

SUPPORTING INFORMATION

Insight into the Composition of Organic Compounds (\geq C6) 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	O₃	SO₂	CO	NO	NO₂	NO_x	T	RH	WD	WS
Unit	$\mu\text{g m}^{-3}$	$\mu\text{g m}^{-3}$	$\mu\text{g m}^{-3}$	$\mu\text{g m}^{-3}$	$\mu\text{g m}^{-3}$	$\mu\text{g m}^{-3}$	$\mu\text{g m}^{-3}$	$\mu\text{g m}^{-3}$	$\mu\text{g m}^{-3}$	$\mu\text{g m}^{-3}$	°C	%	(360° = N)	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	172	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	192	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	159	0.94

From Shi et al. (2018)

Table S2: Concentrations (mean \pm 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 \pm 1.49	1-Octadecanol	1.69 \pm 1.65
1-Tetradecanol	24.2 \pm 88.9	1-Eicosanol	3.71 \pm 2.96
1-Hexadecanol	6.66 \pm 20.7		
Subtotal	38.5\pm110		
II. n-Alkanones			
6-Tetradecanone	1.34 \pm 3.98	8-Pentadecanone	15.0 \pm 22.9
Subtotal	16.4\pm23.0		
III. n-Alkanoic acids			
Hexanoic acid	1.80 \pm 1.54	Nonanoic acid	1.23 \pm 1.37
Heptanoic acid	0.73 \pm 1.05	Decanoic acid	22.8 \pm 25.2
Octanoic acid	2.97 \pm 2.56		
Subtotal	29.5\pm27.0		
IV. Hopanes			
18 α (H)22,29,30-trisnorhopane	2.91 \pm 3.06	17 α (H)21 β (H)-homohopane(22R)	1.32 \pm 1.32
17 α (H)-22,29,30-Trisnorhopane	1.56 \pm 2.74	17 α (H)21 β (H)-homohopane(22S)	0.83 \pm 0.93
17 α (H)21 β (H)-30-norhopane	9.92 \pm 7.63	17 α (H),21 β (H)-bishomohopane(22S)	5.23 \pm 6.51
17 β (H)21 α (H)-hopane(moretane)	5.77 \pm 6.12	17 α (H)21 β (H)-bishomohopane(22R)	1.41 \pm 1.73
17 α (H)21 β (H)-hopane	3.71 \pm 5.49		
Subtotal	32.7\pm24.7		
V. PAHs			
Naphthalene (NAP, 2-rings)	6.03 \pm 4.52	Benzo[k]fluoranthene (BkF, 5-rings)	8.81 \pm 7.68
Acenaphthylene (ACY, 2-rings)	12.7 \pm 9.93	Cyclopenta[cd]pyrene (CcP, 5-rings)	8.60 \pm 10.2
Acenaphthene (ACE, 2-rings)	6.04 \pm 8.94	9,10-Dihydrobenzo[e]pyrene (BePD, 5-rings)	1.60 \pm 1.59
Fluorene (FLU, 3-rings)	16.7 \pm 13.0	Perylene (PER, 5-rings)	3.20 \pm 2.69
Phenanthrene (PHE, 3-rings)	8.59 \pm 8.49	Benzo[b]fluoranthene (BbF, 5-rings)	38.5 \pm 31.8
Anthracene (ANT, 3-rings)	6.14 \pm 6.53	Benzo[a]pyrene (BaP, 5-rings)	13.1 \pm 13.8
Pyrene (PYR, 4-rings)	18.9 \pm 18.2	Benzo[e]pyrene (BeP, 5-rings)	15.4 \pm 10.3
Fluoranthene (FLT, 4-rings)	21.0 \pm 20.4	Dibenzo [a,h]pyrene (DBA, 5-rings)	5.68 \pm 7.35
Chrysene (CHR, 4-rings)	25.5 \pm 19.3	Benzo[ghi]fluoranthene (BghiF, 5-rings)	15.1 \pm 15.8
Benz[a]anthracene (BaA, 4-rings)	17.6 \pm 14.6	Indeno[1,2,3-cd]pyrene (IcdP, 6-rings)	12.3 \pm 8.82
2,3-Dihydro-1H-cyclopenta[1]phenanthrene (DCiP, 4-rings)	1.95 \pm 1.48	Benzo[ghi]perylene (BghiP, 6-rings)	12.4 \pm 11.1
4H-Cyclopenta[def]phenanthrene (CdP, 4 rings)	5.49 \pm 5.31		
Subtotal:	281\pm176		
VI. O-PAHs			
Anthracenedione (AQ)	5.12 \pm 5.97	Xanthone (XaO)	3.15 \pm 2.71
Benzo[a]fluorenone (BaFluO)	5.64 \pm 7.38	Phenanthraquinone (PQ)	1.45 \pm 1.08
Benzanthrone (BAntQ)	4.49 \pm 5.29	5,6-Chrysenequinone (ChryQ)	1.54 \pm 1.56
4,5-Pyrenequinone (4.5-PyrQ)	8.75 \pm 8.57	1-Acenaphthyleneone (AceQ)	0.50 \pm 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)phenanthrene (CdP)	0.67±1.27
5,12-Naphthacenedione (NaphQ)	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	hencicosylbenzene (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-tetradecyl-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
		ng m ⁻³	ng m ⁻³
1	n-Alkanes*	264	577
	Branched Alkanes	234	440
2	n-Alkenes*	132	252
3	n-Alkanols	8.39	59.8
	n-Alkanoic Acids	36.4	24.6
4	Aliphatic carbonyls:		
	n-alkanals*	27.2	42.6
	n-alkan-2-ones*	8.71	24.3
	n-alkan-3-ones*	3.61	8.89
5	Other n-alkanones	11.4	20.0
6	Biomarker:		
	Levoglucosan	238	417
	Cedrol	2.56	2.41
	phytone*	7.47	19.6
	phytane	1.87	1.99
	pristine	2.27	2.22
	Supraene	1.44	2.49
7	Furanones*	8.52	20.52
8	Hopanes	15.2	44.6
9	PAHs	159	364
10	O-PAH	39.7	86.5
11	Alkyl-PAHs & O-PAHs	67.4	118
12	EsterS	89.4	132
13	n-C _n -cyclohexanes	10.8	53.3
14	n-C _n -benzenes	23.3	78.2
15	Alkyl-benzenes	183	200
16	Alkyl-decalins	85.4	126
17	Alkyl-Phe & Ant	11.7	17.1
18	Alkyl-Nap	51.3	133
19	Alkyl-benzaldehyde	31.1	34.3
20	Monoaromatic compounds	17.7	18.2
21	Pyridines	12.0	15.3
22	Quinolines	16.8	16.5
23	Other nitrogen compounds	22.6	34.2
24	Phenolic compounds	14.0	25.9
25	Others	15.3	35.5
	Total	1853	3448

* 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:

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

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	$X \leq 44$	$Y \leq 2.4$	Pentadecane-d32	Low molecular weight: ➤ carbon numbers (n-alkanes) ≤ 17 ; ➤ monoaromatics;
2	$44 < X \leq 63$	$Y \leq 5.0$	Eicosane-d42	Medium molecular weight: ➤ $17 < \text{carbon numbers (n-alkanes)} \leq 23$;
3	$63 < X \leq 80$	$Y \leq 5.0$	Pentacosane-d52	Medium molecular weight: ➤ $23 < \text{carbon numbers (n-alkanes)} \leq 27$;
4	$X > 80$	$Y \leq 5.0$	Triacotane-d62	High molecular weight: ➤ carbon numbers (n-alkanes) ≥ 27 ;
5	$X \leq 44$	$2.4 < Y \leq 4.0$	Nonylbenzene- 2,3,4,5,6-d5	Oxidized monoaromatics;
6	$X \leq 44$	$Y > 4.0$	Biphenyl-d10	2 rings PAHs
7	$X \geq 44$	$Y \geq 5.0$	p-Terphenyl-d14	3-6 rings PAHs and hopanes;

Table S5: Mean \pm s.d. of estimated concentrations in each section of the chromatogram for haze and non-haze conditions.

	Clean	Haze
	ng/m ³	ng/m ³
	Mean \pm SD	Mean \pm SD
1	546 \pm 406	632 \pm 626
2	137 \pm 90	147 \pm 63
3	215 \pm 215	228 \pm 102
4	188 \pm 166	320 \pm 484
5	298 \pm 184	985 \pm 707
6	303 \pm 168	879 \pm 979
7	440 \pm 312	774 \pm 629
Total	2119	3964

References:

Feng, B., Li, L., Xu, H., Wang, T., Wu, R., Chen, J., Zhang, Y., Liu, S., Ho, S.S.H., Cao, J., Huang, W., 2018. PM_{2.5}-bound polycyclic aromatic hydrocarbons (PAHs) in Beijing: Seasonal variations, sources, and risk assessment. *Journal of Environmental Sciences*.

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