Supplement for

The Secondary Formation of Organosulfates under the Interactions between Biogenic Emissions and Anthropogenic Pollutants in Summer of Beijing

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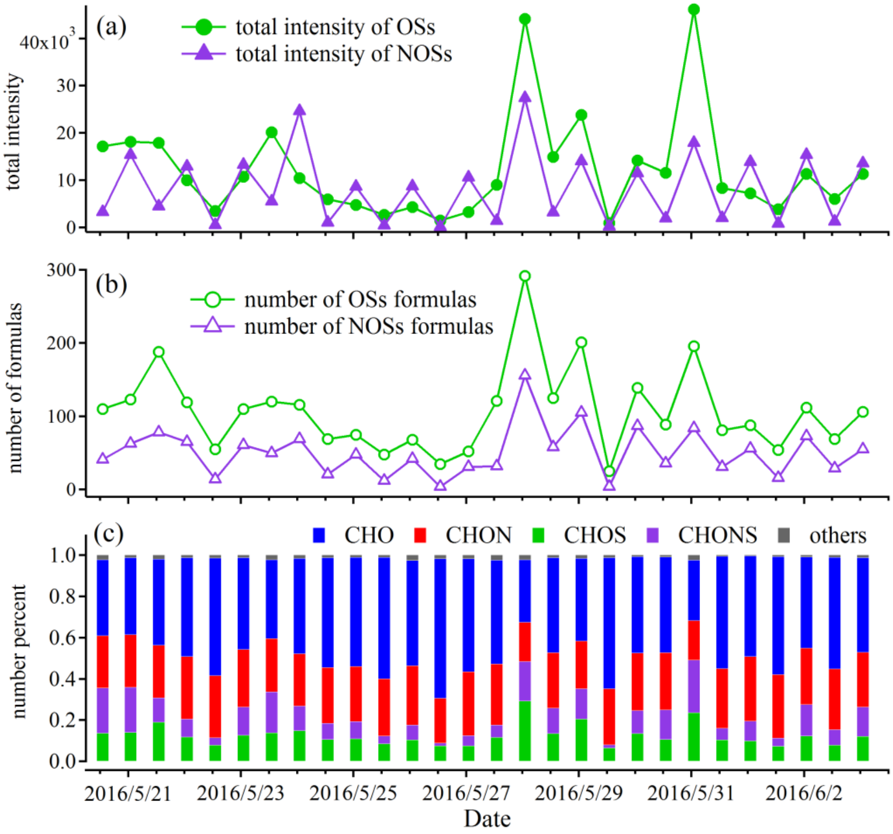

Fig. S1 Temporal variation of the (a) total intensity and (b) total number of OSs and NOSs, and (c) temporal variation of the number percent of different compound categories.

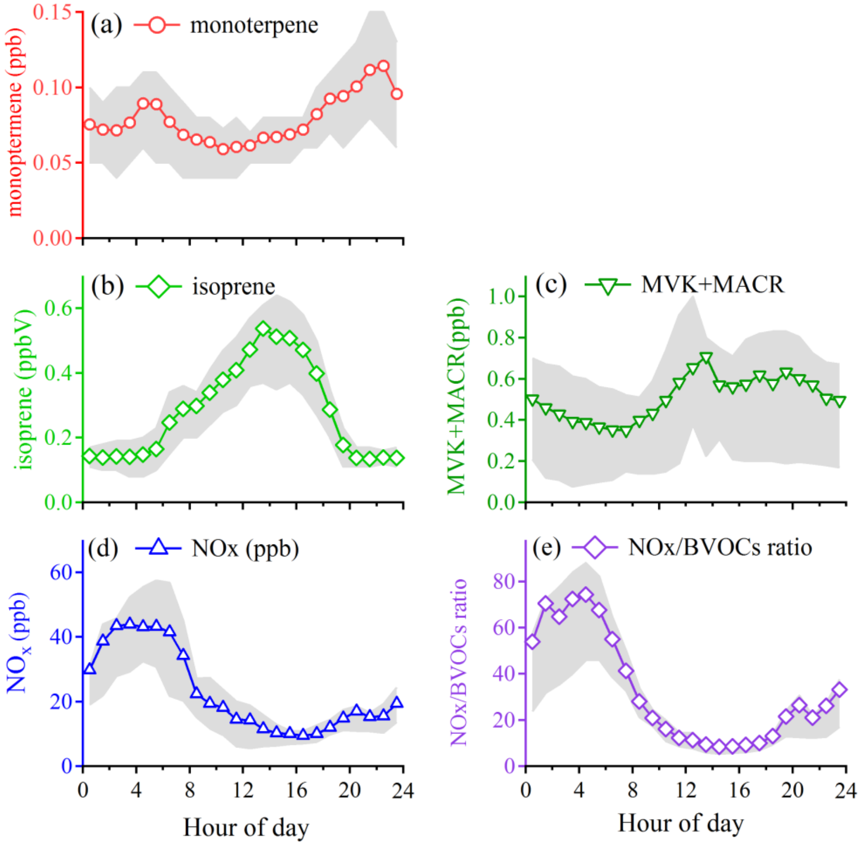

Fig. S2 The diurnal variations of monoterpene, isoprene, NO_x and NO_x/BVOCs ratios

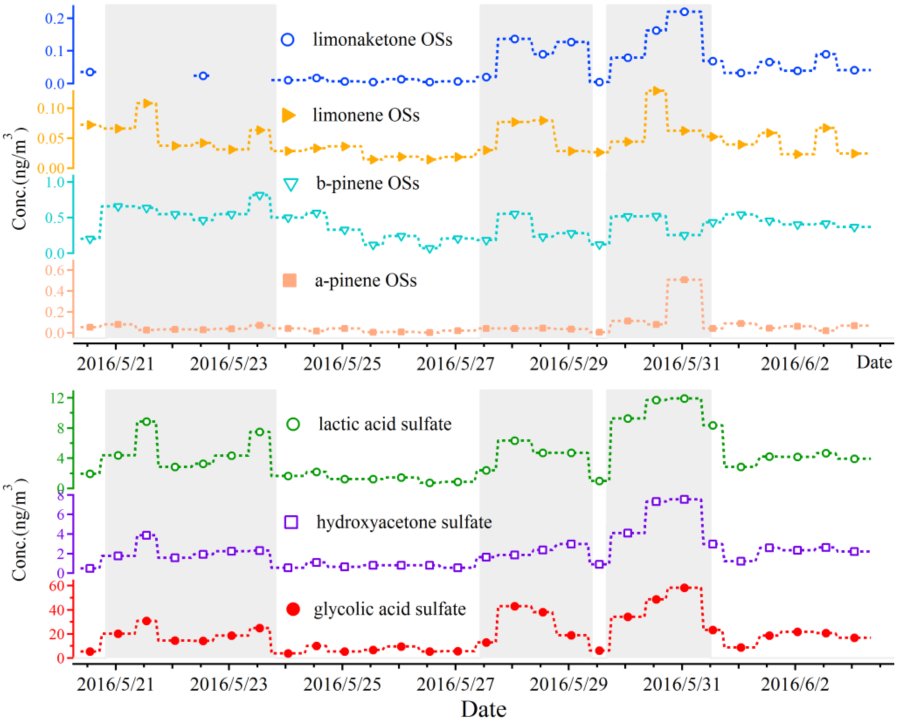

Fig. S3 Time series of α-pinene OSs, β-pinene OSs, limonene OSs, limonaketone OSs, lactic acid sulfate, glycolic acid sulfate and hydroxyacetone sulfate. The pollution episodes were marked by gray shadow.

Table S1 List of some most abundant OSs and NOSs peaks observed in the mass spectra

No.	m/z [M-H]$^-$	Formula [M-H]$^-$	relative intensity (%)			precursor/ formation	references
			05/24N	05/30D	05/30N		
organosulfates							
1	267.05440	$C_9H_{15}SO_7^-$	2.1	19.4	100.0	alkane/ isoprene	(Riva et al., 2016b;Riva et al., 2016a)
2	281.07005	$C_{10}H_{17}SO_7^-$	2.6	13.3	40.0	diesel fuel SOA	(Blair et al., 2017)
3	253.07513	$C_9H_{17}SO_6^-$	2.0	11.1	38.0	diesel fuel SOA	(Blair et al., 2017)
4	239.05948	$C_8H_{15}SO_6^-$		11.1	29.4	diesel fuel SOA	(Blair et al., 2017)
5	309.10135	$C_{12}H_{21}SO_7^-$		11.0	25.7	diesel fuel SOA	(Blair et al., 2017)
6	295.08570	$C_{11}H_{19}SO_7^-$	1.2	9.0	25.6	diesel fuel SOA	(Blair et al., 2017)
7	251.05948	$C_9H_{15}SO_6^-$	3.7	9.5	24.7	monoterpene	(Wang et al., 2017)
8	223.06457	$C_8H_{15}SO_5^-$	3.1	9.7	16.8	diesel fuel SOA	(Blair et al., 2017)
9	279.05440	$C_{10}H_{15}SO_7^-$	3.9	4.8	15.9	alkane	(Riva et al., 2016b)
10	269.07005	$C_9H_{17}SO_7^-$	0.3	4.0	15.8	alkane	(Riva et al., 2016b)
11	225.04383	$C_7H_{13}SO_6^-$	0.4	2.3	14.0	diesel fuel SOA	(Blair et al., 2017)
12	265.07513	$C_{10}H_{17}SO_6^-$	3.0	7.3	13.9	alkane	(Riva et al., 2016b)
13	297.06496	$C_{10}H_{17}SO_8^-$		4.2	13.5	alkane	(Riva et al., 2016b)
14	267.09078	$C_{10}H_{19}SO_6^-$	1.6	6.0	13.4	diesel fuel SOA	(Blair et al., 2017)
15	279.09078	$C_{11}H_{19}SO_6^-$	1.9	5.5	13.3	diesel fuel SOA	(Blair et al., 2017)
16	283.04931	$C_9H_{15}SO_8^-$	0.4	3.2	12.3	diesel fuel SOA	(Blair et al., 2017)
17	151.00705	$C_4H_7SO_4^-$	1.0	4.8	10.3	diesel fuel SOA	(Blair et al., 2017)
18	325.09626	$C_{12}H_{21}SO_8^-$			10.2	diesel fuel SOA	(Blair et al., 2017)
19	293.07005	$C_{11}H_{17}SO_7^-$	0.9		10.1	diesel fuel SOA	(Blair et al., 2017)
20	283.08570	$C_{10}H_{19}SO_7^-$	0.3	3.7	10.1	diesel fuel SOA	(Blair et al., 2017)
21	237.04383	$C_8H_{13}SO_6^-$	1.4	3.3	10.0	diesel fuel SOA	(Blair et al., 2017)
22	307.08570	$C_{12}H_{19}SO_7^-$	0.6		9.7		
23	293.10643	$C_{12}H_{21}SO_6^-$	0.9		9.5		
24	237.08022	$C_9H_{17}SO_5^-$	2.0	5.4	9.4	alkane	(Riva et al., 2016b)
25	351.11191	$C_{14}H_{23}SO_8^-$			9.4	diesel fuel SOA	(Blair et al., 2017)

26	235.06457	$C_9H_{15}SO_5^-$	12.9	8.7	9.1	diesel fuel SOA	(Blair et al., 2017)
27	373.09626	$C_{16}H_{21}SO_8^-$	5.0	9.5	8.7	diesel fuel SOA	(Blair et al., 2017)
28	281.10643	$C_{11}H_{21}SO_6^-$	0.6	3.6	8.2	diesel fuel SOA	(Blair et al., 2017)
29	339.07553	$C_{12}H_{19}SO_9^-$			8.0	diesel fuel SOA	(Blair et al., 2017)
30	321.17412	$C_{15}H_{29}SO_5^-$	1.6	6.0	7.7	diesel fuel SOA	(Blair et al., 2017)
31	307.15847	$C_{14}H_{27}SO_5^-$	2.1		7.6	diesel fuel SOA	(Blair et al., 2017)
32	365.12756	$C_{15}H_{25}SO_8^-$	0.3		7.6	diesel fuel SOA	(Blair et al., 2017)
33	321.10135	$C_{13}H_{21}SO_7^-$	0.5		7.5	diesel fuel SOA	(Blair et al., 2017)
34	251.09587	$C_{10}H_{19}SO_5^-$	1.9	5.3	7.5	alkane	(Riva et al., 2016b)
35	209.04892	$C_7H_{13}SO_5^-$	1.0	2.2	7.4	alkane	(Riva et al., 2016b)
36	307.12208	$C_{13}H_{23}SO_6^-$			7.2		
37	295.04931	$C_{10}H_{15}SO_8^-$	1.0	2.5	7.1	alkane	(Riva et al., 2016b)
38	279.12717	$C_{12}H_{23}SO_5^-$	2.2	3.3	6.5	alkane	(Riva et al., 2016b)
39	295.12208	$C_{12}H_{23}SO_6^-$	0.7	3.2	6.2	diesel fuel SOA	(Blair et al., 2017)
40	249.08022	$C_{10}H_{17}SO_5^-$	2.7	2.6	4.2	monoterpene	(Surratt et al., 2008;Wang et al., 2017)
nitrooxy-organosulfates							
1	294.06530	$C_{10}H_{16}NO_7S^-$	67.3	5.0	82.9	monoterpene	(Surratt et al., 2008)
2	326.05513	$C_{10}H_{16}NO_9S^-$	23.9	4.0	29.2	monoterpene	(Surratt et al., 2008)
3	342.05004	$C_{10}H_{16}NO_{10}S^-$	8.3	3.3	23.3	monoterpene	(Surratt et al., 2008)
4	300.03948	$C_8H_{14}NO_9S^-$	3.9	2.5	19.2		
5	314.05513	$C_9H_{16}NO_9S^-$	1.9		14.6		
6	312.07586	$C_{10}H_{18}NO_8S^-$	10.1		11.5		
7	284.04456	$C_8H_{14}NO_8S^-$	6.9	3.0	10.4		
8	328.07078	$C_{10}H_{18}NO_9S^-$	3.3	2.5	9.4	monoterpene	(Surratt et al., 2008)
9	276.01835	$C_9H_{10}NO_7S^-$	3.2		9.3		
10	296.04456	$C_9H_{14}NO_8S^-$	23.2	1.4	9.0	monoterpene	(Surratt et al., 2008)

Table S2 The pearson correlations between individual OSs and NOSs species quantified by HPLC-MS (n=28)

	$C_3H_5O_5S^-$	$C_2H_3O_6S^-$	$C_3H_5O_6S^-$	$C_4H_7O_7S^-$	$C_5H_7O_7S^-$	$C_5H_{11}O_7S^-$	$C_5H_{10}NO_9S^-$	α-pinene OSs $C_{10}H_{17}O_5S^-$	β-pinene OSs $C_{10}H_{17}O_5S^-$	Limonene OSs $C_{10}H_{17}O_5S^-$	$C_9H_{15}O_6S^-$	$C_{10}H_{16}NO_7S^-$	$C_9H_{14}NO_8S^-$
$C_3H_5O_5S^-$	1.00												
$C_2H_3O_6S^-$	**0.88**	1.00											
$C_3H_5O_6S^-$	**0.92**	**0.91**	1.00										
$C_4H_7O_7S^-$	**0.97**	**0.86**	**0.86**	1.00									
$C_5H_7O_7S^-$	**0.96**	**0.95**	**0.93**	**0.95**	1.00								
$C_5H_{11}O_7S^-$	**0.91**	**0.73**	**0.72**	**0.93**	**0.85**	1.00							
$C_5H_{10}NO_9S^-$	**0.82**	**0.83**	**0.79**	**0.83**	**0.88**	**0.76**	1.00						
α-pinene OS ($C_{10}H_{17}O_5S^-$)	0.68	0.63	0.59	0.67	0.67	**0.71**	**0.84**	1.00					
β-pinene OS ($C_{10}H_{17}O_5S^-$)	0.22	0.29	0.44	0.20	0.31	(0.03)	0.26	0.01	1.00				
Limonene OS ($C_{10}H_{17}O_5S^-$)	0.62	0.69	0.71	0.56	0.67	0.37	0.39	0.20	0.44	1.00			
$C_9H_{15}O_6S^-$	**0.84**	**0.76**	**0.73**	**0.82**	**0.79**	**0.86**	**0.74**	**0.76**	(0.04)	0.48	1.00		
$C_{10}H_{16}NO_7S^-$	0.11	0.26	0.18	0.13	0.25	0.10	0.48	0.40	0.29	(0.14)	0.10	1.00	
$C_9H_{14}NO_8S^-$	0.02	0.07	0.02	0.02	0.10	0.06	0.26	0.32	0.19	(0.18)	0.07	**0.79**	1.00

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