C
ATOM	4	C	MOL	1.821	0.824	0.690	1.00	0.00	C
ATOM	5	C	MOL	-1.864	0.960	0.202	1.00	0.00	C
ATOM	6	O	MOL	3.032	1.216	1.077	1.00	0.00	O
ATOM	7	O	MOL	0.920	1.661	0.573	1.00	0.00	O
ATOM	8	H	MOL	-0.182	0.727	-1.225	1.00	0.00	H
ATOM	9	H	MOL	-0.235	-1.743	-0.084	1.00	0.00	H
ATOM	10	H	MOL	-0.342	-0.836	1.418	1.00	0.00	H
ATOM	11	H	MOL	1.972	-0.817	-0.626	1.00	0.00	H
ATOM	12	H	MOL	2.048	-1.291	1.073	1.00	0.00	H
ATOM	13	H	MOL	-2.549	0.201	0.599	1.00	0.00	H
ATOM	14	H	MOL	-2.365	1.586	-0.538	1.00	0.00	H
ATOM	15	H	MOL	-1.575	1.582	1.061	1.00	0.00	H
ATOM	16	H	MOL	3.637	0.449	1.130	1.00	0.00	H
ATOM	17	O	MOL	-1.771	-0.749	-1.892	1.00	0.00	O
ATOM	18	H	MOL	-2.349	-1.414	-1.472	1.00	0.00	H
ATOM	19	H	MOL	-1.137	-1.279	-2.412	1.00	0.00	H
ATOM	20	O	MOL	1.431	-3.226	0.311	1.00	0.00	O
ATOM	21	H	MOL	0.924	-3.073	1.131	1.00	0.00	H
ATOM	22	H	MOL	2.270	-2.751	0.458	1.00	0.00	H

XYZ coordinates for 1b

ATOM	1	C	MOL	-1.023	-0.169	-0.428	1.00	0.00	C
ATOM	2	C	MOL	0.079	-0.687	0.464	1.00	0.00	C
ATOM	3	C	MOL	1.453	-0.775	-0.196	1.00	0.00	C
ATOM	4	C	MOL	2.069	0.565	-0.517	1.00	0.00	C
ATOM	5	C	MOL	-2.359	0.032	0.229	1.00	0.00	C
ATOM	6	O	MOL	3.119	0.554	-1.363	1.00	0.00	O
ATOM	7	O	MOL	1.704	1.640	-0.054	1.00	0.00	O
ATOM	8	H	MOL	-0.715	0.698	-1.018	1.00	0.00	H
ATOM	9	H	MOL	-0.207	-1.671	0.859	1.00	0.00	H
ATOM	10	H	MOL	0.118	-0.014	1.330	1.00	0.00	H
ATOM	11	H	MOL	1.425	-1.389	-1.105	1.00	0.00	H
ATOM	12	H	MOL	2.152	-1.283	0.484	1.00	0.00	H
ATOM	13	H	MOL	-3.116	0.347	-0.499	1.00	0.00	H
ATOM	14	H	MOL	-2.253	0.833	0.971	1.00	0.00	H
ATOM	15	H	MOL	-2.692	-0.876	0.746	1.00	0.00	H
ATOM	16	H	MOL	3.294	-0.355	-1.676	1.00	0.00	H
ATOM	17	O	MOL	-1.175	-1.236	-1.560	1.00	0.00	O1+
ATOM	18	H	MOL	-1.562	-2.067	-1.202	1.00	0.00	H
ATOM	19	H	MOL	-1.789	-0.918	-2.260	1.00	0.00	H
ATOM	20	O	MOL	0.664	2.109	2.596	1.00	0.00	O
ATOM	21	H	MOL	-0.149	2.640	2.533	1.00	0.00	H
ATOM	22	H	MOL	0.964	2.024	1.666	1.00	0.00	H

XYZ coordinates for TS_{1b}

ATOM 1 C MOL -0.643 0.327 -0.329 1.00 0.00 C
ATOM 2 C MOL 0.033 -0.790 0.388 1.00 0.00 C
ATOM 3 C MOL 1.549 -0.616 0.369 1.00 0.00 C
ATOM 4 C MOL 1.821 0.824 0.690 1.00 0.00 C
ATOM 5 C MOL -1.864 0.960 0.202 1.00 0.00 C
ATOM 6 O MOL 3.032 1.216 1.077 1.00 0.00 O
ATOM 7 O MOL 0.920 1.661 0.573 1.00 0.00 O
ATOM 8 H MOL -0.182 0.727 -1.225 1.00 0.00 H
ATOM 9 H MOL -0.235 -1.743 -0.084 1.00 0.00 H
ATOM 10 H MOL -0.342 -0.836 1.418 1.00 0.00 H
ATOM 11 H MOL 1.972 -0.817 -0.626 1.00 0.00 H
ATOM 12 H MOL 2.048 -1.291 1.073 1.00 0.00 H
ATOM 13 H MOL -2.549 0.201 0.599 1.00 0.00 H
ATOM 14 H MOL -2.365 1.586 -0.538 1.00 0.00 H
ATOM 15 H MOL -1.575 1.582 1.061 1.00 0.00 H
ATOM 16 H MOL 3.637 0.449 1.130 1.00 0.00 H
ATOM 17 O MOL -1.771 -0.749 -1.892 1.00 0.00 O
ATOM 18 H MOL -2.349 -1.414 -1.472 1.00 0.00 H
ATOM 19 H MOL -1.137 -1.279 -2.412 1.00 0.00 H
ATOM 20 O MOL 1.431 -3.226 0.311 1.00 0.00 O
ATOM 21 H MOL 0.924 -3.073 1.131 1.00 0.00 H
ATOM 22 H MOL 2.270 -2.751 0.458 1.00 0.00 H

XYZ coordinates for 1c

ATOM	1	C	MOL	-1.228	0.156	-0.070	1.00 0.00	C
ATOM	2	C	MOL	-0.024	-0.406	0.144	1.00 0.00	C
ATOM	3	C	MOL	1.191	-0.126	-0.700	1.00 0.00	C
ATOM	4	C	MOL	2.426	0.232	0.071	1.00 0.00	C
ATOM	5	C	MOL	-2.467	-0.165	0.700	1.00 0.00	C
ATOM	6	O	MOL	3.588	-0.250	-0.295	1.00 0.00	O1+
ATOM	7	O	MOL	2.461	1.005	1.064	1.00 0.00	O
ATOM	8	H	MOL	-1.327	0.889	-0.876	1.00 0.00	H
ATOM	9	H	MOL	0.096	-1.149	0.937	1.00 0.00	H
ATOM	10	H	MOL	-0.308	1.783	1.425	1.00 0.00	H
ATOM	11	H	MOL	1.005	0.716	-1.385	1.00 0.00	H
ATOM	12	H	MOL	1.424	-0.996	-1.330	1.00 0.00	H
ATOM	13	H	MOL	-3.234	-0.580	0.030	1.00 0.00	H
ATOM	14	H	MOL	-2.902	0.746	1.136	1.00 0.00	H
ATOM	15	H	MOL	-2.275	-0.885	1.503	1.00 0.00	H
ATOM	16	H	MOL	3.491	-0.863	-1.052	1.00 0.00	H
ATOM	17	O	MOL	-1.439	-2.690	-1.976	1.00 0.00	O
ATOM	18	H	MOL	-1.208	-1.917	-1.429	1.00 0.00	H
ATOM	19	H	MOL	-1.745	-2.293	-2.810	1.00 0.00	H
ATOM	20	O	MOL	0.483	2.149	1.875	1.00 0.00	O1+
ATOM	21	H	MOL	0.511	3.098	1.639	1.00 0.00	H
ATOM	22	H	MOL	1.483	1.545	1.399	1.00 0.00	H1+

XYZ cordinates for 2

ATOM 1 C MOL -2.181 1.156 0.155 1.00 0.00 C

ATOM 2 C MOL -0.846 1.903 0.122 1.00 0.00 C

ATOM 3 C MOL 0.289 1.012 -0.338 1.00 0.00 C

ATOM 4 C MOL 0.664 -0.148 0.589 1.00 0.00 C

ATOM 5 C MOL 2.161 -0.314 0.345 1.00 0.00 C

ATOM 6 C MOL 2.607 1.069 -0.063 1.00 0.00 C

ATOM 7 O MOL 3.737 1.526 -0.107 1.00 0.00 O

ATOM 8 O MOL 1.529 1.817 -0.421 1.00 0.00 O

ATOM 9 H MOL -2.162 0.324 0.870 1.00 0.00 H

ATOM 10 H MOL -2.431 0.748 -0.834 1.00 0.00 H

ATOM 11 H MOL -2.990 1.832 0.454 1.00 0.00 H

ATOM 12 H MOL -0.602 2.295 1.120 1.00 0.00 H

ATOM 13 H MOL -0.916 2.763 -0.558 1.00 0.00 H

ATOM 14 H MOL 0.101 0.648 -1.358 1.00 0.00 H

ATOM 15 H MOL 0.086 -1.050 0.364 1.00 0.00 H

ATOM 16 H MOL 0.467 0.126 1.633 1.00 0.00 H

ATOM 17 H MOL 2.370 -0.989 -0.497 1.00 0.00 H

ATOM 18 H MOL 2.737 -0.668 1.205 1.00 0.00 H

ATOM 19 H MOL -0.836 -2.798 -0.180 1.00 0.00 H

ATOM 20 O MOL -1.315 -3.605 -0.478 1.00 0.00 O1+

ATOM 21 H MOL -1.834 -3.373 -1.284 1.00 0.00 H

ATOM 22 H MOL -0.637 -4.273 -0.738 1.00 0.00 H

ATOM 23 O MOL 4.562 -2.747 1.226 1.00 0.00 O

ATOM 24 H MOL 3.898 -1.858 1.202 1.00 0.00 H

ATOM 25 H MOL 5.516 -2.510 0.710 1.00 0.00 H

XYZ cordinates for 2a

ATOM	1	C	MOL	-1.678	1.793	-0.833	1.00	0.00	C
ATOM	2	C	MOL	-1.025	0.892	0.212	1.00	0.00	C
ATOM	3	C	MOL	0.055	-0.008	-0.316	1.00	0.00	C
ATOM	4	C	MOL	0.745	-0.926	0.687	1.00	0.00	C
ATOM	5	C	MOL	2.204	-0.974	0.220	1.00	0.00	C
ATOM	6	C	MOL	2.331	0.293	-0.525	1.00	0.00	C
ATOM	7	O	MOL	3.467	0.799	-0.867	1.00	0.00	O1+
ATOM	8	O	MOL	1.229	0.872	-0.829	1.00	0.00	O
ATOM	9	H	MOL	-2.099	1.201	-1.656	1.00	0.00	H
ATOM	10	H	MOL	-0.958	2.504	-1.257	1.00	0.00	H
ATOM	11	H	MOL	-2.492	2.370	-0.379	1.00	0.00	H
ATOM	12	H	MOL	-1.770	0.203	0.639	1.00	0.00	H
ATOM	13	H	MOL	-0.624	1.478	1.051	1.00	0.00	H
ATOM	14	H	MOL	-0.249	-0.531	-1.229	1.00	0.00	H
ATOM	15	H	MOL	0.271	-1.911	0.696	1.00	0.00	H
ATOM	16	H	MOL	0.683	-0.495	1.692	1.00	0.00	H
ATOM	17	H	MOL	2.401	-1.789	-0.494	1.00	0.00	H
ATOM	18	H	MOL	2.955	-1.048	1.013	1.00	0.00	H
ATOM	19	H	MOL	3.357	1.631	-1.383	1.00	0.00	H
ATOM	20	O	MOL	-2.586	-2.282	1.072	1.00	0.00	O
ATOM	21	H	MOL	-3.406	-2.188	0.558	1.00	0.00	H
ATOM	22	H	MOL	-2.814	-1.883	1.929	1.00	0.00	H
ATOM	23	O	MOL	5.288	0.836	-1.270	1.00	0.00	O
ATOM	24	H	MOL	5.999	1.491	-1.370	1.00	0.00	H
ATOM	25	H	MOL	5.626	0.245	-0.576	1.00	0.00	H

XYZ cordinates for TS_{2a}

ATOM 1 C MOL -1.913 1.510 -0.897 1.00 0.00 C
ATOM 2 C MOL -1.178 0.967 0.322 1.00 0.00 C
ATOM 3 C MOL -0.391 -0.256 0.058 1.00 0.00 C
ATOM 4 C MOL 0.647 -0.769 0.985 1.00 0.00 C
ATOM 5 C MOL 1.995 -0.966 0.279 1.00 0.00 C
ATOM 6 C MOL 2.289 0.225 -0.580 1.00 0.00 C
ATOM 7 O MOL 3.586 0.440 -0.810 1.00 0.00 O
ATOM 8 O MOL 1.383 0.919 -1.046 1.00 0.00 O
ATOM 9 H MOL -2.567 0.748 -1.337 1.00 0.00 H
ATOM 10 H MOL -1.192 1.825 -1.661 1.00 0.00 H
ATOM 11 H MOL -2.528 2.374 -0.625 1.00 0.00 H
ATOM 12 H MOL -1.872 0.744 1.148 1.00 0.00 H
ATOM 13 H MOL -0.497 1.711 0.762 1.00 0.00 H
ATOM 14 H MOL -0.475 -0.731 -0.916 1.00 0.00 H
ATOM 15 H MOL 0.320 -1.756 1.335 1.00 0.00 H
ATOM 16 H MOL 0.750 -0.114 1.857 1.00 0.00 H
ATOM 17 H MOL 1.960 -1.832 -0.398 1.00 0.00 H
ATOM 18 H MOL 2.795 -1.152 1.001 1.00 0.00 H
ATOM 19 H MOL 3.684 1.213 -1.407 1.00 0.00 H
ATOM 20 O MOL -1.894 -1.797 0.524 1.00 0.00 O
ATOM 21 H MOL -2.692 -1.680 -0.027 1.00 0.00 H
ATOM 22 H MOL -2.211 -1.623 1.432 1.00 0.00 H
ATOM 23 O MOL 5.684 1.104 -0.440 1.00 0.00 O
ATOM 24 H MOL 6.073 1.710 -1.285 1.00 0.00 H
ATOM 25 H MOL 6.499 0.923 0.292 1.00 0.00 H

XYZ coordinates for 2b

ATOM	1	C	MOL	-2.247	1.455	-0.789	1.00	0.00	C
ATOM	2	C	MOL	-0.934	0.850	-0.291	1.00	0.00	C
ATOM	3	C	MOL	-0.910	-0.658	-0.288	1.00	0.00	C
ATOM	4	C	MOL	0.331	-1.363	0.205	1.00	0.00	C
ATOM	5	C	MOL	1.662	-0.913	-0.397	1.00	0.00	C
ATOM	6	C	MOL	2.285	0.313	0.220	1.00	0.00	C
ATOM	7	O	MOL	3.152	0.905	-0.622	1.00	0.00	O
ATOM	8	O	MOL	2.093	0.729	1.359	1.00	0.00	O
ATOM	9	H	MOL	-3.099	1.092	-0.201	1.00	0.00	H
ATOM	10	H	MOL	-2.441	1.237	-1.850	1.00	0.00	H
ATOM	11	H	MOL	-2.210	2.547	-0.703	1.00	0.00	H
ATOM	12	H	MOL	-0.764	1.148	0.752	1.00	0.00	H
ATOM	13	H	MOL	-0.086	1.238	-0.872	1.00	0.00	H
ATOM	14	H	MOL	-1.804	-1.077	0.184	1.00	0.00	H
ATOM	15	H	MOL	0.206	-2.441	0.042	1.00	0.00	H
ATOM	16	H	MOL	0.335	-1.233	1.297	1.00	0.00	H
ATOM	17	H	MOL	1.601	-0.778	-1.483	1.00	0.00	H
ATOM	18	H	MOL	2.400	-1.713	-0.246	1.00	0.00	H
ATOM	19	H	MOL	3.573	1.653	-0.146	1.00	0.00	H
ATOM	20	O	MOL	0.373	-0.031	3.497	1.00	0.00	O
ATOM	21	H	MOL	0.995	0.242	2.787	1.00	0.00	H
ATOM	22	H	MOL	-0.385	0.568	3.385	1.00	0.00	H
ATOM	23	O	MOL	-1.063	-1.076	-1.792	1.00	0.00	O1+
ATOM	24	H	MOL	-1.860	-0.646	-2.176	1.00	0.00	H
ATOM	25	H	MOL	-1.204	-2.046	-1.872	1.00	0.00	H

XYZ cordinates for TS_{2b}

ATOM 1 C MOL -2.519 1.163 -0.565 1.00 0.00 C
ATOM 2 C MOL -1.065 0.853 -0.219 1.00 0.00 C
ATOM 3 C MOL -0.777 -0.560 0.109 1.00 0.00 C
ATOM 4 C MOL 0.488 -1.113 0.262 1.00 0.00 C
ATOM 5 C MOL 1.733 -0.506 -0.372 1.00 0.00 C
ATOM 6 C MOL 2.198 0.834 0.143 1.00 0.00 C
ATOM 7 O MOL 2.742 1.582 -0.825 1.00 0.00 O
ATOM 8 O MOL 2.149 1.223 1.313 1.00 0.00 O
ATOM 9 H MOL -3.196 0.801 0.219 1.00 0.00 H
ATOM 10 H MOL -2.805 0.693 -1.513 1.00 0.00 H
ATOM 11 H MOL -2.660 2.245 -0.663 1.00 0.00 H
ATOM 12 H MOL -0.784 1.426 0.686 1.00 0.00 H
ATOM 13 H MOL -0.380 1.205 -1.004 1.00 0.00 H
ATOM 14 H MOL -1.613 -1.168 0.458 1.00 0.00 H
ATOM 15 H MOL 0.508 -2.206 0.326 1.00 0.00 H
ATOM 16 H MOL 0.573 -0.930 1.576 1.00 0.00 H1-
ATOM 17 H MOL 1.609 -0.441 -1.460 1.00 0.00 H
ATOM 18 H MOL 2.580 -1.185 -0.204 1.00 0.00 H
ATOM 19 H MOL 3.083 2.409 -0.420 1.00 0.00 H
ATOM 20 O MOL 1.067 -0.663 2.796 1.00 0.00 O
ATOM 21 H MOL 1.552 0.164 2.489 1.00 0.00 H
ATOM 22 H MOL 0.327 -0.355 3.357 1.00 0.00 H
ATOM 23 O MOL -1.466 -1.447 -2.200 1.00 0.00 O
ATOM 24 H MOL -2.388 -1.747 -2.109 1.00 0.00 H
ATOM 25 H MOL -0.958 -2.277 -2.179 1.00 0.00 H

XYZ coordinates for 2c

ATOM 1 C MOL -2.219 1.611 -0.700 1.00 0.00 C
ATOM 2 C MOL -0.998 1.129 0.095 1.00 0.00 C
ATOM 3 C MOL -1.003 -0.354 0.295 1.00 0.00 C
ATOM 4 C MOL 0.002 -1.220 0.069 1.00 0.00 C
ATOM 5 C MOL 1.370 -0.871 -0.472 1.00 0.00 C
ATOM 6 C MOL 2.116 0.216 0.229 1.00 0.00 C
ATOM 7 O MOL 2.832 0.988 -0.553 1.00 0.00 O
ATOM 8 O MOL 2.145 0.412 1.474 1.00 0.00 O
ATOM 9 H MOL -3.152 1.316 -0.203 1.00 0.00 H
ATOM 10 H MOL -2.222 1.182 -1.711 1.00 0.00 H
ATOM 11 H MOL -2.211 2.703 -0.792 1.00 0.00 H
ATOM 12 H MOL -1.005 1.614 1.085 1.00 0.00 H
ATOM 13 H MOL -0.079 1.461 -0.406 1.00 0.00 H
ATOM 14 H MOL -1.943 -0.774 0.665 1.00 0.00 H
ATOM 15 H MOL -0.168 -2.281 0.254 1.00 0.00 H
ATOM 16 H MOL 0.060 -1.231 2.675 1.00 0.00 H
ATOM 17 H MOL 1.338 -0.616 -1.539 1.00 0.00 H
ATOM 18 H MOL 2.028 -1.752 -0.399 1.00 0.00 H
ATOM 19 H MOL 3.343 1.633 -0.013 1.00 0.00 H
ATOM 20 O MOL 0.979 -1.089 2.982 1.00 0.00 O1+
ATOM 21 H MOL 1.510 -0.381 2.275 1.00 0.00 H
ATOM 22 H MOL 0.908 -0.667 3.862 1.00 0.00 H
ATOM 23 O MOL -0.854 -0.982 -3.174 1.00 0.00 O
ATOM 24 H MOL -1.700 -1.014 -3.654 1.00 0.00 H
ATOM 25 H MOL -1.115 -1.097 -2.242 1.00 0.00 H

XYZ coordinates for 3

ATOM 1 C MOL -0.125 1.624 0.396 1.00 0.00 C
ATOM 2 C MOL -0.115 0.125 0.001 1.00 0.00 C
ATOM 3 C MOL 1.322 -0.304 0.295 1.00 0.00 C
ATOM 4 C MOL 2.110 1.004 0.192 1.00 0.00 C
ATOM 5 O MOL 1.224 2.064 0.189 1.00 0.00 O1+
ATOM 6 O MOL 3.297 1.147 0.120 1.00 0.00 O1-
ATOM 7 H MOL -0.390 1.758 1.453 1.00 0.00 H
ATOM 8 H MOL -0.780 2.240 -0.226 1.00 0.00 H
ATOM 9 H MOL -0.856 -0.401 0.642 1.00 0.00 H
ATOM 10 H MOL -0.325 0.045 -1.079 1.00 0.00 H
ATOM 11 H MOL 1.743 -1.039 -0.397 1.00 0.00 H
ATOM 12 H MOL 1.444 -0.690 1.315 1.00 0.00 H
ATOM 13 O MOL -2.071 -1.926 -0.943 1.00 0.00 O1+
ATOM 14 H MOL -3.012 -1.633 -0.971 1.00 0.00 H
ATOM 15 H MOL -1.464 -1.216 -0.502 1.00 0.00 H
ATOM 16 H MOL -2.001 -2.797 -0.486 1.00 0.00 H
ATOM 17 O MOL 3.595 -1.289 -0.535 1.00 0.00 O
ATOM 18 H MOL 4.150 -0.907 -1.418 1.00 0.00 H
ATOM 19 H MOL 4.096 -2.200 -0.148 1.00 0.00 H

XYZ coordinates for 3a

ATOM	1	C	MOL	-0.622	0.562	0.052	1.00	0.00 C
ATOM	2	C	MOL	0.154	-0.687	-0.340	1.00	0.00 C
ATOM	3	C	MOL	1.571	-0.408	0.183	1.00	0.00 C
ATOM	4	C	MOL	1.596	1.066	0.223	1.00	0.00 C
ATOM	5	O	MOL	0.448	1.637	0.142	1.00	0.00 O1+
ATOM	6	O	MOL	2.674	1.759	0.346	1.00	0.00 O
ATOM	7	H	MOL	-1.064	0.531	1.050	1.00	0.00 H
ATOM	8	H	MOL	-1.336	0.932	-0.682	1.00	0.00 H
ATOM	9	H	MOL	-0.288	-1.583	0.104	1.00	0.00 H
ATOM	10	H	MOL	0.171	-0.804	-1.428	1.00	0.00 H
ATOM	11	H	MOL	2.390	-0.809	-0.422	1.00	0.00 H
ATOM	12	H	MOL	1.723	-0.759	1.216	1.00	0.00 H
ATOM	13	H	MOL	2.488	2.726	0.371	1.00	0.00 H
ATOM	14	O	MOL	-3.366	-1.010	-0.148	1.00	0.00 O
ATOM	15	H	MOL	-3.337	-1.822	0.386	1.00	0.00 H
ATOM	16	H	MOL	-3.201	-1.331	-1.051	1.00	0.00 H
ATOM	17	O	MOL	4.499	-1.511	-0.459	1.00	0.00 O
ATOM	18	H	MOL	4.989	-0.877	0.092	1.00	0.00 H
ATOM	19	H	MOL	4.802	-1.303	-1.359	1.00	0.00 H

XYZ coordinates for TS_{3a}

ATOM 1 C MOL -1.012 0.245 0.032 1.00 0.00 C

ATOM 2 C MOL 0.021 -0.763 -0.368 1.00 0.00 C

ATOM 3 C MOL 1.389 -0.370 0.216 1.00 0.00 C

ATOM 4 C MOL 1.470 1.115 0.182 1.00 0.00 C

ATOM 5 O MOL 0.426 1.784 0.102 1.00 0.00 O

ATOM 6 O MOL 2.678 1.648 0.278 1.00 0.00 O

ATOM 7 H MOL -1.224 0.415 1.083 1.00 0.00 H

ATOM 8 H MOL -1.497 0.886 -0.690 1.00 0.00 H

ATOM 9 H MOL -0.250 -1.748 0.028 1.00 0.00 H

ATOM 10 H MOL 0.078 -0.830 -1.459 1.00 0.00 H

ATOM 11 H MOL 2.228 -0.836 -0.313 1.00 0.00 H

ATOM 12 H MOL 1.480 -0.662 1.273 1.00 0.00 H

ATOM 13 H MOL 2.611 2.628 0.296 1.00 0.00 H

ATOM 14 O MOL -2.771 -0.802 -0.074 1.00 0.00 O

ATOM 15 H MOL -2.742 -1.644 0.421 1.00 0.00 H

ATOM 16 H MOL -2.885 -1.069 -1.007 1.00 0.00 H

ATOM 17 O MOL 2.663 -2.140 -1.024 1.00 0.00 O

ATOM 18 H MOL 2.648 -3.105 -1.136 1.00 0.00 H

ATOM 19 H MOL 3.594 -1.956 -0.808 1.00 0.00 H

XYZ coordinates for 3b

ATOM 1 C MOL -1.456 -0.158 -0.390 1.00 0.00 C

ATOM 2 C MOL -0.385 -0.632 0.551 1.00 0.00 C

ATOM 3 C MOL 1.009 -0.755 -0.059 1.00 0.00 C

ATOM 4 C MOL 1.623 0.560 -0.473 1.00 0.00 C

ATOM 5 O MOL 2.669 0.495 -1.321 1.00 0.00 O

ATOM 6 O MOL 1.261 1.664 -0.078 1.00 0.00 O

ATOM 7 H MOL -1.186 0.720 -0.977 1.00 0.00 H

ATOM 8 H MOL -0.679 -1.594 0.991 1.00 0.00 H

ATOM 9 H MOL -0.377 0.086 1.384 1.00 0.00 H

ATOM 10 H MOL 1.014 -1.443 -0.914 1.00 0.00 H

ATOM 11 H MOL 1.692 -1.195 0.682 1.00 0.00 H

ATOM 12 H MOL 2.848 -0.434 -1.569 1.00 0.00 H

ATOM 13 H MOL -2.426 -0.026 0.092 1.00 0.00 H

ATOM 14 O MOL -1.662 -1.227 -1.466 1.00 0.00 O1+

ATOM 15 H MOL -2.031 -2.050 -1.071 1.00 0.00 H

ATOM 16 H MOL -2.314 -0.923 -2.137 1.00 0.00 H

ATOM 17 O MOL 0.339 2.213 2.587 1.00 0.00 O

ATOM 18 H MOL -0.536 2.633 2.517 1.00 0.00 H

ATOM 19 H MOL 0.596 2.066 1.652 1.00 0.00 H

XYZ coordinates for TS_{3b}

ATOM 1 C MOL -1.381 0.034 -0.136 1.00 0.00 C
ATOM 2 C MOL -0.370 -0.485 0.643 1.00 0.00 C
ATOM 3 C MOL 1.056 -0.589 0.117 1.00 0.00 C
ATOM 4 C MOL 1.647 0.683 -0.449 1.00 0.00 C
ATOM 5 O MOL 2.543 0.552 -1.436 1.00 0.00 O
ATOM 6 O MOL 1.396 1.819 -0.046 1.00 0.00 O
ATOM 7 H MOL -1.174 0.770 -0.912 1.00 0.00 H
ATOM 8 H MOL -0.646 -1.280 1.343 1.00 0.00 H
ATOM 9 H MOL -0.342 0.565 1.515 1.00 0.00 H1-
ATOM 10 H MOL 1.095 -1.385 -0.639 1.00 0.00 H
ATOM 11 H MOL 1.730 -0.908 0.925 1.00 0.00 H
ATOM 12 H MOL 2.647 -0.387 -1.686 1.00 0.00 H
ATOM 13 H MOL -2.417 -0.053 0.184 1.00 0.00 H
ATOM 14 O MOL -1.681 -1.456 -1.828 1.00 0.00 O
ATOM 15 H MOL -2.020 -2.209 -1.310 1.00 0.00 H
ATOM 16 H MOL -2.450 -1.172 -2.356 1.00 0.00 H
ATOM 17 O MOL 0.203 1.498 2.272 1.00 0.00 O
ATOM 18 H MOL -0.468 2.156 2.545 1.00 0.00 H
ATOM 19 H MOL 0.708 1.905 1.504 1.00 0.00 H

XYZ coordinates for 3c

ATOM 1 C MOL -1.714 0.174 0.134 1.00 0.00 C

ATOM 2 C MOL -0.529 -0.409 0.363 1.00 0.00 C

ATOM 3 C MOL 0.670 -0.232 -0.528 1.00 0.00 C

ATOM 4 C MOL 1.935 0.157 0.175 1.00 0.00 C

ATOM 5 O MOL 3.082 -0.336 -0.226 1.00 0.00 O1+

ATOM 6 O MOL 2.011 0.968 1.134 1.00 0.00 O

ATOM 7 H MOL -1.863 0.852 -0.708 1.00 0.00 H

ATOM 8 H MOL -0.407 -1.091 1.207 1.00 0.00 H

ATOM 9 H MOL -0.739 1.802 1.566 1.00 0.00 H

ATOM 10 H MOL 0.486 0.555 -1.277 1.00 0.00 H

ATOM 11 H MOL 0.856 -1.160 -1.089 1.00 0.00 H

ATOM 12 H MOL 2.955 -0.975 -0.957 1.00 0.00 H

ATOM 13 H MOL -2.570 -0.027 0.777 1.00 0.00 H

ATOM 14 O MOL -1.662 -2.737 -1.848 1.00 0.00 O

ATOM 15 H MOL -1.786 -2.031 -1.188 1.00 0.00 H

ATOM 16 H MOL -1.964 -2.326 -2.677 1.00 0.00 H

ATOM 17 O MOL 0.079 2.171 1.967 1.00 0.00 O1+

ATOM 18 H MOL 0.118 3.108 1.685 1.00 0.00 H

ATOM 19 H MOL 1.042 1.535 1.490 1.00 0.00 H1+

XYZ coordinates for 4

ATOM	1	C	MOL	-0.425	1.544	0.304	1.00	0.00	C
ATOM	2	C	MOL	-0.352	0.142	-0.262	1.00	0.00	C
ATOM	3	C	MOL	0.928	-0.538	0.200	1.00	0.00	C
ATOM	4	C	MOL	2.125	0.284	-0.276	1.00	0.00	C
ATOM	5	C	MOL	2.006	1.779	-0.103	1.00	0.00	C
ATOM	6	O	MOL	0.783	2.344	0.054	1.00	0.00	O
ATOM	7	O	MOL	2.971	2.531	-0.158	1.00	0.00	O
ATOM	8	H	MOL	-0.557	1.517	1.392	1.00	0.00	H
ATOM	9	H	MOL	-1.235	2.129	-0.140	1.00	0.00	H
ATOM	10	H	MOL	-0.418	0.159	-1.358	1.00	0.00	H
ATOM	11	H	MOL	-1.241	-0.378	0.125	1.00	0.00	H
ATOM	12	H	MOL	1.002	-1.559	-0.195	1.00	0.00	H
ATOM	13	H	MOL	0.931	-0.612	1.296	1.00	0.00	H
ATOM	14	H	MOL	2.274	0.137	-1.357	1.00	0.00	H
ATOM	15	H	MOL	3.060	-0.025	0.204	1.00	0.00	H
ATOM	16	O	MOL	-3.094	-2.327	-0.160	1.00	0.00	O1+
ATOM	17	H	MOL	-3.677	-2.130	0.610	1.00	0.00	H
ATOM	18	H	MOL	-2.302	-1.738	-0.102	1.00	0.00	H
ATOM	19	H	MOL	-2.781	-3.259	-0.073	1.00	0.00	H
ATOM	20	O	MOL	5.025	-2.533	-0.000	1.00	0.00	O
ATOM	21	H	MOL	5.704	-1.899	0.607	1.00	0.00	H
ATOM	22	H	MOL	4.142	-2.080	0.497	1.00	0.00	H

XYZ coordinates for 4a

ATOM	1	C	MOL	-0.868	1.191	0.179	1.00 0.00	C
ATOM	2	C	MOL	-0.636	-0.166	-0.421	1.00 0.00	C
ATOM	3	C	MOL	0.614	-0.799	0.185	1.00 0.00	C
ATOM	4	C	MOL	1.820	0.090	-0.115	1.00 0.00	C
ATOM	5	C	MOL	1.533	1.536	0.017	1.00 0.00	C
ATOM	6	O	MOL	0.370	2.056	0.126	1.00 0.00	O1+
ATOM	7	O	MOL	2.480	2.428	0.001	1.00 0.00	O
ATOM	8	H	MOL	-1.109	1.160	1.246	1.00 0.00	H
ATOM	9	H	MOL	-1.600	1.800	-0.354	1.00 0.00	H
ATOM	10	H	MOL	-0.537	-0.085	-1.513	1.00 0.00	H
ATOM	11	H	MOL	-1.530	-0.773	-0.221	1.00 0.00	H
ATOM	12	H	MOL	0.793	-1.795	-0.230	1.00 0.00	H
ATOM	13	H	MOL	0.496	-0.907	1.271	1.00 0.00	H
ATOM	14	H	MOL	2.157	-0.039	-1.158	1.00 0.00	H
ATOM	15	H	MOL	2.693	-0.141	0.511	1.00 0.00	H
ATOM	16	O	MOL	-3.461	-2.400	-0.181	1.00 0.00	O
ATOM	17	H	MOL	-3.692	-2.014	0.681	1.00 0.00	H
ATOM	18	H	MOL	3.360	2.004	-0.081	1.00 0.00	H
ATOM	19	H	MOL	-2.885	-3.146	0.057	1.00 0.00	H
ATOM	20	O	MOL	4.619	-2.085	0.150	1.00 0.00	O
ATOM	21	H	MOL	5.673	-1.740	0.194	1.00 0.00	H
ATOM	22	H	MOL	4.899	-3.039	0.642	1.00 0.00	H

XYZ coordinates for TS_{4a}

ATOM 1 C MOL -0.915 -0.448 0.359 1.00 0.00 C

ATOM 2 C MOL -0.122 -1.312 -0.646 1.00 0.00 C

ATOM 3 C MOL 1.381 -1.267 -0.417 1.00 0.00 C

ATOM 4 C MOL 1.925 0.117 -0.506 1.00 0.00 C

ATOM 5 C MOL -0.745 1.015 0.152 1.00 0.00 C

ATOM 6 O MOL 1.217 1.136 -0.571 1.00 0.00 O

ATOM 7 O MOL 3.252 0.203 -0.517 1.00 0.00 O

ATOM 8 H MOL -1.979 -0.684 0.214 1.00 0.00 H

ATOM 9 H MOL 3.511 1.151 -0.535 1.00 0.00 H

ATOM 10 H MOL -0.646 -0.725 1.385 1.00 0.00 H

ATOM 11 H MOL -0.462 -2.346 -0.534 1.00 0.00 H

ATOM 12 H MOL 1.918 -1.888 -1.146 1.00 0.00 H

ATOM 13 H MOL 1.652 -1.667 0.572 1.00 0.00 H

ATOM 14 H MOL -0.297 1.660 0.893 1.00 0.00 H

ATOM 15 H MOL -1.079 1.466 -0.777 1.00 0.00 H

ATOM 16 H MOL -0.356 -1.006 -1.675 1.00 0.00 H

ATOM 17 O MOL -2.498 1.780 1.067 1.00 0.00 O

ATOM 18 H MOL -2.462 1.455 1.988 1.00 0.00 H

ATOM 19 H MOL -3.295 1.360 0.693 1.00 0.00 H

ATOM 20 O MOL 5.380 -3.230 -0.205 1.00 0.00 O

ATOM 21 H MOL 6.059 -2.596 0.402 1.00 0.00 H

ATOM 22 H MOL 4.497 -2.777 0.292 1.00 0.00 H

XYZ coordinates for 4b

ATOM 1 C MOL -0.198 0.362 0.622 1.00 0.00 C

ATOM 2 C MOL -0.010 -0.683 -0.479 1.00 0.00 C

ATOM 3 C MOL 1.356 -1.365 -0.442 1.00 0.00 C

ATOM 4 C MOL 2.517 -0.477 -0.790 1.00 0.00 C

ATOM 5 C MOL -1.555 1.025 0.644 1.00 0.00 C

ATOM 6 O MOL 2.441 0.647 -1.281 1.00 0.00 O

ATOM 7 O MOL 3.703 -1.064 -0.522 1.00 0.00 O

ATOM 8 H MOL 0.003 -0.078 1.612 1.00 0.00 H

ATOM 9 H MOL 4.411 -0.444 -0.801 1.00 0.00 H

ATOM 10 H MOL 0.532 1.175 0.501 1.00 0.00 H

ATOM 11 H MOL -0.770 -1.470 -0.387 1.00 0.00 H

ATOM 12 H MOL 1.384 -2.200 -1.158 1.00 0.00 H

ATOM 13 H MOL 1.552 -1.817 0.540 1.00 0.00 H

ATOM 14 H MOL -1.578 1.887 1.315 1.00 0.00 H

ATOM 15 H MOL -1.900 1.331 -0.348 1.00 0.00 H

ATOM 16 H MOL -0.160 -0.210 -1.460 1.00 0.00 H

ATOM 17 O MOL -2.640 0.132 1.143 1.00 0.00 O1+

ATOM 18 H MOL -2.352 -0.322 1.961 1.00 0.00 H

ATOM 19 H MOL -3.074 -0.620 0.398 1.00 0.00 H

ATOM 20 O MOL 2.475 3.159 0.126 1.00 0.00 O

ATOM 21 H MOL 3.210 3.131 0.763 1.00 0.00 H

ATOM 22 H MOL 2.551 2.312 -0.358 1.00 0.00 H

XYZ coordinates for TS_{4b}

ATOM 1 C MOL -0.052 0.485 0.659 1.00 0.00 C

ATOM 2 C MOL 0.191 -0.505 -0.470 1.00 0.00 C

ATOM 3 C MOL 1.505 -1.280 -0.400 1.00 0.00 C

ATOM 4 C MOL 2.738 -0.568 -0.872 1.00 0.00 C

ATOM 5 C MOL -1.157 1.312 0.664 1.00 0.00 C

ATOM 6 O MOL 2.822 0.609 -1.229 1.00 0.00 O

ATOM 7 O MOL 3.805 -1.384 -0.892 1.00 0.00 O

ATOM 8 H MOL 0.363 0.212 1.636 1.00 0.00 H

ATOM 9 H MOL 4.576 -0.859 -1.195 1.00 0.00 H

ATOM 10 H MOL 0.662 1.609 0.449 1.00 0.00 H1-

ATOM 11 H MOL -0.613 -1.252 -0.426 1.00 0.00 H

ATOM 12 H MOL 1.432 -2.196 -1.003 1.00 0.00 H

ATOM 13 H MOL 1.706 -1.637 0.621 1.00 0.00 H

ATOM 14 H MOL -1.347 1.966 1.511 1.00 0.00 H

ATOM 15 H MOL -1.660 1.557 -0.271 1.00 0.00 H

ATOM 16 H MOL 0.078 -0.015 -1.447 1.00 0.00 H

ATOM 17 O MOL -3.075 0.259 1.368 1.00 0.00 O

ATOM 18 H MOL -2.678 -0.205 2.127 1.00 0.00 H

ATOM 19 H MOL -3.287 -0.456 0.703 1.00 0.00 H

ATOM 20 O MOL 1.603 2.534 0.139 1.00 0.00 O

ATOM 21 H MOL 2.100 2.746 0.954 1.00 0.00 H

ATOM 22 H MOL 2.204 1.961 -0.420 1.00 0.00 H

XYZ coordinates for 4c

ATOM 1 C MOL -0.198 0.362 0.622 1.00 0.00 C

ATOM 2 C MOL -0.010 -0.683 -0.479 1.00 0.00 C

ATOM 3 C MOL 1.356 -1.365 -0.442 1.00 0.00 C

ATOM 4 C MOL 2.517 -0.477 -0.790 1.00 0.00 C

ATOM 5 C MOL -1.555 1.025 0.644 1.00 0.00 C

ATOM 6 O MOL 2.441 0.647 -1.281 1.00 0.00 O

ATOM 7 O MOL 3.703 -1.064 -0.522 1.00 0.00 O

ATOM 8 H MOL 0.003 -0.078 1.612 1.00 0.00 H

ATOM 9 H MOL 4.411 -0.444 -0.801 1.00 0.00 H

ATOM 10 H MOL 0.532 1.175 0.501 1.00 0.00 H

ATOM 11 H MOL -0.770 -1.470 -0.387 1.00 0.00 H

ATOM 12 H MOL 1.384 -2.200 -1.158 1.00 0.00 H

ATOM 13 H MOL 1.552 -1.817 0.540 1.00 0.00 H

ATOM 14 H MOL -1.578 1.887 1.315 1.00 0.00 H

ATOM 15 H MOL -1.900 1.331 -0.348 1.00 0.00 H

ATOM 16 H MOL -0.160 -0.210 -1.460 1.00 0.00 H

ATOM 17 O MOL -2.640 0.132 1.143 1.00 0.00 O1+

ATOM 18 H MOL -2.352 -0.322 1.961 1.00 0.00 H

ATOM 19 H MOL -3.074 -0.620 0.398 1.00 0.00 H

ATOM 20 O MOL 2.475 3.159 0.126 1.00 0.00 O

ATOM 21 H MOL 3.210 3.131 0.763 1.00 0.00 H

ATOM 22 H MOL 2.551 2.312 -0.358 1.00 0.00 H

XYZ coordinates for 5

ATOM	1	C	MOL	0.325	-0.231	-1.309	1.00	0.00	C
ATOM	2	C	MOL	1.546	0.611	-0.925	1.00	0.00	C
ATOM	3	C	MOL	1.239	2.099	-0.582	1.00	0.00	C
ATOM	4	C	MOL	-0.109	2.591	-1.045	1.00	0.00	C
ATOM	5	C	MOL	-0.730	-0.371	-0.206	1.00	0.00	C
ATOM	6	C	MOL	-1.065	0.948	0.479	1.00	0.00	C
ATOM	7	O	MOL	-0.277	3.476	-1.877	1.00	0.00	O
ATOM	8	O	MOL	-1.223	2.037	-0.486	1.00	0.00	O
ATOM	9	H	MOL	0.659	-1.231	-1.614	1.00	0.00	H
ATOM	10	H	MOL	-0.146	0.212	-2.201	1.00	0.00	H
ATOM	11	H	MOL	2.251	0.595	-1.764	1.00	0.00	H
ATOM	12	H	MOL	2.061	0.151	-0.071	1.00	0.00	H
ATOM	13	H	MOL	1.984	2.758	-1.037	1.00	0.00	H
ATOM	14	H	MOL	1.296	2.257	0.504	1.00	0.00	H
ATOM	15	H	MOL	-0.374	-1.059	0.576	1.00	0.00	H
ATOM	16	H	MOL	-1.641	-0.813	-0.630	1.00	0.00	H
ATOM	17	H	MOL	-0.304	1.234	1.213	1.00	0.00	H
ATOM	18	H	MOL	-2.030	0.903	0.991	1.00	0.00	H
ATOM	19	H	MOL	-1.779	-4.165	2.450	1.00	0.00	H
ATOM	20	O	MOL	-0.809	-4.185	2.276	1.00	0.00	O1+
ATOM	21	H	MOL	-0.502	-3.254	2.182	1.00	0.00	H
ATOM	22	H	MOL	-0.373	-4.562	3.076	1.00	0.00	H
ATOM	23	O	MOL	1.622	4.421	-2.937	1.00	0.00	O
ATOM	24	H	MOL	1.252	5.161	-2.197	1.00	0.00	H
ATOM	25	H	MOL	2.732	4.421	-2.937	1.00	0.00	H

XYZ coordinates for 5a

ATOM 1 C MOL 0.323 -1.088 -1.278 1.00 0.00 C

ATOM 2 C MOL 1.543 -0.255 -0.876 1.00 0.00 C

ATOM 3 C MOL 1.250 1.253 -0.577 1.00 0.00 C

ATOM 4 C MOL -0.115 1.687 -0.949 1.00 0.00 C

ATOM 5 C MOL -0.749 -1.232 -0.189 1.00 0.00 C

ATOM 6 C MOL -1.065 0.063 0.531 1.00 0.00 C

ATOM 7 O MOL -0.354 2.634 -1.805 1.00 0.00 O1+

ATOM 8 O MOL -1.190 1.186 -0.456 1.00 0.00 O

ATOM 9 H MOL 0.661 -2.088 -1.573 1.00 0.00 H

ATOM 10 H MO -0.132 -0.651 -2.180 1.00 0.00 H

ATOM 11 H MOL 2.272 -0.283 -1.693 1.00 0.00 H

ATOM 12 H MOL 2.026 -0.688 0.007 1.00 0.00 H

ATOM 13 H MOL 1.974 1.900 -1.080 1.00 0.00 H

ATOM 14 H MOL 1.343 1.454 0.501 1.00 0.00 H

ATOM 15 H MOL -0.416 -1.931 0.591 1.00 0.00 H

ATOM 16 H MOL -1.663 -1.648 -0.628 1.00 0.00 H

ATOM 17 H MOL -0.302 0.361 1.254 1.00 0.00 H

ATOM 18 H MOL -2.039 0.061 1.020 1.00 0.00 H

ATOM 19 H MOL 0.480 2.997 -2.169 1.00 0.00 H

ATOM 20 O MOL -1.222 -1.237 3.452 1.00 0.00 O

ATOM 21 H MOL -0.578 -1.081 4.163 1.00 0.00 H

ATOM 22 H MOL -2.048 -1.414 3.934 1.00 0.00 H

ATOM 23 O MOL -1.603 4.450 -2.329 1.00 0.00 O

ATOM 24 H MOL -1.543 5.293 -3.048 1.00 0.00 H

ATOM 25 H MOL -2.367 4.676 -1.557 1.00 0.00 H

XYZ coordinates for TS_{5a}

ATOM 1 C MOL 0.231 -1.050 -1.104 1.00 0.00 C

ATOM 2 C MOL 1.488 -0.193 -0.934 1.00 0.00 C

ATOM 3 C MOL 1.253 1.274 -0.473 1.00 0.00 C

ATOM 4 C MOL -0.085 1.766 -0.920 1.00 0.00 C

ATOM 5 C MOL -0.611 -1.370 0.153 1.00 0.00 C

ATOM 6 C MOL -1.060 -0.219 0.987 1.00 0.00 C

ATOM 7 O MOL -0.174 2.659 -1.906 1.00 0.00 O

ATOM 8 O MOL -1.152 1.348 -0.441 1.00 0.00 O

ATOM 9 H MOL 0.538 -2.017 -1.518 1.00 0.00 H

ATOM 10 H MOL -0.424 -0.594 -1.856 1.00 0.00 H

ATOM 11 H MOL 1.996 -0.166 -1.906 1.00 0.00 H

ATOM 12 H MOL 2.185 -0.657 -0.226 1.00 0.00 H

ATOM 13 H MOL 2.058 1.921 -0.838 1.00 0.00 H

ATOM 14 H MOL 1.262 1.335 0.622 1.00 0.00 H

ATOM 15 H MOL -0.006 -2.022 0.798 1.00 0.00 H

ATOM 16 H MOL -1.490 -1.942 -0.164 1.00 0.00 H

ATOM 17 H MOL -0.352 0.373 1.556 1.00 0.00 H

ATOM 18 H MOL -2.106 0.039 1.080 1.00 0.00 H

ATOM 19 H MOL 0.721 2.943 -2.188 1.00 0.00 H

ATOM 20 O MOL -1.399 -1.346 2.747 1.00 0.00 O

ATOM 21 H MOL -0.679 -1.122 3.367 1.00 0.00 H

ATOM 22 H MOL -2.194 -0.958 3.164 1.00 0.00 H

ATOM 23 O MOL -1.894 2.939 -0.613 1.00 0.00 O

ATOM 24 H MOL -1.620 3.705 0.142 1.00 0.00 H

ATOM 25 H MOL -1.998 3.421 -1.608 1.00 0.00 H

XYZ coordinates for 5b

ATOM	1	C	MOL	-0.110	-0.724	-0.818	1.00	0.00 C
ATOM	2	C	MOL	1.374	-0.392	-1.003	1.00	0.00 C
ATOM	3	C	MOL	1.825	0.947	-0.383	1.00	0.00 C
ATOM	4	C	MOL	1.101	2.141	-0.945	1.00	0.00 C
ATOM	5	C	MOL	-0.509	-0.974	0.640	1.00	0.00 C
ATOM	6	C	MOL	-1.963	-1.288	0.836	1.00	0.00 C
ATOM	7	O	MOL	1.288	2.412	-2.256	1.00	0.00 O
ATOM	8	O	MOL	0.351	2.876	-0.309	1.00	0.00 O
ATOM	9	H	MOL	-0.332	-1.619	-1.415	1.00	0.00 H
ATOM	10	H	MOL	-0.735	0.082	-1.232	1.00	0.00 H
ATOM	11	H	MOL	1.609	-0.397	-2.076	1.00	0.00 H
ATOM	12	H	MOL	1.990	-1.183	-0.555	1.00	0.00 H
ATOM	13	H	MOL	2.900	1.079	-0.571	1.00	0.00 H
ATOM	14	H	MOL	1.680	0.948	0.702	1.00	0.00 H
ATOM	15	H	MOL	-0.340	-0.077	1.257	1.00	0.00 H
ATOM	16	H	MOL	0.107	-1.770	1.084	1.00	0.00 H
ATOM	17	H	MOL	-2.636	-0.586	0.340	1.00	0.00 H
ATOM	18	H	MOL	-2.246	-1.442	1.879	1.00	0.00 H
ATOM	19	H	MOL	1.918	1.778	-2.651	1.00	0.00 H
ATOM	20	O	MOL	-2.279	-2.608	0.120	1.00	0.00 O1+
ATOM	21	H	MOL	-3.246	-2.789	0.132	1.00	0.00 H
ATOM	22	H	MOL	-1.846	-3.363	0.577	1.00	0.00 H
ATOM	23	O	MOL	-0.335	2.224	2.348	1.00	0.00 O
ATOM	24	H	MOL	0.491	2.241	2.860	1.00	0.00 H
ATOM	25	H	MOL	-0.055	2.483	1.438	1.00	0.00 H

XYZ coordinates for TS_{5b}

ATOM 1 C MOL -0.047 -0.639 -0.764 1.00 0.00 C
ATOM 2 C MOL 1.430 -0.317 -0.992 1.00 0.00 C
ATOM 3 C MOL 1.895 1.018 -0.380 1.00 0.00 C
ATOM 4 C MOL 1.147 2.198 -0.932 1.00 0.00 C
ATOM 5 C MOL -0.444 -0.863 0.686 1.00 0.00 C
ATOM 6 C MOL -1.775 -0.973 1.039 1.00 0.00 C
ATOM 7 O MOL 1.367 2.524 -2.219 1.00 0.00 O
ATOM 8 O MOL 0.327 2.870 -0.301 1.00 0.00 O
ATOM 9 H MOL -0.272 -1.574 -1.297 1.00 0.00 H
ATOM 10 H MOL -0.697 0.124 -1.217 1.00 0.00 H
ATOM 11 H MOL 1.627 -0.321 -2.073 1.00 0.00 H
ATOM 12 H MOL 2.056 -1.112 -0.565 1.00 0.00 H
ATOM 13 H MOL 2.966 1.154 -0.577 1.00 0.00 H
ATOM 14 H MOL 1.765 1.009 0.707 1.00 0.00 H
ATOM 15 H MOL -0.533 0.290 1.334 1.00 0.00 H1-
ATOM 16 H MOL 0.274 -1.413 1.304 1.00 0.00 H
ATOM 17 H MOL -2.538 -0.474 0.445 1.00 0.00 H
ATOM 18 H MOL -2.052 -1.270 2.050 1.00 0.00 H
ATOM 19 H MOL 2.040 1.933 -2.612 1.00 0.00 H
ATOM 20 O MOL -2.505 -2.904 -0.005 1.00 0.00 O
ATOM 21 H MOL -3.434 -3.131 0.183 1.00 0.00 H
ATOM 22 H MOL -1.997 -3.602 0.447 1.00 0.00 H
ATOM 23 O MOL -0.527 1.604 1.901 1.00 0.00 O
ATOM 24 H MOL 0.092 1.663 2.654 1.00 0.00 H
ATOM 25 H MOL -0.163 2.208 1.185 1.00 0.00 H

XYZ coordinates for 5c

ATOM	1	C	MOL	-0.009	-0.760	-0.853	1.00 0.00	C
ATOM	2	C	MOL	1.442	-0.292	-1.029	1.00 0.00	C
ATOM	3	C	MOL	1.805	1.003	-0.264	1.00 0.00	C
ATOM	4	C	MOL	1.103	2.206	-0.791	1.00 0.00	C
ATOM	5	C	MOL	-0.366	-1.119	0.558	1.00 0.00	C
ATOM	6	C	MOL	-1.537	-0.844	1.161	1.00 0.00	C
ATOM	7	O	MOL	1.430	2.697	-1.965	1.00 0.00	O1+
ATOM	8	O	MOL	0.168	2.815	-0.205	1.00 0.00	O
ATOM	9	H	MOL	-0.130	-1.665	-1.470	1.00 0.00	H
ATOM	10	H	MOL	-0.723	-0.025	-1.253	1.00 0.00	H
ATOM	11	H	MOL	1.659	-0.166	-2.097	1.00 0.00	H
ATOM	12	H	MOL	2.126	-1.068	-0.663	1.00 0.00	H
ATOM	13	H	MOL	2.884	1.184	-0.361	1.00 0.00	H
ATOM	14	H	MOL	1.589	0.897	0.804	1.00 0.00	H
ATOM	15	H	MOL	-0.788	0.989	1.855	1.00 0.00	H
ATOM	16	H	MOL	0.393	-1.677	1.116	1.00 0.00	H
ATOM	17	H	MOL	-2.334	-0.309	0.638	1.00 0.00	H
ATOM	18	H	MOL	-1.743	-1.182	2.177	1.00 0.00	H
ATOM	19	H	MOL	2.180	2.206	-2.359	1.00 0.00	H
ATOM	20	O	MOL	-2.505	-3.861	0.007	1.00 0.00	O
ATOM	21	H	MOL	-3.347	-3.556	-0.372	1.00 0.00	H
ATOM	22	H	MOL	-2.084	-3.036	0.316	1.00 0.00	H
ATOM	23	O	MOL	-0.664	1.970	1.906	1.00 0.00	O1+
ATOM	24	H	MOL	-0.083	2.141	2.673	1.00 0.00	H
ATOM	25	H	MOL	-0.170	2.388	0.831	1.00 0.00	H1+