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Insight into the composition of organic compounds ($\geq C_6$) in $PM_{2.5}$ in wintertime in Beijing, China

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Table S1: Average concentrations of major pollutants and weather condition parameters during the winter sampling campaign.

	$PM_{2.5}$	BC	OC	EC	O_3	SO_2	CO	NO	NO_2	NO_x	T	RH	WS
Unit	μg m^{-3}	μg m^{-3}	μg m^{-3}	μg m^{-3}	μg m^{-3}	μg m^{-3}	μg m^{-3}	μg m^{-3}	μg m^{-3}	μg m^{-3}	ºC	%	m s^{-1}
Averages	99.5	6.54	18. 9	4. 86	16.6	14.9	1.52	51.8	69.5	121	5.23	49.6	1.15
Non-haze days	35.3	2.42	9. 37	1. 39	26.6	7.67	0.81	23.9	47.9	71.8	4.00	39.8	1.44
Haze days	141	9.21	25. 0	7. 12	9.75	19.9	2.00	70.9	84.2	155	6.07	56.3	0.94

From Shi et al. (2018)

Table S2: Concentrations (mean ± s.d.) of specific compounds measured in Beijing aerosol samples (n = 33).

Compound name	ng m-3	Compound name	ng m-3
I. n-Alkanols			
1-Dodecanol	2.27±1.49	1-Octadecanol	1.69±1.65
1-Tetradecanol	24.2±88.9	1-Eicosanol	3.71±2.96
1-Hexadecanol	6.66±20.7		
Subtotal	**38.5±110**		
II. n-Alkanones			
6-Tetradecanone	1.34±3.98	8-Pentadecanone	15.0±22.9
Subtotal	**16.4±23.0**		
III. n-Alkanoic acids			
Hexanoic acid	1.80±1.54	Nonanoic acid	1.23±1.37
Heptanoic acid	0.73±1.05	Decanoic acid	22.8±25.2
Octanoic acid	2.97±2.56		
Subtotal	**29.5±27.0**		
IV. Hopanes			
18α(H)22,29,30-trisnorneohopane	2.91±3.06	17α(H)21β(H)-homohopane(22R)	1.32±1.32
17α(H)-22,29,30-Trisnorhopane	1.56±2.74	17α(H)21β(H)-homohopane(22S)	0.83±0.93
17α(H)21β(H)-30-norhopane	9.92±7.63	17α(H),21β(H)-bishomohopane(22S)	5.23±6.51
17β(H)21α(H)-hopane(moretane)	5.77±6.12	17α(H)21β(H)-bishomohopane(22R)	1.41±1.73
17α(H)21β(H)-hopane	3.71±5.49		
Subtotal	**32.7±24.7**		
V. PAHs			
Naphthalene (NAP,2-rings)	6.03±4.52	Benzo[k]fluoranthene (BkF, 5-rings)	8.81±7.68
Acenaphthylene (ACY, 2-rings)	12.7±9.93	Cyclopenta[cd]pyrene (CcP, 5-rings)	8.60±10.2
Acenaphthene (ACE, 2-rings)	6.04±8.94	9,10-Dihydrobenzo[e]pyrene (BePD, 5-rings)	1.60±1.59
Fluorene (FLU, 3-rings)	16.7±13.0	Perylene (PER, 5-rings)	3.20±2.69
Phenanthrene (PHE, 3-rings)	8.59±8.49	Benzo[b]fluoranthene (BbF, 5-rings)	38.5±31.8
Anthracene (ANT, 3-rings)	6.14±6.53	Benzo[a]pyrene (BaP, 5-rings)	13.1±13.8
Pyrene (PYR, 4-rings)	18.9±18.2	Benzo[e]pyrene (BeP, 5-rings)	15.4±10.3
Fluoranthene (FLT, 4-rings)	21.0±20.4	Dibenzo [a,h]pyrene (DBA, 5-rings)	5.68±7.35
Chrysene (CHR, 4-rings)	25.5±19.3	Benzo[ghi]fluoranthene (BghiF, 5-rings)	15.1±15.8
Benz[a]anthracene (BaA, 4-rings)	17.6±14.6	Indeno[1,2,3-cd]pyrene (IcdP, 6-rings)	12.3±8.82
2,3-Dihydro-1H-cyclopenta[l]phenanthrene (DCiP, 4-rings)	1.95±1.48	Benzo[ghi]perylene (BghiP, 6-rings)	12.4±11.1
4H-Cyclopenta[def]phenanthrene (CdP, 4 rings)	5.49±5.31		
Subtotal:	**281±176**		
VI. O-PAHs			
Anthracenedione (AQ)	5.12±5.97	Xanthone (XaO)	3.15±2.71
Benzo[a]fluorenone (BaFluO)	5.64±7.38	Phenanthraquinone (PQ)	1.45±1.08
Benzanthrone (BAntQ)	4.49±5.29	5,6-Chrysenequinone (ChryQ)	1.54±1.56
4,5-Pyrenequinone (4.5-PyrQ)	8.75±8.57	1-Acenaphthylenone (AceQ)	0.50±0.36

Compound name	ng m-3	Compound name	ng m-3
1,8-Pyrenequinone (1.8-PyrQ)	3.74±3.58	Acenaphthylenedione (AcPQ)	0.24±0.20
1,6-Pyrenequinone (1.6-PyrQ)	7.38±6.79	1-indanone (IndO)	0.46±0.36
9-Fluorenone (9-FluQ)	3.78±4.01	Benzo[b]naphtho[2,3-d]furan (BbN-2,3-F)	4.48±5.08
7,12-Benz[a]anthracenequinone (BaAQ)	4.09±3.61	Benzo(b)naphtho(1,2-d)furan (BbN-1,2-F)	6.75±13.1
Aceanthrenequinone (AceAntQ)	2.41±2.89	Cyclopenta(def)phenanthrenone (CdP)	0.67±1.27
5,12-Naphthacenedione (NapthQ)	3.29±3.09		
Subtotal:	**67.9±58.5**		
VII. Alkylated-PAHs and Alkylated-OPAHs			
Pyrene, 1-methyl-	21.5±21.5	Phenanthrene, 2,3,5-trimethyl-	6.94±7.28
Pyrene, 2-methyl-	6.68±7.95	Phenanthrene, 9,10-dimethyl-	2.95±2.87
Pyrene, 4-methyl-	12.3±12.9	Phenanthrene, 1-methyl-	5.29±5.38
Pyrene, 1,3-dimethyl-	9.00±10.8	Phenanthrene, 3,6-dimethyl-	4.24±4.16
2-Methylanthraquinone	1.91±3.98	10-Methylbenzo(a)pyrene	8.10±9.86
Dibenzo[def,mno]chrysene	4.59±8.01	Retene	14.4±17.5
1-Methylanthraquinone	1.92±1.76	2-Methylnaphthalene	1.76±3.57
Subtotal:	**102±79.7**		
VIII. Monoaromatic compounds			
Benzyl alcohol	2.97±3.22	Benzeneacetaldehyde	1.09±1.43
Benzaldehyde	8.38±8.19	1,2-Benzenedicarboxylic acid	2.66±4.43
1,2,4-Trimethoxybenzene	1.84±2.44	Acetophenone	1.06±1.28
Subtotal:	**18.0±14.0**		
IX. n-C_n-benzenes			
decylbenzene (C10)	0.51±0.41	octadecylbenzene (C18)	6.81±6.63
undecylbenzene (C11)	2.43±2.55	nonadecylbenzene (C19)	6.23±5.84
Dodecylbenzene (C12)	5.56±16.4	eicosylbenzene (C20)	4.07±3.60
tridecylbenzene (C13)	2.07±6.59	henicosylbenzene (C21)	2.35±1.80
tetradecylbenzene (C14)	8.85±33.2	docosylbenzene (C22)	2.00±1.39
pentadecylbenzene (C15)	2.85±2.74	tricosylbenzene (C23)	1.03±0.88
hexadecylbenzene (C16)	3.57±2.94	tetracosylbenzene (C24)	1.24±0.42
heptadecylbenzene (C17)	6.61±5.93	pentacosylcyclohexane (C25)	0.36±0.29
Subtotal	**56.6±73.0**		
X. n-C_n-cyclohexanes			
n-tetradeyl-cyclohexane (C20)	0.65±1.02	n-eicosyl-clohexane (C26)	8.15±10.1
n-pentadecyl-cyclohexane (C21)	0.83±0.85	n-heneicosyl-cyclohexane (C27)	2.45±4.11
n-hexadecyl-cyclohexane (C22)	0.90±0.53	n-docosyl-cyclohexane (C28)	1.99±1.62
n-heptadecyl-cyclohexane (C23)	6.69±9.65	n-tricosyl-cyclohexane (C29)	1.59±0.92
n-octadecyl-cyclohexane (C24)	6.41±6.98	n-tetracosyl-cyclohexane (C30)	1.32±0.75
n-nonadecyl-cyclohexane (C25)	8.47±8.93		
Subtotal	**39.4±37.1**		
XI. Esters			
Dibutyl phthalate (DBP)	16.9±15.5	Di(2-ethylhexyl)-phthalate (DEHP)	16.0±12.6
Diethyl Phthalate (DEP)	2.67±2.91	Benzoic acid, 4-ethoxy-, ethyl ester	1.74±4.27

Compound name	ng m-3	Compound name	ng m-3
Diisooctyl phthalate	49.7±43.2	Butanedioic acid, bis(2-methylpropyl) ester	2.10±2.04
Dimethyl phthalate	2.58±2.80	Hexanedioic acid, bis(2-methylpropyl) ester	20.0±16.8
Glutaric acid, di(isobutyl) ester	5.35±4.91		
Subtotal	**117±82.1**		
XII. Biomarkers			
levoglucosan	355±232	phytane	1.94±1.05
Cedrol	2.55±3.77	pristane	2.24±1.69
phytone	14.7±11.7	Supraene	2.13±1.75
Subtotal:	**511±317**		
XIII. Pyridines			
Pyridine, 2-propyl- (C8)	1.98±2.74	Pyridine, 2-dodecyl- (C17)	0.52±0.26
Pyridine, 2-butyl- (C9)	0.71±0.70	Pyridine, 2-tridecyl- (C18)	2.33±1.81
Pyridine, 2-pentyl- (C10)	0.28±0.14	Pyridine, 2-tetradecyl- (C19)	0.59±1.20
Pyridine, 2-hexyl- (C11)	3.03±2.52	Pyridine, 2-pentadecyl- (C20)	1.42±1.16
Pyridine, 2-heptyl- (C12)	0.41±0.21	Pyridine, 2,3,5-trimethyl- (C8)	1.14±1.64
Pyridine, 2-octyl- (C13)	0.31±0.15	Pyridine, 2,3,6-trimethyl- (C8)	0.62±0.90
Pyridine, 2-nonyl- (C14)	0.83±2.73	Pyridine, 2,4,6-trimethyl- (C8)	1.45±1.52
Pyridine, 2-decyl- (C15)	0.39±0.64	Pyridine, 4-ethyl-2,6-dimethyl- (C9)	1.22±2.75
Pyridine, 2-undecyl- (C16)	0.20±0.17		
Subtotal	17.4±7.58		
XIV. Quinolines			
Quinoline	3.25±5.29	Quinoline, 5-methyl-	2.96±2.45
Quinoline, 2-methyl-	2.04±2.60	Quinoline, 6-methyl-	1.00±1.52
Quinoline, 3-methyl-	1.24±1.83	Quinoline, 7-methyl-	1.00±1.13
Quinoline, 4-methyl-	3.64±5.32	Quinoline, 8-methyl-	1.44±1.33
Subtotal	**16.6±15.0**		
XV. Other nitrogen compounds (Nitro，amine，heterocyclic compounds)			
5-Methyl-2-nitrophenol	1.85±2.03	Phthalimide	0.91±0.87
Phenol, 4-nitro-	1.66±1.77	Acridine	1.99±1.98
Benzenamine, 2,3-dimethyl-	0.47±0.53	Ellipticine	10.5±10.7
Benzenamine, 2,4-dimethyl-	0.65±0.78	Phenanthridine	1.96±2.66
Benzenamine, 2,5-dimethyl-	1.36±5.42	Carbazole	1.83±1.82
Benzenamine, 3,5-dimethyl-	0.28±0.29	Benzo[f]quinoline	4.40±4.66
9H-Carbazole, 9-methyl-	1.35±1.77	Isoquinoline	0.80±0.83
Subtotal:	**30.0±23.1**		
XVI. Phenolic compounds			
Phenol, 2,5-dimethyl-	0.88±0.91	1-Naphthalenol, 4-methoxy-	0.71±1.04
Phenol, 3,4-dimethyl-	0.59±0.74	1-Naphthalenol, 4-methyl-	2.49±2.14
Phenol, 2-ethyl-4-methyl-	0.41±0.27	2-Dibenzofuranol	1.84±2.09
Benzaldehyde, 2-hydroxy-	1.35±1.78	7-Methyl-1-naphthol	1.00±1.33
1-Naphthalenol	1.56±5.61	2-Hydroxyfluorene	1.08±1.07

Compound name	ng m-3	Compound name	ng m-3
1-Naphthalenol, 2-methyl-	1.28±1.52	Methoxyphenols	7.29±7.11
2-Naphthalenol	1.15±1.21		
Subtotal:	**21.6±17.0**		
XVII. Others			
2,2'-Binaphthalene	1.97±2.64	1-Naphthalenecarboxaldehyde	1.71±1.53
1,2'-Binaphthalene	1.11±1.16	Terphenyl-m+p+o	1.81±1.69
Naphthalene, 2-phenyl-	4.41±4.72	Benzo[kl]xanthene	6.40±7.88
Naphthalic anhydride	9.62±13.4		
Subtotal:	**27.0±26.1**		
XVIII. Graphics method			
1) alkyl-benzenes	193±142	2) alkyl-Nap	103±252
3) alkyl-decalins	110±95.4	4) alkyl-benzaldehydes	39.1±36.6
5) alkyl-Phe & Ant	15.4±11.3		

6) Branched alkanes

NO	Concentrations	NO	Concentrations	NO	Concentrations	NO	Concentrations
C12	7.89±7.96	C19	5.70±4.13	C26	25.1±21.8	C33	5.36±4.93
C13	12.8±13.7	C20	15.5±13.8	C27	20.5±17.4	C34	3.59±2.65
C14	3.39±2.21	C21	17.8±14.1	C28	14.6±10.6	C35	3.23±2.26
C15	23.7±29.4	C22	29.2±21.2	C29	19.6±13.4	C36	3.62±1.91
C16	5.35±5.14	C23	24.7±19.1	C30	22.4±34.5		
C17	12.3±7.66	C24	27.3±22.0	C31	13.7±10.1		
C18	4.53±2.60	C25	24.2±14.3	C32	10.0±9.77		
Subtotal	**356±173**						

alkyl-Phenanthrene & Anthracene (alkyl-Phe&Ant)

alkyls-Naphthalene (alkyl-Nap)

Table S3: The concentrations of organic compounds, ng m^{-3}.

NO	Groups	Non-haze	Haze	Ratio
		ng m^{-3}	ng m^{-3}	
1	n-Alkanes*	264	577	2.19
	Branched Alkanes	234	440	1.88
2	n-Alkenes*	132	252	1.91
3	n-Alkanols	8.39	59.8	7.13
	n-Alkanoic Acids	36.4	24.6	0.68
4	Aliphatic carbonyls:			
	n-alkanals*	27.2	42.6	1.57
	n-alkan-2-ones*	8.71	24.3	2.79
	n-alkan-3-ones*	3.61	8.89	2.46
5	Other n-alkanones	11.4	20.0	1.75
6	Biomarker:			
	Levoglucosan	238	417	1.75
	Cedrol	2.56	2.41	0.94
	phytone*	7.47	19.6	2.62
	phytane	1.87	1.99	1.06
	pristine	2.27	2.22	0.98
	Supraene	1.44	2.49	1.73
7	Furanones*	8.52	20.52	2.41
8	Hopanes	15.2	44.6	2.93
9	PAHs	159	364	2.29
10	O-PAH	39.7	86.5	2.18
11	Alkylated-(PAHs & O-PAHs)	67.4	118	1.75
12	EsterS	89.4	132	1.48
13	n-C_n-cyclohexanes	10.8	53.3	4.94
14	n-C_n-benzenes	23.3	78.2	3.36
15	Alkyl-benzenes	183	200	1.09
16	Alkyl-decalins	85.4	126	1.48
17	Alkyl-Phe & Ant	11.7	17.1	1.46
18	Alkyl-Nap	51.3	133	2.59
19	Alkyl-benzaldehyde	31.1	34.3	1.10
20	Monoaromatic compounds	17.7	18.2	1.03
21	Pyridines	12.0	15.3	1.28
22	Quinolines	16.8	16.5	0.98
23	Other nitrogen compounds	22.6	34.2	1.51
24	Phenolic compounds	14.0	25.9	1.85
25	Others	15.3	35.5	2.32
	Total	**1853**	**3448**	1.86

* The data have been reported by Lyu et al. (2018)

1. Estimate method of unidentified organic compounds

Unidentified compounds in the chromatograms were estimated according to the chemical and physical properties of compounds. The retention time I (min) and retention time II (sec) were used to separate all unidentified compounds according to the criteria in Table S4. Seven internal standards (IS) were used in the method, with 3 ng for each of them. The mass concentrations of undefined compounds were calculated by the ratio of the intensity of volume (IV) for the compound and the adjacent IS; the equation is as follows:

$$Mass\ (unknown\ compounds) = \frac{IV_{unknown\ compounds}}{IV_{IS}}\ x\ 3\ ng$$

Table S4: Detailed criteria of coordinate and reference internal standards (IS) for each section of the chromatogram.

NO	Retention I	Retention II	IS	Characteristics of unidentified organic compounds
	min	sec		
1	X ≤ 44	Y ≤ 2.4	Pentadecane-d32	Low molecular weight: ➢ carbon numbers (n-alkanes) ≤ 17; ➢ monoaromatics;
2	44 < X ≤ 63	Y ≤ 5.0	Eicosane-d42	Medium molecular weight: ➢ 17 < carbon numbers (n-alkanes) ≤ 23);
3	63< X ≤ 80	Y ≤ 5.0	Pentacosane-d52	Medium molecular weight: ➢ 23 < carbon numbers (n-alkanes) ≤ 27);
4	X > 80	Y ≤ 5.0	Triacontane-d62	High molecular weight: ➢ carbon numbers (n-alkanes) ≥ 27;
5	X ≤ 44	2.4 < Y ≤ 4.0	Nonylbenzene-2,3,4,5,6-d5	Oxidized monoaromatics;
6	X ≤ 44	Y > 4.0	Biphenyl-d10	2 rings PAHs
7	X ≥ 44	Y ≥ 5.0	p-Terphenyl-d14	3-6 rings PAHs and hopanes;

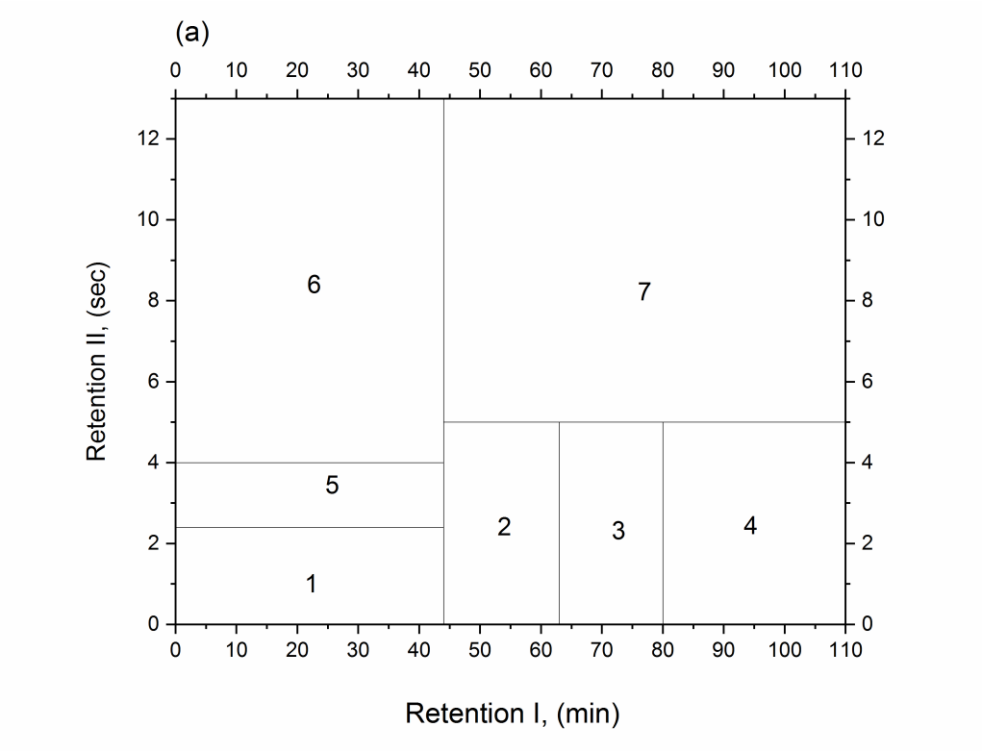

Figure S1: The separated chromatogram from the GC × GC-TOFMS.

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