

Ultraviolet and Free Chlorine Aqueous-phase Advanced Oxidation Process: Kinetic Simulations and
Experimental Validation

Prepared for Environmental Science: Water Research & Technology

Supporting Information

7 Figures

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1 Text

Optimized structures and xyz-matrix

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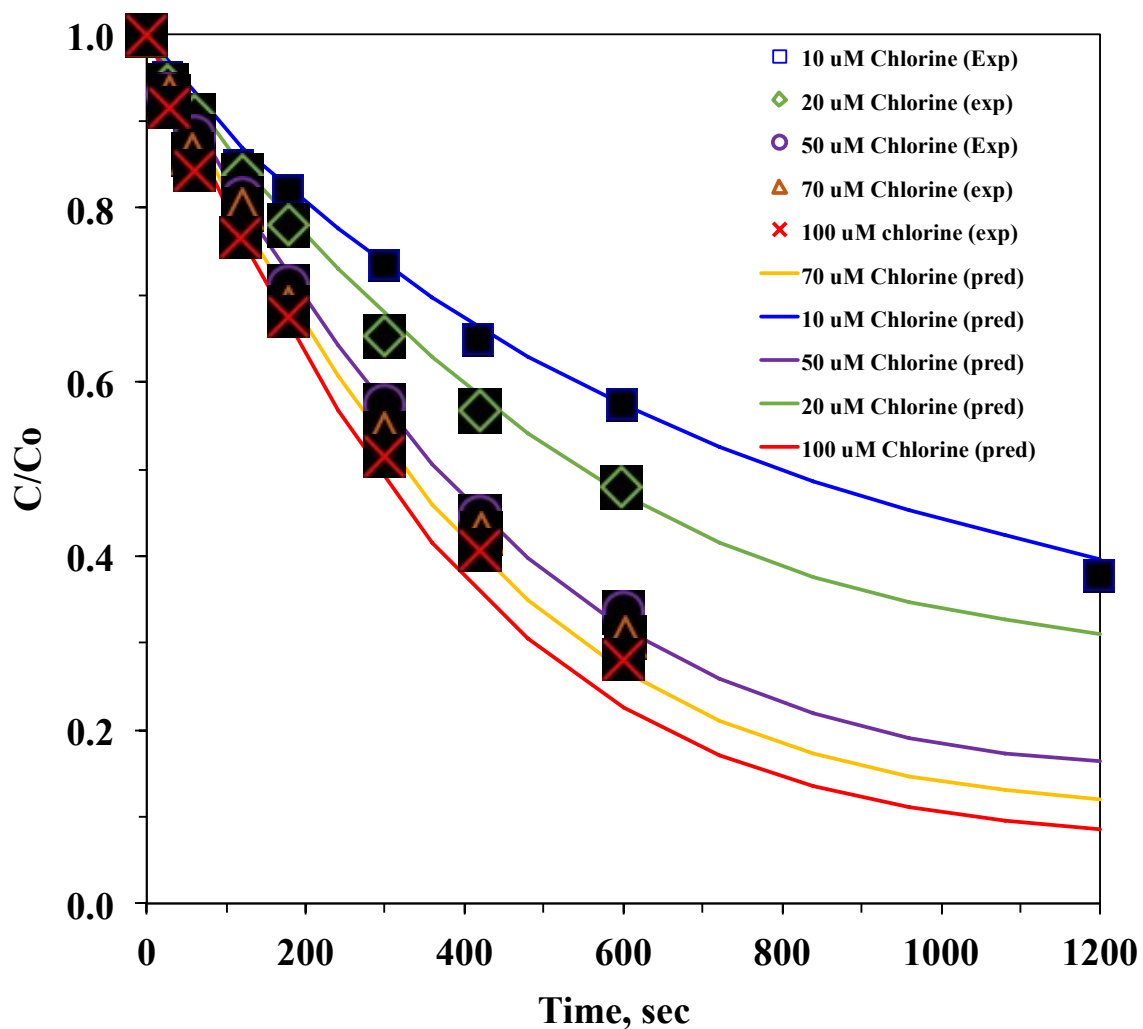


Figure S1: Experimental and predicted time-dependent concentration profiles of benzoic acid at various initial free chlorine concentrations. Experiments from Fang et al. (2014)

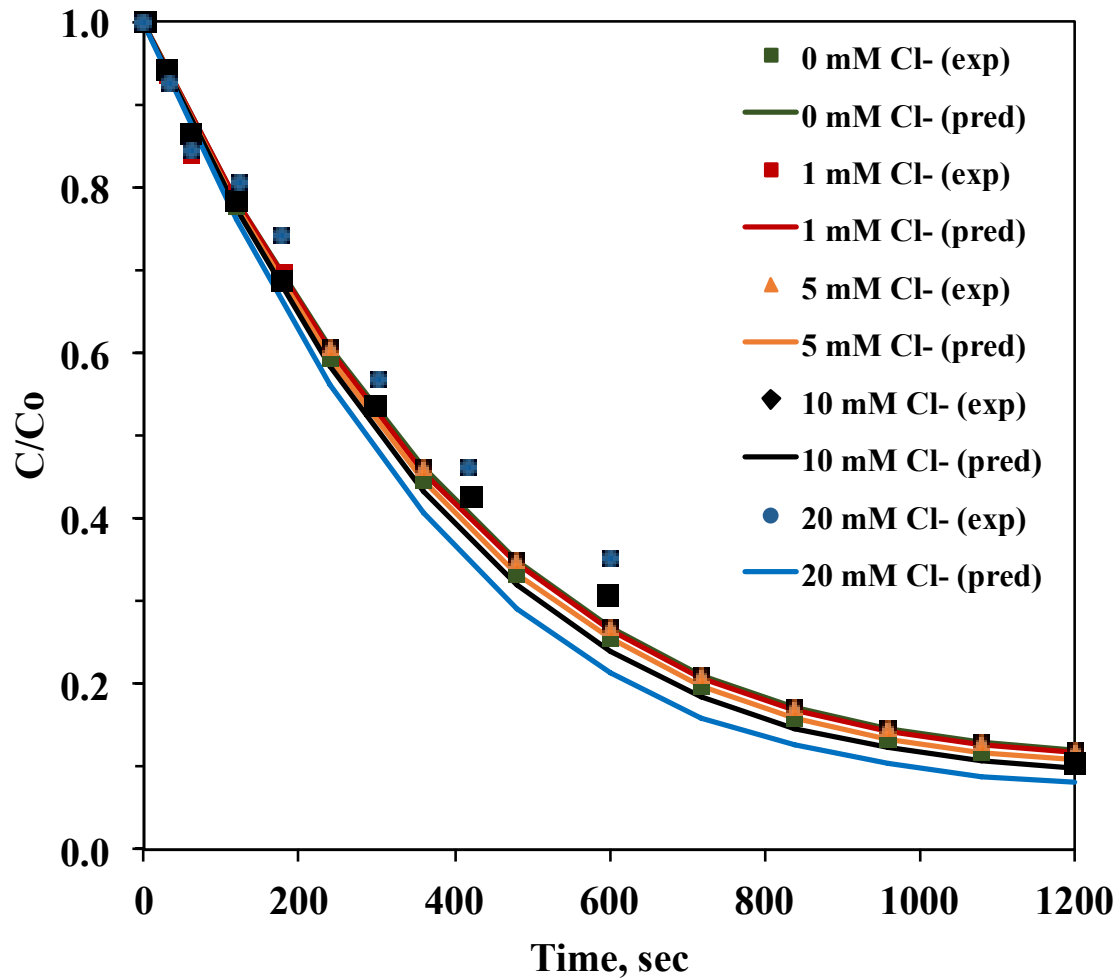


Figure S2: Experimental and predicted time-dependent concentration profiles of benzoic acid at various initial chloride concentrations. Experiments from Fang et al. (2014)

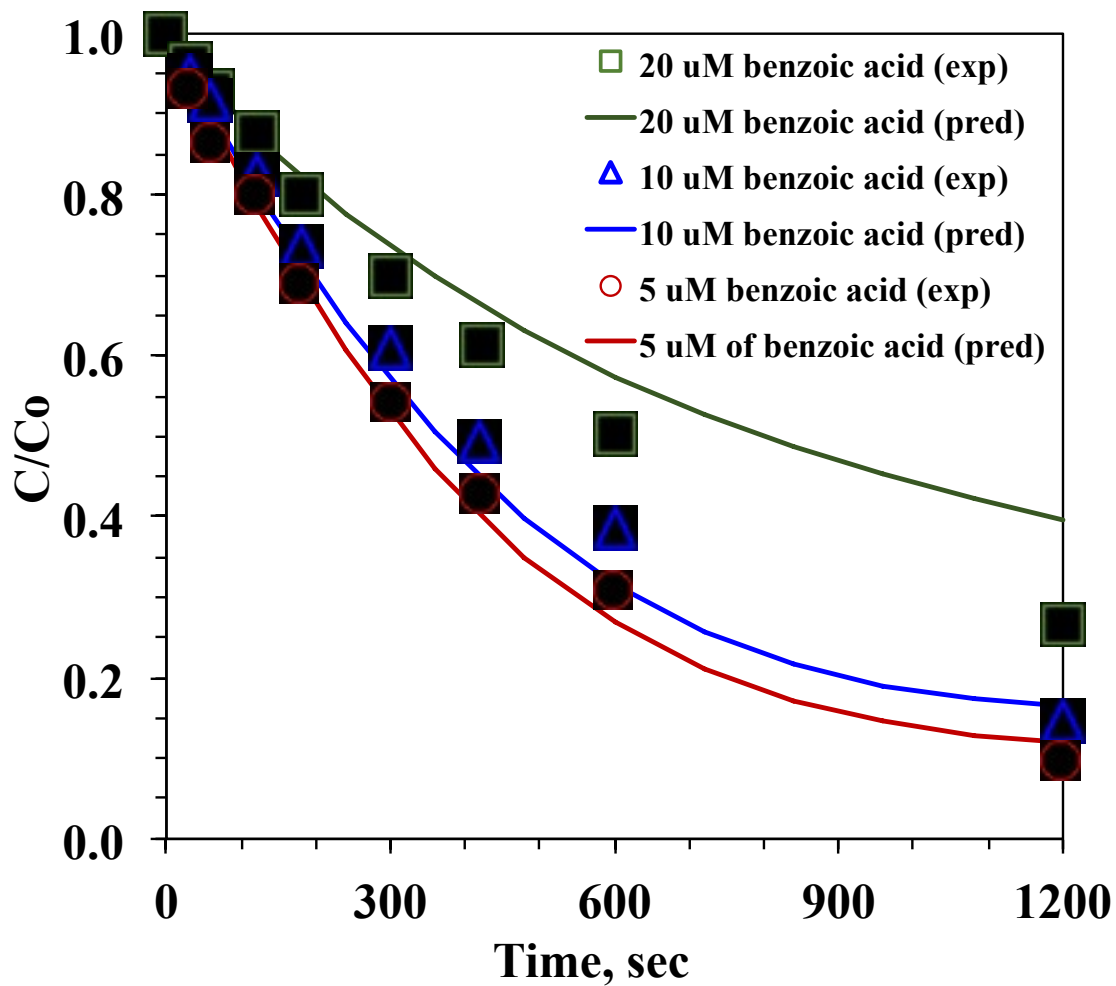


Figure S3: Experimental and predicted time-dependent concentration profiles of benzoic acid at various initial benzoic acid concentrations. Experiments from Fang et al. (2014)

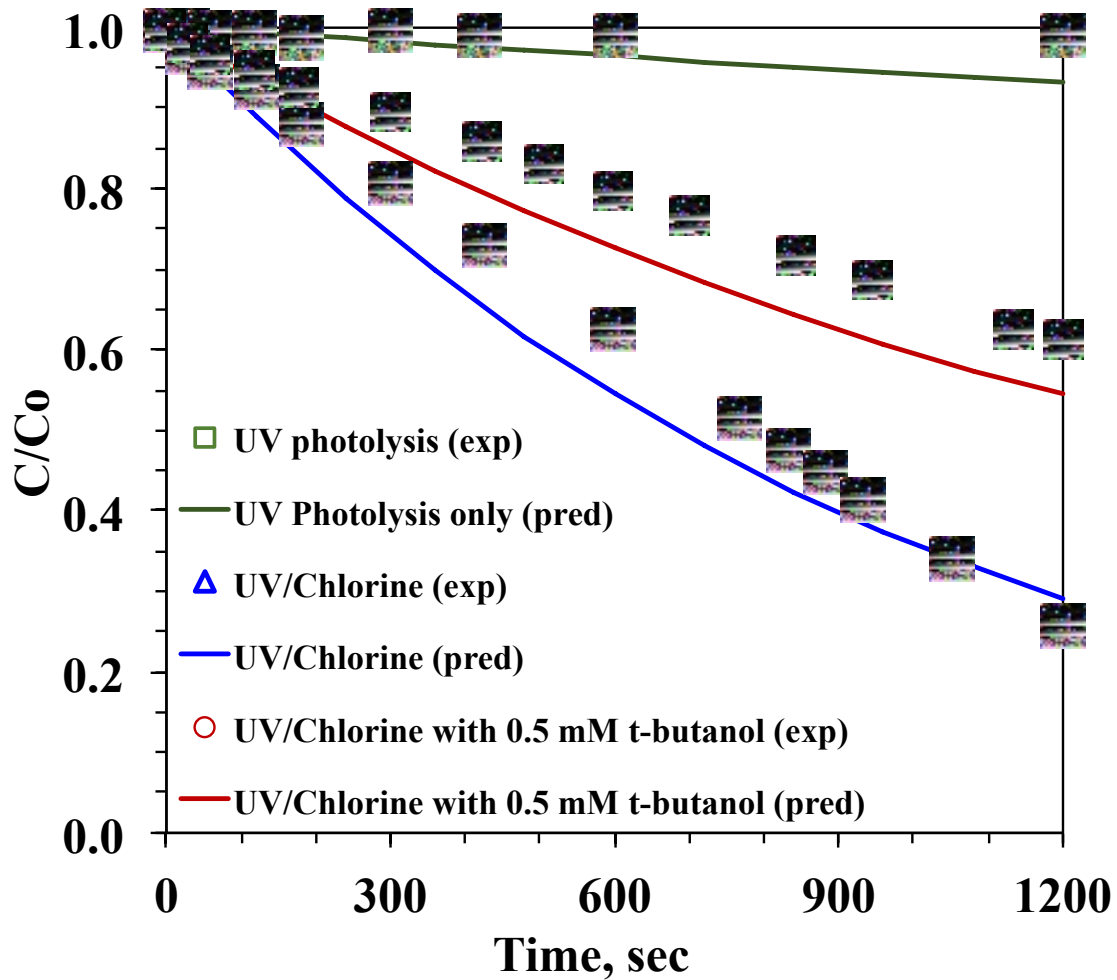


Figure S4: Experimental and predicted time-dependent concentration profiles of benzoic acid induced by photolysis and UV/free chlorine in the presence or absence of *tert*-butanol. Experiments from Fang et al. (2014)

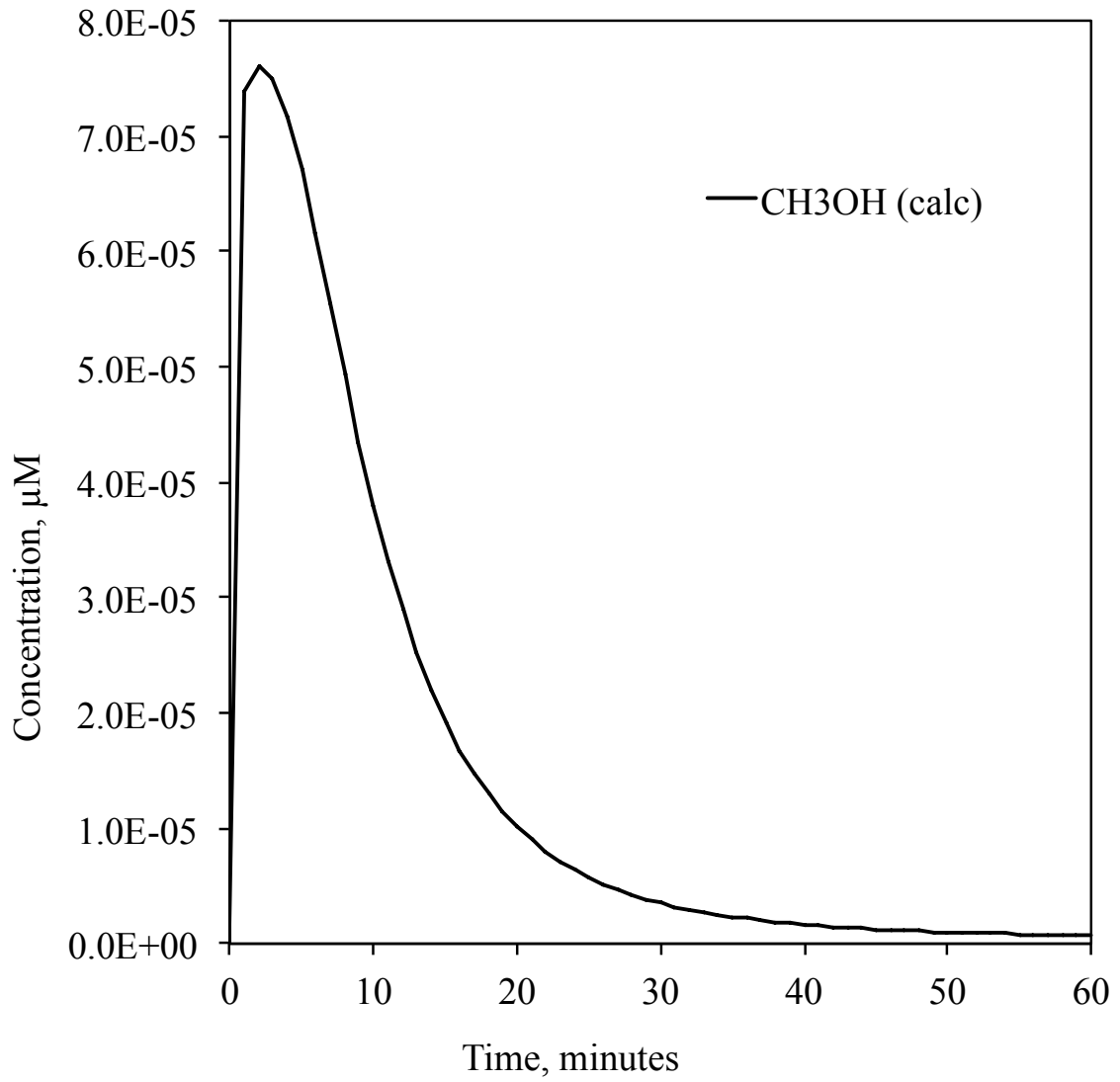


Figure S5: Predicted time-dependent concentration profile of CH₃OH

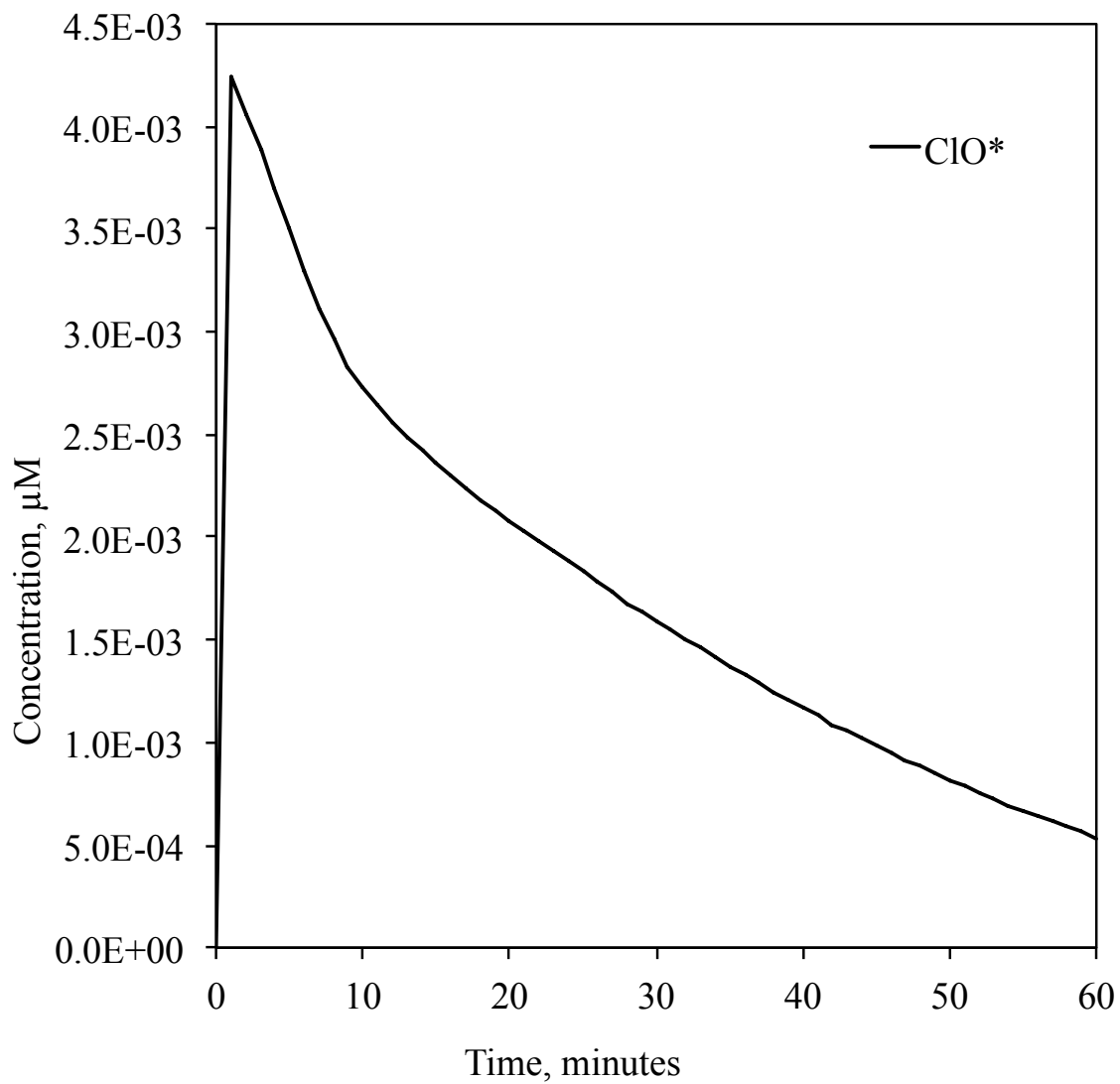


Figure S6: Predicted time-dependent concentration profile of ClO•

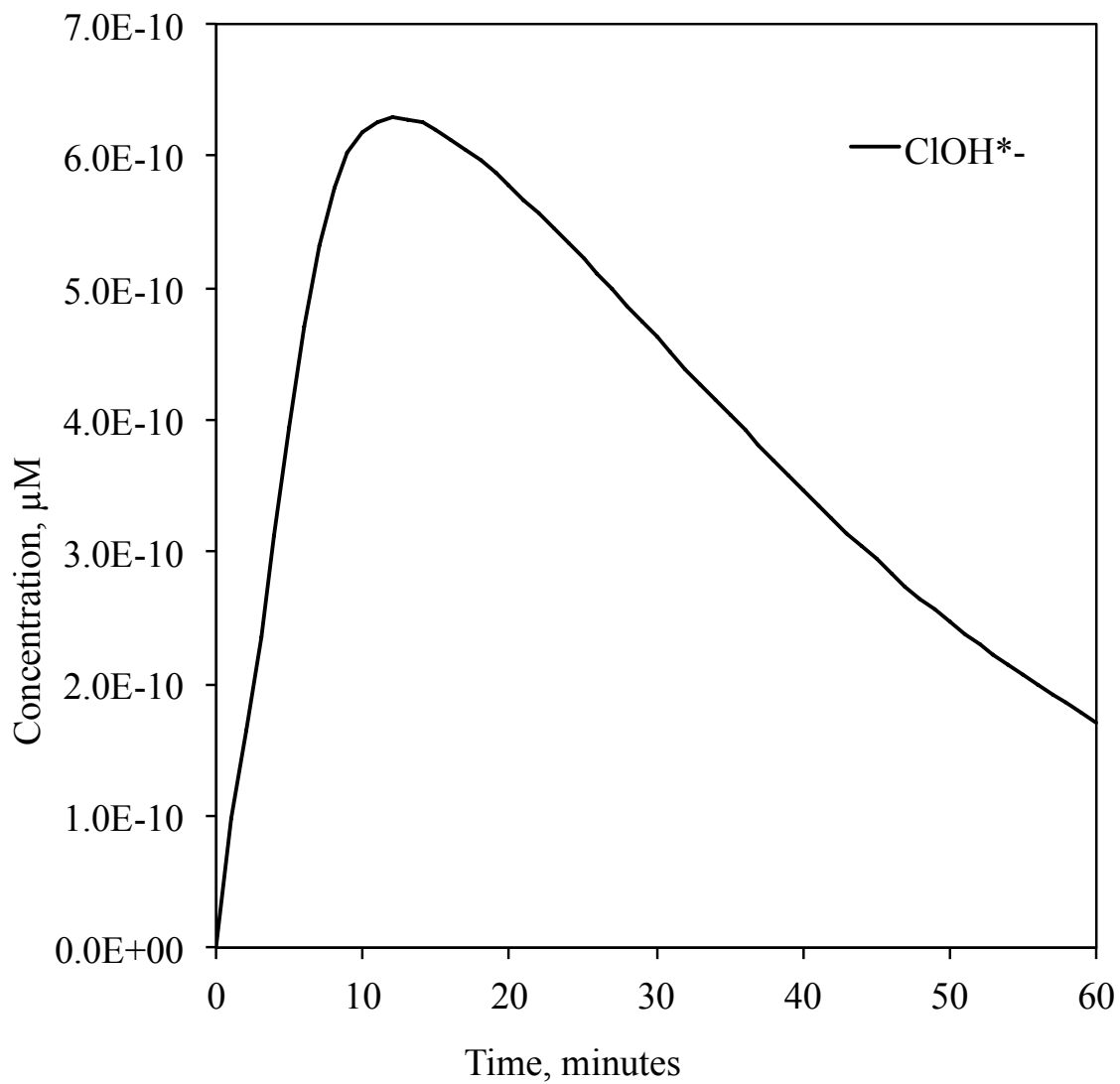


Figure S7: Predicted time-dependent concentration profile of ClOH*⁻

Table S1: Theoretically identified elementary reaction pathways and predicted reaction rate constants for Cl-derived radical reactions with organic compounds.

No.	Elementary reaction	$k_{\text{exp}}, \text{M}^{-1}\text{s}^{-1}$	References
0	$\text{HOC/OCI} + \text{UV} \rightarrow \text{HO}^{\bullet}/\text{O}^{\bullet} + \text{Cl}^{\bullet}$	$\epsilon=59/66 \text{ M}^{-1}\text{s}^{-1}, \Phi \approx 1.5$	
1	$\text{HOCl} + \text{Cl}^{\bullet} \rightarrow \bullet\text{OCl} + \text{HCl}$ $\text{HOCl} + \text{Cl}^{\bullet} \rightarrow \text{Cl}_2 + \text{HO}^{\bullet}$ $\text{HOCl} + \text{Cl}^{\bullet} \rightarrow \text{HOCl}(\text{Cl}^{\bullet})$	3×10^9	Kläning and Wolff, 1985
2	$\text{HOCl} + \text{HO}^{\bullet} \rightarrow \bullet\text{OCl} + \text{H}_2\text{O}$ $\text{HOCl} + \text{HO}^{\bullet} \rightarrow \text{HO}^{\bullet} + \text{HOCl}$ $\text{HOCl} + \text{HO}^{\bullet} \rightarrow \text{HOCl}(\text{HO}^{\bullet})$	$8.46 \times 10^4 - 2.0 \times 10^9$	Watt and Linden, 2007; Zuo <i>et al.</i> , 1997; Connick 1947
3	$\text{OCl} + \text{Cl}^{\bullet} \rightarrow \bullet\text{OCl} + \text{Cl}^{\bullet}$	8.2×10^9	Klaning and Wolff, 1985
4	$\text{OCl} + \text{HO}^{\bullet} \rightarrow \bullet\text{OCl} + \text{HO}^{\bullet}$	8.8×10^9	Buxton and Subhani, 1972
5	$\text{Cl}^{\bullet} + \text{Cl}^{\bullet} \rightarrow \text{Cl}_2^{\bullet}$	$6.5-8.5 \times 10^9$	Yu and Barker, 2003; Klaning and Wolff, 1985
6	$\text{Cl}^{\bullet} + \text{Cl}_2 \rightarrow \text{Cl}_3^{\bullet}$	2.0×10^4	Ershov, 2004
7	$\text{Cl}_2^{\bullet} \rightarrow \text{Cl}^{\bullet} + \text{Cl}^{\bullet}$	$5.2 \times 10^4 - 1.4 \times 10^5$	Yu and Barker, 2003; Jayson <i>et al.</i> , 1973
8	$\text{Cl}^{\bullet} + \text{Cl}_2^{\bullet} \rightarrow \text{Cl}_2 + \text{Cl}^{\bullet}$	$(2.1 \pm 0.05) \times 10^9$	Yu and Barker, 2004
9	$\text{Cl}_2^{\bullet} + \text{Cl}_2^{\bullet} \rightarrow \text{Cl}_2 + 2\text{Cl}^{\bullet} \text{ (or } \text{Cl}_3^{\bullet} + \text{Cl}^{\bullet})$	$(0.9-9.0) \times 10^9$	Yu and Barker, 2003; Navaratnam <i>et al.</i> , 1980; Woods <i>et al.</i> , 1975
10	$\text{Cl}_2^{\bullet} + \text{HO}^{\bullet} \rightarrow \text{HOCl} + \text{Cl}^{\bullet}$	1×10^9	Ross <i>et al.</i> , 1998
11	$\text{Cl}_3^{\bullet} \rightarrow \text{Cl}_2 + \text{Cl}^{\bullet}$	1.1×10^5	Ershov, 2004
12	$\text{HO}^{\bullet} + \text{Cl}^{\bullet} \rightarrow \bullet\text{OHCl}$	$(4.3 \pm 0.4) \times 10^9$	Ross <i>et al.</i> , 1998
13	$\text{Cl}^{\bullet} + \text{H}_2\text{O} \rightarrow \bullet\text{OHCl} + \text{H}^{\bullet}$	$(1.6 \pm 0.2) \times 10^5$	Jayson <i>et al.</i> , 1973
14	$\text{Cl}^{\bullet} + \text{OH}^{\bullet} \rightarrow \bullet\text{OHCl}$	1.8×10^{10}	Klaning and Wolff, 1985
15	$\text{Cl}_2^{\bullet} + \text{OH}^{\bullet} \rightarrow \bullet\text{OHCl} + \text{Cl}^{\bullet}$	4.5×10^7	Grigor'ev <i>et al.</i> , 1987
16	$\bullet\text{OHCl} \rightarrow \text{HO}^{\bullet} + \text{Cl}^{\bullet}$	$(6.1 \pm 0.8) \times 10^9$	Jayson <i>et al.</i> , 1973
17	$\bullet\text{OHCl} + \text{H}^{\bullet} \rightarrow \text{Cl}^{\bullet} + \text{H}_2\text{O}$	$(2.6 \pm 0.6) \times 10^{10}$	Jayson <i>et al.</i> , 1973
18	$\bullet\text{OHCl} + \text{Cl}^{\bullet} \rightarrow \text{Cl}_2^{\bullet} + \text{OH}^{\bullet}$	1.0×10^5	Grigor'ev <i>et al.</i> , 1987
19	$\text{Cl}^{\bullet} + \text{H}_2\text{O} \rightarrow \bullet\text{Cl}(\text{H}_2\text{O})$	2.5×10^5	McElroy, 1990
20	$\text{Cl}_2^{\bullet} + \text{H}_2\text{O} \rightarrow \bullet\text{Cl}(\text{H}_2\text{O}) + \text{Cl}^{\bullet}$	1.3×10^3	McElroy, 1990
21	$\bullet\text{Cl}(\text{H}_2\text{O}) + \text{Cl}^{\bullet} \rightarrow \text{Cl}_2^{\bullet} + \text{H}_2\text{O}$	5×10^9	McElroy, 1990
22	$\bullet\text{OCl} + \bullet\text{OCl} + \text{H}_2\text{O} \rightarrow \text{HClO} + \text{HClO}_2$	$2.5 - 7.5 \times 10^9$	Buxton and Subhani, 1972; Kläning and Wolff 1985
23	$\text{HO}^{\bullet} + \text{ClO}_2^{\bullet} \rightarrow \text{ClO}_2^{\bullet} + \text{OH}^{\bullet}$	1.0×10^9	Stanford <i>et al.</i> , 2011
24	$\text{HO}^{\bullet} + \text{ClO}_2^{\bullet} \rightarrow \text{ClO}_3^{\bullet} + \text{H}^{\bullet}$	4.0×10^9	Stanford <i>et al.</i> , 2011
25	$\text{ClO}^{\bullet} + \text{ClO}_2^{\bullet} \rightarrow \text{ClO}^{\bullet} + \text{ClO}_2^{\bullet}$	9.4×10^8	Stanford <i>et al.</i> , 2011
26	$\text{O}^{\bullet} + \text{H}_2\text{O} \rightarrow \text{HO}^{\bullet} + \text{OH}^{\bullet}$	1.8×10^6	Buxton <i>et al.</i> , 1988
27	$\text{HO}^{\bullet} + \text{OH}^{\bullet} \rightarrow \text{O}^{\bullet} + \text{H}_2\text{O}$	1.3×10^{10}	Buxton <i>et al.</i> , 1988
28	$\text{HO}_2^{\bullet} + \text{Cl}_2^{\bullet} \rightarrow 2\text{Cl}^{\bullet} + \text{H}^{\bullet} + \text{O}_2$	3.0×10^9	Neta <i>et al.</i> , 1988
29	$\text{O}_2^{\bullet} + \text{Cl}_2^{\bullet} \rightarrow 2\text{Cl}^{\bullet} + \text{H}^{\bullet} + \text{O}_2$	2.0×10^8	Stanford <i>et al.</i> , 2011
30	$\text{H}_2\text{O}_2 + \text{Cl}_2^{\bullet} \rightarrow \text{HO}_2^{\bullet} + \text{H}^{\bullet} + 2\text{Cl}^{\bullet}$	1.4×10^5	Stanford <i>et al.</i> , 2011
31	$\text{Cl}^{\bullet} + \text{Cl}^{\bullet} \rightarrow \text{Cl}_2 + \text{Cl}^{\bullet}$	8.8×10^7	Wu <i>et al.</i> , 1980

Text S1: Example of how to calculate the sample deviation for free chlorine in equation (1)

Time, min	Exp	Calc	Diff
0	148.7676	149	2.44025E-06
2	106.5141	99.3	0.004587207
5	100.3521	85.7	0.021318049
8	77.46479	76.3	0.000226092
11	62.5	68.2	0.00831744
15	44.01408	58.6	0.109820658
18	28.16901	52.1	0.721735203
22	31.69014	44.2	0.155831949
26	23.76761	37.3	0.324174184
30	22.88732	31.3	0.135107139
36	20.42254	23.8	0.027350316
40	15.49296	19.7	0.073736934
45	11.26761	15.4	0.134505563
56	5.633803	8.91	0.338171326
60	2.957746	7.26	2.115778041
			4.17066254
			0.545806254

Reference

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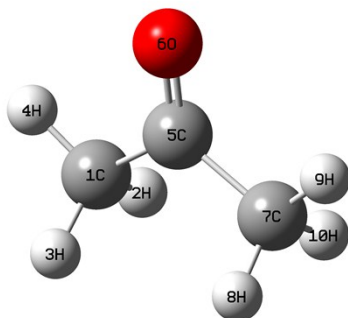
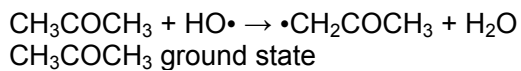
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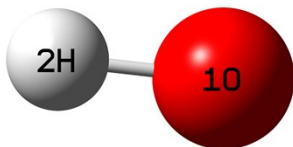
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Aqueous-phase optimized electronic structures and xyz-coordinate



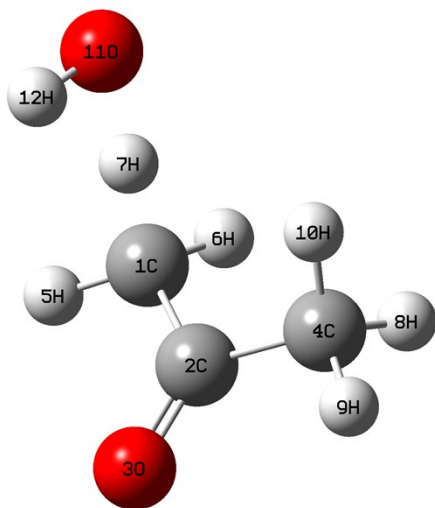
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HO• radical



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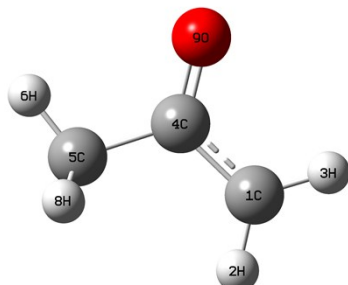
Transition state



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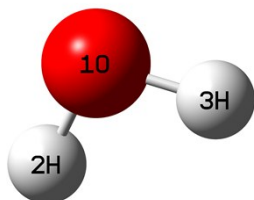
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•CH₂COCH₃ ground state



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5	No	Show	5	C	4	1	2	1.5120062	118.0496378	0.0485394
6	No	Show	6	H	5	4	1	1.0910809	110.2735572	-179.4130436
7	No	Show	7	H	5	4	1	1.0953107	110.2606421	-58.2316960
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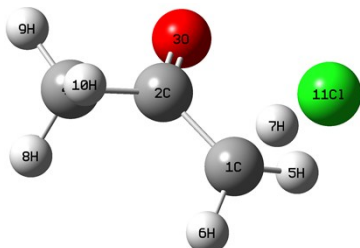
H₂O ground state



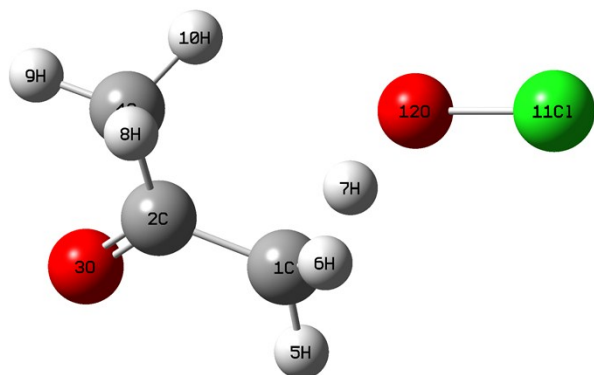
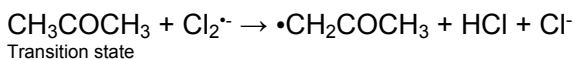
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CH₃COCH₃ + Cl• → •CH₂COCH₃ + HCl

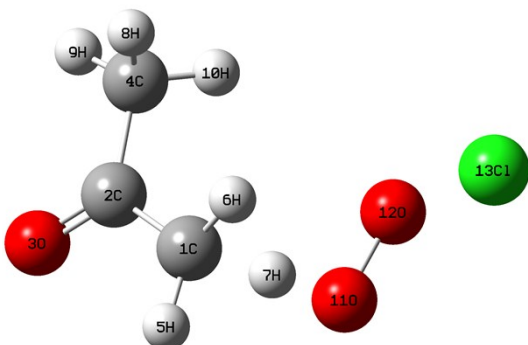
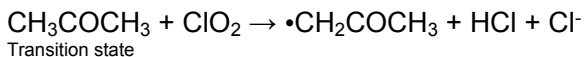
Transition state



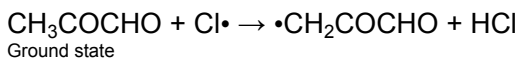
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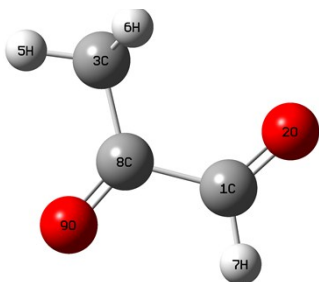


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9	No	Show	9	H	4	2	1	1.0906120	110.6738708	174.1459500
10	No	Show	10	H	4	2	1	1.0953423	109.4901022	52.2714783
11	No	Show	11	Cl	1	2	3	3.4500711	126.9744052	123.4153680
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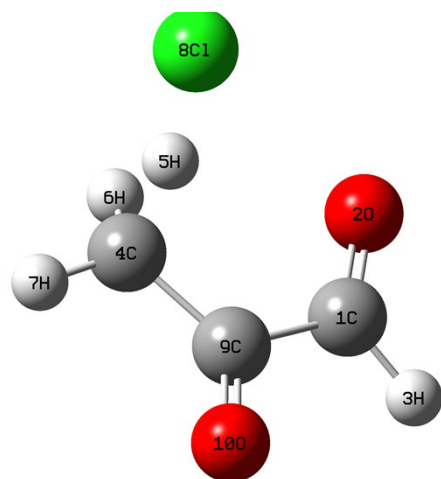
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5	No	Show	5	H	1	2	3	1.0888132	116.0666135	-8.6630372
6	No	Show	6	H	1	2	3	1.0891755	117.6656112	-153.0135663
7	No	Show	7	H	1	2	3	1.3971333	102.3070063	99.3597324
8	No	Show	8	H	4	2	1	1.0956959	109.7454952	-63.0752073
9	No	Show	9	H	4	2	1	1.0907248	110.5973957	175.7504626
10	No	Show	10	H	4	2	1	1.0956455	109.6765284	54.1146157
11	No	Show	11	O	1	2	3	2.5618253	104.2250423	99.2350533
12	No	Show	12	O	11	1	2	1.3310660	108.4375663	67.8803796
13	No	Show	13	Cl	12	11	1	1.8080605	112.1927459	87.6526648



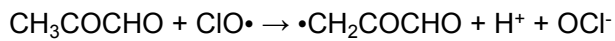


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	O	1			1.2071474		
3	No	Show	3	C	1			2.5874140	92.3332719	
4	No	Show	4	H	3	1	2	1.0957020	91.4184658	53.3377767
5	No	Show	5	H	3	1	2	1.0901642	142.2152429	-179.9662180
6	No	Show	6	H	3	1	2	1.0956938	91.3956931	-53.2999666
7	No	Show	7	H	1	2	3	1.1064189	123.3294393	179.9816565
8	No	Show	8	C	3	1	2	1.4949906	31.7476463	179.9909602
9	No	Show	9	O	8	3	1	1.2152663	125.4641816	179.9887314

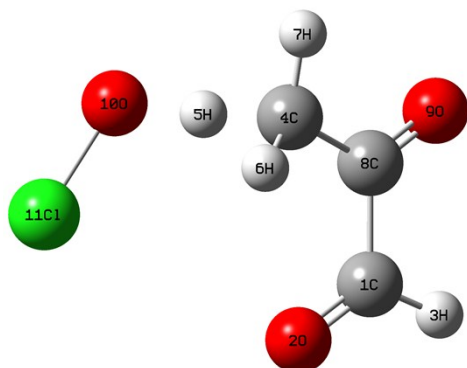
Transition state



Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	O	1			1.2044962		
3	No	Show	3	H	1	2		1.1036864	124.0648387	
4	No	Show	4	C	1	2	3	2.5638424	91.6556191	-175.4056202
5	No	Show	5	H	4	1	2	1.3580391	95.4824933	-63.9422265
6	No	Show	6	H	4	1	2	1.0881018	87.6994208	36.1862860
7	No	Show	7	H	4	1	2	1.0880949	146.9961710	175.2175643
8	No	Show	8	Cl	4	1	2	2.8582720	100.2780589	-61.7705791
9	No	Show	9	C	4	1	2	1.4717942	32.1815981	-168.6917444
10	No	Show	10	O	9	4	1	1.2173305	123.7001339	179.5935258

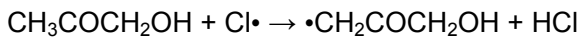


Transition state

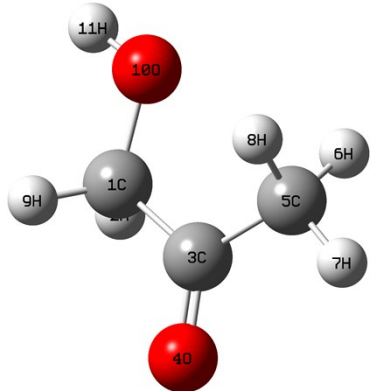


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
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1	No	Show	1	C				1.2058668		
2	No	Show	2	O	1			1.1047674	123.6107018	
3	No	Show	3	H	1	2		2.5680167	92.3875230	-176.3243589
4	No	Show	4	C	1	2	3	1.2982474	96.6316892	-64.7580768
5	No	Show	5	H	4	1	2	1.0891636	87.6468253	36.5857978
6	No	Show	6	H	4	1	2	1.0889222	145.5259208	170.8932298
7	No	Show	7	H	4	1	2	1.4724645	32.0182779	-170.8110567
8	No	Show	8	C	4	1	2	1.2185596	124.3982033	178.7858203
9	No	Show	9	O	8	4	1	2.5300579	100.6815303	-62.8515301
10	No	Show	10	O	4	1	2	1.6620970	110.1160977	57.9313186
11	No	Show	11	Cl	10	4	1			

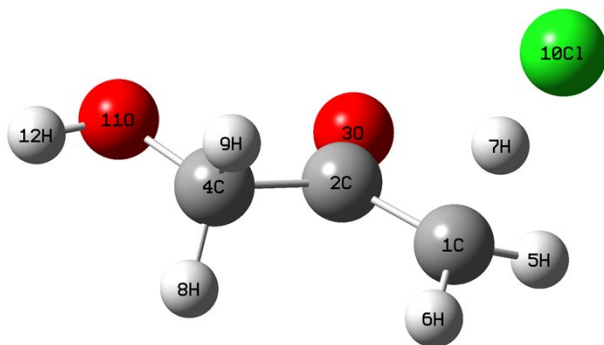


Ground state

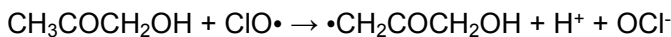


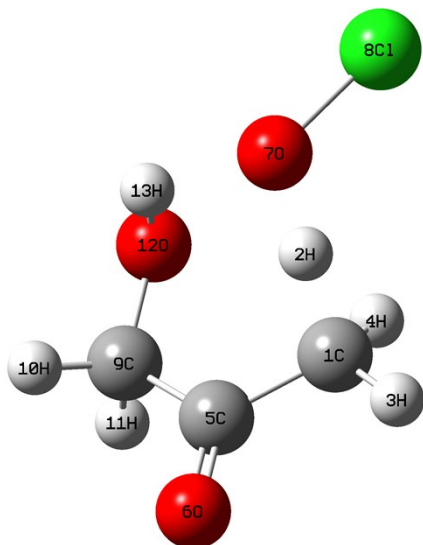
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	H	1			1.0999082		
3	No	Show	3	C	1	2		1.5198853	107.0559572	
4	No	Show	4	O	3	1	2	1.2194913	118.7760540	-57.2512248
5	No	Show	5	C	3	1	4	1.5021887	118.2911194	179.9993900
6	No	Show	6	H	5	3	1	1.0953385	109.8038585	-58.3424055
7	No	Show	7	H	5	3	1	1.0906721	110.2595416	179.9969323
8	No	Show	8	H	5	3	1	1.0953355	109.8052399	58.3339992
9	No	Show	9	H	1	3	4	1.0999076	107.0562747	57.2473281
10	No	Show	10	O	1	3	4	1.4161665	111.4175672	179.9982494
11	No	Show	11	H	10	1	3	0.9637464	107.4395814	180.0000000

Transition state

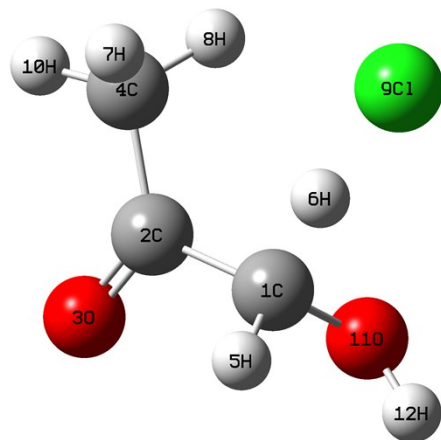
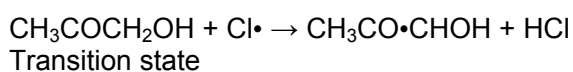


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	C	1			1.4809509		
3	No	Show	3	O	2	1		1.2202881	120.9751120	
4	No	Show	4	C	2	1	3	1.5107412	116.1089234	179.0632435
5	No	Show	5	H	1	2	3	1.0884060	115.7929518	-11.5335709
6	No	Show	6	H	1	2	3	1.0888983	117.8959595	-156.1149923
7	No	Show	7	H	1	2	3	1.3915837	102.5821070	95.4950499
8	No	Show	8	H	4	2	1	1.1005297	107.8640306	-59.2435720
9	No	Show	9	H	4	2	1	1.1029870	107.1778664	55.0957685
10	No	Show	10	Cl	1	2	3	2.8727194	106.6063191	95.5305258
11	No	Show	11	O	4	2	1	1.4094135	109.5547604	177.8849211
12	No	Show	12	H	11	4	2	0.9641291	107.2874429	171.4183436

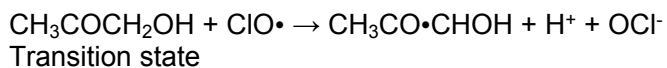


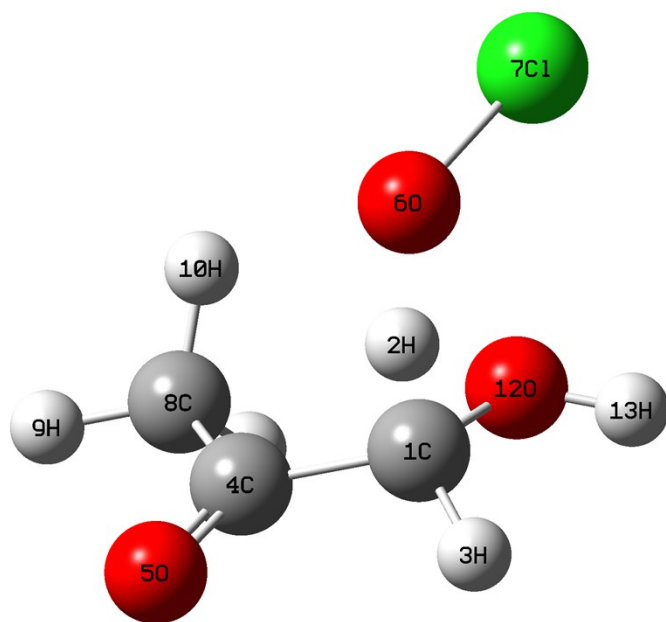


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	H	1			1.2960016		
3	No	Show	3	H	1	2		1.0893902	104.9071877	
4	No	Show	4	H	1	3	2	1.0905826	115.1020054	109.9779076
5	No	Show	5	C	1	3	4	1.4846121	114.5345544	137.2112456
6	No	Show	6	O	5	1	3	1.2208114	121.0465022	0.6354825
7	No	Show	7	O	1	5	6	2.5383027	103.1095010	-115.6859323
8	No	Show	8	Cl	7	1	5	1.6677734	108.8995680	-154.0298585
9	No	Show	9	C	5	1	6	1.5239724	118.2930417	-179.2243160
10	No	Show	10	H	9	5	1	1.0978534	107.5275222	-137.3514585
11	No	Show	11	H	9	5	1	1.0962453	107.1545814	107.5881674
12	No	Show	12	O	9	5	1	1.4131478	114.4915298	-11.3985906
13	No	Show	13	H	12	9	5	0.9664433	107.9571350	-67.3828713

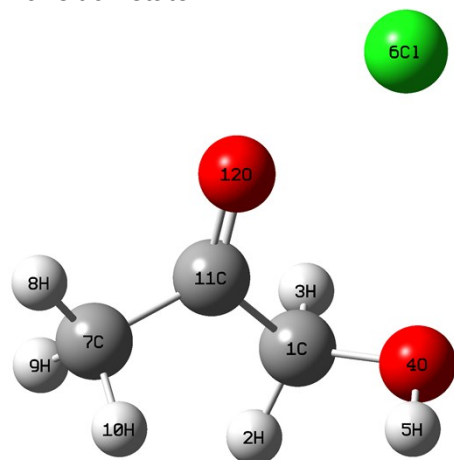
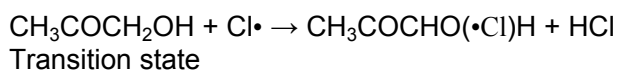


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	C	1			1.5524393		
3	No	Show	3	O	2	1		1.2102629	115.2992491	
4	No	Show	4	C	2	1	3	1.4896255	119.5025395	179.6493414
5	No	Show	5	H	1	2	3	1.0952385	111.4565424	-58.1006154
6	No	Show	6	H	1	2	3	1.2229507	107.4691270	-170.9116829
7	No	Show	7	H	4	2	1	1.0960725	109.2202828	-58.6576913
8	No	Show	8	H	4	2	1	1.0960944	109.2693440	57.6559427
9	No	Show	9	Cl	1	2	3	2.9337648	112.3642169	-169.3782732
10	No	Show	10	H	4	2	1	1.0902014	110.6643508	179.6764265
11	No	Show	11	O	1	2	3	1.3715206	110.5512973	69.9393235
12	No	Show	12	H	11	1	2	0.9683559	109.4038551	-147.2517538

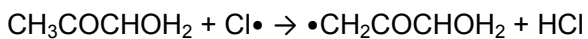




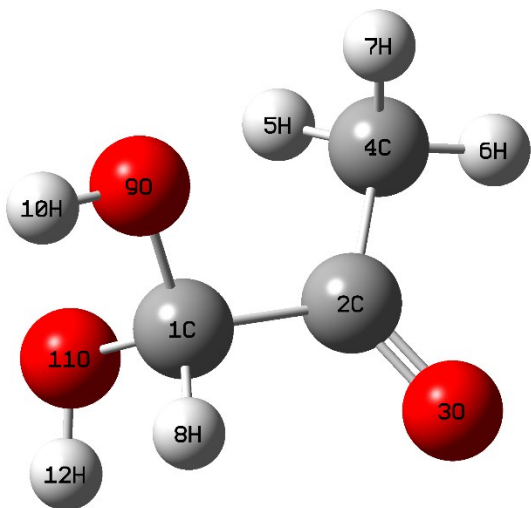
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	H	1			1.2055298		
3	No	Show	3	H	1	2		1.0944450	103.8670159	
4	No	Show	4	C	1	3	2	1.5128741	112.6511728 -109.9087370	
5	No	Show	5	O	4	1	3	1.2176594	118.5555005 31.3741410	
6	No	Show	6	O	1	4	5	2.6207610	106.5692265 -84.2076422	
7	No	Show	7	Cl	6	1	4	1.6494860	100.9406016 -122.7237043	
8	No	Show	8	C	4	1	5	1.5007202	117.6395817 178.3675238	
9	No	Show	9	H	8	4	1	1.0904236	109.9892745 -174.7031600	
10	No	Show	10	H	8	4	1	1.0951456	109.9378230 -52.9508570	
11	No	Show	11	H	8	4	1	1.0952637	109.5619037 64.1759180	
12	No	Show	12	O	1	4	5	1.3826189	113.5995058 163.7469078	
13	No	Show	13	H	12	1	4	0.9670004	109.1048815 -157.8015778	



Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	H	1			1.0937928		
3	No	Show	3	H	1	2		1.0943369	109.4169072	
4	No	Show	4	O	1	2	3	1.4112631	112.0827960 -119.8065816	
5	No	Show	5	H	4	1	2	0.9660565	107.6712761 -46.8034607	
6	No	Show	6	Cl	4	1	2	3.3691808	79.4678128 173.6128195	
7	No	Show	7	C	1	4	5	2.5957892	124.1861384 43.7599519	
8	No	Show	8	H	7	1	4	1.0892037	143.2945474 75.1972931	
9	No	Show	9	H	7	1	4	1.0968353	89.4665234 -159.2069616	
10	No	Show	10	H	7	1	4	1.0960709	90.5081334 -52.3062855	
11	No	Show	11	C	7	1	4	1.4973930	31.6752214 73.6339618	
12	No	Show	12	O	11	7	1	1.2206514	120.3627423 -179.4614512	

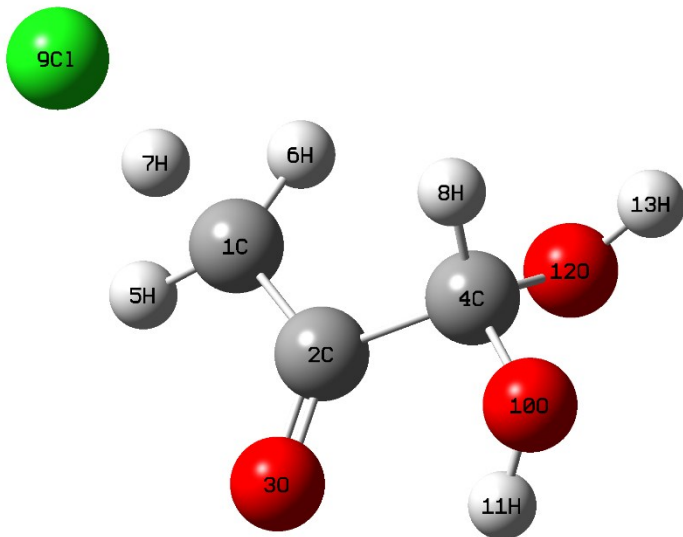


Ground state



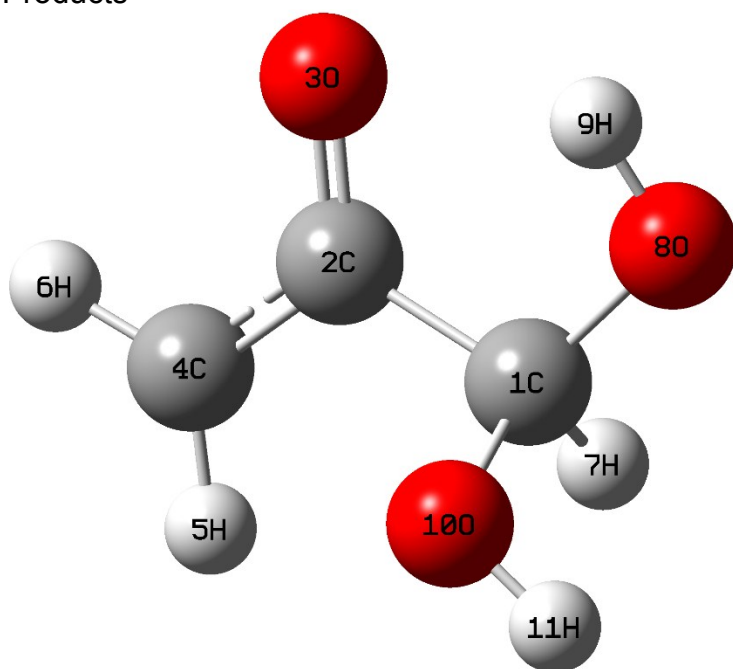
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	C	1			1.5372308		
3	No	Show	3	O	2	1		1.2169041	119.3796958	
4	No	Show	4	C	2	1	3	1.5025186	117.0097781	177.3762320
5	No	Show	5	H	4	2	1	1.0943054	109.9600895	-48.9936505
6	No	Show	6	H	4	2	1	1.0907081	110.4020327	-170.9891624
7	No	Show	7	H	4	2	1	1.0950939	109.3508328	68.1891661
8	No	Show	8	H	1	2	3	1.0967943	108.8915545	14.7097772
9	No	Show	9	O	1	2	3	1.3985976	108.1562539	137.0727264
10	No	Show	10	H	9	1	2	0.9665322	107.7744458	-171.0908489
11	No	Show	11	O	1	9	2	1.4193944	109.0013478	-117.2647568
12	No	Show	12	H	11	1	9	0.9657593	107.9606779	-152.1043653

Transition state

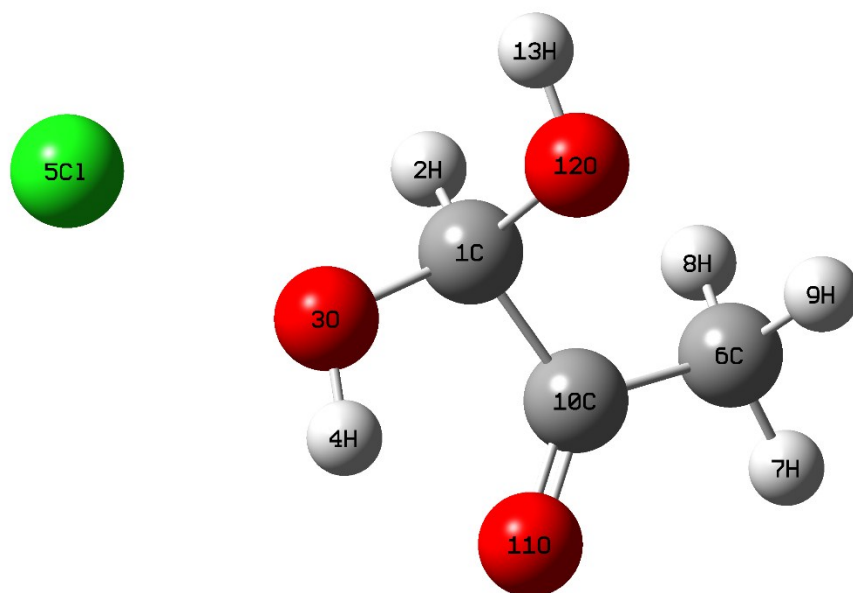
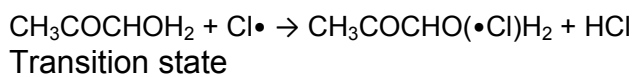


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	C	1			1.4773311		
3	No	Show	3	O	2	1		1.2185139	121.8625255	
4	No	Show	4	C	2	1	3	1.5375227	117.5759716	178.3645825
5	No	Show	5	H	1	2	3	1.0883165	115.6995690	-10.1373675
6	No	Show	6	H	1	2	3	1.0877748	117.2736714	-154.1150007
7	No	Show	7	H	1	2	3	1.3604169	102.6531313	97.9308943
8	No	Show	8	H	4	2	1	1.0967060	109.3367924	54.7128246
9	No	Show	9	Cl	1	2	3	2.8590429	106.9220858	97.9749813
10	No	Show	10	O	4	2	1	1.3992415	110.8201965	172.6684237
11	No	Show	11	H	10	4	2	0.9696612	107.1970356	33.2189508
12	No	Show	12	O	4	2	1	1.4120553	105.3525496	-64.2144081
13	No	Show	13	H	12	4	2	0.9657757	107.5713113	160.7230676

Products



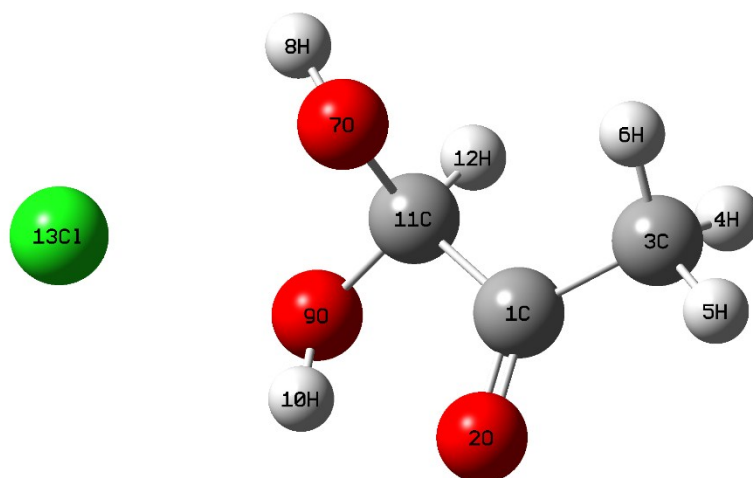
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	C	1			1.5390112		
3	No	Show	3	O	2	1		1.2404813	118.6256284	
4	No	Show	4	C	2	1	3	1.4217049	118.3704230 -179.0822915	
5	No	Show	5	H	4	2	1	1.0834264	121.0599510 -1.6595822	
6	No	Show	6	H	4	2	1	1.0842258	119.3980742 178.7460146	
7	No	Show	7	H	1	2	3	1.0962448	110.5426297 -129.5260938	
8	No	Show	8	O	1	2	3	1.4017587	109.9242452 -10.7370937	
9	No	Show	9	H	8	1	2	0.9722811	105.7321391 22.6206057	
10	No	Show	10	O	1	8	2	1.4146002	113.0793205 -117.5636347	
11	No	Show	11	H	10	1	8	0.9656473	107.4824552 -75.9160448	



Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	H	1			1.0947644		
3	No	Show	3	O	1	2		1.4037432	107.8743063	
4	No	Show	4	H	3	1	2	0.9738441	109.5418843 138.3790969	

5	No	Show	5	Cl	3	1	2	2.4466260	128.3223618	-44.1013804
6	No	Show	6	C	1	3	4	2.5919055	139.3622578	22.0207217
7	No	Show	7	H	6	1	3	1.0905728	142.3731468	4.2791255
8	No	Show	8	H	6	1	3	1.0949526	88.6969946	127.2794651
9	No	Show	9	H	6	1	3	1.0951749	93.7865985	-125.8398307
10	No	Show	10	C	6	1	3	1.4958556	32.2639454	-5.3724560
11	No	Show	11	O	10	6	1	1.2147047	124.4219221	-178.8864555
12	No	Show	12	O	1	3	10	1.4048754	112.7925397	-117.7350005
13	No	Show	13	H	12	1	3	0.9653943	108.0891053	-84.8984674

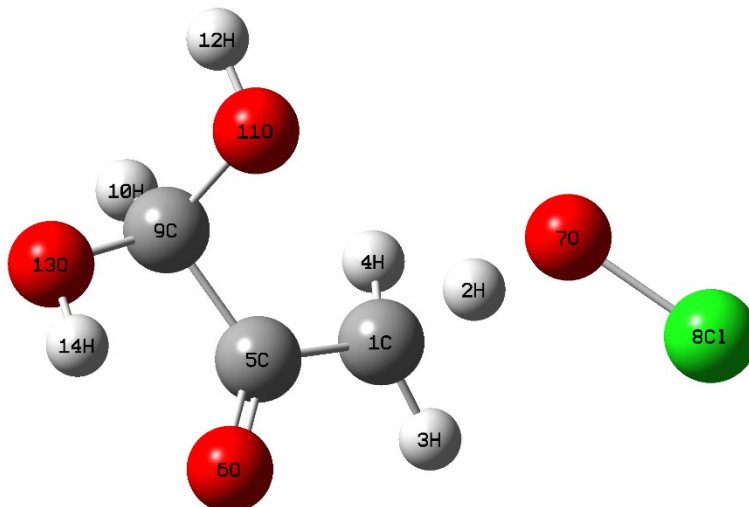
Products



Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	O	1			1.2141803		
3	No	Show	3	C	1	2		1.4934756	124.9702572	
4	No	Show	4	H	3	1	2	1.0968677	108.6686115	114.8864670
5	No	Show	5	H	3	1	2	1.0904488	110.6799238	-5.8936618
6	No	Show	6	H	3	1	2	1.0943483	109.8814325	-128.5350649
7	No	Show	7	O	1	2	3	2.3442788	119.4773734	-138.1587206
8	No	Show	8	H	7	1	2	0.9666710	145.1463212	-125.7119670
9	No	Show	9	O	7	1	2	2.3607874	61.3768866	-64.5954024
10	No	Show	10	H	9	7	1	0.9773729	100.2448524	64.3328896
11	No	Show	11	C	7	1	2	1.4007040	39.6061520	-98.3136385
12	No	Show	12	H	11	7	1	1.0930488	111.8398015	-121.9680967
13	No	Show	13	Cl	9	7	1	2.4563556	85.2329966	160.6434317

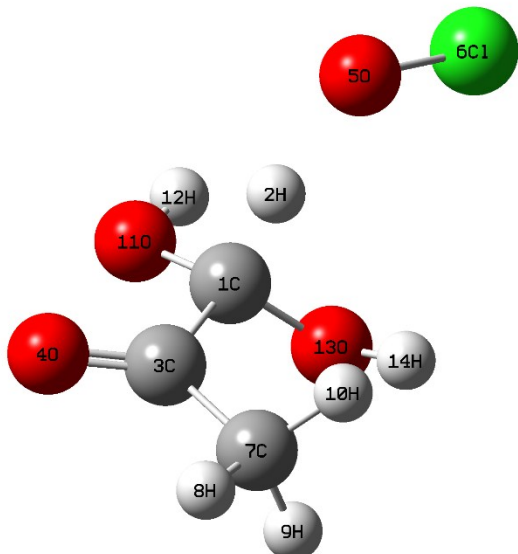
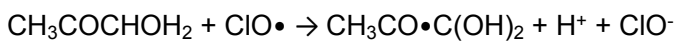


Transition state

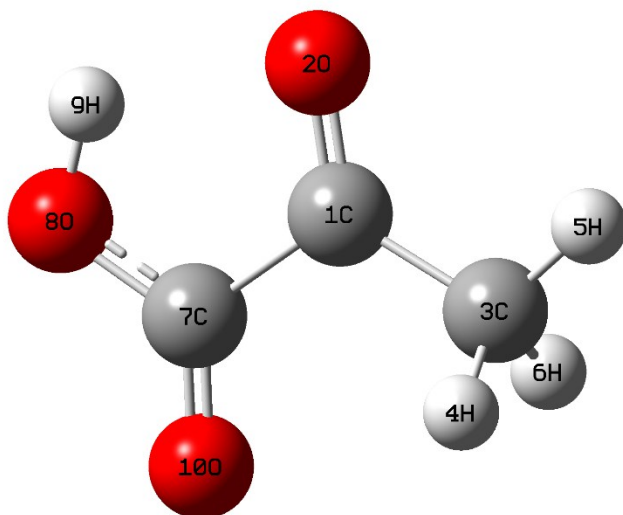
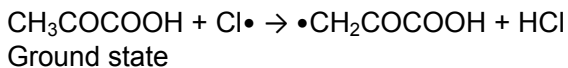


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	H	1			1.2945811		
3	No	Show	3	H	1	2		1.0896841	102.3738381	
4	No	Show	4	H	1	3	2	1.0892084	115.4295641	109.5153611
5	No	Show	5	C	1	4	3	1.4758603	116.2155346	-138.7201165
6	No	Show	6	O	5	1	4	1.2194295	122.8467647	153.5716173
7	No	Show	7	O	1	5	6	2.5319898	105.2998047	-96.4747736
8	No	Show	8	Cl	7	1	5	1.6636211	109.1455662	125.8629576

9	No	Show	9	C	5	1	6	1.5383537	117.2477600	177.9868135
10	No	Show	10	H	9	5	1	1.0960714	109.9039691	58.7103511
11	No	Show	11	O	9	5	1	1.4127989	105.1672704	-59.9754434
12	No	Show	12	H	11	9	5	0.9653782	107.9407091	156.4661248
13	No	Show	13	O	9	5	1	1.4003880	110.5270958	177.3130440
14	No	Show	14	H	13	9	5	0.9706418	106.7624500	25.0542865



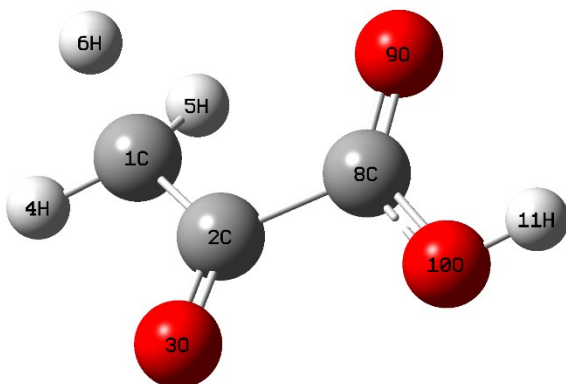
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	H	1			1.1705476		
3	No	Show	3	C	1	2		1.5513818	102.9238888	
4	No	Show	4	O	3	1	2	1.2096596	119.3130720	98.2008459
5	No	Show	5	O	1	3	4	2.6933753	110.1975554	102.0067187
6	No	Show	6	Cl	5	1	3	1.6422635	101.2227579	152.8072016
7	No	Show	7	C	3	1	4	1.4990792	115.8242008	-177.8013490
8	No	Show	8	H	7	3	1	1.0901830	110.2010913	170.3165205
9	No	Show	9	H	7	3	1	1.0958723	109.2517919	-68.9387227
10	No	Show	10	H	7	3	1	1.0958567	109.9306004	48.4707933
11	No	Show	11	O	1	3	4	1.3763717	109.8371035	-19.7716729
12	No	Show	12	H	11	1	3	0.9686674	107.8532830	-175.4704402
13	No	Show	13	O	1	11	3	1.3936908	109.9490621	127.7694555
14	No	Show	14	H	13	1	11	0.9679803	109.8065806	168.7272759



Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	O	1			1.2144357		

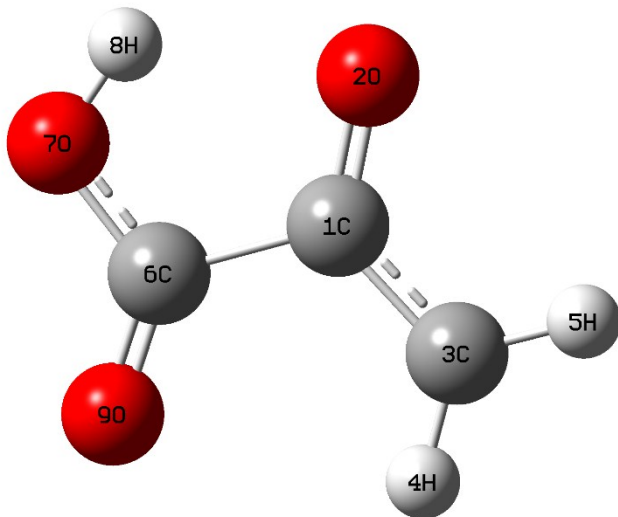
3	No	Show	3	C	1	2		1.4890866	125.8707975	
4	No	Show	4	H	3	1	2	1.0955175	109.4059470	121.8402042
5	No	Show	5	H	3	1	2	1.0897314	110.4196125	0.0266716
6	No	Show	6	H	3	1	2	1.0955232	109.4054909	-121.7845950
7	No	Show	7	C	1	2	3	1.5461468	117.2682658	-179.9710113
8	No	Show	8	O	7	1	2	1.3306721	113.2332141	0.0217543
9	No	Show	9	H	8	7	1	0.9775310	107.2469927	-0.0080937
10	No	Show	10	O	7	1	2	1.2078411	123.6031771	179.9978411

Transition state

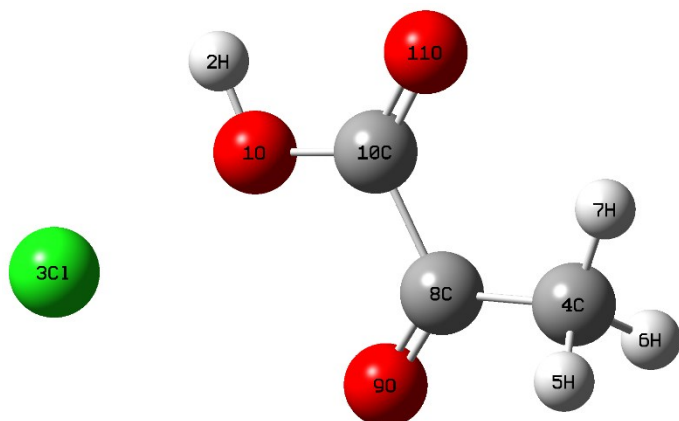
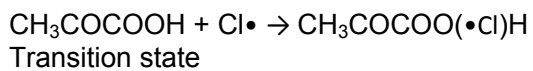


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	C	1			1.4727541		
3	No	Show	3	O	2	1		1.2140374	123.0380450	
4	No	Show	4	H	1	2	3	1.0879380	115.0020998	-4.7142550
5	No	Show	5	H	1	2	3	1.0884537	116.7146549	-146.2419231
6	No	Show	6	H	1	2	3	1.3507528	103.8341597	105.2673512
7	No	Show	7	Cl	1	2	3	2.8527504	109.2877160	104.7961893
8	No	Show	8	C	2	1	3	1.5375312	115.6947740	-179.7236882
9	No	Show	9	O	8	2	1	1.2080736	121.7330641	14.4116634
10	No	Show	10	O	8	2	1	1.3268988	111.8366393	-166.8118122
11	No	Show	11	H	10	8	2	0.9735115	108.8812007	-179.4583541

Product

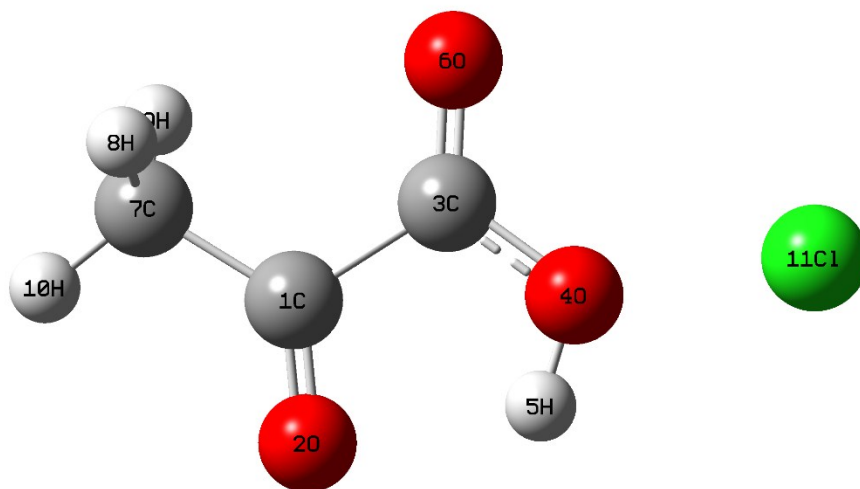


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	O	1			1.2439721		
3	No	Show	3	C	1	2		1.4128443	124.4532579	
4	No	Show	4	H	3	1	2	1.0821458	120.8670544	179.9620445
5	No	Show	5	H	3	1	2	1.0837323	119.1044793	-0.0390500
6	No	Show	6	C	1	2	3	1.5351065	117.3093968	179.9238850
7	No	Show	7	O	6	1	2	1.3317027	112.8494618	0.0353439
8	No	Show	8	H	7	6	1	0.9780149	107.0337509	0.0267622
9	No	Show	9	O	6	1	2	1.2089807	124.2525527	-179.9177777

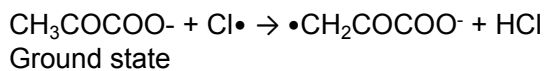


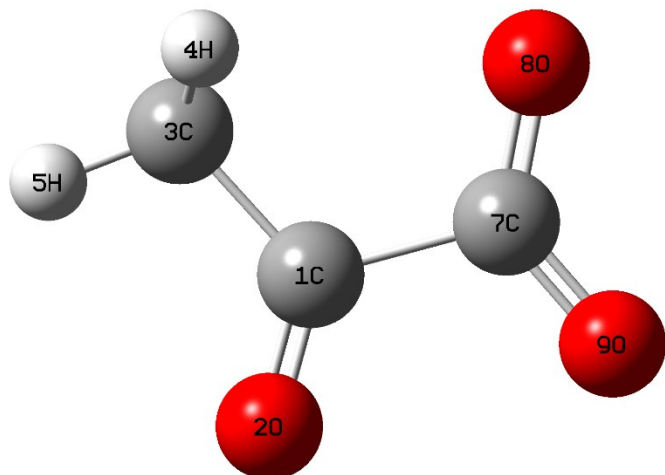
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	O						
2	No	Show	2	H	1			0.9753341		
3	No	Show	3	Cl	1	2		2.5920209	97.7919014	
4	No	Show	4	C	1	2	3	3.7549177	132.7140388	-122.2189837
5	No	Show	5	H	4	1	2	1.0948028	117.7077483	116.3586386
6	No	Show	6	H	4	1	2	1.0949755	118.4676037	-111.6734555
7	No	Show	7	H	4	1	2	1.0883387	92.2350130	2.4063392
8	No	Show	8	C	4	1	2	1.4983623	20.0837585	-176.3108523
9	No	Show	9	O	8	4	1	1.2087861	124.9047927	-178.2587504
10	No	Show	10	C	1	8	4	1.3492578	36.6674195	3.6926351
11	No	Show	11	O	10	1	8	1.2037432	123.6725872	178.9252022

Product



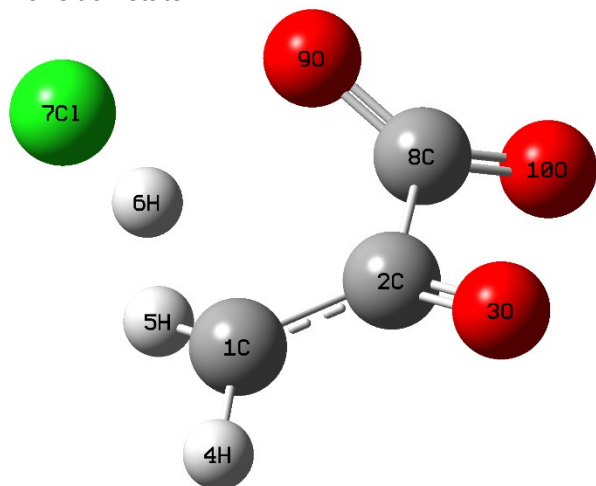
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	O	1			1.2118926		
3	No	Show	3	C	1	2		1.5516337	117.0770277	
4	No	Show	4	O	3	1	2	1.3420552	112.6523248	-5.1207796
5	No	Show	5	H	4	3	1	0.9799477	107.8087971	12.7199086
6	No	Show	6	O	3	1	2	1.2017747	124.4253874	174.7539983
7	No	Show	7	C	1	2	3	1.4884585	126.3766393	179.9320961
8	No	Show	8	H	7	1	2	1.0962148	109.0122203	119.6205237
9	No	Show	9	H	7	1	2	1.0949290	109.7357248	-123.8593613
10	No	Show	10	H	7	1	2	1.0896684	110.2427440	-1.6235545
11	No	Show	11	Cl	4	3	1	2.5785685	116.9793457	122.2706381





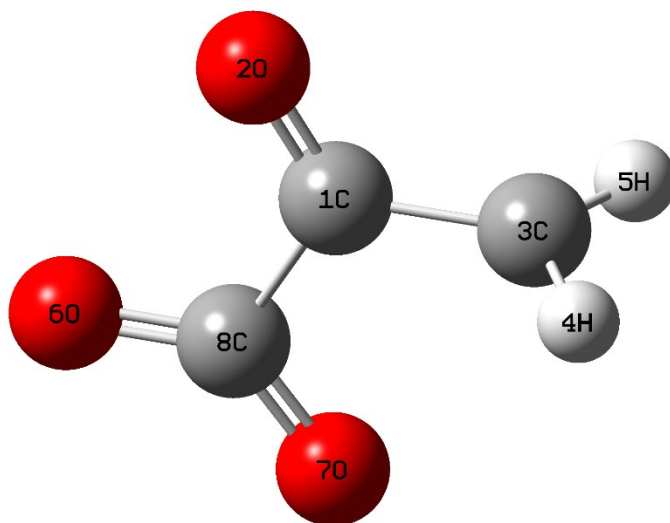
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	O	1			1.2182729		
3	No	Show	3	C	1	2		1.5053620	122.5400129	
4	No	Show	4	H	3	1	2	1.0950696	109.6449365	121.6521740
5	No	Show	5	H	3	1	2	1.0915722	110.8566922	-0.1398902
6	No	Show	6	H	3	1	2	1.0949621	109.6833647	-121.9886460
7	No	Show	7	C	1	2	3	1.5659464	120.2980665	-179.9982131
8	No	Show	8	O	7	1	2	1.2549642	115.6785577	179.6591705
9	No	Show	9	O	7	1	2	1.2518380	115.9311412	-0.3203450

Transition state

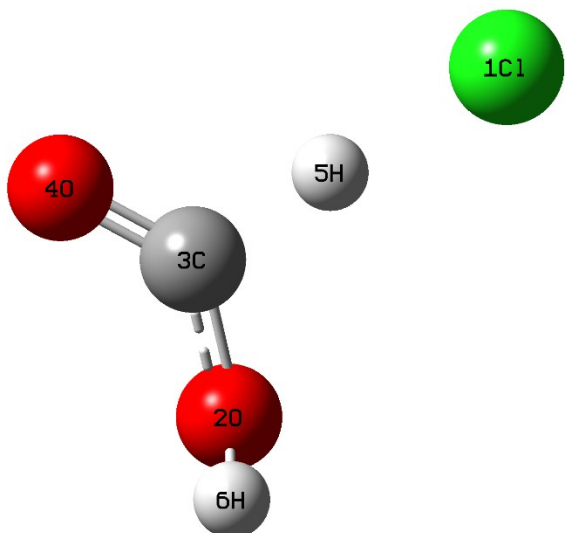
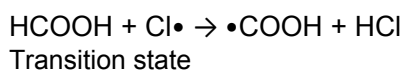


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	C	1			1.4165121		
3	No	Show	3	O	2	1		1.2331336	127.0339909	
4	No	Show	4	H	1	2	3	1.0873338	118.4536107	-16.2434634
5	No	Show	5	H	1	2	3	1.0831887	118.9635608	-171.7948051
6	No	Show	6	H	1	2	3	1.8251427	97.2055744	89.4120458
7	No	Show	7	Cl	1	2	3	3.1625975	100.8234628	88.2065022
8	No	Show	8	C	2	1	3	1.5909178	114.7303156	179.2357050
9	No	Show	9	O	8	2	1	1.2479346	110.7610080	47.7460142
10	No	Show	10	O	8	2	1	1.2372771	116.7892869	-134.5839441

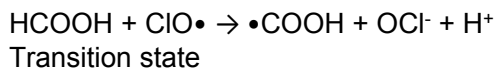
Product

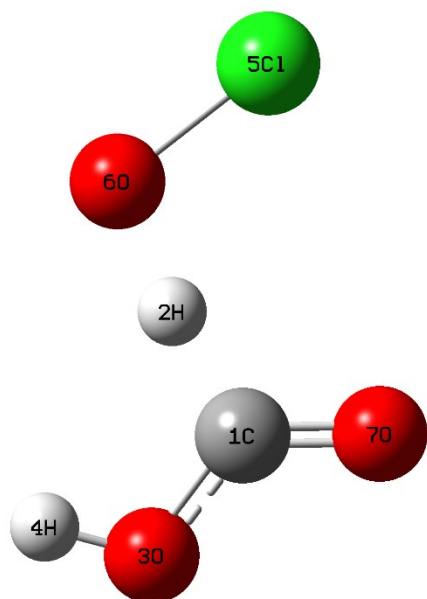


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	O	1			1.2197208		
3	No	Show	3	C	1	2		1.4775383	122.5380652	
4	No	Show	4	H	3	1	2	1.0847926	120.0849395	95.2152802
5	No	Show	5	H	3	1	2	1.0847926	120.0849395	-95.2152802
6	No	Show	6	O	1	2	3	2.3975810	92.8127681	180.0000000
7	No	Show	7	O	6	1	2	2.2597440	61.4466258	180.0000000
8	No	Show	8	C	6	1	2	1.2490349	35.8403221	180.0000000

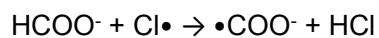


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	Cl						
2	No	Show	2	O	1			3.5592245		
3	No	Show	3	C	2	1		1.3265666	49.8884343	
4	No	Show	4	O	3	2	1	1.1840899	131.5506151	174.3586193
5	No	Show	5	H	3	2	1	1.2779522	110.6362324	-0.6038554
6	No	Show	6	H	2	1	3	0.9756441	109.4963909	-103.0206882

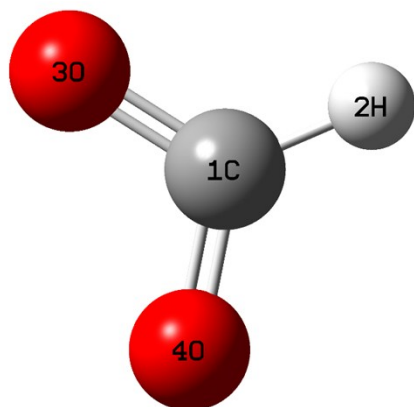




Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	H	1			1.2801005		
3	No	Show	3	O	1	2		1.3178199	114.3750998	
4	No	Show	4	H	3	1	2	0.9719453	110.4735573	-0.0456612
5	No	Show	5	Cl	1	3	4	3.3276104	146.9094768	-0.1549633
6	No	Show	6	O	1	3	4	2.5417403	117.6628464	-0.0975553
7	No	Show	7	O	1	3	6	1.1946281	126.3141802	-179.9147444

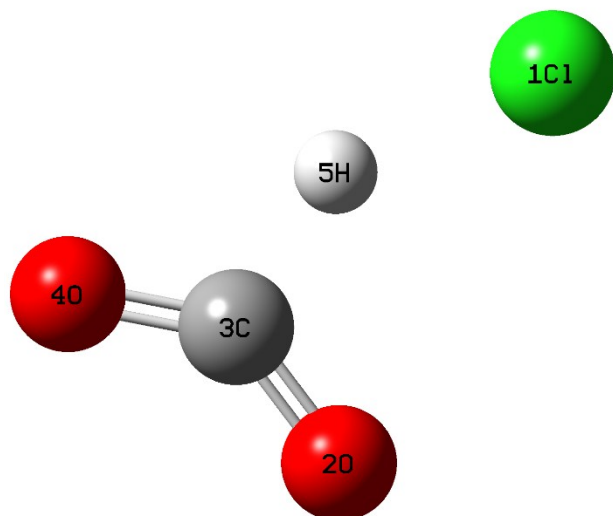


Ground state

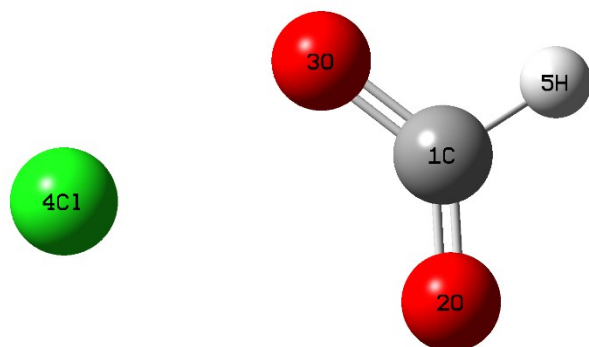
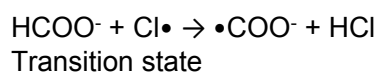


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	H	1			1.0944200		
3	No	Show	3	O	1	2		1.2568211	124.4587828	
4	No	Show	4	O	1	3	2	1.2568211	111.0824343	180.0000000

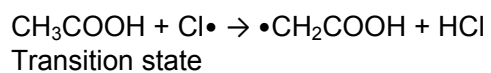
Transition state

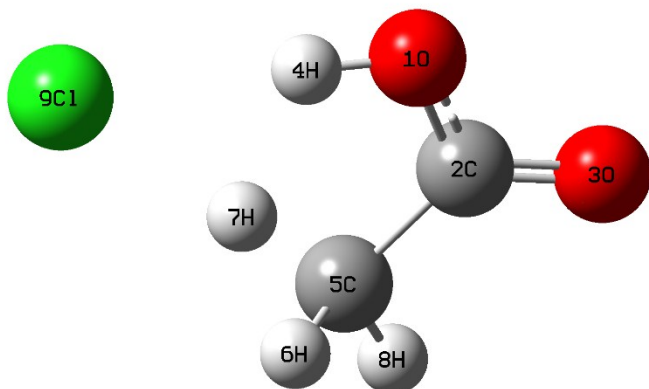


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	Cl						
2	No	Show	2	O	1			3.2010821		
3	No	Show	3	C	2	1		1.2231278	65.6195665	
4	No	Show	4	O	3	2	1	1.2267180	137.9789668	-179.9934986
5	No	Show	5	H	3	2	1	1.3255105	110.4148600	0.0042015

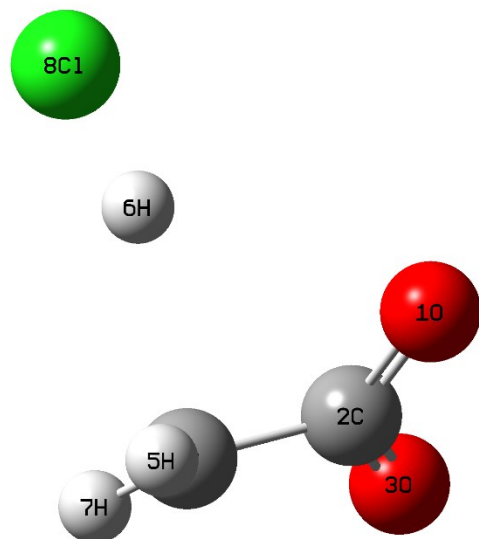
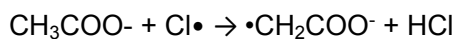


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	O	1			1.2282704		
3	No	Show	3	O	1	2		1.2804649	130.9007266	
4	No	Show	4	Cl	3	1	2	2.4433874	113.6690877	-0.0034951
5	No	Show	5	H	1	2	3	1.1180341	119.5921724	179.9951297

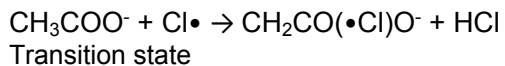


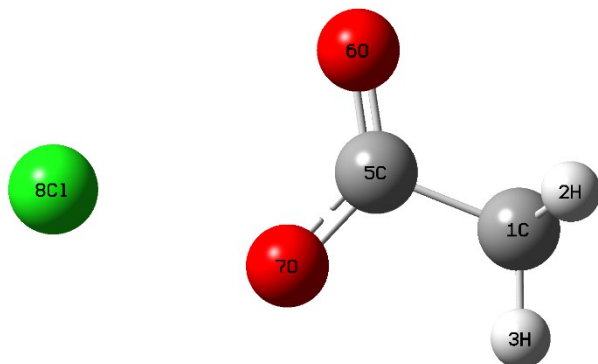


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	O						
2	No	Show	2	C	1			1.3390695		
3	No	Show	3	O	2	1		1.2124571	119.7622807	
4	No	Show	4	H	1	2	3	0.9692070	111.3026600	-177.4807953
5	No	Show	5	C	2	1	3	1.5036606	117.7386566	178.5743541
6	No	Show	6	H	5	2	1	1.0939625	111.0658902	-61.7827401
7	No	Show	7	H	5	2	1	1.1294187	109.1846823	55.2756730
8	No	Show	8	H	5	2	1	1.0889690	111.2651789	173.6432091
9	No	Show	9	Cl	5	2	1	3.1360915	109.1848604	55.2789935

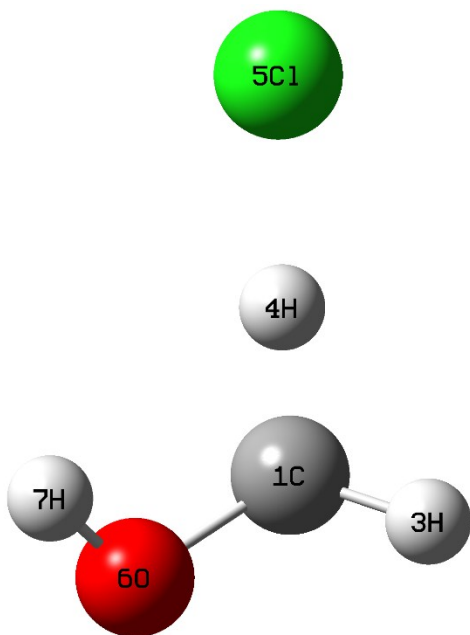
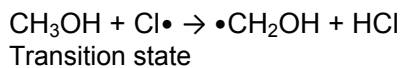


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	O						
2	No	Show	2	C	1			1.2677413		
3	No	Show	3	O	2	1		1.2633781	126.0733181	
4	No	Show	4	C	2	1	3	1.4812706	116.5730884	-179.3225753
5	No	Show	5	H	4	2	1	1.0864733	120.2352801	-33.1833214
6	No	Show	6	H	4	2	1	2.1071418	87.9235574	49.3799147
7	No	Show	7	H	4	2	1	1.0857482	120.7847252	156.2181046
8	No	Show	8	Cl	4	2	1	3.3878199	93.4278775	52.0529502

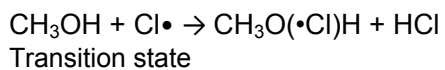


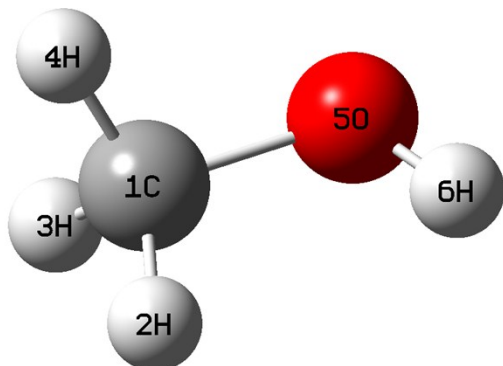


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	H	1			1.0939461		
3	No	Show	3	H	1	2		1.0903380	109.6029213	
4	No	Show	4	H	1	3	2	1.0939840	109.5766443	118.4744439
5	No	Show	5	C	1	3	4	1.5344063	112.7015963	120.7466612
6	No	Show	6	O	5	1	3	1.2322452	120.1462687	179.8110381
7	No	Show	7	O	5	1	6	1.2899058	111.8801266	179.9805874
8	No	Show	8	Cl	7	5	1	2.4647355	115.5862292	179.8826962

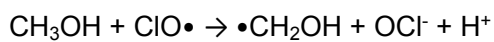


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
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2	No	Show	2	H	1			1.0957256		
3	No	Show	3	H	1	2		1.0957256	113.7158094	
4	No	Show	4	H	1	2	3	1.2215020	102.1704591	109.2871899
5	No	Show	5	Cl	1	2	4	2.9023064	101.5717317	-1.0113649
6	No	Show	6	O	1	2	4	1.3855184	113.4692625	119.0340043
7	No	Show	7	H	6	1	2	0.9653028	112.3961055	-114.1002540

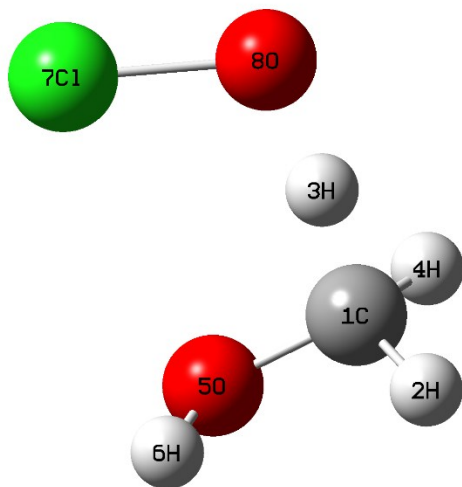




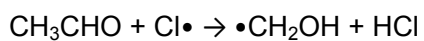
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	H	1			1.0910024		
3	No	Show	3	H	1	2		1.0932749	110.3637471	
4	No	Show	4	H	1	2	3	1.0923979	109.7224799	120.2926269
5	No	Show	5	O	1	2	4	1.4395751	110.6243818	121.2468547
6	No	Show	6	H	5	1	2	0.9681134	108.6730540	-11.9528287
7	No	Show	7	Cl	5	1	2	2.4217234	111.0696364	-106.3200471



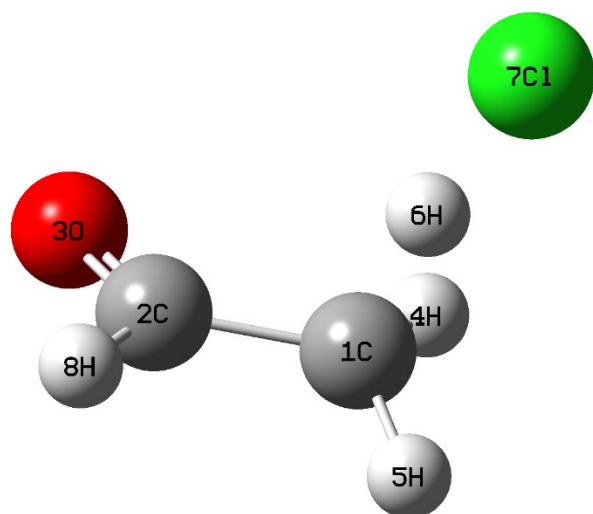
Transition state



Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C						
2	No	Show	2	H	1			1.0940778		
3	No	Show	3	H	1	2		1.2450235	103.6418087	
4	No	Show	4	H	1	2	3	1.0918638	114.4442536	112.5179566
5	No	Show	5	O	1	4	2	1.3803670	110.2302144	-131.2296091
6	No	Show	6	H	5	1	4	0.9676371	109.0614734	163.9961297
7	No	Show	7	Cl	5	1	4	3.3082274	79.8727461	-115.8907831
8	No	Show	8	O	1	5	6	2.5807751	105.1963785	-82.4961463



Transition state



Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	No	Show	1	C	1			1.4716497		
2	No	Show	2	C	1			1.2187380	122.1034019	
3	No	Show	3	O	2	1		1.0889264	116.3509178 -6.5235823	
4	No	Show	4	H	1	2	3	1.0894558	116.7408125 -150.7906856	
5	No	Show	5	H	1	2	3	1.3667031	101.2073839 102.5543817	
6	No	Show	6	H	1	2	3	2.8635058	105.3703686 102.5321491	
7	No	Show	7	Cl	1	2	3	1.1027467	116.2769514 178.6228740	
8	No	Show	8	H	2	1	3			