Supplement of Atmos. Chem. Phys., 19, 8741–8758, 2019
https://doi.org/10.5194/acp-19-8741-2019-supplement

Atmospheric Chemistry and Physics
Open Access
EGU

Supplement of

Variability of polycyclic aromatic hydrocarbons and their oxidative derivatives in wintertime Beijing, China

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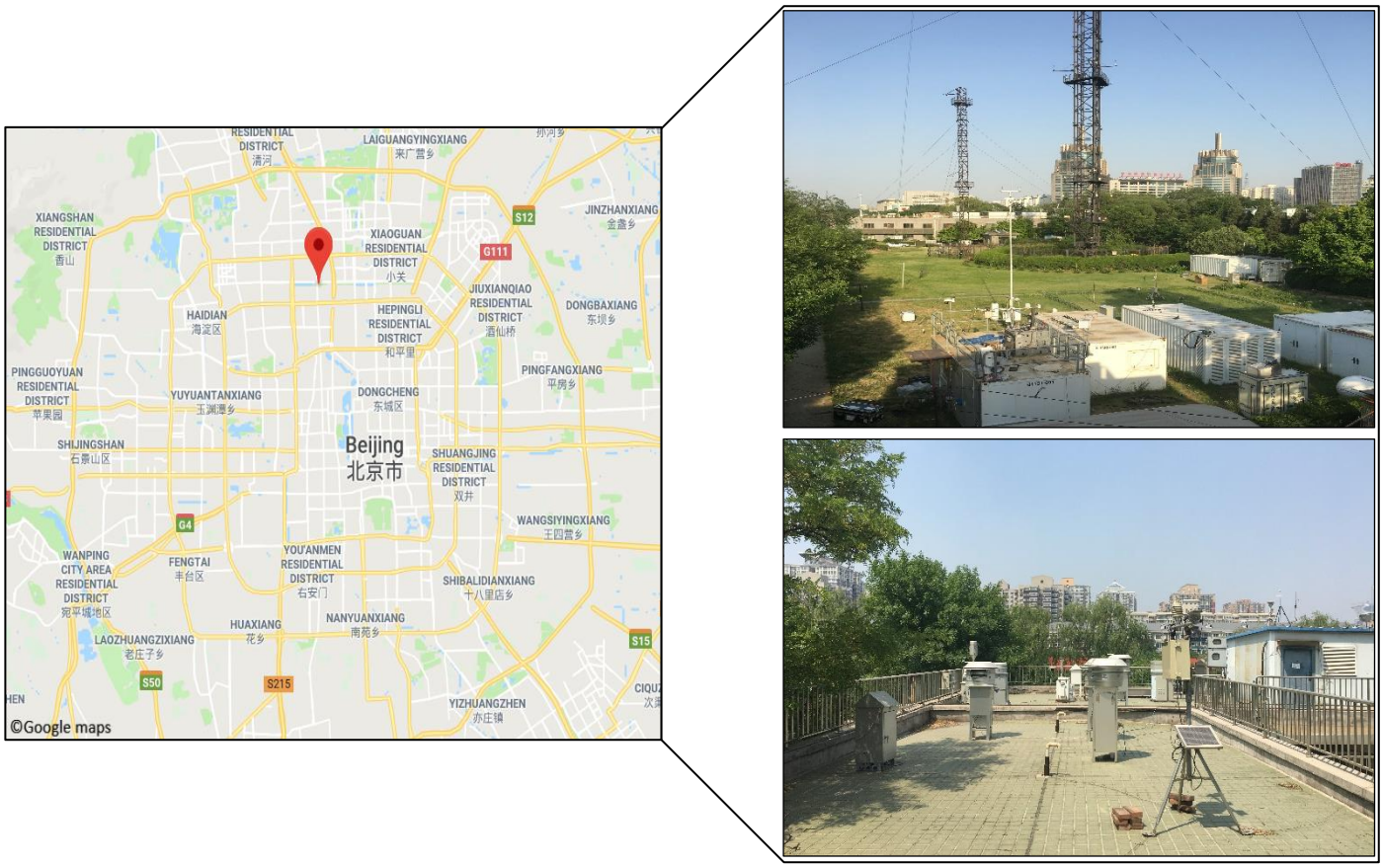

Figure S1. Map with the location of measurements site, the red mark corresponds to 39° 58' 28" North, 116° 22' 15" East.

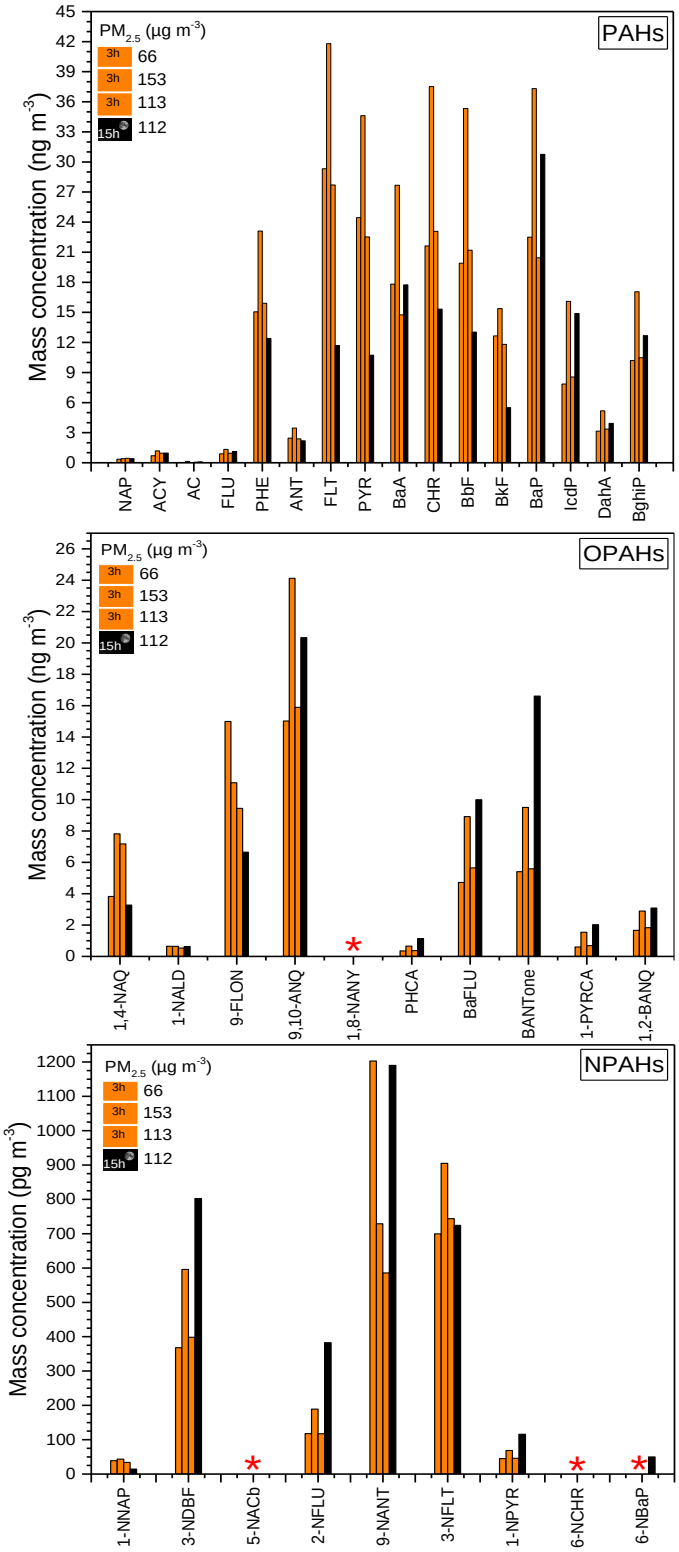

Figure S2. Column distributions illustrating the highest concentrations recorded during the sampling campaign (29 Nov 2016) for individual 16 PAHs, 10 OPAHs and 9 NPAHs in the 3 h (day) and 15 h (night) samples. The first 3 h ($PM_{2.5}$ = 66 µg m^{-3}) correspond to the first sampled filter at 8:30 in the morning and so forth. Asterisk (*) means below LOQ except for 1,8-NANY, it represents outside the dynamic range.

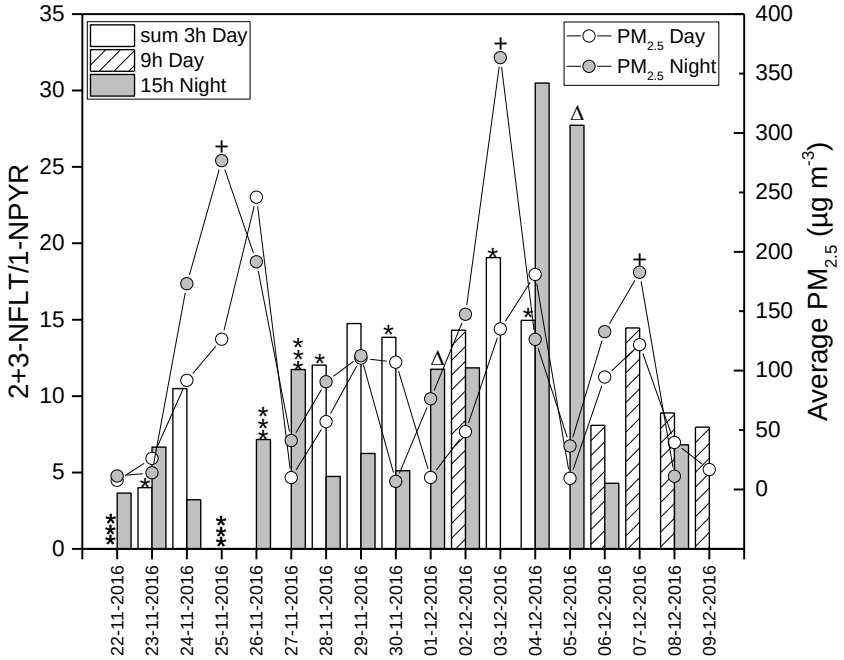

Figure S3. Ratio of 2+3-Nitrofluoranthene/1-Nitropyrene in $PM_{2.5}$ during daytime and night-time samples. One asterisk (*) means 1-NPYR < LOQ in one sample of 3 h, hence the ratios are overestimated; three asterisks mean below LOQ in three samples of 3 h (daytime data not available); (Δ) symbols refer to 1-NPYR < LOQ in the 9 h day samples (daytime data not available); (+) symbols mean night-time data not available.

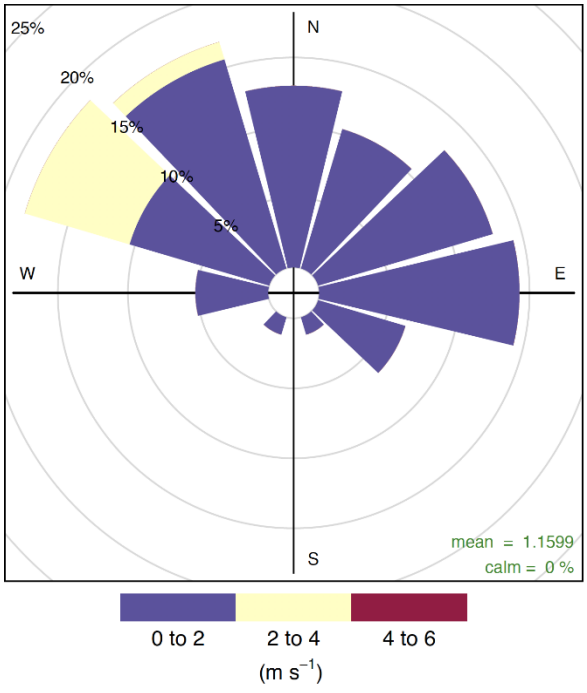

Figure S4. Wind-rose plot for the measurement period from 22 November 2016 to 9 December 2017 in Beijing.

Table S1. Pearson correlation coefficients between ∑PAHs, ∑OPAHs, ∑NPAHs and O_3, CO, NO, NO_2, SO_2, HONO, temperature and relative humidity during the daytime (18 days with 3 h and 9 h sampling time) and night-time (14 nights with 15 h sampling time). Strong positive correlation (0.8-1) are shown in Bold ($P<0.05$).

	Time	∑PAHs	∑OPAHs	∑NPAHs
O_3	3 h	-0.60	-0.59	-0.47
	9 h	-0.78	-0.85	-0.80
	15 h	-0.79	-0.64	-0.75
CO	3 h	0.60	0.62	0.44
	9 h	**0.90**	**0.92**	**0.92**
	15 h	**0.88**	**0.86**	0.56
NO	3 h	0.60	0.55	0.38
	9 h	**0.97**	**0.98**	**0.98**
	15 h	**0.84**	0.73	0.37
NO_2	3 h	0.48	0.58	0.43
	9 h	**0.84**	**0.89**	**0.90**
	15 h	**0.87**	**0.82**	0.68
SO_2	3 h	0.72	0.74	0.59
	9 h	**0.90**	**0.89**	**0.90**
	15 h	**0.85**	**0.86**	0.58
HONO	3 h	**0.87**	**0.94**	**0.94**
	9 h	**0.95**	**0.87**	**0.88**
	15 h	**0.85**	0.77	0.52
T°	3 h	0.04	0.18	0.07
	9 h	-0.17	-0.23	-0.20
	15 h	0.09	0.07	0.16
RH	3 h	0.73	0.71	0.59
	9 h	0.66	0.59	0.63
	15 h	0.50	0.58	0.34

Table S2. Pearson correlation coefficients between individual NPAHs in $PM_{2.5}$ and HONO. (n) correspond to the number of data in common between each NPAHs and HONO concentrations. Values in Bold correspond to strong correlation with high significance levels (R=0.8-1; P<0.05, 95% level of confidence).

	Time	n	HONO	P value
	3 h	**15**	**0.94**	**<0.001**
1-NNAP	9 h	5	0.82	>0.05
	15 h	10	0.59	>0.05
	3 h	**15**	**0.93**	**<0.001**
3-NDBF*	9 h	5	0.82	>0.05
	15 h	10	0.66	<0.05
	3 h	1	NA	
5-NAC	9 h	0	NA	
	15 h	4	0.89	>0.05
	3 h	**16**	**0.92**	**<0.001**
2-NFLU	9 h	5	0.84	>0.05
	15 h	**10**	**0.83**	**<0.01**
	3 h	**16**	**0.90**	**<0.001**
9-NANT*	9 h	5	0.78	>0.05
	15 h	10	0.15	>0.05
	3 h	**13**	**0.93**	**<0.001**
3-NFLT*	**9 h**	**5**	**0.98**	**<0.01**
	15 h	10	0.65	<0.05
	3 h	**6**	**0.90**	**<0.01**
1-NPYR	9 h	4	0.81	>0.05
	15 h	**9**	**0.94**	**<0.001**
	3 h	1	NA	
6-NCHR	9 h	0	NA	
	15 h	2	NA	
	3 h	0	NA	
6-NBaP	9 h	1	NA	
	15 h	6	0.3	>0.05

* Major compounds in NPAHs
(NA) not available.

Table S3. Toxicity Equivalency Factor (TEFs) for individual PAHs, OPAHs and Nitro-PAHs.

Compound	TEF	References
PAHs		
Napthalene	0.001	Nisbet and LaGoy., 1992
Acenaphthylene	0.001	Nisbet and LaGoy., 1992
Acenaphthene	0.001	Nisbet and LaGoy., 1992
Fluorene	0.0005	Larsen et al., 1998
Phenanthrene	0.0005	Larsen et al., 1998
Anthracene	0.0005	Larsen et al., 1998
Fluoranthene	0.05	Larsen et al., 1998
Pyrene	0.001	Larsen et al., 1998
Benzo[a]anthracene	0.082	Durant et al., 1996
Chrysene	0.017	Durant et al., 1996
Benzo[b]fluoranthene	0.25	Durant et al., 1996
Benzo[k]fluoranthene	0.11	Durant et al., 1996
Benzo[a]pyrene	1	OEHHA., 1994
Indeno[1,2,3-cd]pyrene	0.1	Larsen et al., 1998
Dibenzo[a,h]anthracene	1.1	Larsen et al., 1998
Benzo[g,h,i]perylene	0.02	Larsen et al., 1998
OPAHs		
7H-Benz[de]anthracene-7-one	0.0039	Durant et al., 1996
Nitro-PAHs		
5-Nitroacenaphthene	0.01	OEHHA., 1994
2-Nitrofluorene	0.01	OEHHA., 1994
9-Nitroanthracene	0.0032	Durant et al., 1996
3-Nitrofluoranthene	0.0026	Durant et al., 1996
1-Nitropyrene	0.1	OEHHA., 1994
6-Nitrochrysene	10	OEHHA., 1994

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