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*Supplement of*

## **Compositional evolution of particle-phase reaction products and water in the heterogeneous OH oxidation of model aqueous organic aerosols**

**Man Mei Chim et al.**

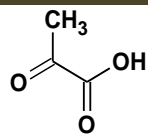
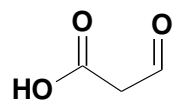
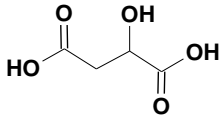
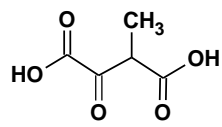
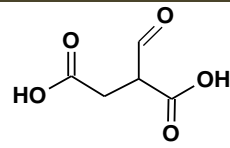
*Correspondence to:* Man Nin Chan (mnchan@cuhk.edu.hk)

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**Table S1. Experimental data obtained from the hygroscopicity measurement.**

<b>Relative Humidity (%)</b>	<b>Refractive Index (650nm)</b>	<b>Refractive Index (589nm)</b>	<b>Mass fraction of solute, <i>mfs</i></b>
87.0	1.411	1.417	0.595
83.4	1.418	1.424	0.642
72.8	1.433	1.439	0.743
68.0	1.440	1.446	0.791
65.6	1.444	1.450	0.818
63.0	1.446	1.452	0.831
85.8	1.415	1.421	0.622
83.2	1.421	1.427	0.662
80.8	1.425	1.431	0.689
78.3	1.428	1.434	0.710
75.8	1.432	1.438	0.737
73.4	1.435	1.441	0.757
71.0	1.438	1.444	0.777
68.5	1.439	1.445	0.784
66.1	1.442	1.447	0.801
63.7	1.444	1.449	0.814
61.3	1.446	1.452	0.831
58.9	1.447	1.453	0.838
56.5	1.450	1.456	0.858
54.2	1.451	1.457	0.865
51.8	1.453	1.459	0.879
49.4	1.455	1.461	0.892
47.1	1.456	1.462	0.899
44.5	1.458	1.463	0.909
41.8	1.459	1.464	0.916
39.0	1.460	1.466	0.926
36.2	1.463	1.469	0.946
33.4	1.464	1.470	0.953
30.7	1.465	1.471	0.960
28.0	1.467	1.473	0.973
25.3	1.468	1.474	0.980

Table S2. Minor reaction products observed in the heterogeneous OH oxidation of aqueous methylsuccinic acid droplet. The relative abundance is reported at the maximum OH exposure ( $1.47 \times 10^{12}$  molecule  $\text{cm}^{-3}$  s) at ionization efficiency = 1.

Chemical Formula	Molecular Weight	Relative Abundance (%)	Proposed Chemical Structure	
$\text{C}_3\text{H}_4\text{O}_3$	87	1.1	 <p>1<sup>st</sup> generation fragmentation product (Scheme 1, Path A)</p>	 <p>1<sup>st</sup> generation fragmentation product (Scheme 1, Path C)</p>
$\text{C}_3\text{H}_4\text{O}_4$	103	1.3	Possible 2 <sup>nd</sup> generation product	
$\text{C}_4\text{H}_4\text{O}_4$	115	1.1	Possible 2 <sup>nd</sup> generation product	
$\text{C}_4\text{H}_6\text{O}_4$	117	1.1	Possible 2 <sup>nd</sup> generation product	
$\text{C}_4\text{H}_6\text{O}_5$	133	1.8	 <p>1<sup>st</sup> generation fragmentation product (Scheme 1, Path C)</p>	
$\text{C}_5\text{H}_6\text{O}_5$	145	1.1	 <p>1<sup>st</sup> generation ketone functionalization product (Scheme 1, Path B)</p>	 <p>1<sup>st</sup> generation ketone functionalization product (Scheme 1, Path C)</p>
$\text{C}_5\text{H}_8\text{O}_6$	163	1.0	Possible 2 <sup>nd</sup> generation product	

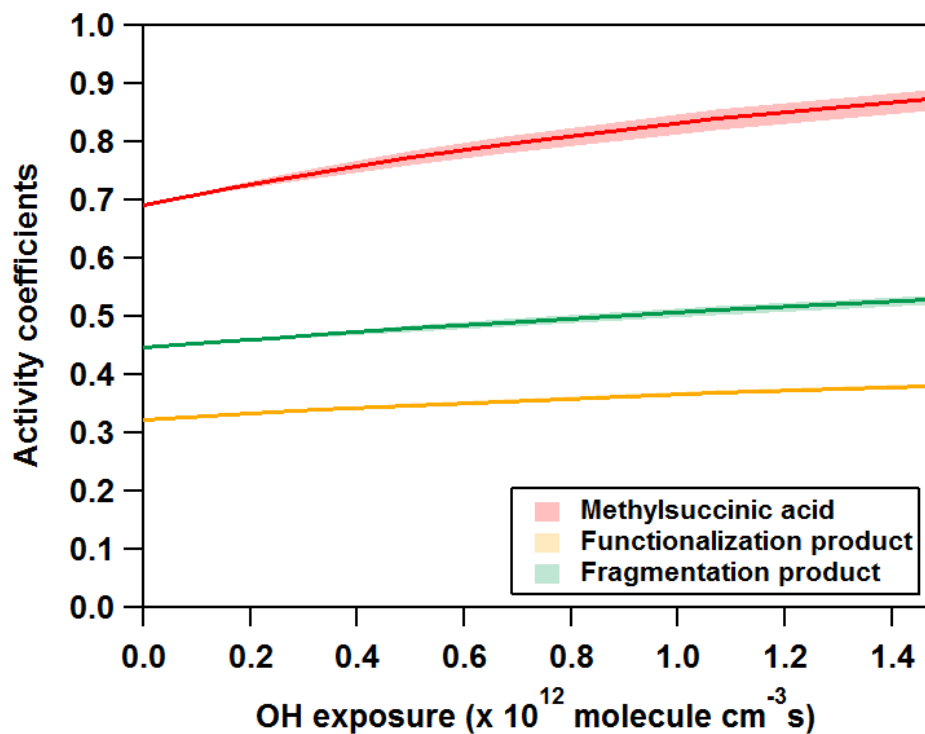


Figure S1. Simulated change of activity coefficients ( $\gamma_i$ ) of parent ( $C_5H_8O_4$ ), major functionalization ( $C_5H_8O_5$ ) and major fragmentation ( $C_4H_6O_3$ ) products (listed in Scheme 2) estimated by the AIOMFAC model. It is noted that no reaction products are formed prior to oxidation (i.e. OH exposure of 0 molecule  $cm^{-3}$  s). The results show the simulated activity coefficients of the two reaction products once the oxidation is initiated. The shaded region shows the error of the effective OH uptake coefficient ( $\gamma_{eff}$ ) measurement in the model simulation.