Supplementary Information

Kinetic and mechanistic insights into the degradation of clofibric acid in saline wastewater by Co^{2+}/PMS process: A modeling and theoretical study

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Text S1 Identification of CA intermediates by GC-MS analysis.

Samples were pretreated by the solid phase extraction (SPE) method (with BOJIN® HLB SPE Column) and the silylation method (using pyridine hexamethyldisilazane and chlorotrimethylsilane). A gas chromatograph was equipped with an HB-5 MS capillary column (30 m × 250 μm × 0.25 μm film thickness). The column oven temperature was held at 60 °C for 3 min, ramp to 250 °C at a rate of 10 $°C\cdot min^{-1}$, then to 310 °C at 20 $°C\cdot min^{-1}$, and maintained for 13 min. Electron impact (EI) mode at 70 eV was used with a mass range scanned at 40-800 m/z. The intermediates were referred to the NIST08 mass spectral library database.

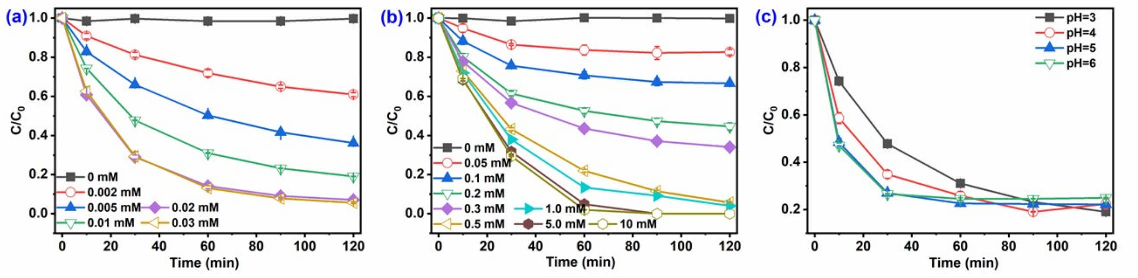


Fig. S1 Effect of (a) Co^{2+} concentration, (b) PMS concentration and (c) pH on CA degradation. Experimental conditions. $[CA]_0$ = 0.1 mM, (a, b) pH = 3.0, (a, c) $[PMS]_0$ = 0.5 mM; (b, c) $[Co^{2+}]_0$ = 0.01 mM.

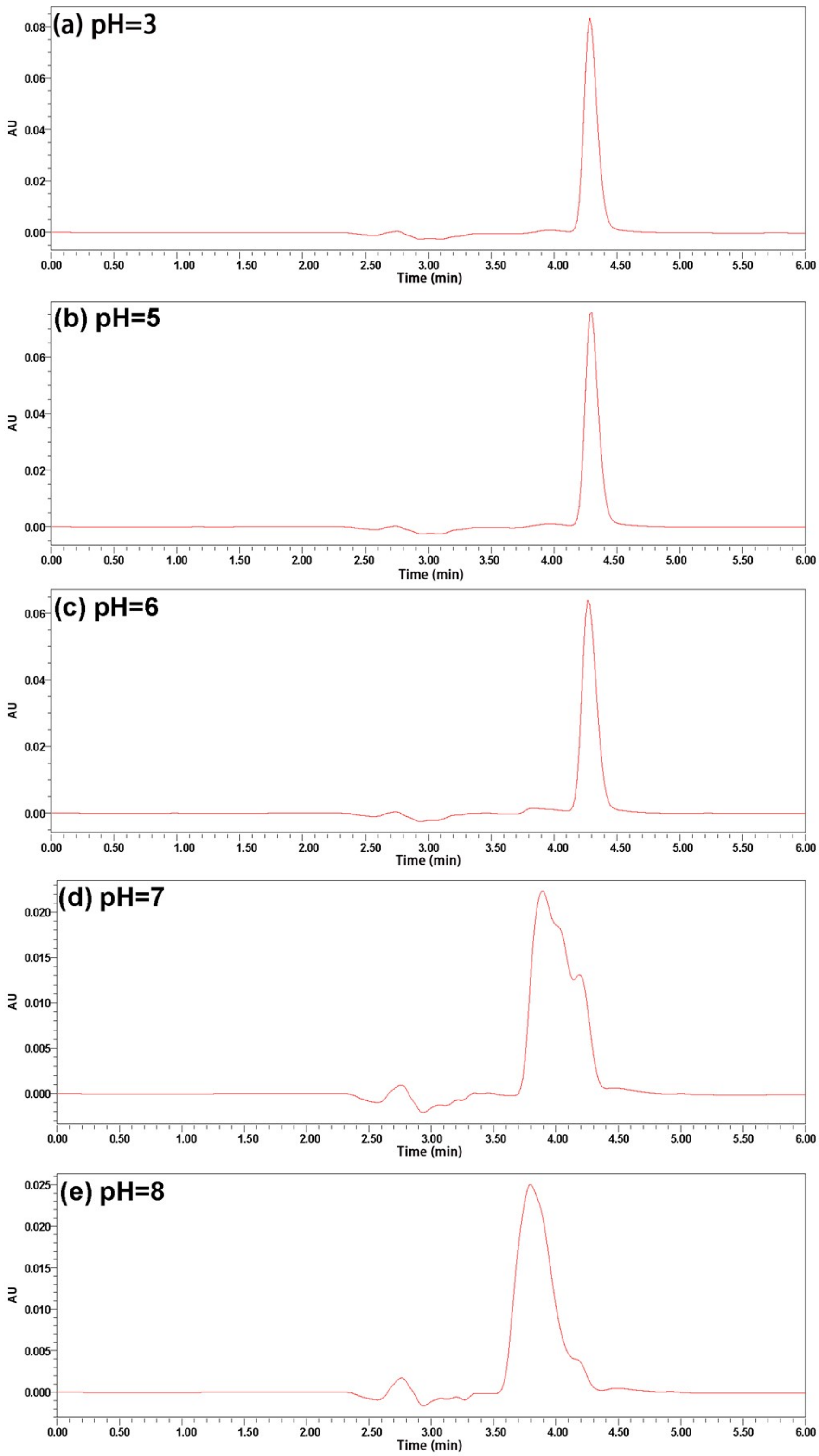


Fig. S2 The HPLC chromatogram of CA under different pH conditions. Experimental conditions: $[CA]_0$ = 0.1 mM, $[Co^{2+}]_0$ = 0.01 mM, $[PMS]_0$ = 0.5 mM.

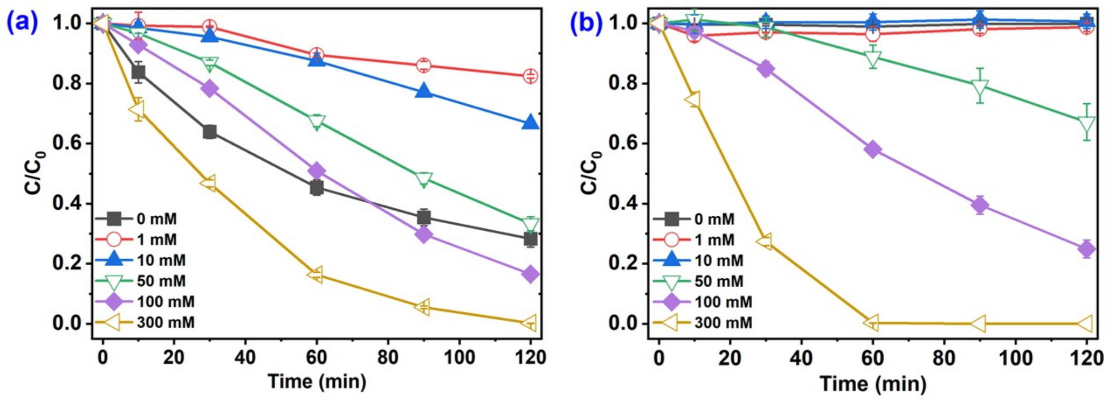


Fig. S3 Effect of chloride ions concentration on CA degradation in the (a) Co^{2+}/PMS system and only (b) PMS process. Experimental conditions: $[CA]_0$ = 0.1 mM, $[Co^{2+}]_0$ = 0.01 mM, $[PMS]_0$ = 0.5 mM, pH 3.0.

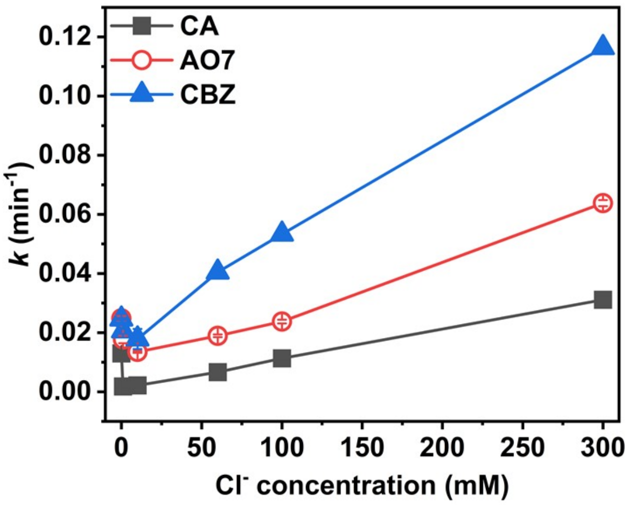


Fig. S4 Effect of Cl^{-} concentrations on the rate constant *k* of CA, AO7 and CBZ degradation in Co^{2+}/PMS system. Experimental conditions: $[CA]_0 = [AO7]_0 = [CBZ]_0 = 0.1$ mM, $[Co^{2+}]_0 = 0.01$ mM, $[PMS]_0 = 0.5$ mM, pH 3.0.

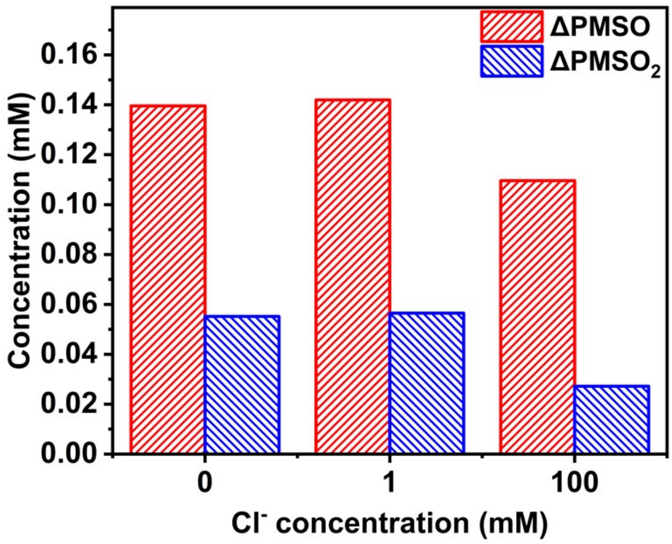


Fig. S5 The further consumption of PMSO and the further formation of $PMSO_2$ in the Co^{2+}PMS system under different Cl^- concentrations. Experimental conditions: $[CA]_0$ = 0 mM, $[PMS]_0$ = 0.5 mM, pH 3.0.

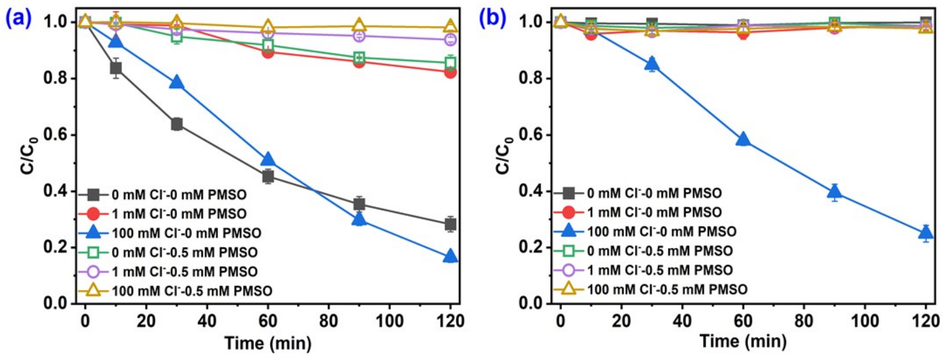


Fig. S6 The degradation of CA in the (a) Co^{2+}/PMS/Cl^- and (b) PMS/Cl^- system under different Cl^- concentrations (0, 1 or 100 mM) and PMSO concentrations (0 or 0.5 mM). Experimental conditions: $[CA]_0 = 0.1$ mM, $[PMS]_0 = 0.5$ mM, pH 3.0, (a) $[Co^{2+}]_0 = 0.01$ mM, (b) $[Co^{2+}]_0 = 0$ mM.

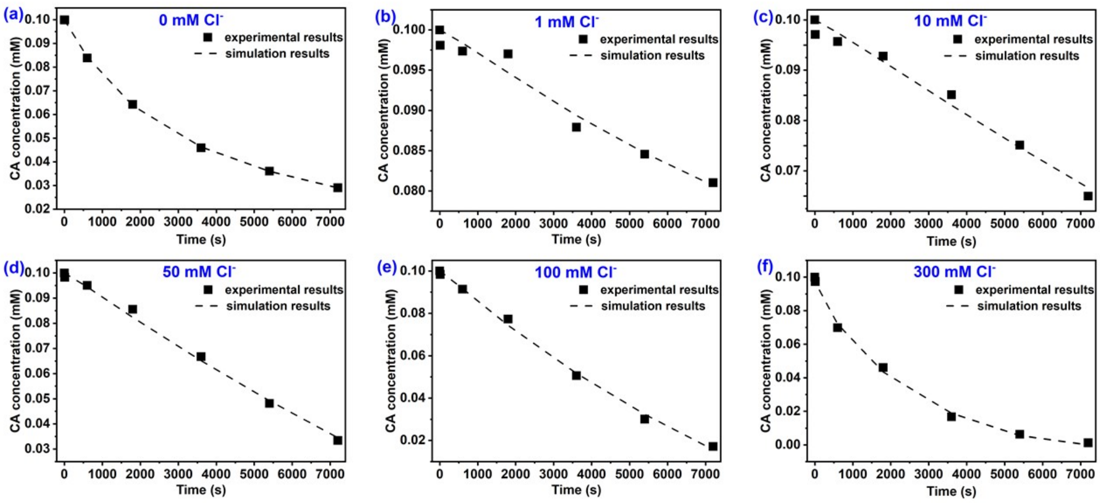


Fig. S7 Model fits to data for oxidation of CA at different Cl^- concentrations in the Co^{2+}/PMS system (Data points represent the average from at least two experiments). Experimental conditions: $[CA]_0$ = 0.1 mM, $[Co^{2+}]_0$ = 0.01 mM, $[PMS]_0$ = 0.5 mM, pH 3.0.

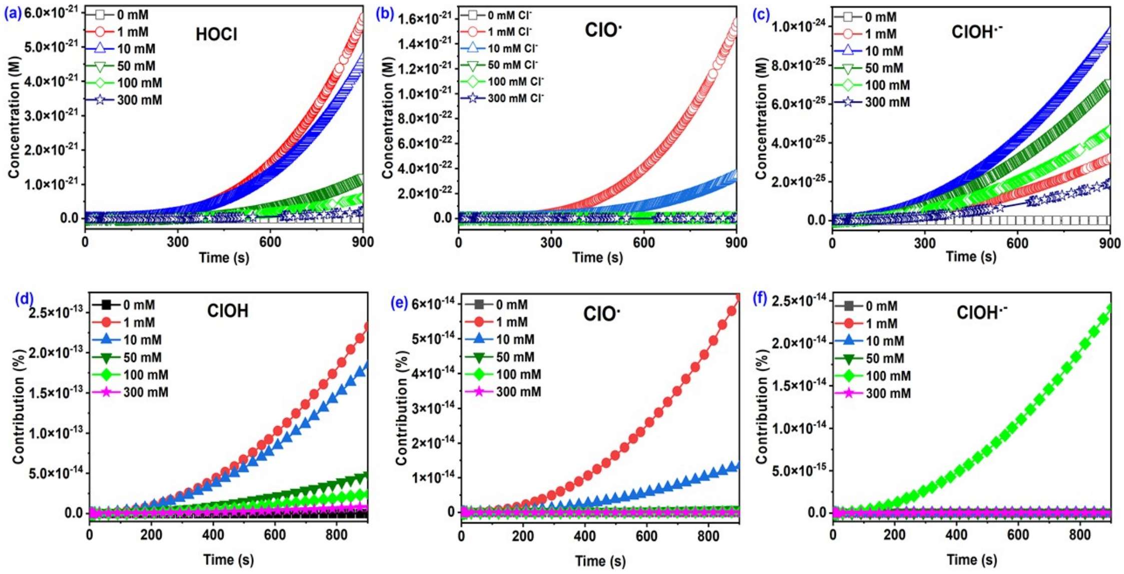


Fig. S8 The (a-c) concentration and (d-f) contribution of reactive species at different Cl^- concentrations in the Co^{2+}/PMS/Cl^- system. Experimental conditions: $[CA]_0$ = 0.1 mM, $[Co^{2+}]_0$ = 0.01 mM, $[PMS]_0$ = 0.5 mM, pH 3.0.

Table S1 The kinetic model for Co^{2+}/PMS process.

No.	Reaction	Rate Constant	Reference
1	$Co^{2+} + HSO_5^- \rightarrow Co^{3+} + SO_4^{\bullet-} + OH^-$	4.72×10^{-1} $M^{-1}s^{-1}$	*fitted*
2	$Co^{2+} + SO_4^{\bullet-} \rightarrow Co^{3+} + SO_4^{2-}$	2.0×10^{6} $M^{-1}s^{-1}$	1
3	$SO_4^{\bullet-} + SO_4^{\bullet-} \rightarrow S_2O_8^{2-}$	4.0×10^{8} $M^{-1}s^{-1}$	2
4	$SO_4^{\bullet-} + HSO_5^- \rightarrow SO_5^{\bullet-} + HSO_4^-$	1.0×10^{5} $M^{-1}s^{-1}$	3
5	$SO_4^{\bullet-} + S_2O_8^{2-} \rightarrow SO_4^{2-} + S_2O_8^{\bullet-}$	6.1×10^{5} $M^{-1}s^{-1}$	3
6	$SO_4^{\bullet-} + H_2O \rightarrow HSO_4^- + {}^{\bullet}OH$	5.0×10^{2} $M^{-1}s^{-1}$	2
7	$Co^{3+} + HSO_5^- \rightarrow Co^{2+} + SO_5^{\bullet-} + H^+$	1.94 $M^{-1}s^{-1}$	*fitted*
8	$2SO_5^{\bullet-} \rightarrow 2SO_4^{\bullet-} + O_2$	1.0×10^{8} $M^{-1}s^{-1}$	2
9	$HSO_4^- + {}^{\bullet}OH \rightarrow SO_4^{\bullet-} + H_2O$	6.9×10^{5} $M^{-1}s^{-1}$	2
10	$HSO_4^- \rightarrow SO_4^{2-} + H^+$	1.2×10^{-2} $M^{-1}s^{-1}$	2
11	$HSO_5^- \rightarrow SO_5^{2-} + H^+$	1.0×10^{-5} $M^{-1}s^{-1}$	2
12	$H_2O \rightarrow H^+ + OH^-$	1.0×10^{-3} $M^{-1}s^{-1}$	4
13	$H^+ + OH^- \rightarrow H_2O$	1.0×10^{11} $M^{-1}s^{-1}$	4
14	$SO_4^{\bullet-} + OH^- \rightarrow {}^{\bullet}OH + SO_4^{2-}$	6.5×10^{7} $M^{-1}s^{-1}$	2
15	${}^{\bullet}OH + {}^{\bullet}OH \rightarrow H_2O_2$	5.2×10^{9} $M^{-1}s^{-1}$	4
16	${}^{\bullet}OH + SO_4^{\bullet-} \rightarrow HSO_5^-$	1.0×10^{10} $M^{-1}s^{-1}$	2
17	${}^{\bullet}OH + H_2O_2 \rightarrow HO_2^{\bullet} + H_2O$	2.7×10^{7} $M^{-1}s^{-1}$	2

18	$HO_2^{\bullet} + HO_2^{\bullet} \rightarrow H_2O_2 + O_2$	$8.3\times10^{5}\ M^{-1}s^{-1}$	5
19	$HO_2^{\bullet} \rightarrow O_2^{\bullet-} + H^+$	$7.0\times10^{5}\ M^{-1}s^{-1}$	6
20	$H_2O_2 \rightarrow HO_2^- + H^+$	$1.3\times10^{-1}\ M^{-1}s^{-1}$	4
21	$HO_2^- + H^+ \rightarrow H_2O_2$	$5.0\times10^{10}\ M^{-1}s^{-1}$	4
22	$Co^{2+} + HSO_5^- \rightarrow SO_4^{2-} + H^+ + Co^{4+}$	$1.85\times10^{-1}\ M^{-1}s^{-1}$	*fitted*
23	$O_2^{\bullet-} + H^+ \rightarrow HO_2^{\bullet}$	$5.0\times10^{10}\ M^{-1}s^{-1}$	4
24	$HO_2^{\bullet} + O_2^{\bullet-} \rightarrow HO_2^- + O_2$	$9.7\times10^{7}\ M^{-1}s^{-1}$	4
25	$^{\bullet}OH + HO_2^{\bullet} \rightarrow H_2O + O_2$	$7.1\times10^{9}\ M^{-1}s^{-1}$	4
26	$^{\bullet}OH + O_2^{\bullet-} \rightarrow OH^- + O_2$	$1.0\times10^{10}\ M^{-1}s^{-1}$	4
27	$^{\bullet}OH + HO_2^- \rightarrow H_2O + O_2^{\bullet-}$	$7.5\times10^{9}\ M^{-1}s^{-1}$	2
28	$^{\bullet}OH + HSO_5^- \rightarrow SO_5^{\bullet-} + H_2O$	$1.7\times10^{7}\ M^{-1}s^{-1}$	2
29	$^{\bullet}OH + SO_4^{2-} \rightarrow SO_4^{\bullet-} + OH^-$	$1.2\times10^{6}\ M^{-1}s^{-1}$	2
30	$SO_4^{\bullet-} + Cl^- \rightarrow SO_4^{2-} + Cl^{\bullet}$	$2.7\times10^{8}\ M^{-1}s^{-1}$	7
31	$Cl^- + {}^{\bullet}OH \rightarrow HOCl^{\bullet-}$	$4.3\times10^{9}\ M^{-1}s^{-1}$	4
32	$HOCl^{\bullet-} + Cl^- \rightarrow Cl_2^{\bullet-} + OH^-$	$1.0\times10^{5}\ M^{-1}s^{-1}$	4
33	$H^+ + Cl^- \rightarrow HCl$	$5.0\times10^{10}\ M^{-1}s^{-1}$	4
34	$HCl \rightarrow H^+ + Cl^-$	$8.6\times10^{16}\ s^{-1}$	4
35	$HOCl^{\bullet-} \rightarrow Cl^- + {}^{\bullet}OH$	$6.1\times10^{9}\ s^{-1}$	4
36	$HOCl^{\bullet-} + H^+ \rightarrow Cl^{\bullet} + H_2O$	$2.1\times10^{10}\ M^{-1}s^{-1}$	4

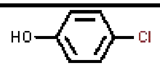
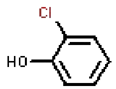
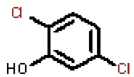
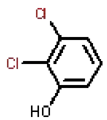
37	$Cl^- + Cl^\bullet \rightarrow Cl_2^{\bullet-}$	$6.5\times10^9\ M^{-1}s^{-1}$	4
38	$Cl^- + Cl_2 \rightarrow Cl_3^-$	$2.0\times10^4\ M^{-1}s^{-1}$	4
39	$Cl^- + HOCl \rightarrow Cl_2OH^-$	$1.5\times10^4\ M^{-1}s^{-1}$	4
40	$Cl^\bullet + H_2O_2 \rightarrow HCl + HO_2^\bullet$	$4.0\times10^9\ M^{-1}s^{-1}$	4
41	$Cl^\bullet + OH^- \rightarrow HOCl^{\bullet-}$	$4.3\times10^9\ M^{-1}s^{-1}$	4
42	$Cl^\bullet + Cl^\bullet \rightarrow Cl_2$	$1.0\times10^8\ M^{-1}s^{-1}$	4
43	$Cl^\bullet + H_2O \rightarrow HClOH$	$2.5\times10^5\ M^{-1}s^{-1}$	4
44	$Cl^\bullet + H_2O \rightarrow HOCl^{\bullet-} + H^+$	$1.6\times10^5\ M^{-1}s^{-1}$	4
45	$Cl_2^{\bullet-} + O_2^{\bullet-} \rightarrow 2Cl^- + O_2$	$1.0\times10^9\ M^{-1}s^{-1}$	4
46	$Cl_2^{\bullet-} + OH^- \rightarrow HOCl^{\bullet-} + Cl^-$	$4.5\times10^7\ M^{-1}s^{-1}$	4
47	$Cl_2^{\bullet-} \rightarrow Cl^\bullet + Cl^-$	$1.1\times10^5\ s^{-1}$	4
48	$Cl_2^{\bullet-} + Cl_2^{\bullet-} \rightarrow Cl_2 + 2Cl^-$	$8.3\times10^8\ M^{-1}s^{-1}$	4
49	$Cl_2^{\bullet-} + H_2O_2 \rightarrow 2Cl^- + HO_2^\bullet + H^+$	$1.4\times10^5\ M^{-1}s^{-1}$	4
50	$Cl_2^{\bullet-} + H_2O \rightarrow HClOH + Cl^-$	$1.3\times10^3\ M^{-1}s^{-1}$	4
51	$Cl_2^{\bullet-} + {}^\bullet OH \rightarrow HOCl + Cl^-$	$1.0\times10^9\ M^{-1}s^{-1}$	4
52	$HOCl \rightarrow H^+ + ClO^-$	$1.6\times10^3\ s^{-1}$	4
53	$H^+ + ClO^- \rightarrow HOCl$	$5.0\times10^{10}\ M^{-1}s^{-1}$	4
54	$HClOH \rightarrow HOCl^{\bullet-} + H^+$	$1.0\times10^8\ s^{-1}$	4
55	$HClOH \rightarrow Cl^\bullet + H_2O$	$1.0\times10^2\ s^{-1}$	4

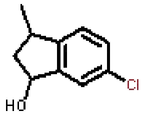
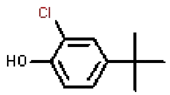
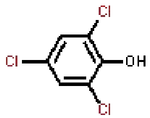
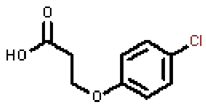
56	$HClOH + Cl^- \rightarrow Cl_2^{\bullet -} + H_2O$	5.0×10^9 $M^{-1}s^{-1}$	4
57	$Cl_3^- + HO_2^\bullet \rightarrow Cl_2^{\bullet -} + HCl + O_2$	1.0×10^9 $M^{-1}s^{-1}$	4
58	$Cl_3^- + O_2^{\bullet -} \rightarrow Cl_2^{\bullet -} + Cl^- + O_2$	3.8×10^9 $M^{-1}s^{-1}$	4
59	$Cl_3^- \rightarrow Cl_2 + Cl^-$	1.1×10^5 s^{-1}	4
60	$Cl_2 + O_2^{\bullet -} \rightarrow Cl_2^{\bullet -} + O_2$	1.0×10^9 $M^{-1}s^{-1}$	4
61	$Cl_2 + HO_2^\bullet \rightarrow Cl_2^{\bullet -} + H^+ + O_2$	1.0×10^9 $M^{-1}s^{-1}$	4
62	$Cl_2 + H_2O \rightarrow Cl_2OH^- + H^+$	1.5×10^1 $M^{-1}s^{-1}$	4
63	$Cl_2 + H_2O_2 \rightarrow 2HCl + O_2$	1.3×10^4 $M^{-1}s^{-1}$	4
64	$Cl_2OH^- + H^+ \rightarrow Cl_2 + H_2O$	2.0×10^{10} $M^{-1}s^{-1}$	4
65	$Cl_2OH^- \rightarrow HOCl + Cl^-$	5.5×10^9 s^{-1}	4
66	$HOCl + {}^\bullet OH \rightarrow ClO^\bullet + H_2O$	2.0×10^9 $M^{-1}s^{-1}$	4
67	$HOCl + O_2^{\bullet -} \rightarrow Cl^\bullet + OH^- + O_2$	7.5×10^6 $M^{-1}s^{-1}$	4
68	$HOCl + HO_2^\bullet \rightarrow Cl^\bullet + H_2O + O_2$	7.5×10^6 $M^{-1}s^{-1}$	4
69	$HOCl + H_2O_2 \rightarrow HCl + H_2O + O_2$	1.1×10^4 $M^{-1}s^{-1}$	4
70	$ClO^- + {}^\bullet OH \rightarrow ClO^\bullet + OH^-$	8.8×10^9 $M^{-1}s^{-1}$	4
71	$ClO^- + H_2O_2 \rightarrow Cl^- + H_2O + O_2$	1.7×10^5 $M^{-1}s^{-1}$	4
72	$ClO^- + O_2^{\bullet -} + H_2O \rightarrow Cl^\bullet + 2OH^- + O_2$	2.0×10^8 $M^{-1}s^{-1}$	4
73	$Cl_2^{\bullet -} + HO_2^{\bullet -} \rightarrow 2Cl^- + H^+ + O_2$	3.0×10^9 $M^{-1}s^{-1}$	4

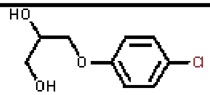
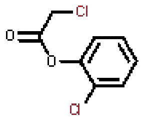
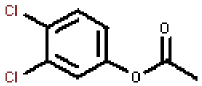
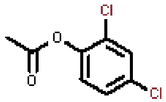
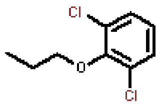
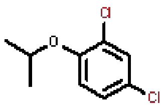
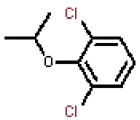
74	$Cl_2 + H_2O \rightarrow HOCl + H^+ + Cl^-$	1.0×10^{-3} $M^{-1}s^{-1}$	4
75	$SO_4^{2-} + Cl^\bullet \rightarrow SO_4^{\bullet-} + Cl^-$	2.5×10^{8} $M^{-1}s^{-1}$	8
76	$HSO_4^- + {}^\bullet OH \rightarrow SO_4^{\bullet-} + H_2O$	6.9×10^{5} $M^{-1}s^{-1}$	2
77	$SO_4^{\bullet-} + H_2O_2 \rightarrow SO_4^{2-} + H^+ + HO_2^\bullet$	1.2×10^{7} $M^{-1}s^{-1}$	9
78	$SO_4^{\bullet-} + HO_2^\bullet \rightarrow SO_4^{2-} + H^+ + O_2$	3.5×10^{9} $M^{-1}s^{-1}$	9
79	$Cl^\bullet + ClO^- \rightarrow ClO^\bullet + Cl^-$	8.2×10^{9} $M^{-1}s^{-1}$	4
80	$Cl^\bullet + HOCl \rightarrow ClO^\bullet + H^+ + Cl^-$	3.0×10^{9} $M^{-1}s^{-1}$	10
81	$H^+ + SO_4^{2-} \rightarrow HSO_4^-$	3.5 $M^{-1}s^{-1}$	4
82	${}^\bullet OH$ + CA → pro1	2.8×10^{9} $M^{-1}s^{-1}$	11
83	$SO_4^{\bullet-}$ + CA → pro2 + SO_4^{2-}	2.3×10^{9} $M^{-1}s^{-1}$	12
84	$Cl_2^{\bullet-}$ + CA → pro3	1.41×10^{8} $M^{-1}s^{-1}$	12
85	$Cl^\bullet$ + CA → pro4	5.5×10^{9} $M^{-1}s^{-1}$	12
86	$ClO^\bullet$ + CA → pro5	1.0×10^{6} $M^{-1}s^{-1}$	11
87	$HOCl^{\bullet-}$ + CA → pro6	2.56 $M^{-1}s^{-1}$	fitted
88	HOCl + CA → pro7	1.45×10^{-1} $M^{-1}s^{-1}$	fitted
89	Cl_2 + CA → pro8	5.06×10^{-2} $M^{-1}s^{-1}$	fitted
90	Co^{4+} + CA → pro9 + Co^{2+}	2.82×10^{-2} $M^{-1}s^{-1}$	fitted

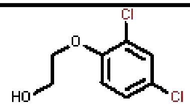
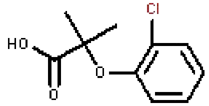
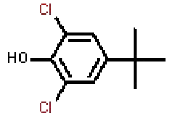
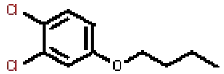
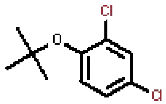
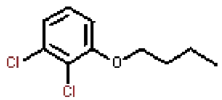
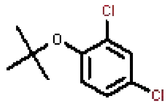
fitted **means the reaction rate constant was calculated by Kintecus 6.51.**

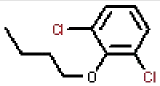
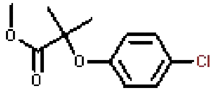
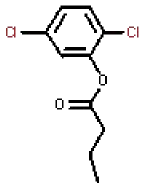
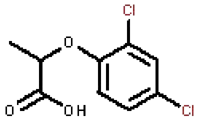
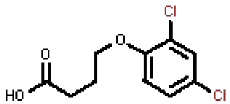
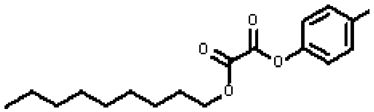
Table S2 Major chlorinated by-products of CA in Co^{2+}/PMS system.

NO.	Compound	Proposed Structure	Formula	MW (g/mol)	0 mM Cl^- 30min	0 mM Cl^- 120min	1 mM Cl^- 30min	1 mM Cl^- 120min	100 mM Cl^- 30min	100 mM Cl^- 120min
1	4-chlorophenol		C_6H_8ClO	128	✓	✓	✓	✓	✓	✓
2	3-chlorophenol		C_6H_8ClO	128.56	✓	✓	✓	✓		
3	2-chlorophenol		C_6H_8ClO	128.56				✓		
4	2,4-dichloro-phenol		$C_6H_4Cl_2O$	163	✓	✓	✓	✓	✓	✓
5	2,5-dichloro-phenol		$C_6H_4Cl_2O$	163				✓	✓	✓
6	2,3-dichloro-phenol		$C_6H_4Cl_2O$	163				✓	✓	✓
7	3,4-dichloro-phenol		$C_6H_4Cl_2O$	163						✓

8	1-chloro-4-isopropenyloxy-benzene		C_9H_9ClO	168.62				✓		
9	acetic acid-4-chlorophenyl ester		$C_8H_7ClO_2$	170.59	✓	✓	✓			
10	acetic acid-3-chlorophenyl ester		$C_8H_7ClO_2$	170.59		✓				
11	6-chloro-3-methyl-1-indanol		$C_{12}H_{15}ClO_3$	182.05		✓	✓			
12	4-tert-butyl-2-chlorophenol		$C_{10}H_{13}ClO$	184.66				✓	✓	
13	2,4,6-trichloro-phenol		$C_6H_3Cl_3O$	197.45			✓	✓		✓
14	3-(p-chlorophenoxy) propionic acid		$C_9H_9ClO_3$	200.62			✓			

15	3-(4-chloro-phenoxy)-propane-1,2-diol		$C_9H_{11}ClO_3$	202.63		✓			
16	o-chlorophenol chloroacetate		$C_8H_6Cl_2O_2$	205.04		✓			
17	3,4-dichloro-phenol acetate		$C_8H_6Cl_2O_2$	205.04				✓	
18	2,4-dichloro-phenol acetate		$C_8H_6Cl_2O_2$	205.04				✓	✓
19	2,6-dichlorophenol n-propyl ether		$C_9H_{10}Cl_2O$	205.08	✓				
20	2,4-dichlorophenol isopropyl ether		$C_9H_{10}Cl_2O$	205.08			✓	✓	
21	2,6-dichlorophenol isopropyl ether		$C_9H_{10}Cl_2O$	205.08					✓

22	2-(2,4-dichlorophenoxy)-ethanol		$C_8H_8Cl_2O2$	207.05					✓	✓
23	2-(2-chloro-phenoxy)-2-methyl-propionic acid		$C_{10}H_{11}ClO_3$	214.65	✓					✓
24	2,6-dichloro-4-(1,1-dimethylethyl) phenol		$C_{10}H_{12}Cl_2O$	219.11			✓			✓
25	3,4-dichlorophenol n-butyl ether		$C_{10}H_{12}Cl_2O$	219.11					✓	
26	2,4-dichlorophenol tert-butyl ether		$C_{10}H_{12}Cl_2O$	219.11				✓	✓	✓
27	2,3-dichlorophenol n-butyl ether		$C_{10}H_{12}Cl_2O$	219.11						✓
28	2,4-dichlorophenol tert-butyl ether		$C_{10}H_{12}Cl_2O$	219.11				✓	✓	✓

29	2,6-dichlorophenol n-butyl ether		$C_{10}H_{12}Cl_2O$	219.11						✓
30	2-(4-chlorophenoxy)-2-methyl- propanoic acid methyl ester		$C_{11}H_{13}ClO_3$	228.67	✓	✓	✓	✓	✓	✓
31	butyric acid 2,5-dichloro-phenyl ester		$C_{10}H_{10}Cl_2O_2$	233.09						✓
32	2-(2,4-dichloro-phenoxy)-propionic acid		$C_9H_8Cl_2O_3$	235.06		✓		✓	✓	
33	4-(2,4-dichlorophenoxy)-butanoic acid		$C_{10}H_{10}Cl_2O_3$	249.09		✓	✓	✓		✓
34	oxalic acid 4-chlorophenyl nonyl ester		$C_{17}H_{23}ClO_4$	326.82			✓			

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