Electronic Supplementary Material to: Highly Oxidized Molecules Make a Significant Contribution to Enhanced Aromatic-Derived Secondary Organic Aerosol under a Humid Environment*

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Table S1. Mixing time scale (τ_m) of organic molecules within toluene SOA under different RH conditions.

RH conditions	D_p (nm)[1]	D_{org} ($cm^2\ s^{-1}$)[2]	τ_m (min)	SOA
High RH (~70%)	228 ± 6	1×10^{-12}	0.69 ± 0.04	Liquid
Medium RH	167 ± 22	2×10^{-15}	188 ± 49	Semisolid
Low RH (~8%)	111± 14	3×10^{-17}	5578 ±1404	Solid or semisolid

[1]The diameter of SOA at the reaction time of 240 min.
[2]The values were extracted from the studies of Song et al. (2016) and Li et al. (2018).

* The online version of this article can be found at https://doi.org/10.1007/s00376-024-4085-y.

Table S2. Unique CHO compounds in toluene SOA under different RH conditions.

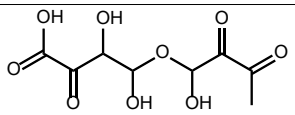
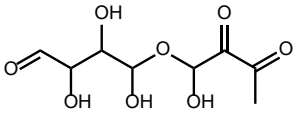
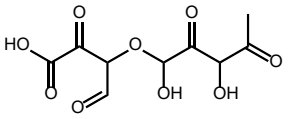
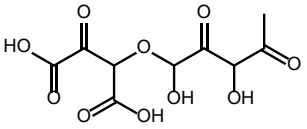
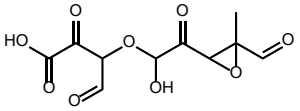
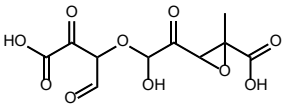
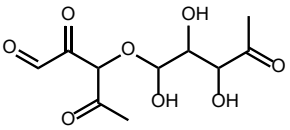
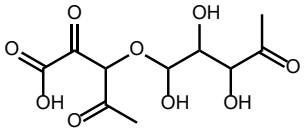
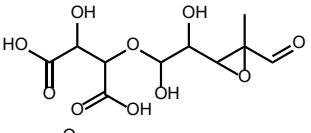
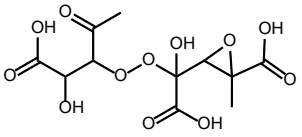
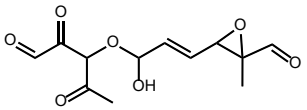
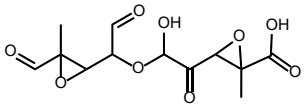
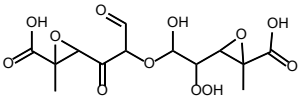
[M–H]⁻	Suggested molecular formula	~70% RH		~8% RH		Proposed molecular structure
		Absolute intensity	Relative intensity (%)	Absolute intensity	Relative intensity (%)	
249.02426	$C_8H_{10}O_9$	3992	2.3	–	–	
235.04422	$C_8H_{12}O_8$	5057	3.0	–	–	
261.02361	$C_9H_{10}O_9$	6513	3.8	–	–	
277.01873	$C_9H_{10}O_{10}$	3272	1.9	–	–	
273.02350	$C_{10}H_{10}O_9$	6296	3.7	–	–	
289.01780	$C_{10}H_{10}O_{10}$	3342	2.0	–	–	
261.05937	$C_{10}H_{14}O_8$	4258	2.5	–	–	
277.05404	$C_{10}H_{14}O_9$	4761	2.8	–	–	
293.04883	$C_{10}H_{14}O_{10}$	4013	2.4	–	–	
337.03957	$C_{11}H_{14}O_{12}$	3139	1.8	–	–	
269.06463	$C_{12}H_{14}O_7$	4583	2.7	–	–	
301.05448	$C_{12}H_{14}O_9$	9276	5.4	–	–	
363.05497	$C_{13}H_{16}O_{12}$	6675	3.9	–	–	

Table S2. (Continued.)

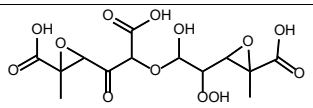
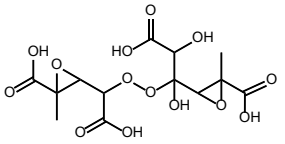
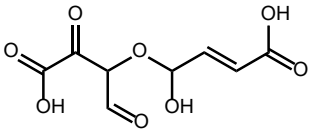
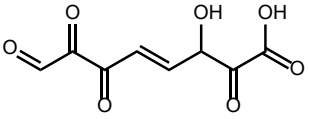
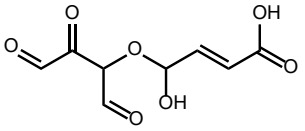
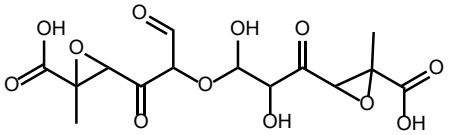
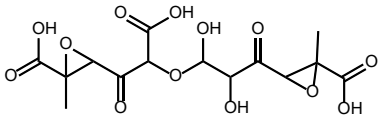
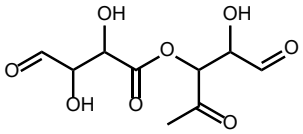
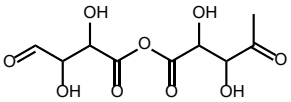
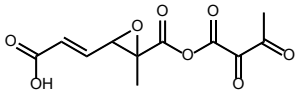
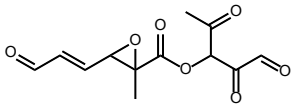
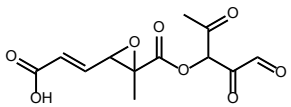
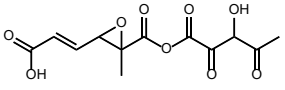
[M–H]⁻	Suggested molecular formula	~70% RH		~8% RH		Proposed molecular structure
		Absolute intensity	Relative intensity (%)	Absolute intensity	Relative intensity (%)	
379.05015	$C_{13}H_{16}O_{13}$	4210	2.5	–	–	
395.04585	$C_{13}H_{16}O_{14}$	2119	1.2	–	–	
231.01342	$C_8H_8O_8$	4448	2.6	–	–	
213.00480	$C_8H_6O_7$	3532	2.1	–	–	
215.01850	$C_8H_8O_7$	7565	4.4	–	–	
375.05595	$C_{14}H_{16}O_{12}$	6640	3.9	–	–	
391.05031	$C_{14}H_{16}O_{13}$	5002	2.9	–	–	
247.04456	$C_9H_{12}O_8$	–	–	3675	2.4	
263.03959	$C_9H_{12}O_9$	–	–	2420	1.6	
269.02978	$C_{11}H_{10}O_8$	–	–	3838	2.5	
267.05028	$C_{12}H_{12}O_7$	–	–	5118	3.3	
283.04538	$C_{12}H_{12}O_8$	–	–	5088	3.3	
299.04069	$C_{12}H_{12}O_9$	–	–	4130	2.7	

Table S2. (Continued.)

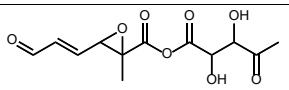
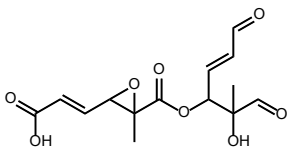
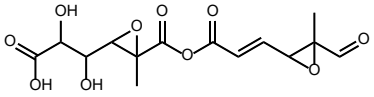
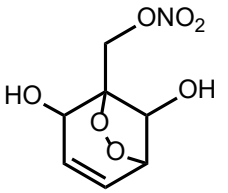
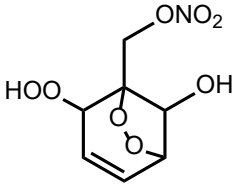
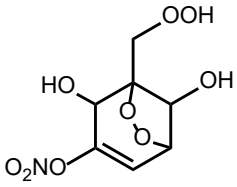
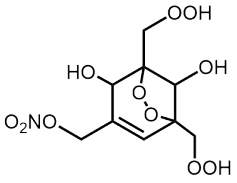
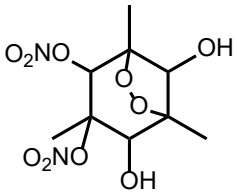
[M–H]⁻	Suggested molecular formula	~70% RH		~8% RH		Proposed molecular structure
		Absolute intensity	Relative intensity (%)	Absolute intensity	Relative intensity (%)	
285.05997	$C_{12}H_{14}O_8$	–	–	4925	3.2	
311.07503	$C_{14}H_{16}O_8$	–	–	3140	2.0	
343.06514	$C_{14}H_{16}O_{10}$	–	–	3786	2.4	

Table S3. Highly oxidized nitrates only observed in SOA formed under 70% RH.

Measured [M–H]⁻	Theoretical [M–H]⁻	Suggested molecular formula	Error (ppm)	Proposed molecular structure
		Toluene-derived SOA		
218.03107	218.03063	$C_7H_9NO_7$	–2.03	
234.02582	234.02554	$C_7H_9NO_8$	–1.18	
250.02032	250.02045	$C_7H_9NO_9$	0.53	
		1,3,5-Trimethylbenzene-derived SOA		
310.04138	310.04158	$C_9H_{13}NO_{11}$	0.66	
309.05723	309.05757	$C_9H_{14}N_2O_{10}$	1.10	

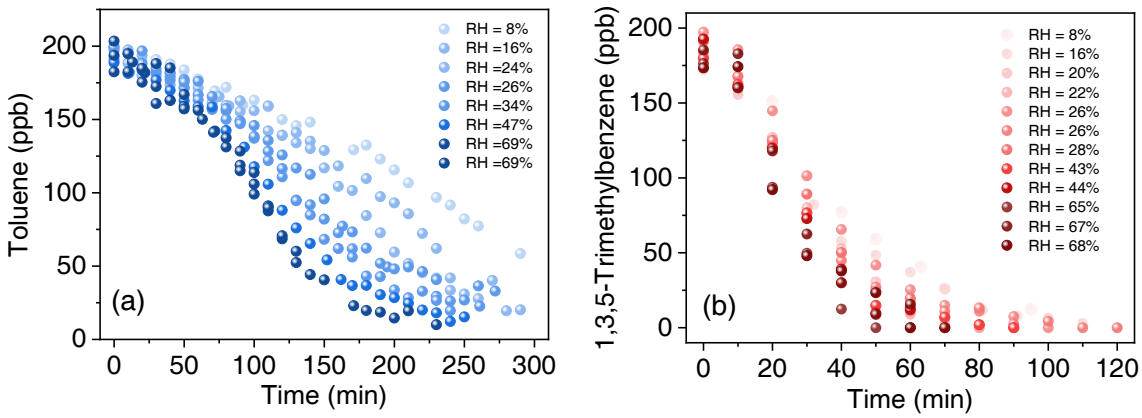
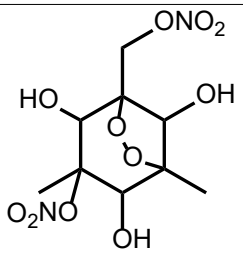


Fig. S1. Concentrations of (a) toluene and (b) 1,3,5-trimethylbenzene as a function of reaction time under different RH conditions.

Table S3. (Continued.)

Measured $[M–H]^-$	Theoretical $[M–H]^-$	Suggested molecular formula	Error (ppm)	Proposed molecular structure
325.05140	325.05248	$C_9H_{14}N_2O_{11}$	3.32	

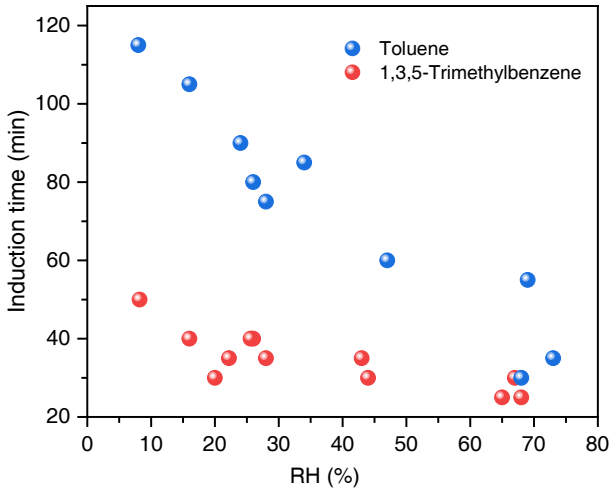


Fig. S2. Induction time of SOA formed from the photooxidation of toluene and 1,3,5-trimethylbenzene as a function of RH.

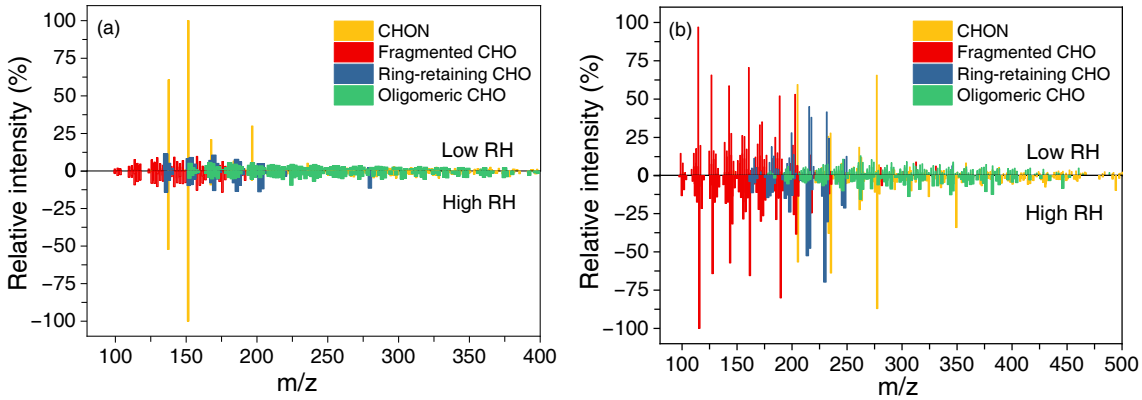


Fig. S3. Negative ion mode mass spectra of SOA formed from the photooxidation of (a) toluene and (b) 1,3,5-trimethylbenzene under low RH (~8%) and high RH (~70%) conditions.

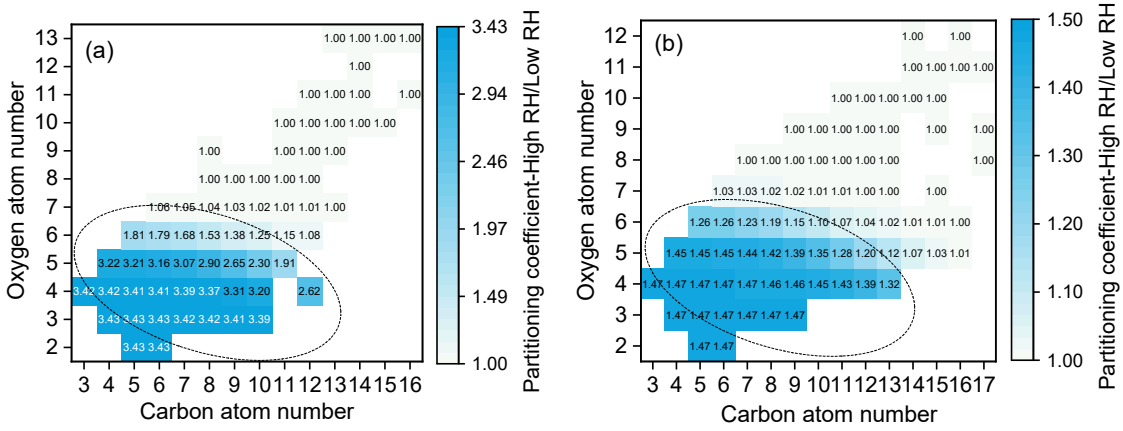


Fig. S4. Ratios of partitioning coefficients of common CHO compounds under low RH (~8%) and high RH (~70%) conditions. (a) Toluene SOA; (b) 1,3,5-trimethylbenzene SOA.

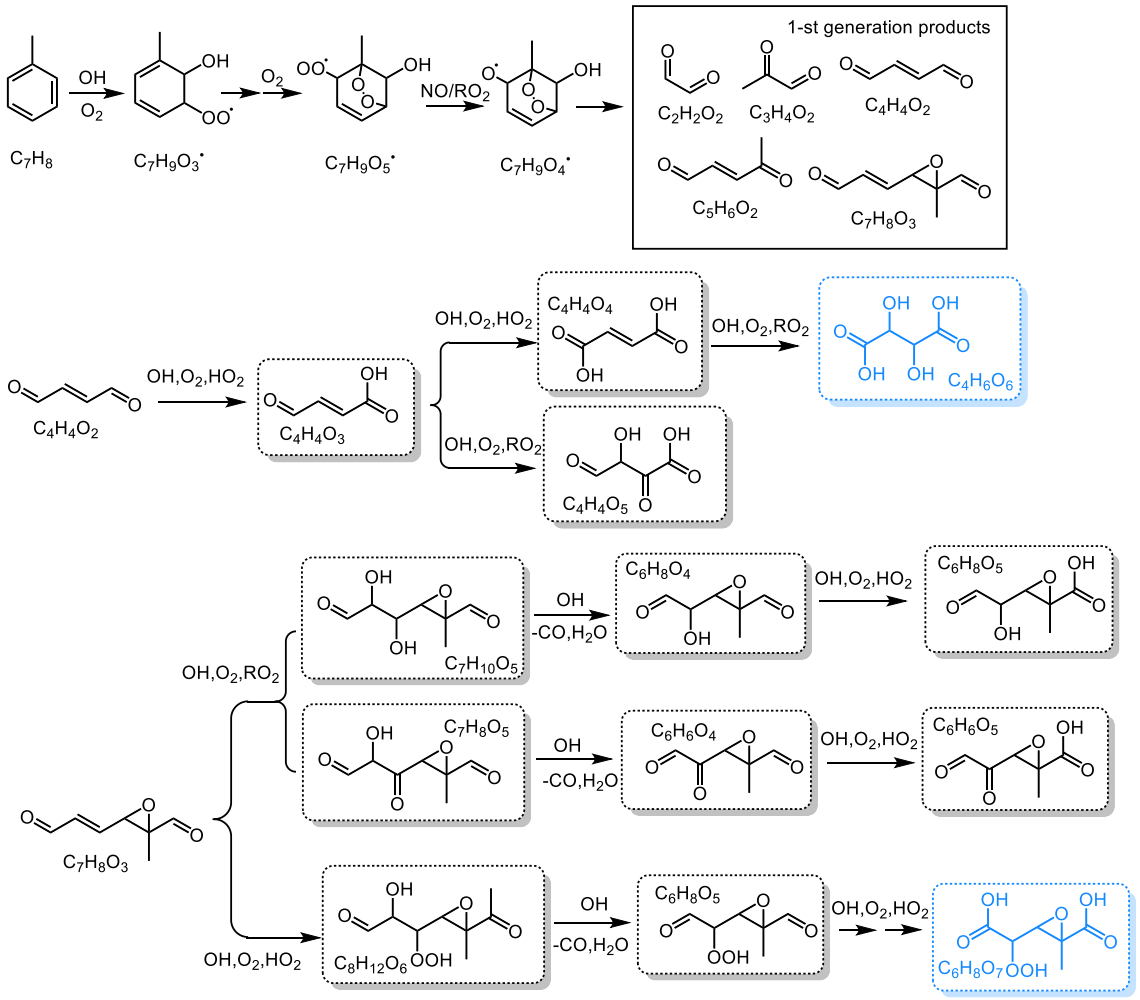


Fig. S5. Formation mechanism of monomeric CHO compounds identified in toluene SOA. Products in the black dashed boxes are CHO compounds observed under both low RH (~8%) and high RH (~70%) conditions, while the products in the blue dashed boxes were only detected under high RH condition.

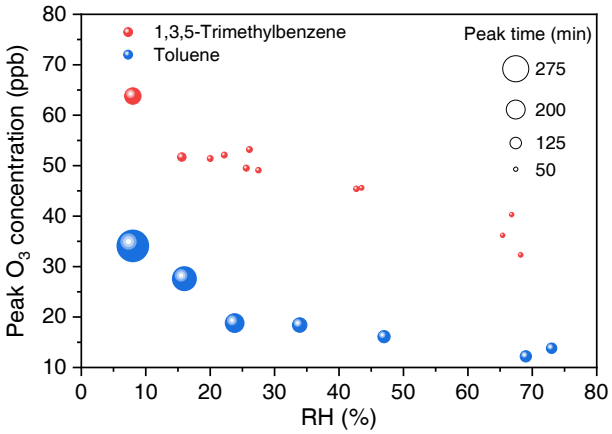


Fig. S6. Peak concentration of O_3 formed from the photooxidation of toluene and 1,3,5-trimethylbenzene as a function of RH. Data sizes represent the time required for O_3 to reach its peak concentration.

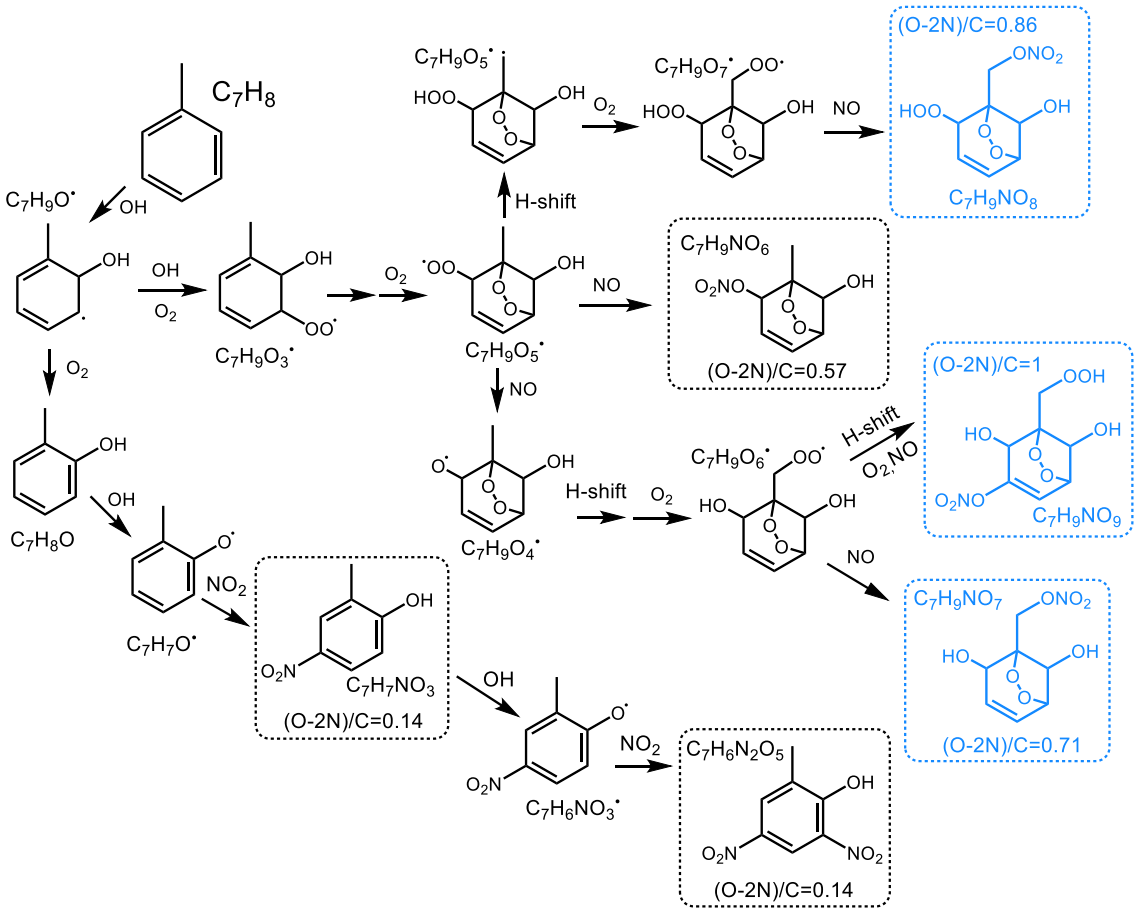


Fig. S7. Proposed formation mechanism of CHON compounds observed in toluene SOA. Products in the black dashed boxes are CHON compounds observed under low RH (~8%) and high RH (~70%) conditions, while the products in the blue dashed boxes were only detected under high RH condition.

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