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Supplement of

Relationship between chemical composition and oxidative potential of secondary organic aerosol from polycyclic aromatic hydrocarbons

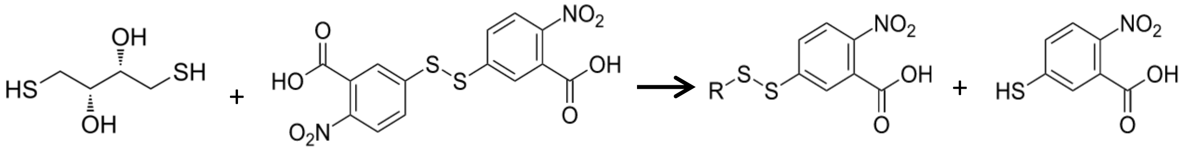
Shunyao Wang et al.

Correspondence to: Arthur W. H. Chan (arthurwh.chan@utoronto.ca)

Section S1. Additional chemical information.

Dithiothreitol (99 %), 5,5’-dithio-bis (2-nitrobenzoicacid) (98 %), phosphate buffer (0.1 M, pH 7.4 (25 ℃), hydrogen peroxide (30 wt. % in H_2O, ACS reagent), cumene peroxide (technical grade, 80 %), tert-Butyl peroxide (98 %), benzoyl peroxide (reagent grade, ≥98 %),1,4 – naphthoquinone (≥96.5 %, HPLC grade), 1,2-nathphoquinone (97 %), 5-hydroxy-1,4-nathphoquinone (97 %), Anthraquinone (≥99.0 % HPLC grade), 1,3-dihydroxynaphthalene (≥99 %), 2,3-dihydroxynaphthalene (≥98 %), copper (II) sulfate (≥99.99 %) were purchased from Sigma Aldrich.

Section S2. Supporting figures and tables



Dithiothreitol (DTT) 5,5'-dithiobis-2-nitrobenzoic acid (DTNB) 2-nitro-5-thiobenzoate (TNB)

Figure S1. Scheme of the DTT assay (Cleland, 1964; Ellman, 1959).

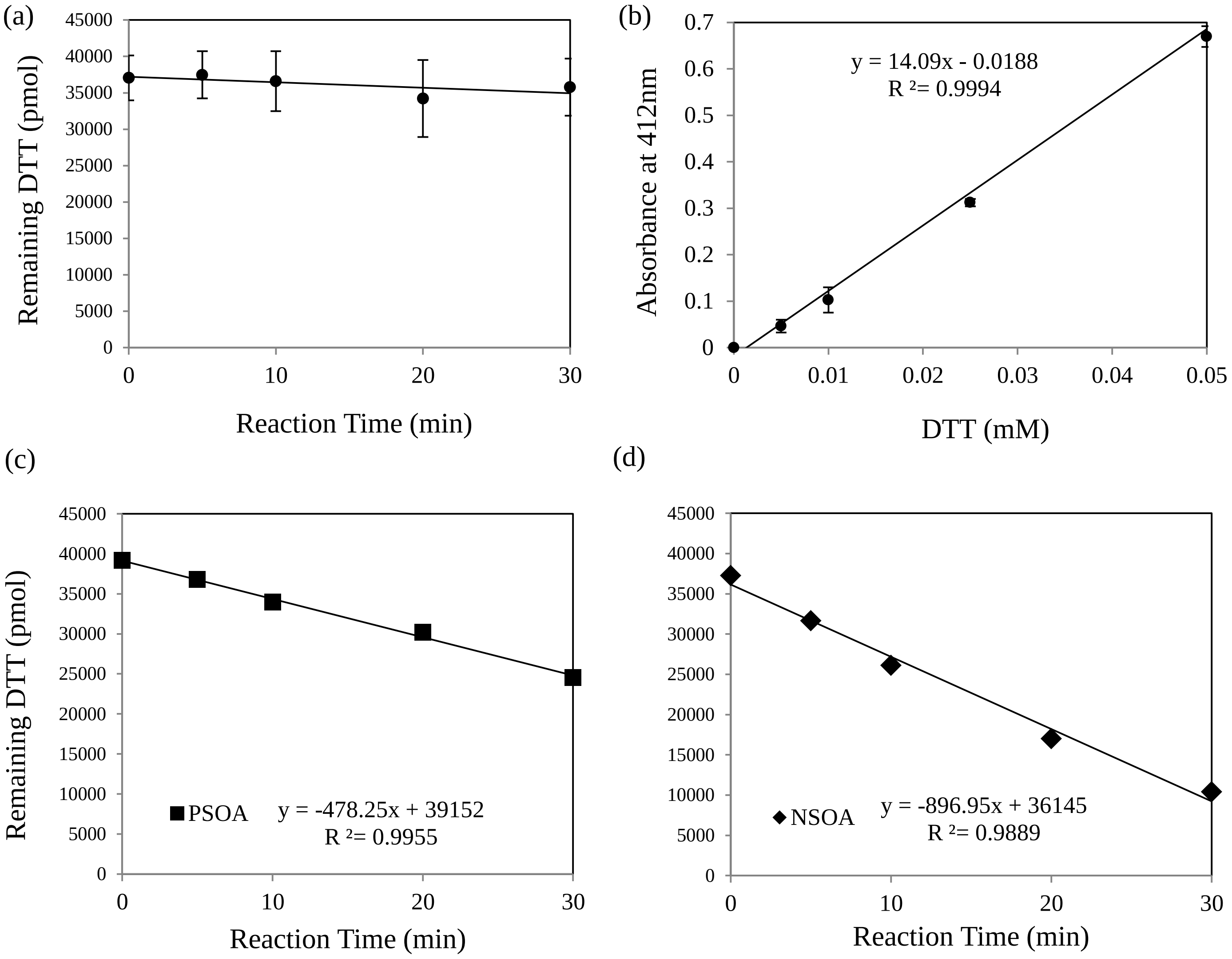


Figure S2. (a) Blank control for DTT assay. (b) Calibration curve used in DTT assay. Slope is determined from the averaged linear regression of the triplicates. Error bar of each data point represents the standard deviation of replicates (n=3). (c) DTT activity of PSOA. (d) DTT activity of NSOA.

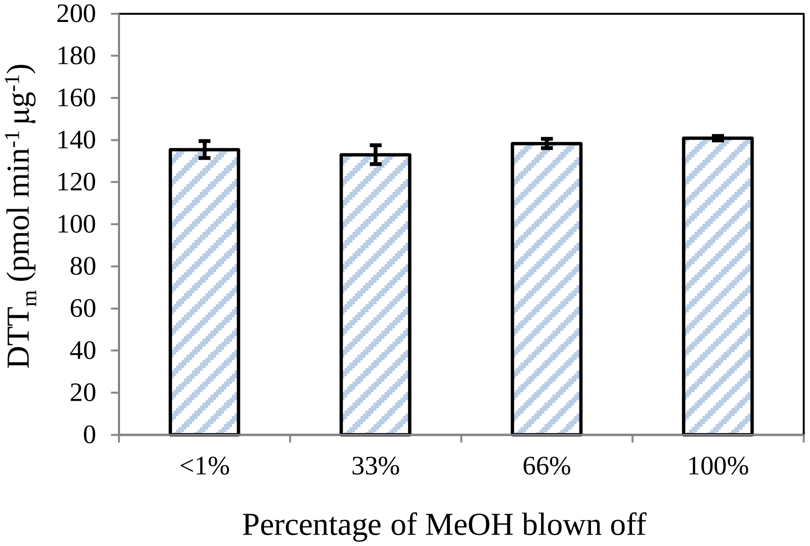


Figure S3. DTT results of four sets of NSOA methanol solutions (with the same SOA amount extracted) evaporated under the N_2 blow-off system to various extents, with which 100 %, 66 %, 33 %, <1 % of the original methanol remained. All the solutions were then replenished with methanol to the same total volume and reconstituted to the experimental concentration with phosphate buffer for the measurement of DTT activity. Despite the difference in degree of evaporation, there was no significant change in the DTT_m of NSOA in this study. Thus, we deduced the evaporation of volatile SOA compounds during N_2 blow-off procedure did not lead to a significant underestimation of the OP of SOA here.

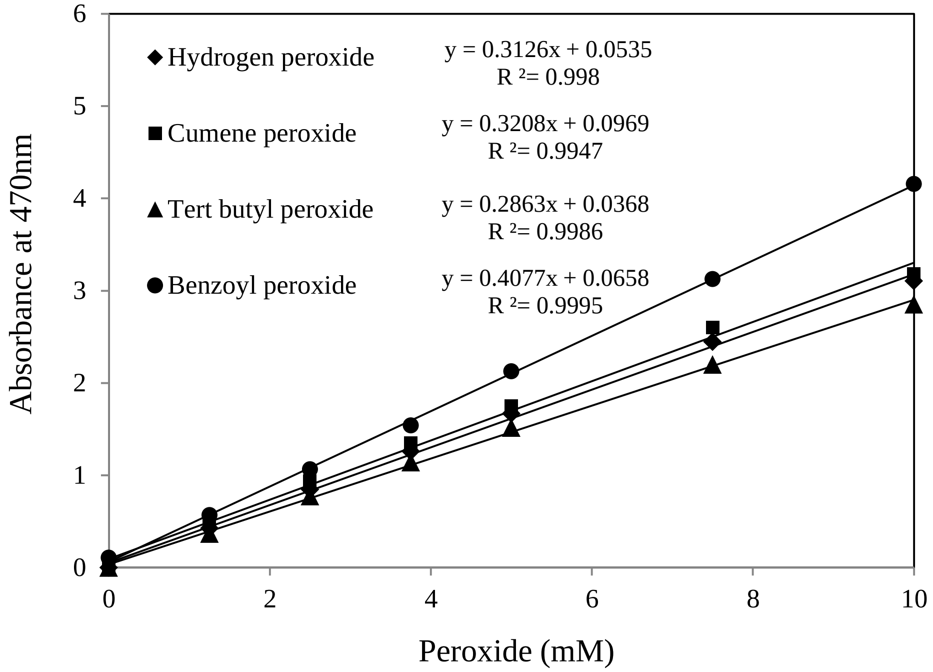


Figure S4. KI calibration curves for hydrogen peroxide (30 % in H_2O), cumene hydroperoxide (80 %), tert-Butyl peroxide (98 % in H_2O), benzoyl peroxide (98 %) at a series of concentration of 0 mM, 1.25 mM, 2.5 mM, 3.75 mM, 5 mM, 7.5 mM and 10 mM.

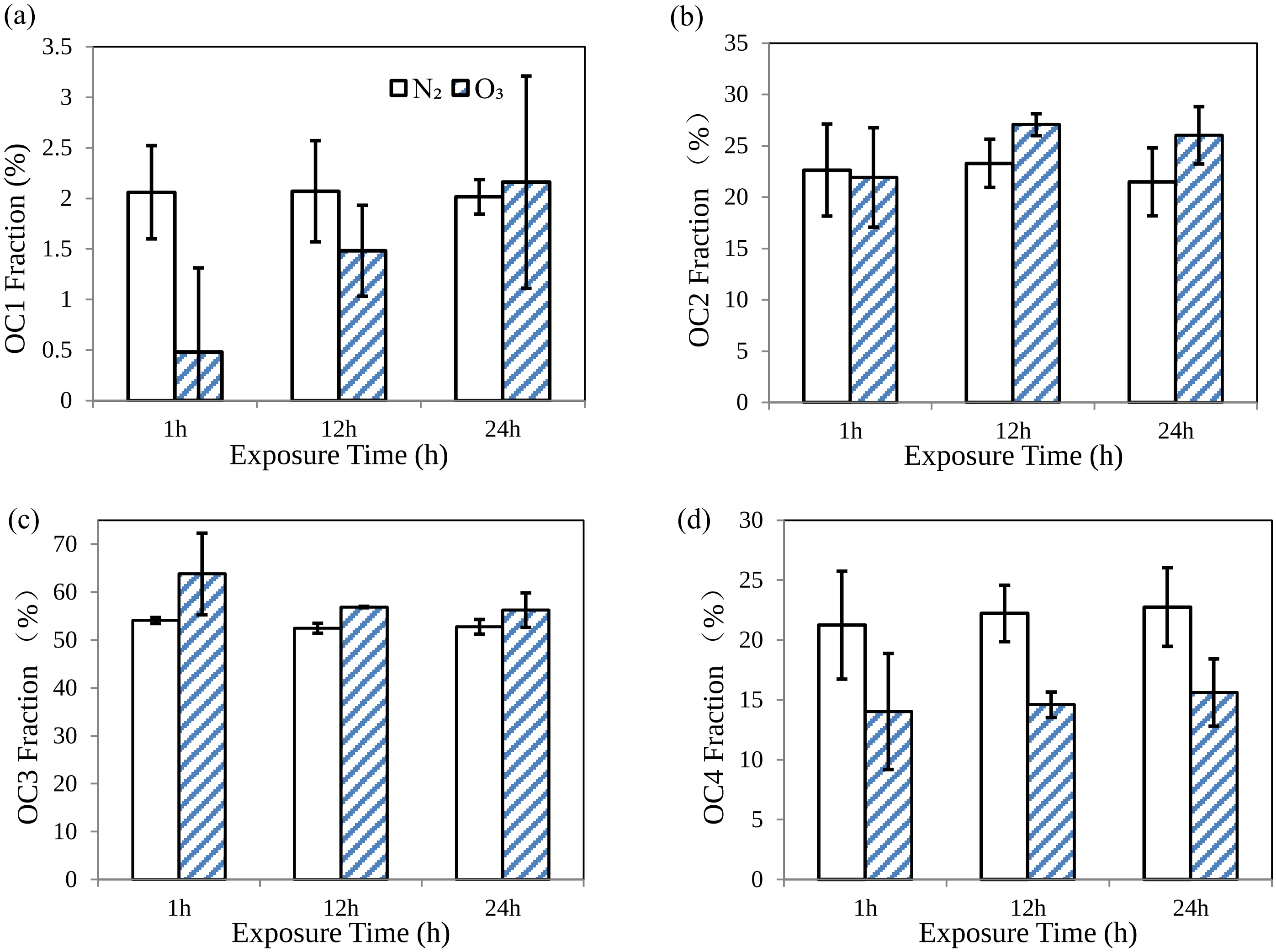


Figure S5. Changes in OC fractions (a)OC1, (b)OC2, (c)OC3, (d)OC4 (Chow et al., 1993) of NSOA filters exposed to N_2/O_3 for 1 h, 12 h and 24 h. Error bar of each data point represents standard deviation of the replicates (n=3).

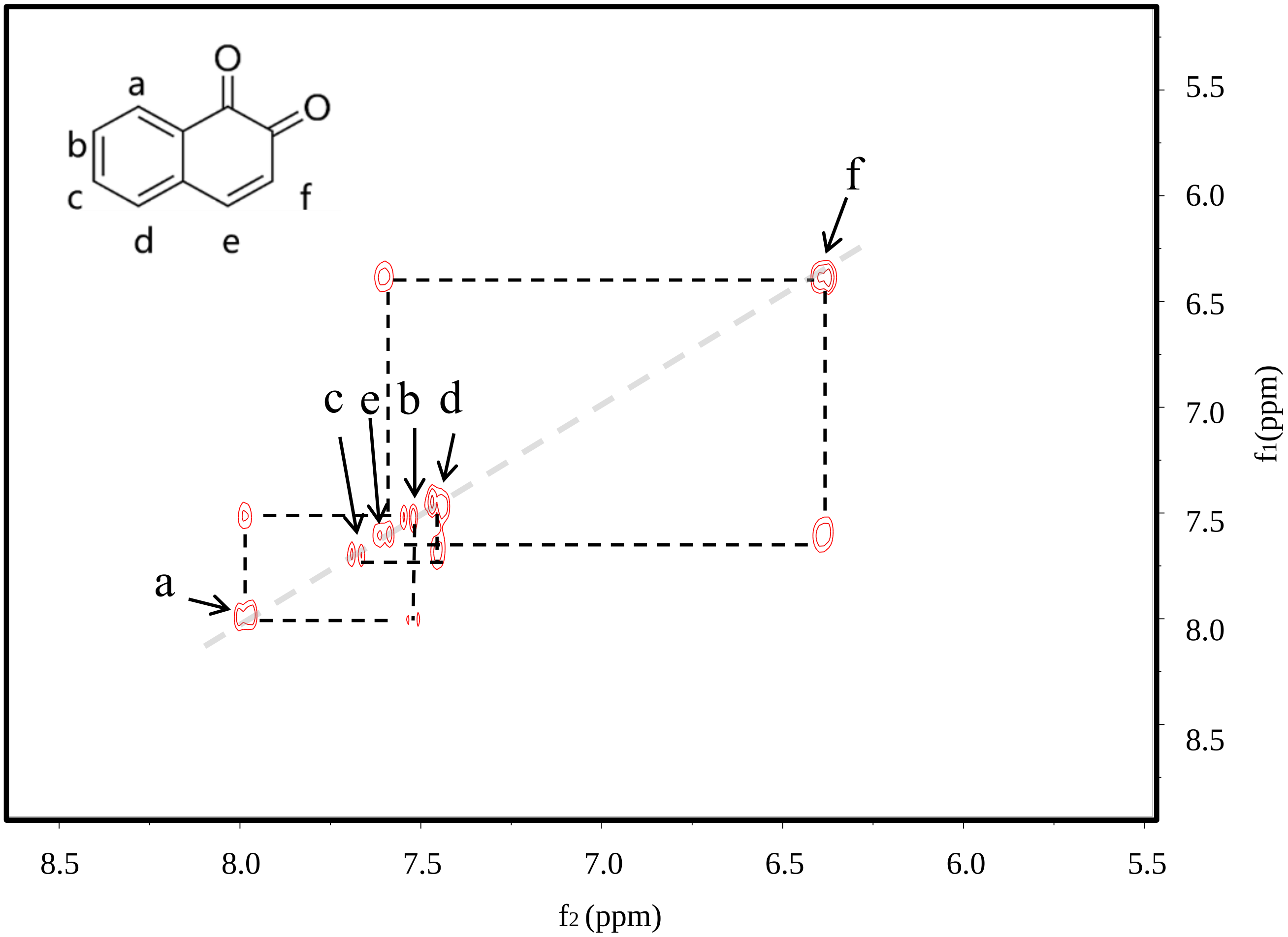


Figure S6. COSY spectra for 1,2-NQN, which were used for proton peak assignment. Proton peaks a, b, c, d, e, f could be assigned based on the coupling between ab, ef and cd. COSY NMR experiments were done in non-phase-sensitive mode, using gradients for coherence selection. 96 transients and 2048 data points were collected for each of the 196 increments in the F1. Both dimensions were processed using an unshifted sine-squared function, zero filling factor of 2 and a magnitude mode was used for projection.

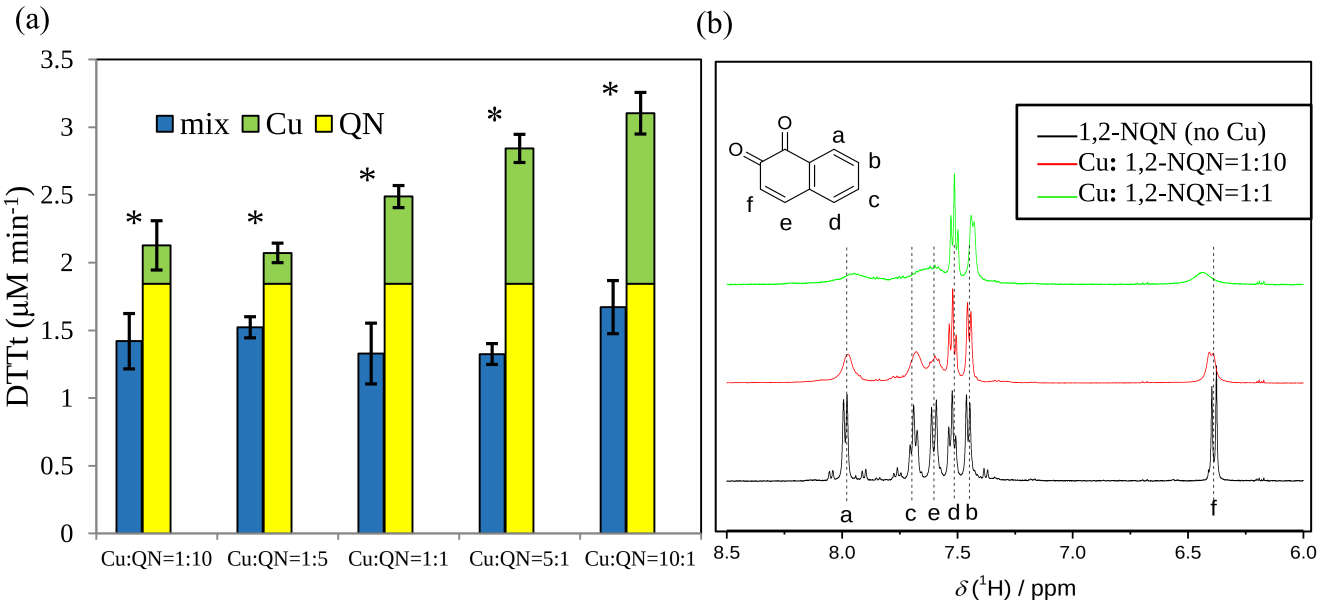


Figure S7. (a) Result of DTT assay on a series of mixture with the same amount of quinone but an increasing amount of Cu (II). Molar ratio of Cu (II):1,2-NQN ranges from 1:10, 1:5, 1:1, 5:1 to 10:1. The asterisk indicates significant difference between a pair of bars at the 95 % confidence level. An increasing trend of OP depletion was observed with increasing ratios of Cu (II) to 1,2-NQN, which corresponded well with (b) an increasing extent of peak broadening observed in 1D ^{1}H NMR spectra (Rehmann and Barton, 1990;Kowalewski and Maler, 2006).

Table S1. ^{1}H NMR T1, T2 relaxation value for individual proton on 1,2-NQN (peak assignment shown in Fig. 9).

^{1}H peak	T_1 (s)			T_2 (s)		
	1,2-NQN	Cu:1,2-NQN 1:10	Cu:1,2-NQN 1:1	1,2-NQN	Cu:1,2-NQN 1:10	Cu:1,2-NQN 1:1
a	1.76	0.73	0.4	0.14	0.029	0.018
b	1.51	0.68	0.37	0.13	0.036	0.015
c	1.4	0.57	0.37	0.12	0.026	0.019
d	1.52	0.74	0.59	0.13	0.045	0.035
e	1.49	0.76	0.61	0.15	0.059	0.039
f	1.82	0.61	0.37	0.12	0.027	0.013

References:

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