



Supplement of

Organic peroxide and OH formation in aerosol and cloud water: laboratory evidence for this aqueous chemistry

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Table S1. Reactions and rate/equilibrium constants used in the full kinetic model of unified glyoxal/methylglyoxal + OH

	Reactions	Rate constants (M ¹⁻ⁿ s ⁻¹)	Ref
1	H ₂ O ₂ → 2OH	1.1e-4×Trans ^a	T, e
2	OH + H ₂ O ₂ → HO ₂ + H ₂ O	2.7e7	T
3	HO ₂ + H ₂ O ₂ → OH + H ₂ O + O ₂	3.7	T
4	2 HO ₂ → H ₂ O ₂ + O ₂	8.3e5	T
5	OH + HO ₂ → H ₂ O + O ₂	7.1e9	T
6	HO ₂ + O ₂ ⁻ + H ⁺ → H ₂ O ₂ + O ₂	1e8	T
7	2OH → H ₂ O ₂	5.5e9	T
8	OH + O ₂ ⁻ → OH ⁻ + O ₂	1e10	T
9	O _{2g} ↔ O ₂	K _{eq} = 1.3e-3 k _r = 5.3e2	T, W
10	CO _{2g} ↔ CO ₂	K _{eq} = 3.4e-2 k _r = 5.3e2	T, W
11	CO ₂ ↔ H ⁺ + HCO ₃ ⁻	K _{eq} = 4.3e-7 k _r = 5.6e4	T
12	HCO ₃ ⁻ → H ⁺ + CO ₃ ⁻²	K _{eq} = 4.69e-11 k _r = 5.0e10	T
13	CO ₂ ⁻ + O ₂ → O ₂ ⁻ + CO ₂	2.4e9	T
14	HCO ₃ ⁻ + OH → CO ₃ ⁻² + H ₂ O	1e7	T
15	CO ₃ ⁻ + O ₂ ⁻ → CO ₃ ⁻² + O ₂	6.5e8	T
16	CO ₃ ⁻ + HCO ₂ ⁻ → HCO ₃ ⁻ + CO ₂ ⁻	1.5e5	T
17	CO ₃ ⁻ + H ₂ O ₂ → HCO ₃ ⁻ + HO ₂	8e5	T
18	GCOLAC + OH → GCOLAC* + H ₂ O	6.0e8	T
19	GCOLAC* + O ₂ → GCOLACOO*	1e6	G, L'
20	GCOLACOO* → GLYAC + HO ₂	5e1	C
21	2GCOLACOO* → 2GCOLACO* + O ₂	3e8*0.95	L', e
22	2GCOLACOO* → GLYAC + OXLAC + O ₂	3e8*0.05	L', e
23	GCOLACO* → HCO ₂ H + CO ₂	I	Gi, e
24	GCOLACO* → GLYAC*	1e7	Gi, e
25	GCOLAC ↔ H ⁺ + GCOLAC ⁻	K _{eq} = 1.48e-4 k _r = 2.0e10	T
26	GCOLAC ⁻ + OH → GCOLAC* + H ₂ O	6.0e8	T
27	GCOLAC* + O ₂ → GCOLACOO*	1e6	G, L'
28	GCOLACOO* → GLYAC ⁻ + HO ₂	5e1	C
29	2GCOLACROO* → 2GCOLACO* + O ₂	3e8×0.95	L', e
30	2 GCOLACROO* → GLYAC ⁻ + OXLAC + O ₂	3e8×0.05	L', e
31	GCOLACO* → HCO ₂ H + CO ₂ ⁻	I	Gi, e
32	GCOLACO* → GLYAC*	1e7	Gi, e
33	GLY + OH → GLY* + H ₂ O	1.1e9	T
34	GLY* + O ₂ → GLYOO*	1e6	G, L'
35	GLYOO* → GLYAC + HO ₂	5e1	C
36	2GLYOO* → 2*CHOHOH + 2CO ₂ + O ₂ + 2H ₂ O	3e8	L'
37	*CHOHOH + O ₂ → HCO ₂ H + HO ₂	5e6	G, L'
38	GLYAC + OH → GLYAC* + H ₂ O	3.62e8	T
39	GLYAC* + O ₂ → GLYACOO*	1e6	G, L'
40	GLYACOO* → OXLAC + HO ₂	5e1	C
41	2GLYACOO* → 2CO ₂ + 2COOH	3e8	L'
42	*COOH + O ₂ → CO ₂ + HO ₂	5e6	G, L'

43	$\text{GLYAC} \leftrightarrow \text{H}^+ + \text{GLYAC}^-$	$K_{\text{eq}} = 3.47\text{e-}4$ $K_r = 2.0\text{e}10$	T
44	$\text{GLYAC}^- + \text{OH} \rightarrow \text{GLYAC}^{*-} + \text{H}_2\text{O}$	1.28e7	T
45	$\text{GLYAC}^- + \text{OH} \rightarrow \text{GLYAC}^* + \text{OH}^-$	2.9e9	T
46	$\text{GLYAC}^{*-} + \text{O}_2 \rightarrow \text{GLYACOO}^{*-}$	1e6	G, L'
47	$\text{GLYACOO}^{*-} \rightarrow \text{OXLAC}^- + \text{HO}_2$	1e2	C, L'
48	$2\text{GLYACOO}^{*-} \rightarrow 2\text{CO}_2^- + 2^*\text{COOH}$	3e8	L'
49	$\text{MGLY} + \text{OH} \rightarrow \text{MGLY}^* + \text{H}_2\text{O}$	7.0e8×0.92	T
50	$\text{MGLY} + \text{OH} \rightarrow ^*\text{MGLY} + \text{H}_2\text{O}$	7.0e8×0.08	T
51	$\text{MGLY}^* + \text{O}_2 \rightarrow \text{MGLYOO}^*$	1e6	G, L'
52	$\text{MGLYOO}^* \rightarrow \text{PYRAC} + \text{HO}_2$	5e1	C
53	$2\text{MGLYOO}^* \rightarrow 2\text{CO}_2 + 2\text{CH}_3\text{CO}_2\text{H} + \text{O}_2$	3e8	L'
54	$^*\text{MGLY} + \text{O}_2 \rightarrow ^*\text{OOMGLY}$	1e6	G, L'
55	$2^*\text{OOMGLY} \rightarrow 2^*\text{OMGLY} + \text{O}_2$	3e8×0.95	L', e
56	$2^*\text{OOMGLY} \rightarrow \text{HOMGLY} + \text{OMGLY} + \text{O}_2$	3e8×0.05	L', e
57	$^*\text{OMGLY} \rightarrow \text{HCHO} + \text{GLY}^*$	I	Gi, e
58	$^*\text{OMGLY} \rightarrow ^*\text{HOMGLY}$	1e7	Gi, e
59	$\text{HOMGLY} + \text{OH} \rightarrow ^*\text{HOMGLY} + \text{H}_2\text{O}$	4.10e7	M
60	$^*\text{HOMGLY} + \text{O}_2 \rightarrow ^*\text{OOHOMGLY}$	1e6	G, L'
61	$^*\text{OOHOMGLY} \rightarrow \text{OMGLY} + \text{HO}_2$	5e1	C
62	$\text{OMGLY} + \text{OH} \rightarrow ^*\text{OMGLY} + \text{H}_2\text{O}$	6.17e9	M
63	$^*\text{OMGLY} + \text{O}_2 \rightarrow ^*\text{OOMGLY}$	5e1	C
64	$\text{GLY}^* + ^*\text{CHOHOH} \rightarrow \text{C3D}$	1.3e9	G, L'
65	$2\text{GLY}^* \rightarrow \text{C4D}$	1.3e9	G, L'
66	$\text{GLY}^* + ^*\text{COOH} \rightarrow \text{C3D}$	1.3e9	G, L'
67	$\text{GLYAC}^* + ^*\text{COOH} \rightarrow \text{C3D}$	1.3e9	G, L'
68	$\text{GLYAC}^* + ^*\text{CHOHOH} \rightarrow \text{C3D}$	1.3e9	G, L'
69	$2\text{GLYAC}^* \rightarrow \text{C4D}$	1.3e9	G, L'
70	$\text{GLYAC}^* + \text{GLY}^* \rightarrow \text{C4D}$	1.3e9	G, L'
71	$\text{GLYAC}^{*-} + \text{GLY}^* \rightarrow \text{C4D}$	1.3e9	G, L'
72	$\text{GLYAC}^{*-} + \text{GLYAC}^* \rightarrow \text{C4D}$	1.3e9	G, L'
73	$2\text{GLYAC}^{*-} \rightarrow \text{C4D}$	1.3e9	G, L'
74	$\text{GLYAC}^{*-} + ^*\text{COOH} \rightarrow \text{C3D}$	1.3e9	G, L'
75	$\text{GLYAC}^{*-} + ^*\text{CHOHOH} \rightarrow \text{C3D}$	1.3e9	G, L'
76	$\text{GLYCOL}^{*1} + ^*\text{CHOHOH} \rightarrow \text{C3D}$	1.3e9	G, L'
77	$\text{GLYCOL}^{*1} + \text{GLY}^* \rightarrow \text{C4D}$	1.3e9	G, L'
78	$\text{GLYCOL}^{*1} + ^*\text{COOH} \rightarrow \text{C3D}$	1.3e9	G, L'
79	$\text{GLYCOL}^{*1} + \text{GLYAC}^* \rightarrow \text{C4D}$	1.3e9	G, L'
80	$\text{GLYCOL}^{*1} + \text{GLYAC}^{*-} \rightarrow \text{C4D}$	1.3e9	G, L'
81	$\text{GLYCOL}^{*2} + ^*\text{CHOHOH} \rightarrow \text{C3D}$	1.3e9	G, L'
82	$\text{GLYCOL}^{*2} + \text{GLY}^* \rightarrow \text{C4D}$	1.3e9	G, L'
83	$\text{GLYCOL}^{*2} + ^*\text{COOH} \rightarrow \text{C3D}$	1.3e9	G, L'
84	$\text{GLYCOL}^{*2} + \text{GLYAC}^* \rightarrow \text{C4D}$	1.3e9	G, L'
85	$\text{GCOLAC}^* + ^*\text{CHOHOH} \rightarrow \text{C3D}$	1.3e9	G, L'
86	$\text{GCOLAC}^* + \text{GLY}^* \rightarrow \text{C4D}$	1.3e9	G, L'
87	$\text{GCOLAC}^* + ^*\text{COOH} \rightarrow \text{C3D}$	1.3e9	G, L'
88	$\text{GCOLAC}^* + \text{GLYAC}^* \rightarrow \text{C4D}$	1.3e9	G, L'
89	$\text{GCOLAC}^* + \text{GLYAC}^{*-} \rightarrow \text{C4D}$	1.3e9	G, L'
90	$\text{GCOLAC}^* + \text{GLYCOL}^{*1} \rightarrow \text{C4D}$	1.3e9	G, L'
91	$\text{GCOLAC}^* + \text{GLYCOL}^{*2} \rightarrow \text{C4D}$	1.3e9	G, L'

92	$\text{GCOLAC}^* + \text{GCOLAC}^* \rightarrow \text{C4D}$	1.3e9	G, L'
93	$\text{GCOLAC}^{*-} + * \text{CHOHOH} \rightarrow \text{C3D}$	1.3e9	G, L'
94	$\text{GCOLAC}^{*-} + \text{GLY}^* \rightarrow \text{C4D}$	1.3e9	G, L'
95	$\text{GCOLAC}^{*-} + * \text{COOH} \rightarrow \text{C3D}$	1.3e9	G, L'
96	$\text{GCOLAC}^{*-} + \text{GLYAC}^* \rightarrow \text{C4D}$	1.3e9	G, L'
97	$\text{GCOLAC}^{*-} + \text{GLYAC}^{*-} \rightarrow \text{C4D}$	1.3e9	G, L'
98	$\text{GCOLAC}^{*-} + \text{GLYAC}^{*-} \rightarrow \text{C4D}$	1.3e9	G, L'
99	$\text{GCOLAC}^{*-} + \text{GLYCOL}^{*1} \rightarrow \text{C4D}$	1.3e9	G, L'
100	$\text{GCOLAC}^{*-} + \text{GLYCOL}^{*2} \rightarrow \text{C4D}$	1.3e9	G, L'
101	$\text{GCOLAC}^{*-} + \text{GCOLAC}^* \rightarrow \text{C4D}$	1.3e9	G, L'
102	$2 \text{GCOLAC}^{*-} \rightarrow \text{C4D}$	1.3e9	G, L'
103	$2 \text{MGLY}^* \rightarrow \text{C6D}$	1.3e9	G, L'
104	$\text{MGLY}^* + * \text{CHOHOH} \rightarrow \text{C4D}$	1.3e9	G, L'
105	$\text{MGLY}^* + \text{GLY}^* \rightarrow \text{C5D}$	1.3e9	G, L'
106	$\text{MGLY}^* + * \text{COOH} \rightarrow \text{C4D}$	1.3e9	G, L'
107	$\text{MGLY}^* + \text{GLYAC}^* \rightarrow \text{C5D}$	1.3e9	G, L'
108	$\text{MGLY}^* + \text{GLYAC}^{*-} \rightarrow \text{C5D}$	1.3e9	G, L'
109	$\text{MGLY}^* + \text{GLYCOL}^{*1} \rightarrow \text{C5D}$	1.3e9	G, L'
110	$\text{MGLY}^* + \text{GLYCOL}^{*2} \rightarrow \text{C5D}$	1.3e9	G, L'
111	$\text{MGLY}^* + \text{GCOLAC}^* \rightarrow \text{C5D}$	1.3e9	G, L'
112	$\text{MGLY}^* + \text{GCOLAC}^{*-} \rightarrow \text{C5D}$	1.3e9	G, L'
113	$\text{MGLY}^* + \text{CH}_3\text{CO}^* \rightarrow \text{C5D}$	1.3e9	G, L'
114	$\text{MGLY}^* + * \text{HOPYRAC} \rightarrow \text{C6D}$	1.3e9	G, L'
115	$2 * \text{HOPYRAC} \rightarrow \text{C6D}$	1.3e9	G, L'
116	$\text{MGLY}^* + * \text{HOPYRAC}^- \rightarrow \text{C6D}$	1.3e9	G, L'
117	$* \text{HOPYRAC}^- + * \text{HOPYRAC}^- \rightarrow \text{C6D}$	1.3e9	G, L'
118	$* \text{HOPYRAC} + * \text{HOPYRAC}^- \rightarrow \text{C6D}$	1.3e9	G, L'
119	$\text{CH}_3\text{CO}^* + * \text{HOPYRAC} \rightarrow \text{C6D}$	1.3e9	G, L'
120	$\text{CH}_3\text{CO}^* + * \text{HOPYRAC}^- \rightarrow \text{C6D}$	1.3e9	G, L'
121	$2 \text{LA}^* \rightarrow \text{C6D}$	1.3e9	G, L'
122	$\text{LA}^* + \text{MGLY}^* \rightarrow \text{C6D}$	1.3e9	G, L'
123	$\text{LA}^* + * \text{CHOHOH} \rightarrow \text{C4D}$	1.3e9	G, L'
124	$\text{LA}^* + \text{GLY}^* \rightarrow \text{C5D}$	1.3e9	G, L'
125	$\text{LA}^* + * \text{COOH} \rightarrow \text{C4D}$	1.3e9	G, L'
126	$\text{LA}^* + \text{GLYAC}^* \rightarrow \text{C5D}$	1.3e9	G, L'
127	$\text{LA}^* + \text{GLYAC}^{*-} \rightarrow \text{C5D}$	1.3e9	G, L'
128	$\text{LA}^* + \text{GLYCOL}^{*1} \rightarrow \text{C5D}$	1.3e9	G, L'
129	$\text{LA}^* + \text{GLYCOL}^{*2} \rightarrow \text{C5D}$	1.3e9	G, L'
130	$\text{LA}^* + \text{GCOLAC}^* \rightarrow \text{C5D}$	1.3e9	G, L'
131	$\text{LA}^* + \text{GCOLAC}^{*-} \rightarrow \text{C5D}$	1.3e9	G, L'
132	$\text{LA}^* + \text{CH}_3\text{CO}^* \rightarrow \text{C5D}$	1.3e9	G, L'
133	$2 \text{CH}_3\text{CO}^* \rightarrow \text{C4D}$	1.3e9	G, L'
134	$\text{LA}^* + * \text{HOPYRAC} \rightarrow \text{C6D}$	1.3e9	G, L'
135	$\text{LA}^* + * \text{HOPYRAC}^- \rightarrow \text{C6D}$	1.3e9	G, L'
136	$\text{OXLAC} + \text{OH} \rightarrow \text{COOH} + \text{CO}_2 + \text{H}_2\text{O}$	1.4e6	T
137	$\text{OXLAC} \leftrightarrow \text{H}^+ + \text{OXLAC}^-$	$K_{\text{eq}} = 5.67\text{e-}2$ $k_r = 5.0\text{e}10$	T
138	$\text{OXLAC}^- + \text{OH} \rightarrow \text{COOH} + \text{CO}_2^- + \text{H}_2\text{O}$	2.0e7	T, L'
139	$\text{OXLAC}^- \leftrightarrow \text{H}^+ + \text{OXLAC}^{-2}$	$K_{\text{eq}} = 5.42\text{e-}5$ $k_r = 5\text{e}10$	T
140	$\text{OXLAC}^{-2} + \text{OH} \rightarrow * \text{COOH} + \text{CO}_2^- + \text{OH}^-$	4.0e7	T, L'

141	$LA + OH \rightarrow LA^* + H_2O$	4.3e8	H
142	$LA^* + O_2 \rightarrow LAOO^*$	1e6	G, L'
143	$LAROO^* \rightarrow PYRAC + HO_2$	5e1	C
144	$LA \leftrightarrow LA^- + H^+$	$K_{eq} = 1.38e-4$ $k_r = 5.0e10$	E&C
145	$LA^- + OH \rightarrow LA^{*-} + H_2O$	3e8	B
146	$LA^{*-} + O_2 \rightarrow LAOO^{*-}$	1e6	G, L'
147	$LAOO^{*-} \rightarrow PYRAC^- + HO_2$	5e1	C
148	$PYRAC + OH \rightarrow PYRAC^* + H_2O$	6.0e7×0.85	T
149	$PYRAC + OH \rightarrow CH_3CO^* + CO_2 + H_2O$	6.0e7×0.15	T
150	$CH_3CO^* + O_2 \rightarrow CH_3C(O)OO^*$	1e6	G, L'
151	$CH_3C(O)OO^* \rightarrow CH_3CO_2H + HO_2$	5e1	C
152	$2CH_3C(O)OO^* \rightarrow 2CH_3C(O)O^* + O_2$	3e8	L'
153	$CH_3C(O)O^* \rightarrow CO_2 + HCHO$	1e7	Gi
154	$PYRAC^* + O_2 \rightarrow PYRACOO^*$	1e6	G, L'
144	$2PYRACOO^* \rightarrow 2PYRACO^* + O_2$	3e8×0.95	L', e
145	$2PYRACOO^* \rightarrow HOPYRAC + OPYRAC + O_2$	3e8×0.15	L', e
146	$PYRACO^* \rightarrow HCHO + GLYAC^*$	I	Gi, e
147	$PYRACO^* \rightarrow *HOPYRAC$	1e7	Gi, e
148	$HOPYRAC + OH \rightarrow *HOPYRAC + H_2O$	3.6e8	H
149	$*HOPYRAC + O_2 \rightarrow *OOHOPYRAC$	1e6	G, L'
150	$*OOHOPYRAC \rightarrow OPYRAC + HO_2$	5e1	C
151	$OPYRAC + OH \rightarrow *OPYRAC + H_2O$	5e7	e
152	$*OPYRAC + O_2 \rightarrow *OO(O)PYRAC$	1e6	G, L'
153	$*OO(O)PYRAC \rightarrow MOXLAC + HO_2$	5e1	C
154	$PYRAC \leftrightarrow PYRAC^- + H^+$	$K_{eq} = 3.2e-3$ $k_r = 2e10$	T
155	$PYRAC^- + OH \rightarrow PYRAC^{*-} + H_2O$	6.0e7×0.95	T
156	$PYRAC^- + OH \rightarrow CH_3CO^* + CO_2 + OH^-$	6.0e7×0.05	T
157	$PYRAC^{*-} + O_2 \rightarrow PYRACOO^{*-}$	5e1	C
158	$2PYRACOO^{*-} \rightarrow 2PYRACO^{*-} + O_2$	3e8×0.95	L', e
159	$2PYRACOO^{*-} \rightarrow HOPYRAC^- + OPYRAC^- + O_2$	3e8×0.05	L', e
160	$PYRACO^{*-} \rightarrow HCHO + GLYAC^{*-} + O_2$	I	Gi, e
161	$PYRACO^{*-} \rightarrow *HOPYRAC^-$	1e7	Gi, e
162	$HOPYRAC \leftrightarrow HOPYRAC^- + H^+$	$K_{eq} = 3.2e-3$ $k_r = 2e10$	e
163	$OPYRAC \leftrightarrow OPYRAC^- + H^+$	$K_{eq} = 3.2e-3$ $k_r = 2e10$	e
164	$HOPYRAC^- + OH \rightarrow *HOPYRAC^- + H_2O$	2.6e9	H
165	$*HOPYRAC^- + O_2 \rightarrow *OOHOPYRAC^-$	1e6	G, L'
166	$*OOHOPYRAC^- \rightarrow OPYRAC^- + HO_2$	5e1	C
167	$OPYRAC^- + OH \rightarrow *OPYRAC^- + H_2O$	5e7	M
168	$*OPYRAC^- + O_2 \rightarrow *OO(O)PYRAC^-$	1e6	G, L'
169	$*OO(O)PYRAC^- \rightarrow MOXLAC^- + HO_2$	5e1	C
170	$MOXLAC^- + OH \rightarrow GLYAC^* + CO_2 + H_2O$	5.7e7	Gl
171	$MOXLAC^- + OH \rightarrow GLYAC^{*-} + CO_2 + H_2O$	7.85e7	e
172	$MOXLAC^{-2} + OH \rightarrow GLYAC^{*-} + CO_2 + OH^-$	1.0e8	H
173	$MOXLAC \leftrightarrow MOXLAC^- + H^+$	$K_{eq} = 3.16e-3$ $k_r = 5e10$	H
174	$MOXLAC^- \leftrightarrow MOXLAC^{-2} + H^+$	$K_{eq} = 1.5e-2$	V

		$k_r = 5e10$	
175	$\text{CH}_3\text{CO}_2\text{H} + \text{OH} \rightarrow * \text{CH}_2\text{CO}_2\text{H} + \text{H}_2\text{O}$	1.36e7	T
176	$\text{CH}_3\text{CO}_2\text{H} + \text{OH} \rightarrow \text{CO}_2 + \text{HCHO} + \text{HO}_2 + \text{H}_2\text{O}$	2.40e6	T
177	$* \text{CH}_2\text{CO}_2\text{H} + \text{O}_2 \rightarrow * \text{OOCH}_2\text{CO}_2\text{H}$	1e6	G, L'
178	$2 * \text{OOCH}_2\text{CO}_2\text{H} \rightarrow 2 * \text{OCH}_2\text{CO}_2\text{H} + \text{O}_2$	$3e8 * 0.95$	L', e
179	$2 * \text{OOCH}_2\text{CO}_2\text{H} \rightarrow \text{GLYAC} + \text{GCOLAC} + \text{O}_2$	$3e8 * 0.05$	L', e
180	$* \text{OCH}_2\text{CO}_2\text{H} \rightarrow 2 \text{CO}_2 + 2 \text{HCHO}$	I	Gi, e
181	$* \text{OCH}_2\text{CO}_2\text{H} \rightarrow \text{GCOLAC}^*$	1e7	Gi, e
182	$\text{CH}_3\text{CO}_2\text{H} \leftrightarrow \text{CH}_3\text{CO}_2^- + \text{H}^+$	$K_{\text{eq}} = 1.75e-5$ $k_r = 5.0e10$	T
183	$\text{CH}_3\text{CO}_2^- + \text{OH} \rightarrow * \text{CH}_2\text{CO}_2^- + \text{H}_2\text{O}$	7.23e7	T
184	$\text{CH}_2\text{CO}_2^- + \text{OH} \rightarrow \text{CO}_2 + \text{HCHO} + \text{HO}_2 + \text{OH}^-$	1.28e7	T
185	$* \text{CH}_2\text{CO}_2^- + \text{O}_2 \rightarrow * \text{OOCH}_2\text{CO}_2^-$	1e6	G, L'
186	$2 * \text{OOCH}_2\text{CO}_2^- \rightarrow 2 * \text{OCH}_2\text{CO}_2^- + \text{O}_2$	$3e8 \times 0.95$	L', e
187	$2 * \text{OOCH}_2\text{CO}_2^- \rightarrow \text{GLYAC}^- + \text{GCOLAC}^- + \text{O}_2$	$3e8 \times 0.05$	L', e
188	$* \text{OCH}_2\text{CO}_2^- \rightarrow 2 \text{CO}_2^- + 2 \text{HCHO}$	I	Gi, e
189	$* \text{OCH}_2\text{CO}_2^- \rightarrow \text{GCOLAC}^*$	1e7	Gi, e
190	$\text{H}_2\text{O} \leftrightarrow \text{H}^+ + \text{OH}^-$	$K_{\text{eq}} = 1.0e-14$ $k_r = 1.4e11$	T
191	$\text{HO}_2 \leftrightarrow \text{H}^+ + \text{O}_2^-$	$K_{\text{eq}} = 1.6e-5$ $k_r = 5.0e10$	T
192	$\text{HCO}_2\text{H} + \text{OH} \rightarrow * \text{COOH} + \text{H}_2\text{O}$	1e8	T
193	$\text{HCO}_2^- + \text{OH} \rightarrow \text{CO}_2^- + \text{H}_2\text{O}$	2.4e9	T
194	$\text{HCO}_2\text{H} \leftrightarrow \text{H}^+ + \text{HCO}_2^-$	$K_{\text{eq}} = 1.77e-4$ $k_r = 5.0e10$	T
195	$\text{GLYAC} + \text{H}_2\text{O}_2 \rightarrow \text{HCO}_2\text{H} + \text{CO}_2 + \text{H}_2\text{O}$	0.3	T
196	$\text{PYRAC} + \text{H}_2\text{O}_2 \rightarrow \text{CH}_2\text{CO}_2\text{H} + \text{H}_2\text{O} + \text{CO}_2$	0.11	T
197	$\text{PYRAC}^- + \text{H}_2\text{O}_2 \rightarrow \text{CH}_2\text{CO}_2^- + \text{H}_2\text{O} + \text{CO}_2$	0.11	T
198	$\text{MOXLAC} + \text{H}_2\text{O}_2 \rightarrow \text{OXLAC} + \text{CO}_2 + \text{H}_2\text{O}$	0.5	T
199	$\text{MOXLAC}^- + \text{H}_2\text{O}_2 \rightarrow \text{OXLAC}^- + \text{CO}_2 + \text{H}_2\text{O}$	0.5	T
200	$\text{HCO}_2\text{H} + \text{OH} \rightarrow \text{COOH} + \text{H}_2\text{O}$	1e8	T
201	$\text{HCO}_2^- + \text{OH} \rightarrow \text{CO}_2^- + \text{H}_2\text{O}$	2.4e9	T
202	$\text{HCO}_2\text{H} \leftrightarrow \text{H}^+ + \text{HCO}_2^-$	$K_{\text{eq}} = 1.77e-4$ $k_r = 5.0e10$	T
203	$2 * \text{CHOHOH} \rightarrow \text{GLY}$	1.3e9	G, L'
204	$* \text{CHOHOH} + * \text{COOH} \rightarrow \text{GLYAC}$	1.3e9	G, L'
205	$2 * \text{COOH} \rightarrow \text{OXLAC}$	1.3e9	G, L'
206	$\text{C3D} \leftrightarrow \text{MA} + \text{H}_2\text{O}$	$K_{\text{eq}} = 1e5$ $k_r = 1e-8$	L'
207	$\text{MA} + \text{OH} \rightarrow \text{C3D}^* + \text{H}_2\text{O}$	1.6e7	E
208	$\text{TA} + \text{OH} \rightarrow \text{C4D}^* + \text{H}_2\text{O}$	3.1e8	M
209	$2 * \text{COOH} \rightarrow \text{OXLAC}$	1.3e9	G, L'
210	$\text{CO}_2^- + * \text{COOH} \rightarrow \text{OXLAC}^-$	1.3e9	G, L'
211	$2 \text{CO}_2^- \rightarrow \text{OXLAC}^{-2}$	1.3e9	G, L'
212	$\text{PYRAC}^- \rightarrow 0.45 \text{CH}_3\text{CO}_2^-^b$	$1e-4^b$	C, e
213	$\text{GCOLACOO}^* + \text{HO}_2 \rightarrow \text{GCOLACOOH} + \text{O}_2$	$3e6^c$	e
214	$\text{GCOLACOO}^* + \text{HO}_2 \rightarrow \text{GCOLACOOH} + \text{O}_2$	$3e6^c$	e
215	$* \text{OOMGLY} + \text{HO}_2 \rightarrow \text{HOOMGLY} + \text{O}_2$	$3e6^c$	e
216	$\text{PYRACOO}^* + \text{HO}_2 \rightarrow \text{PYRACOOH} + \text{O}_2$	$3e6^c$	e
217	$\text{PYRACOO}^* + \text{HO}_2 \rightarrow \text{PYRACOOH} + \text{O}_2$	$3e6^c$	e
218	$* \text{OOCH}_2\text{COOH} + \text{HO}_2 \rightarrow \text{HOCH}_2\text{COOH} + \text{O}_2$	$3e6^c$	e

219	$*\text{OOCH}_2\text{COO}^- + \text{HO}_2 \rightarrow \text{HOCH}_2\text{COO}^- + \text{O}_2$	$3\text{e}6^c$	e
220	$\text{GCOLACOOH} + \text{OH} \rightarrow \text{products}$	$6\text{e}8^d$	e
221	$\text{GCOLACOOH} + \text{OH} \rightarrow \text{products}$	$6\text{e}8^d$	e
222	$\text{HOOMGLY} + \text{OH} \rightarrow \text{products}$	$7\text{e}8^d$	e
223	$\text{PYRACOOH} + \text{OH} \rightarrow \text{products}$	$6\text{e}7^d$	e
224	$\text{PYRACOOH} + \text{OH} \rightarrow \text{products}$	$6\text{e}7^d$	e
225	$\text{HOCH}_2\text{COOH} + \text{OH} \rightarrow \text{products}$	$1.4\text{e}7^d$	e
226	$\text{MGLY} \leftrightarrow \text{DeMGLY}^c$	$K_{\text{eq}} = 2700$ $k_r = 6$	M S
227	$\text{DeMGLY} + \text{OH} \rightarrow \text{MGLY}^* + \text{H}_2\text{O}$	$7\text{e}8 \times 0.92^f$	T
228	$\text{DeMGLY} + \text{OH} \rightarrow * \text{MGLY} + \text{H}_2\text{O}$	$7\text{e}8 \times 0.08^f$	T
229	$\text{ROOH} + \text{DeMGLY} \leftrightarrow \text{PHA}$	$K_{\text{eq}} = 6.25$ $k_r = 1.6\text{e}-4$	T'
230	$\text{ROOH} \rightarrow \text{RO}^* + \text{OH}$	$k = 1.1\text{e}-4^h$	e
231	$\text{PHA} + \text{OH} \rightarrow \text{products}$	$7\text{e}8^g$	T
232	$\text{OH}_g \leftrightarrow \text{OH}$	$K_{\text{eq}} = 30^i$ $k_r = 3.5\text{e}5^j$	L W
233	$\text{HO}_{2g} \leftrightarrow \text{HO}_2$	$K_{\text{eq}} = 4\text{e}3^k$ $k_r = 4.2\text{e}5^l$	L W
234	$\text{ROOH}_g^m \leftrightarrow \text{ROOH}$	$K_{\text{eq}} = 1000^n$ $k_r = 5.7\text{e}2^o$	L W

^aTrans = Transmittance = $10^{-18.4 \times 0.80 \times [\text{H}_2\text{O}_2]}$; * = radical (e.g., glyoxal* = glyoxal radical); ⁿ = radical type n (e.g., GLYCOLAC*¹ = glycolic acid radical type 1); O* (or *O) = alkoxy radical; OO* (or *OO) = peroxy radical; C_nD = C_n dimer (e.g., C₂D = C₂ dimer); X_g = X in the gas phase (e.g., O_{2g} = O₂ in the gas phase); MGLY = methylglyoxal, PYRAC = pyruvic acid, GLYAC = glyoxylic acid, GLYCOL = glycolaldehyde, GLYCOLAC = glycolic acid, LA = lactic acid, MOXLAC = mesoxalic acid, OXLAC = oxalic acid; n = nth order; K_{eq} = the equilibrium constant (M), k_r = the reverse rate constant for corresponding K_{eq}. Thus, the forward rate constant can be calculated by K_{eq} × k_r; (g) = in the gas phase; I (= the decomposition rate constant from alkoxy radicals) = 5e6 s⁻¹ for ~10 μM acetic acid/methylglyoxal, 8e6 s⁻¹ for ~10² μM acetic acid/methylglyoxal, and 2e7 s⁻¹ for ~10³ μM acetic acid/ 3.2e7 s⁻¹ for ~10³ μM methylglyoxal; ^b PYRAC is assumed to photolyze to produce only 45% acetic acid with 5 times slower than the literature value (Carlton et al., 2006). ^c The rate constant for ROO* + HO₂ is assumed to be similar to that for HO₂ + HO₂ (ROO* = peroxy radical). ^d The rate constant for ROOH + OH is assumed to be that of the parent organic compound + OH (e.g. GCOLAC + OH for GCOLACOOH + OH). ^e DeMGLY = dehydrated MGLY (containing an aldehyde moiety). Therefore, MGLY is a hydrated form of methylglyoxal. ^f The rate constant for DeMGLY + OH is assumed to be the same as that for MGLY + OH. ^g The rate constant for PHA + OH is assumed to be the same as that for MGLY + OH. ^h The ROOH photolysis rate is assumed to be the same as the H₂O₂ photolysis rate. ⁱ Henry's law constant for OH. ^j diffusion-controlled transfer coefficient for OH. However, these h and j values are changed to maintain ~1e-14 M of OH; otherwise, OH is ~1e-12 M. ^k Henry's law constant for OH₂. ^l diffusion-controlled transfer coefficient for OH₂. ^m It is assumed that [ROOH]_g = 1ppb. ⁿ Henry's law constant for ROOH. ^o diffusion-controlled transfer coefficient for ROOH (based on the estimation by Lim et al, 2005).

Reference

T = Tan et al., 2009, 2010 and 2012
G = Guzman et al., JPCA, 2006
C = Carter et al., JPC, 1979
H = Herrmann et al., AE, 2005
E = Ervens et al., PCCP, 2003
M = Monod et al., AE, 2005, 2008
L = Lim et al., EST, 2005
L' = Lim et al., ACP, 2010
W = Warneck, PCCP, 1999

E&C = Eyal and Canari, *Ind. Eng. Chem. Res.*, 1995

B = Buxton et al., *JPCRD*, 1988

Gi = Gilbert et al., 1976 and 1981

V = Volgger et al., *J. Chrom. A*, 1997

e = Estimation

S = Sareen et al., *PNAS*, 2013

T' = Tran and Ziemann, unpublished data, 2006

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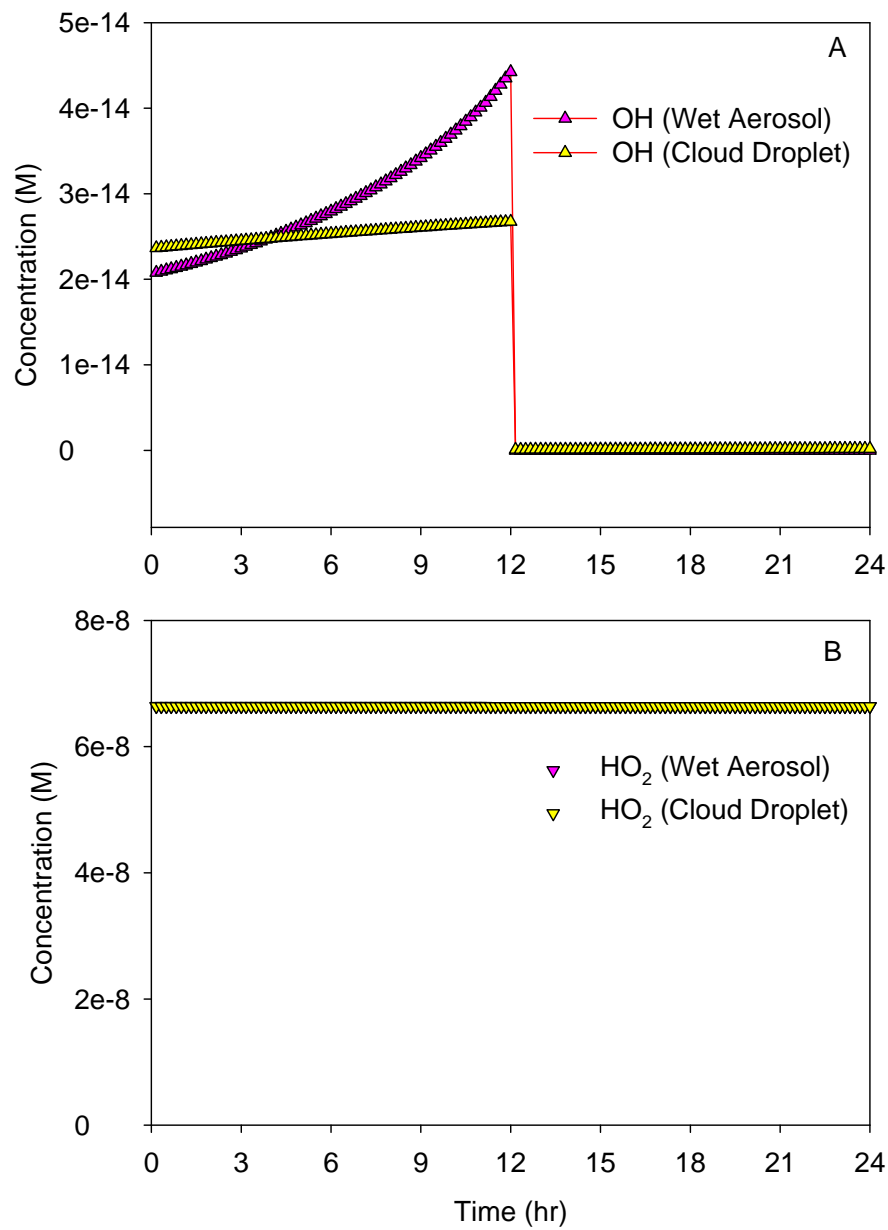


Fig. S1. The atmospheric simulated concentrations of OH (A) and HO₂ (B) in wet aerosols and cloud droplets for 24 hours (The first 12 hrs are daytime)

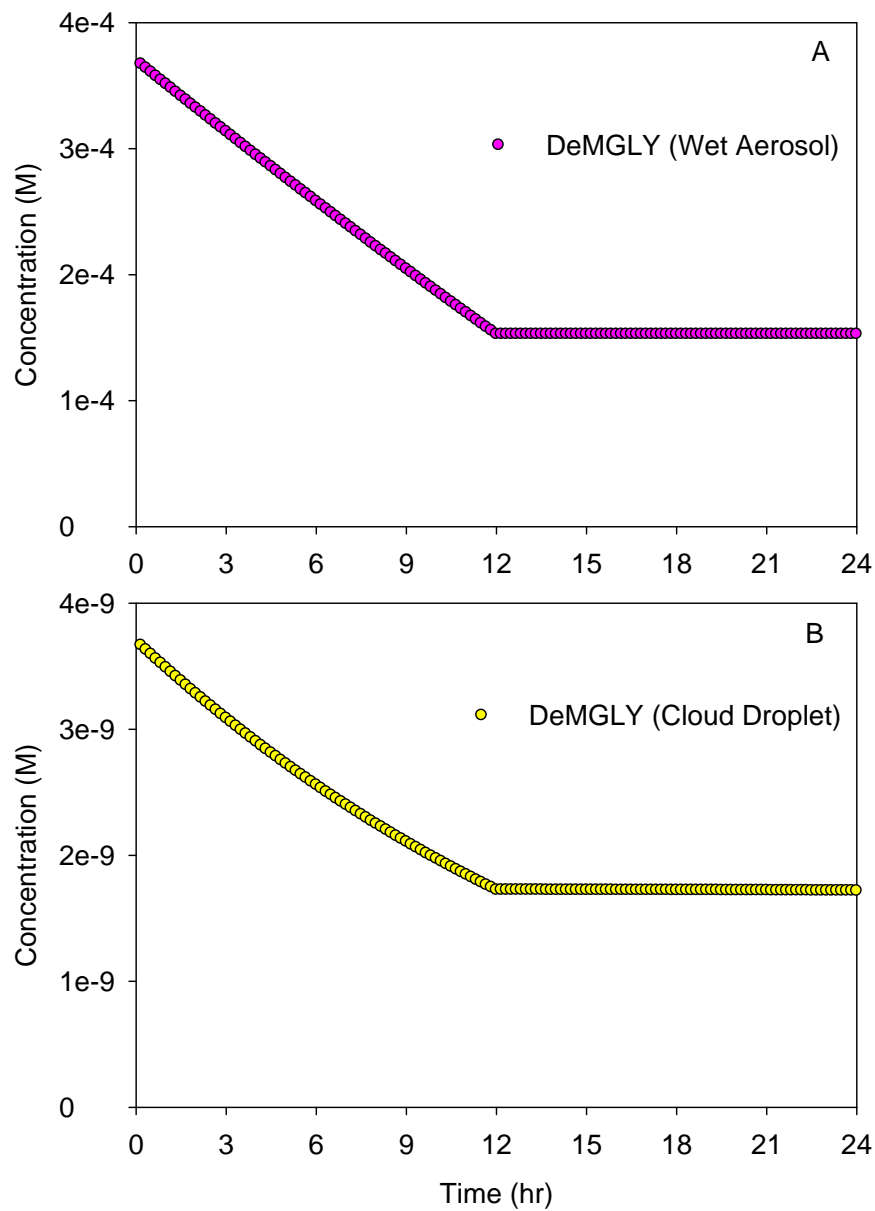


Fig. S2. The atmospheric simulated concentrations of DeMGLY (dehydrated methylglyoxal) in wet aerosols (A) and cloud droplets (B) for 24 hours (The first 12 hrs are daytime)

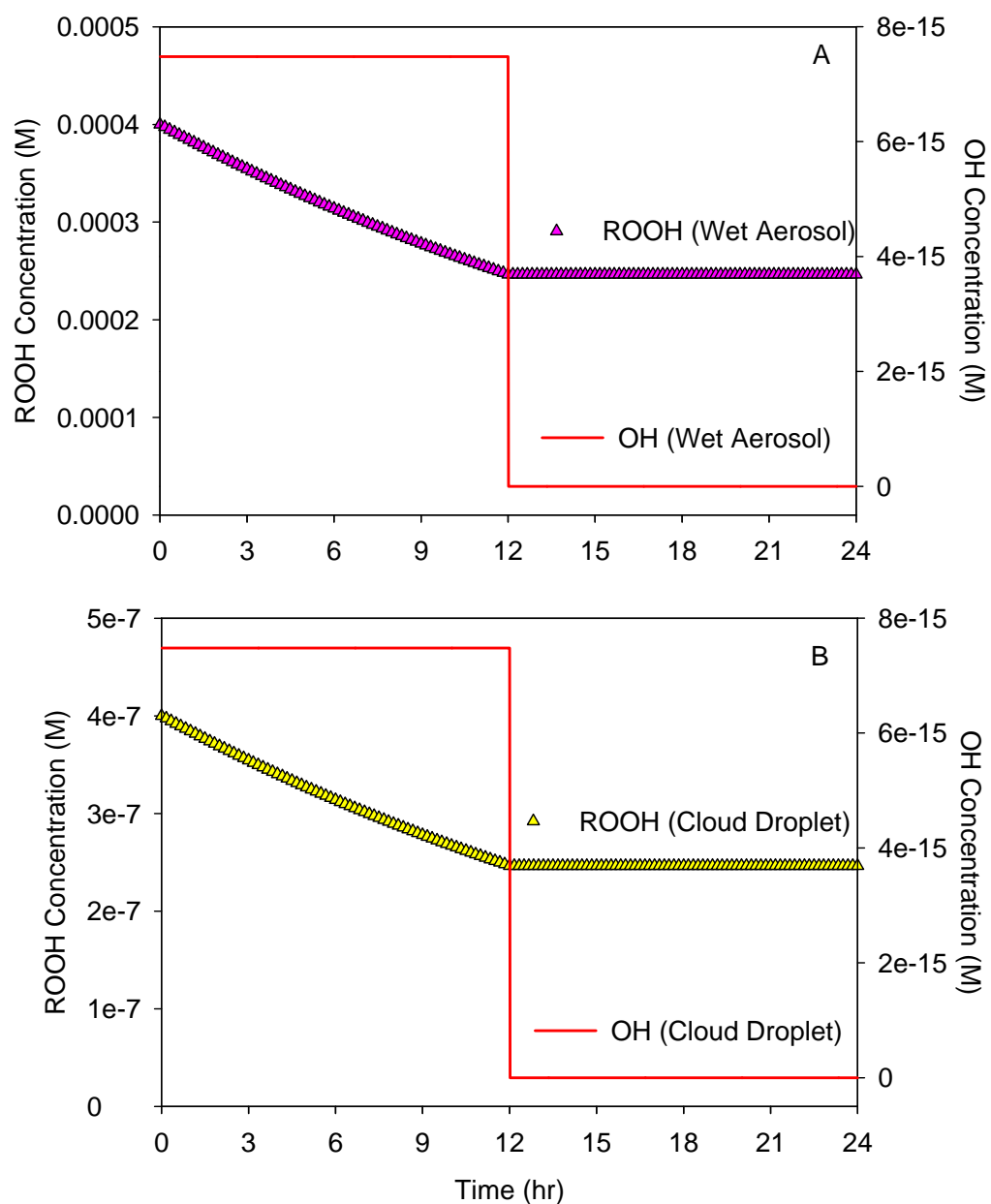


Fig. S3. The atmospheric simulated concentrations of ROOH and OH in wet aerosols (A) and cloud droplets (B) for 24 hours (The first 12 hrs are daytime)