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Supplement of

Increase of nitrooxy organosulfates in firework-related urban aerosols during Chinese New Year's Eve

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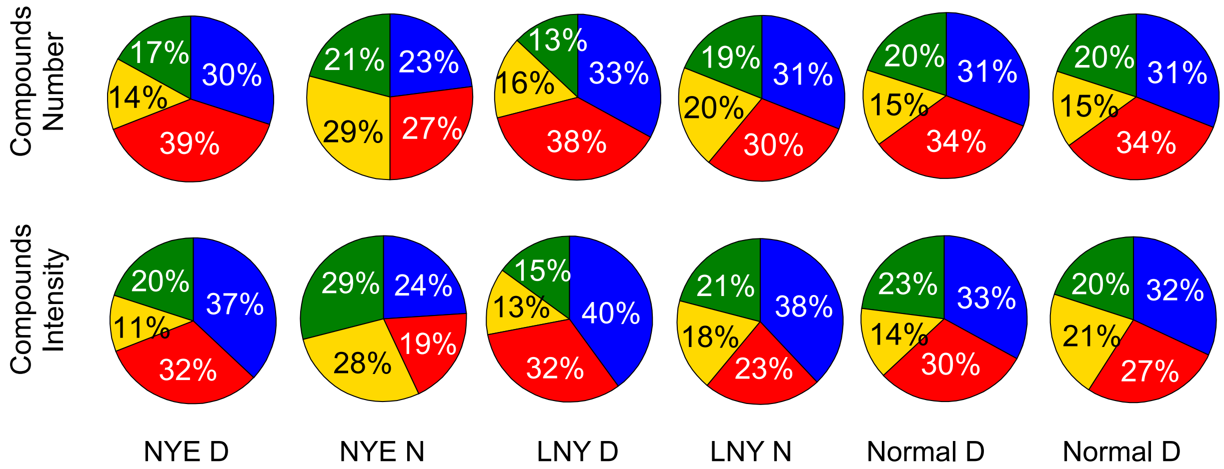


Figure S1: Number, and intensity percentages of CHO, CHNO, CHOS and CHNOS compound categories in WSOC isolated from aerosol samples detected in ESI^- FT-ICRMS. D=daytime; N=nighttime.

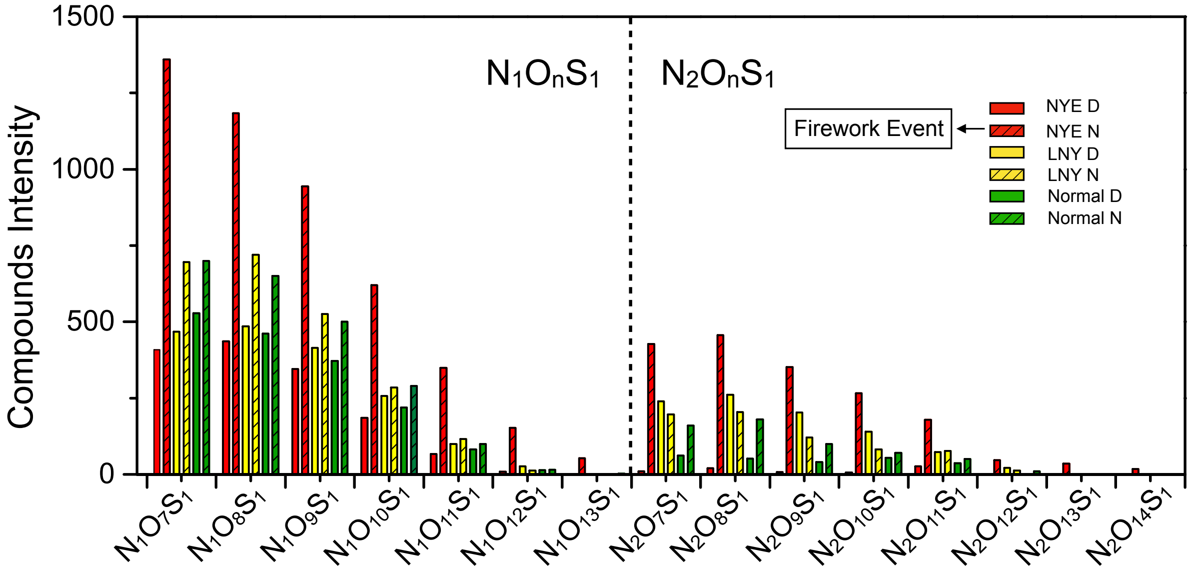


Figure S2: Intensity of nitrooxy-OSs species in different subgroups according to the numbers of N, S and O atoms in their molecules.

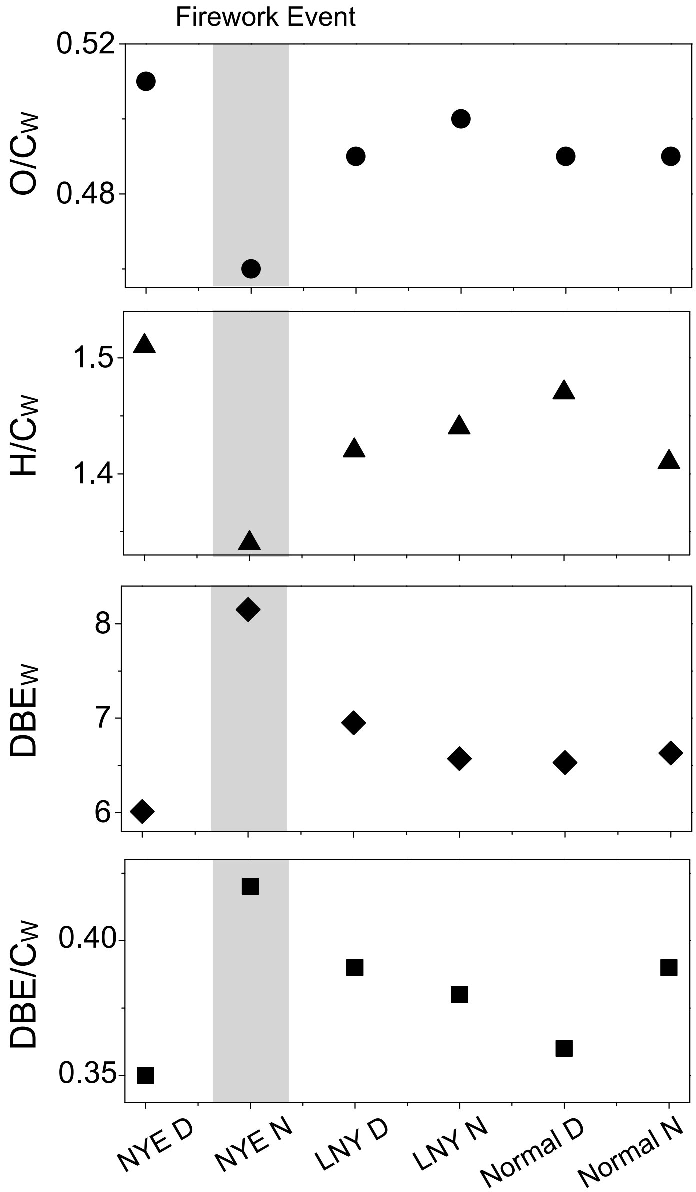


Figure S3: The weighted mean elemental ratio of total nitrooxy-OSs for each sample.

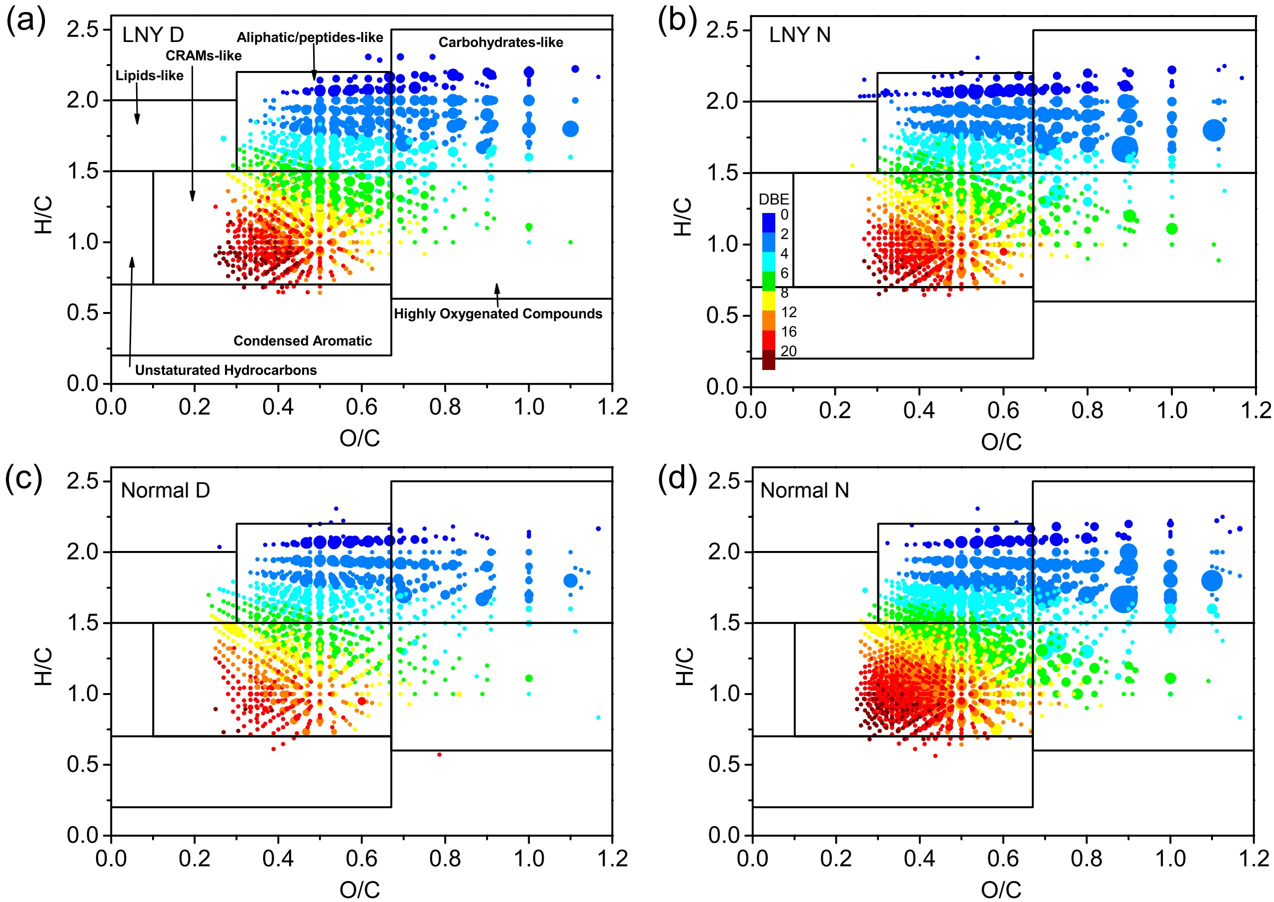


Figure S4: Van Krevelen plots for samples LNY D (a) and LNY N (b), and samples Normal D (c) and Normal N (d). The color bar denotes the number of DBE. Black lines show class identification. The stoichiometric ranges set as boundaries of the classifications are showed in Table S3. The size of the symbols reflects the relative peak intensities of molecular formulae on a logarithmic scale.

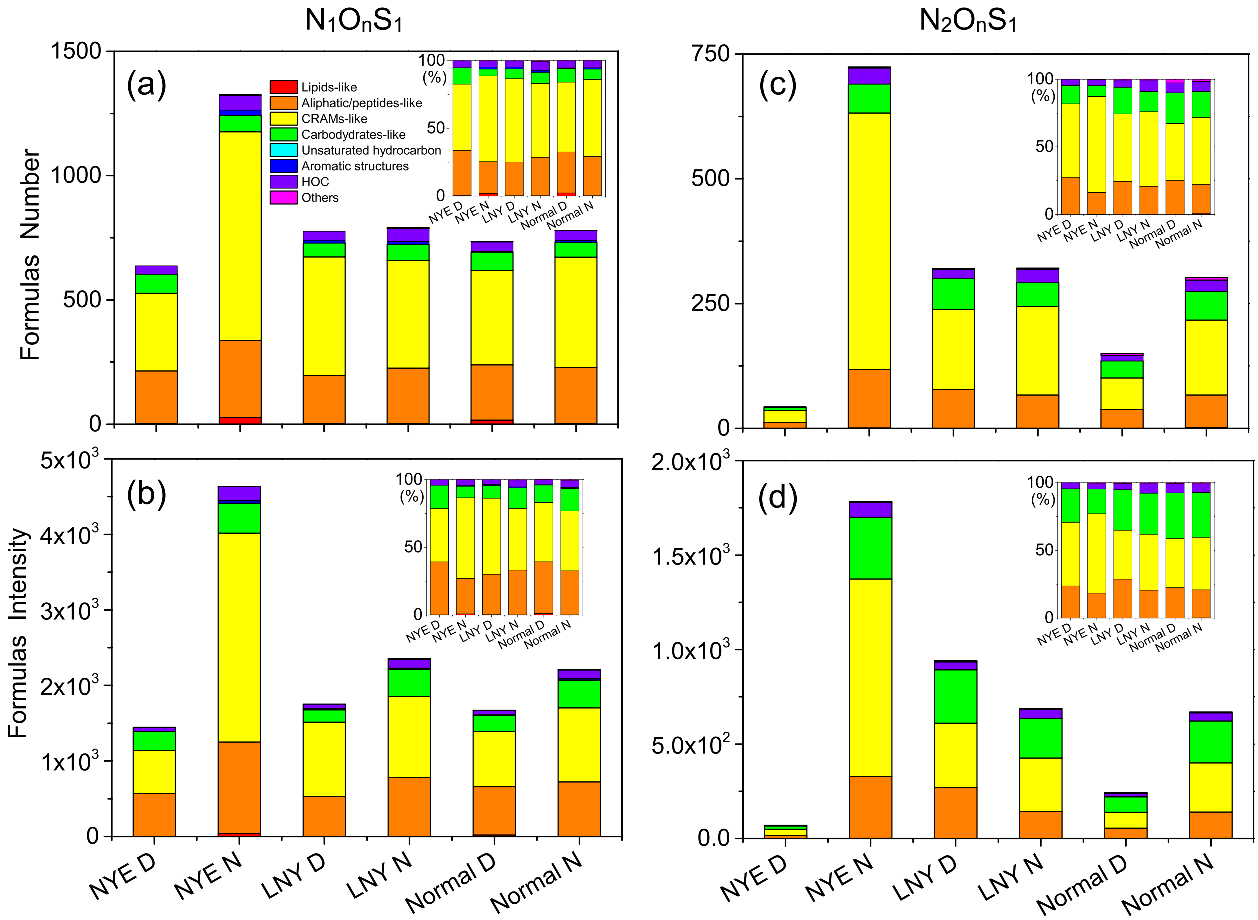


Figure S5: The number and intensity contribution of $N_1O_nS_1$ and $N_2O_nS_1$ species of nitrooxy-OSs in VK classes in samples. The bar diagrams in top right represent the relative contribution of them.

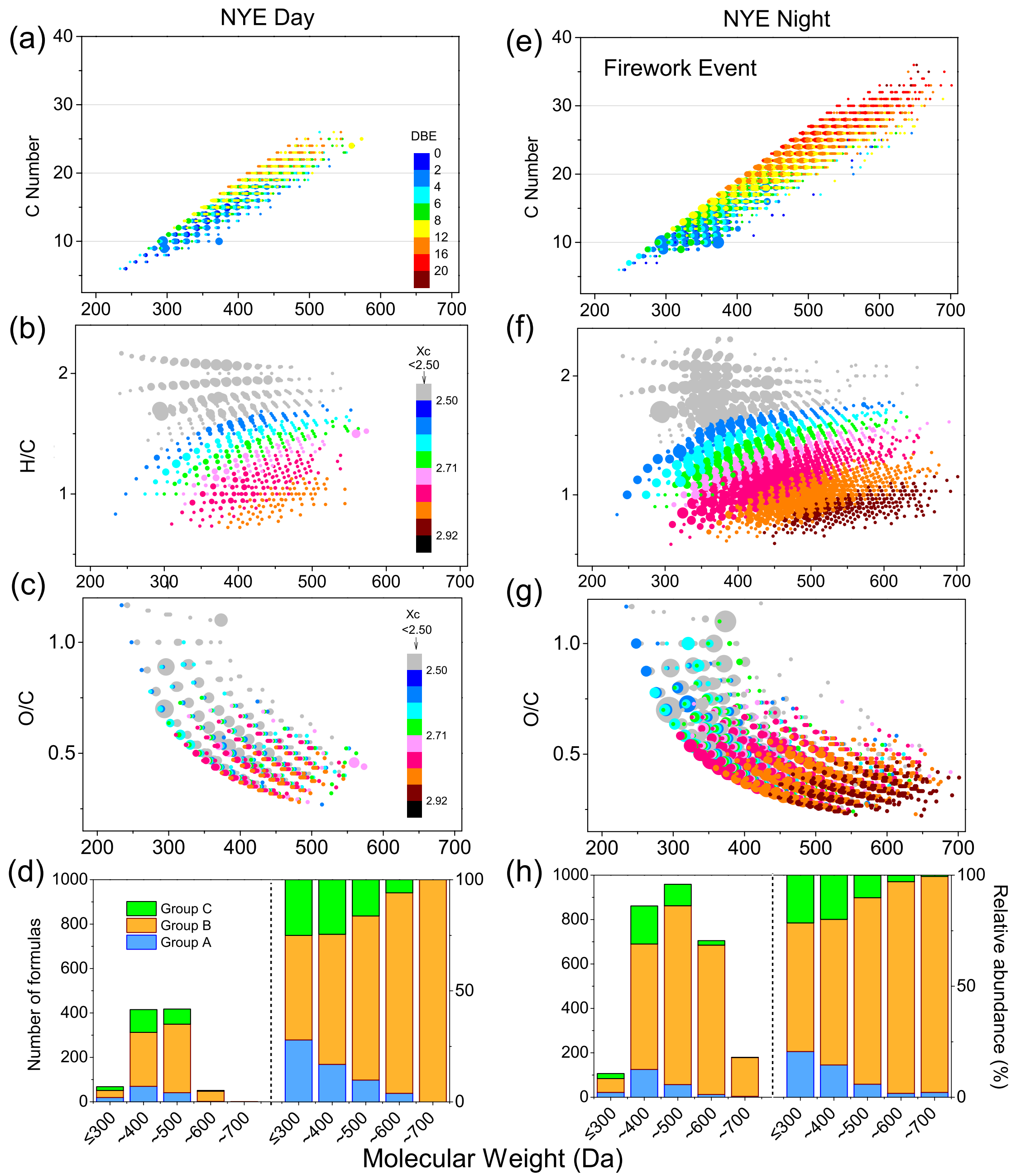


Figure S6: The carbon chain length (a and e), H/C (b and f)) and O/C (c and g) ratios, different groups (d and h) distributions via molecular weights of nitrooxy-OSs in NYE D (during the before-FW periods) and NYE N (during the FW periods) aerosols. Group A includes the aliphatic nitrooxy-OSs with DBE≤2; Group B includes the aromatic-like nitrooxy-OSs with X_c>2.5; Group C includes the biogenic derived nitrooxy-OSs.

Table S1. Sampling date and the concentrations of chemical components of the Beijing aerosols collected in January 2012 (Xie et al., 2020).

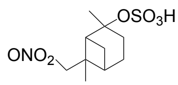
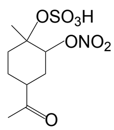
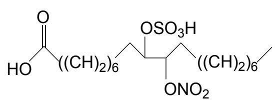
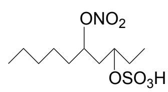
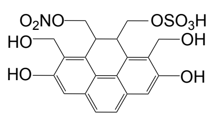
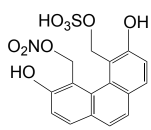
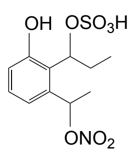
Sample ID	Sampling Date and Time	OC ($\mu g\ m^{-3}$)	EC ($\mu g\ m^{-3}$)	WSOC ($\mu gC\ m^{-3}$)	WSON ($\mu gN\ m^{-3}$)	ΣPAHs* ($ng\ m^{-3}$)	Ion concentrations ($\mu g\ m^{-3}$)						
							SO_4^{2-}	NO_3^-	Cl^-	NH_4^+	K^+	Mg^{2+}	Ca^{2+}
Normal D	21st Jan 7:00 ~ 18:00	11.9	3.93	2.81	0.07	39.2	5.18	2.27	1.14	0.71	0.51	0.23	1.60
Normal N	21st 18:30 ~ 22nd Jan 6:30	9.27	2.32	2.70	0.12	71.7	4.65	2.03	1.56	0.61	0.65	0.16	0.67
NYE D	22nd Jan 7:00 ~ 18:00	13.0	3.22	5.10	0.36	44.4	5.66	4.19	2.49	2.00	1.90	0.24	1.38
NYE N	22nd 18:30 ~23th Jan 6:30	23.3	8.65	11.6	1.36	165.7	65.4	5.34	55.2	0.17	102	2.92	2.25
LNY D	23th Jan 7:00 ~ 18:00	11.2	3.20	3.83	0.16	29.7	6.43	3.16	3.54	0.95	3.99	0.53	1.39
LNY N	23th18:30 ~24th Jan 6:30	14.1	4.73	5.14	0.58	50.9	11.6	3.31	6.49	0.47	11.0	0.83	1.13

*: ΣPAHs; The total concentration of eighteen detected PAHs. NYE: new year eve (detailed days). LNY: lunar New Year's Day (detailed days).

Table S2. The stoichiometric classification ranges of VK classes **(Bianco et al., 2018; Wozniak et al., 2008)**.

Class	H/C	O/C
Lipids-like	1.5<H/C≤2.0	0≤O/C≤0.3
Aliphatic/peptides-like	1.5<H/C≤2.2	0.3<O/C≤0.67
CRAMs-like / lignin-like	0.67<H/C≤1.5	0.1≤O/C<0.67
Carbohydrates-like	1.5<H/C≤2.5	0.67<O/C<1.2
Unsaturated hydrocarbons	0.67<H/C≤1.5	O/C<0.1
Aromatic structures	0.2≤H/C≤0.67	O/C<0.67
tannins-like / HOC	0.6<H/C≤1.5	0.67≤O/C≤1.2

Table S3. The relative intensities of seven different nitrooxy-OSs in each sample.

Formula	Proposed structure	Relative Intensity (%)						Potential precursor
		NYE D	NYE N	LNY D	LNY N	Normal D	Normal N	
(1) $C_{10}H_{17}NO_7S$		26	95	16	37	17	86	Pinene (Surratt et al., 2008)
(2) $C_9H_{15}NO_8S$		20	25	8.4	79	9.7	95	Limonene (Surratt et al., 2008)
(3) $C_{18}H_{35}NO_9S$		7.3	21	8.5	15	7.5	10	Oleic acid
(4) $C_{12}H_{25}NO_7S$		4.1	11	4.2	3.1	5.2	5.5	Alkane
(5) $C_{18}H_{15}NO_{11}S$		0	1.8	0	0	0	0	Aromatics /PAHs
(6) $C_{16}H_{13}NO_9S$		1.1	3.3	2.2	2.5	1.4	2.2	Aromatics /PAHs
(7) $C_{11}H_{15}NO_8S$		2.4	19	3.8	14	3.0	12	Aromatics /PAHs

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