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Molecular characterization of firework-related urban aerosols using Fourier transform ion cyclotron resonance mass spectrometry

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Table S1. Number of compounds in each subgroup and arithmetic and weighted mean elemental ratio for each subgroup in LNY D and LNY N samples.

		All	CHO	CHNO	CHOS
LNY D	Number frequency	9511	3120	3604	1249
	Molecular weight (Da)	448±97	456±120	472±112	402±82
	O/C	0.35±0.14	0.31±0.12	0.33±0.11	0.40±0.13
	O/C_w	0.36	0.31	0.33	0.39
	H/C	1.18±0.36	1.14±0.37	1.08±0.29	1.37±0.43
	H/C_w	1.18	1.10	1.05	1.46
	OM/OC	1.65±0.22	1.50±0.17	1.60±0.16	1.80±0.21
	OM/OC_w	1.66	1.50	1.60	1.79
	DBE	11.2±4.98	12.2±5.95	13.2±4.97	7.21±4.65
	DBE_w	10.8	11.8	13.1	6.05
	DBE/C	0.47±0.17	0.47±0.18	0.53±0.14	0.37±0.21
	DBE/C_w	0.48	0.50	0.55	0.33
LNY N	Number frequency	8426	2618	2515	1626
	Molecular weight (Da)	413±85	420±100	415±86	402±78
	O/C	0.34±0.13	0.28±0.12	0.34±0.11	0.34±0.16
	O/C_w	0.35	0.28	0.34	0.31
	H/C	1.28±0.38	1.24±0.40	1.14±0.34	1.42±0.42
	H/C_w	1.28	1.24	1.08	1.50
	OM/OC	1.66±0.20	1.47±0.16	1.61±0.17	1.71±0.25
	OM/OC_w	1.67	1.48	1.61	1.68
	DBE	9.19±4.8	9.98±5.23	11.0±4.50	6.80±4.30
	DBE_w	8.71	9.38	11.3	5.81
	DBE/C	0.43±0.20	0.42±0.20	0.51±0.17	0.34±0.21
	DBE/C_w	0.43	0.43	0.54	0.31

Table S2. Number of compounds in each subgroup and arithmetic and weighted mean elemental ratio for each subgroup in Normal D and Normal N samples.

		All	CHO	CHNO	CHOS
Normal D	Number frequency	5945	2168	2378	1399
	Molecular weight (Da)	405±80	400±90	406±79	405±83
	O/C	0.36±0.15	0.31±0.12	0.34±0.10	0.38±0.15
	O/C_w	0.36	0.31	0.34	0.36
	H/C	1.26±0.38	1.14±0.38	1.10±0.34	1.44±0.40
	H/C_w	1.29	1.12	1.11	1.54
	OM/OC	1.69±0.22	1.51±0.15	1.62±0.16	1.77±0.24
	OM/OC_w	1.69	1.51	1.62	1.76
	DBE	9.01±4.25	10.6±4.95	11.0±4.26	6.49±4.06
	DBE_w	8.59	10.6	10.9	5.38
	DBE/C	0.44±0.19	0.47±0.19	0.53±0.17	0.34±0.20
	DBE/C_w	0.42	0.49	0.52	0.29
Normal N	Number frequency	5454	2071	2140	1243
	Molecular weight (Da)	416±88	408±99	414±89	395±81
	O/C	0.37±0.14	0.31±0.11	0.34±0.11	0.41±0.14
	O/C_w	0.38	0.31	0.34	0.41
	H/C	1.24±0.36	1.19±0.37	1.11±0.30	1.36±0.42
	H/C_w	1.23	1.16	1.09	1.40
	OM/OC	1.70±0.19	1.51±0.15	1.61±0.17	1.81±0.22
	OM/OC_w	1.72	1.51	1.61	1.82
	DBE	9.71±4.47	10.2±4.77	11.6±4.20	7.17±4.48
	DBE_w	9.20	10.0	11.4	6.49
	DBE/C	0.46±0.18	0.45±0.18	0.52±0.15	0.38±0.20
	DBE/C_w	0.46	0.47	0.53	0.36

Table S3. Comparison of chemical characterization of water-soluble organic compounds in aerosol samples.

Sampling site	Compounds	O/C	H/C	DBE	DBE/C	Ref.
Non-firework	All	0.37±0.14	1.24±0.37	9.36±4.42	0.45±0.18	This study
Firework	All	0.37±0.13	1.23±0.37	10.1±4.82	0.45±0.18	This study
Free tropospheric	All	0.53±0.2	1.48±0.3	6.18±3.0	NA	(Mazzoleni et al., 2012)
Free tropospheric	All	0.46±0.13	1.17±0.26	10.7±4.0	0.47±0.14	(Dzepina et al., 2015)
Rural	All	0.46 ± 0.23	1.34 ± 0.39	5.3 ± 2.6	0.45 ± 0.21	(Lin et al., 2012)
Rural	All	0.28–0.32	1.37–1.46	6.30–7.45	0.33–0.38	(Wozniak et al., 2008)
Marin boundary layer	All	0.36–0.42	1.49–1.56	5.88–6.76	0.28–0.32	(Wozniak et al., 2014)
Remote	All	0.39–0.42	1.30–1.34	7.71–8.38	0.41–0.42	(An et al., 2019)
Free tropospheric	CHO	0.47 ± 0.2	0.47 ± 0.2	0.47 ± 0.2	NA	(Mazzoleni et al., 2012)
Free tropospheric	CHO	0.47 ± 0.14	1.19 ± 0.27	10.8 ± 4.3	0.46 ± 0.14	(Dzepina et al., 2015)
Rural	CHO	0.40 ± 0.21	1.29 ± 0.35	5.6 ± 2.4	0.44 ± 0.18	(Lin et al., 2012)
Urban (hazy)	CHO	0.41 ± 0.19	1.19 ± 0.38	8.0 ± 3.9	0.47 ± 0.19	(Jiang et al., 2016)
Free tropospheric	CHNO	0.57 ± 0.2	0.57 ± 0.2	6.72 ± 2	NA	(Mazzoleni et al., 2012)
Free tropospheric	CHNO	0.45±0.10	1.14±0.22	10.3±2.9	0.51±0.12	(Dzepina et al., 2015)
Rural	CHNO	0.41 ± 0.19	1.15 ± 0.31	6.4 ± 2.1	0.59 ± 0.16	(Lin et al., 2012)
Urban (hazy)	CHNO	0.45 ± 0.22	1.13 ± 0.38	8.8 ± 4.0	0.55 ± 0.19	(Jiang et al., 2016)
Free tropospheric	CHOS	0.56 ± 0.2	1.64 ± 0.3	1.64 ± 0.3	NA	(Mazzoleni et al., 2012)
Free tropospheric	CHOS	0.50±0.11	1.75±0.31	3.5±2.6	0.2±0.14	(Dzepina et al., 2015)
Rural	CHOS	0.55 ± 0.17	1.67 ± 0.31	3.0 ± 1.9	0.25 ± 0.16	(Lin et al., 2012)
Urban (hazy)	CHOS	0.65 ± 0.28	1.64 ± 0.37	3.4 ± 2.4	0.26 ± 0.18	(Jiang et al., 2016)

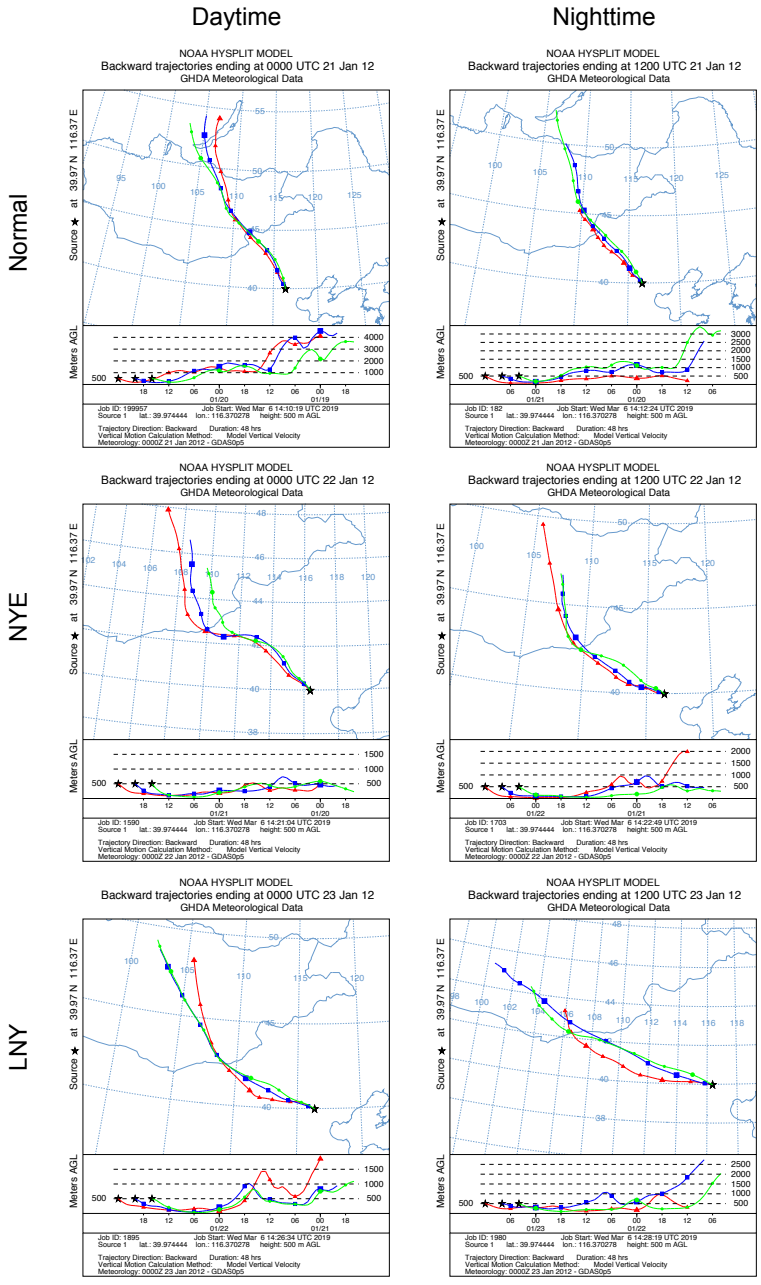

Figure S1: The clustering air mass two-day backward trajectories.

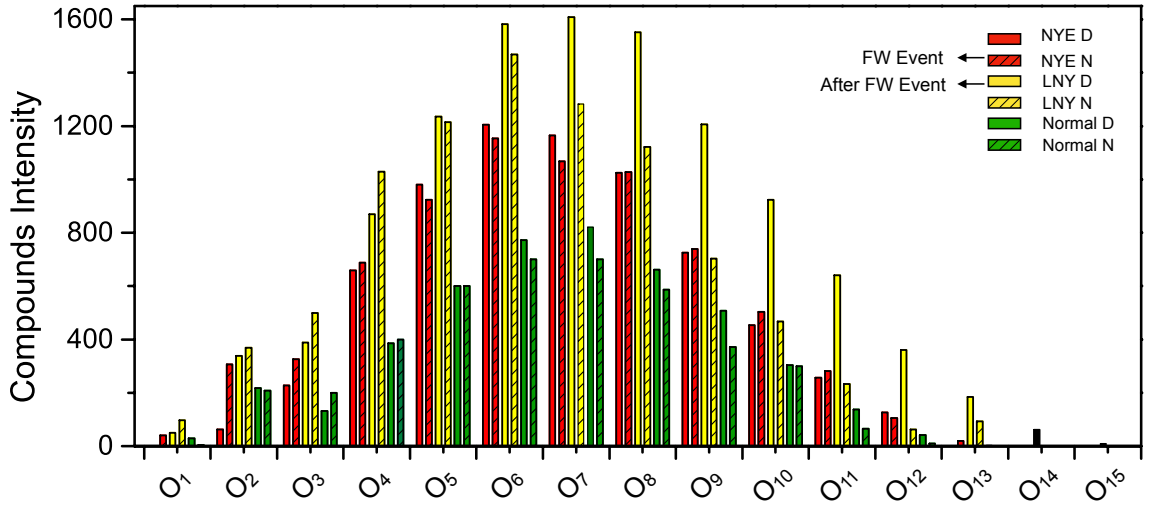

Figure S2: Intensity of CHO species of subgroups according to the number of O atoms in their molecules.

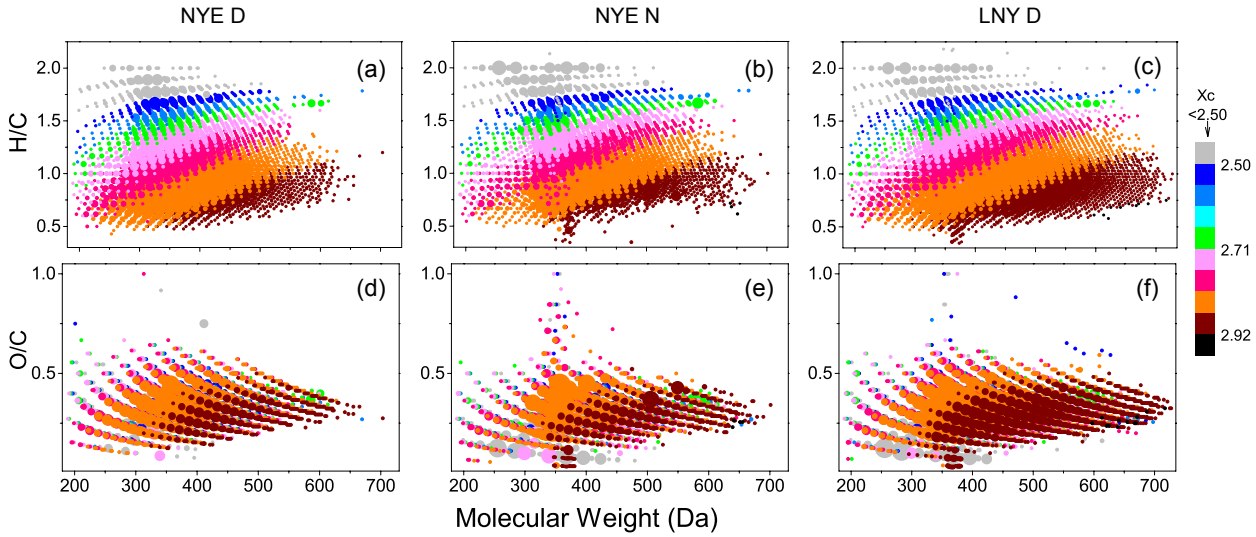

Figure S3: The H/C (**a, b, c**) and O/C (**d, e, f**) ratios of CHO formulae are shown as a function of their neutral mass from NYE D (**a, d**), NYE N (**b, e**) and LNY D (**c, f**) samples with their X_c values color-coded. Grey data points indicate non-aromatic compounds (X_c<2.5), blue to green data (2.5<X_c<2.71) are mono-aromatic compounds and pink to black data (X_c>2.71) includes PAHs. The size of the symbols reflects the relative peak intensities of molecular formulae on a logarithmic scale.

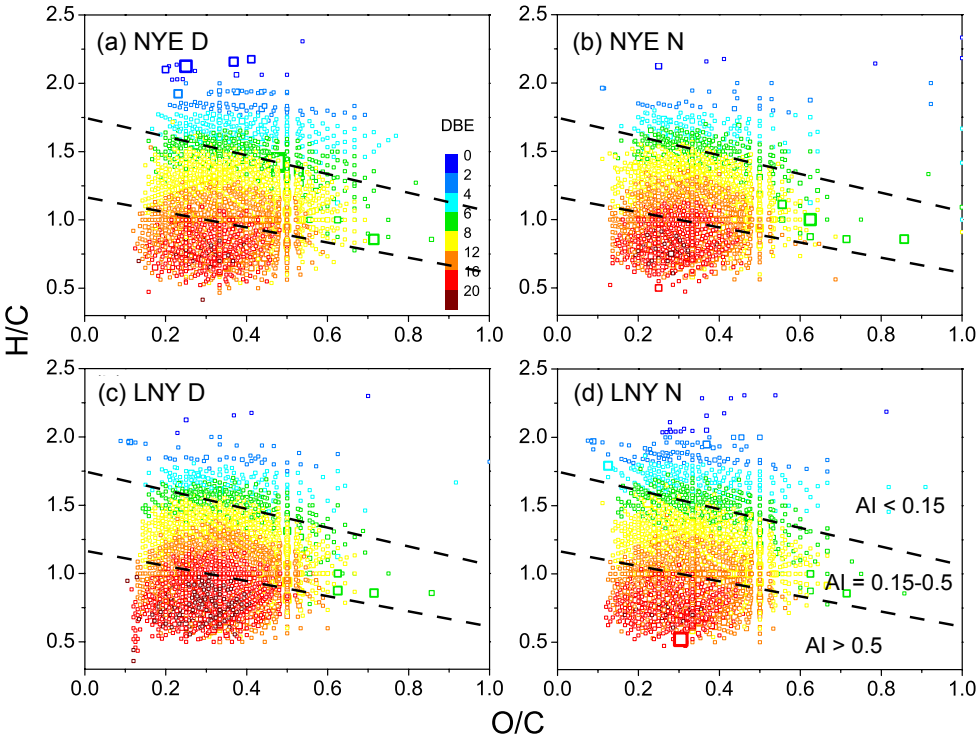

Figure S4: Van Krevelen diagrams (the H/C via O/C ratios) for the CHNO compounds with various aromatic index (AI) values ranges. The dashes lines separate the different AI regions. The size of the symbols reflects the relative peak intensities of compounds on a logarithmic scale.

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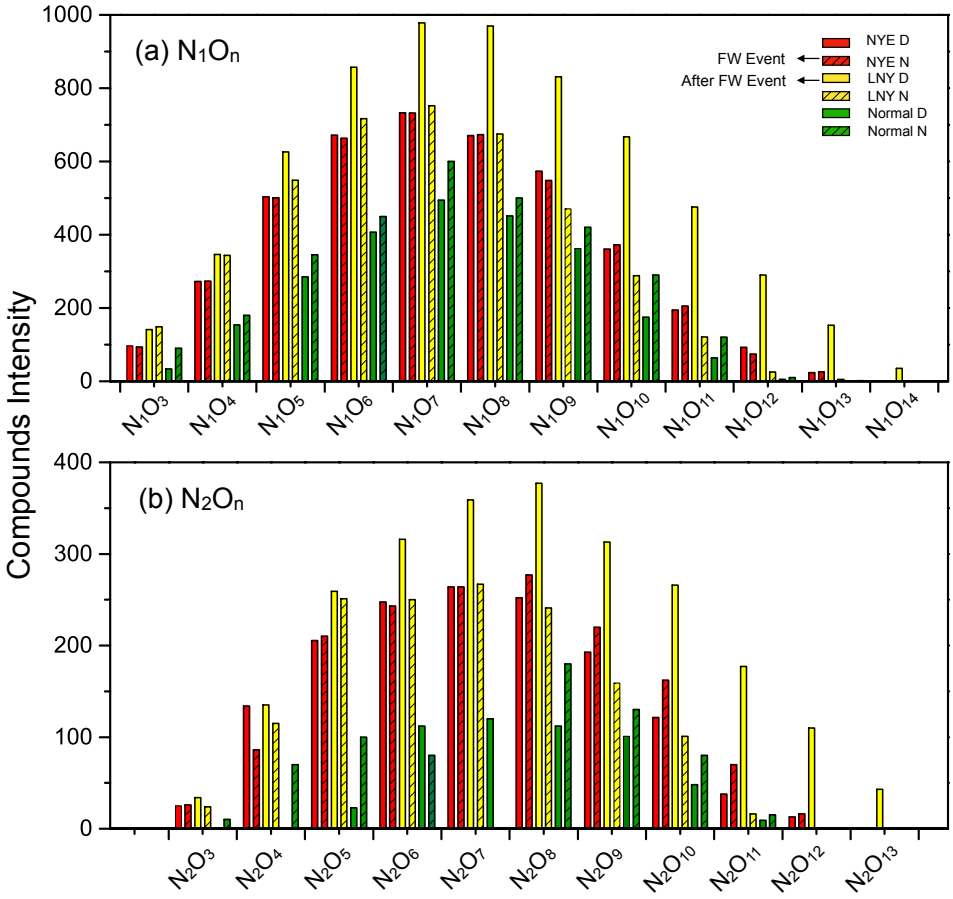

Figure S5: Intensity of CHNO species of subgroups according to the number of N and O atoms in their molecules.

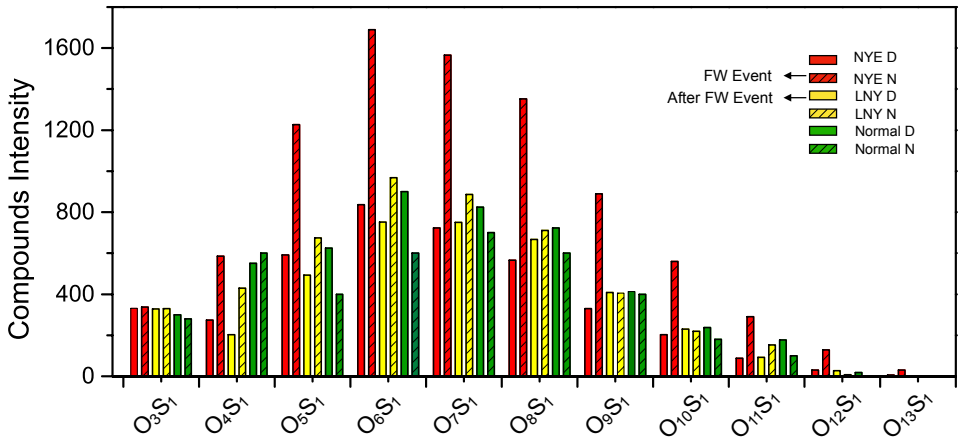

Figure S6: Intensity of CHOS species of subgroups according to the number of O and S atoms in their molecules.

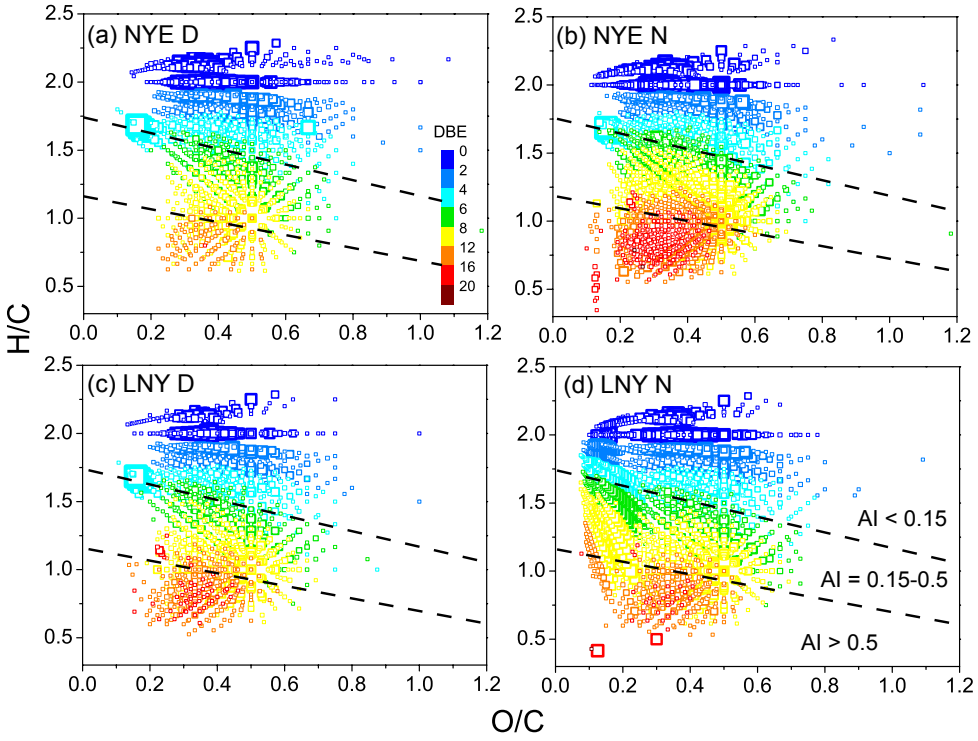

Figure S7: Van Krevelen diagrams (the H/C via O/C ratios) for the CHOS compounds with various aromatic index (AI) values ranges. The dashes lines separate the different AI regions. The size of the symbols reflects the relative peak intensities of compounds on a logarithmic scale.

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