Supplement of Atmos. Chem. Phys., 21, 3685–3697, 2021
https://doi.org/10.5194/acp-21-3685-2021-supplement

Atmospheric Chemistry and Physics
Open Access
EGU

Supplement of

Measurement report: $PM_{2.5}$-bound nitrated aromatic compounds in Xi'an, Northwest China – seasonal variations and contributions to optical properties of brown carbon

Wei Yuan et al.

Correspondence to: Ru-Jin Huang (rujin.huang@ieecas.cn)

Table S1. List of input compounds and their abbreviations measured in this study for PMF source apportionment.

Compounds	Abbreviation
NACs	
4-Nitrophenol	4NP
4-Nitro-1-naphthol	4N1N
2-Methyl-4-nitrophenol	2M4NP
3-Methyl-4-nitrophenol	3M4NP
2,6-Dimethyl-4-nitropheol	2,6DM4NP
4-Nitrocatechol	4NC
3-Methyl-5-nitrocatechol	3M5NC
4-Methyl-5-nitrocatechol	4M5NC
3-Nitrosalicylic acid	3NSA
5-Nitrosalicylic acid	5NSA
PAHs	
Fluoranthene	FLU
Pyrene	PYR
Chrysene	CHR
Benzo(a)anthracene	BaA
Benzo(a)pyrene	BaP
Benzo(b)fluoranthene	BbF
Benzo(k)fluoranthene	BkF
Indeno[1,2,3-cd]pyrene	IcdP
Benzo(ghi)perylene	BghiP
Picene	PI
MOPs	
Syringyl acetone	SyA
Vanillin	VAN
Vanillic acid	VaA
Hopanes	
17α(H),21β(H)-30-Norhopane	HP1
17α(H),21β(H)-Hopane	HP2
17α(H),21β(H)-(22S)-Homohopane	HP3
17α(H),21β(H)-(22R)-Homohopane	HP4
Others	
Levoglucosan	LEV
Phthalic acid	*o*-ph

Table S2. Method performance parameters for nitrated aromatic compounds, including GC retention time (min), instrument detection limit (IDL), instrument quantitation limit (IQL), and mean extraction recoveries (n = 3).

Nitrated aromatic compounds	Retention time (min)	Quan. Ion (m/z)	Linear range (ug L^{-1})	Linear regression R^2	IDL (ug L^{-1})	IQL (ug L^{-1})	Extraction recovery (%)
4NP-2,3,5,6-d_4 (IS)	11.4	200	-	-	-	-	-
4NP	11.5	196	50-5000	0.999	16.4	55	85(7.2)
3M4NP	12.0	210	10-3000	0.999	2.9	9.8	102(5.4)
2M4NP	12.5	210	10-5000	0.999	3.2	10.7	84(3.3)
2,6DM4NP	13.9	224	50-5000	0.999	20	68	79(0.8)
4NC	14.1	73	10-3000	0.997	1.9	6.4	81(2.8)
4M5NC	14.4	313	10-5000	0.997	2.2	7.3	76(3.3)
3NSA	14.8	312	50-3000	0.996	21	69	88(5.1)
3M5NC	15.0	73	10-3000	0.997	3.5	11.5	87(4.5)
5NSA	15.6	312	100-2000	0.996	53	176	74(7.9)
4N1N	16.7	229	50-3000	0.996	16.8	56	95(4.4)

Table S3. *F* matrix elements constrained in the ME-2/chemical species 4 factors solution. The profiles are normalized to the $Abs_{365,MSOC}$. The 0s value denote the $f_{h,j}$ values constrained in ME-2c, while hyphens denote unconstrained elements.

Species	Secondary Formation	Biomass burning	Coal Burning	Vehicle emission
4NP	-	-	-	-
2M4NP	-	-	-	-
3M4NP	-	-	-	-
2,6DM4NP	-	-	-	-
4NC	-	-	-	-
3M5NC	-	-	-	-
4M5NC	-	-	-	-
3NSA	-	-	-	-
5NSA	-	-	-	-
4N1N	-	-	-	-
o-ph	-	0	0	0
HP1	0	0	-	-
HP2	0	0	-	-
HP3	0	0	-	-
HP4	0	0	-	-
PI	0	-	-	-
FLU	0	-	-	-
PYR	0	-	-	-
CHR	0	-	-	-
BaA	0	-	-	-
BaP	0	-	-	-
BbF	0	-	-	-
BkF	0	-	-	-
IcdP	0	-	-	-
BghiP	0	-	-	-
LEV	0	-	0	0
VaA	0	-	0	0
VAN	0	-	0	0
SyA	0	-	0	0

Table S4. Seasonal and annual mean concentrations and standard deviation (value in parentheses) of measured individual NACs in this study and the percentage of NACs to OC and $Abs_{NACs,365}$ to $Abs_{BrC,365}$.

Compound(ng m-3)	Spring Ave(SD)	Summer Ave(SD)	Fall Ave(SD)	Winter Ave(SD)	Annual Ave(SD)
4NP	1.19(0.36)	0.45(0.28)	3.6(2.6)	15.6(6.6)	5.2(7.1)
2M4NP	0.24(0.08)	0.10(0.10)	0.73(0.54)	4.5(1.72)	1.38(2.0)
3M4NP	0.18(0.05)	0.07(0.06)	0.44(0.35)	3.4(1.52)	1.02(1.59)
2,6DM4NP	-	-	-	0.55(0.39)	0.55(0.39)
4NC	0.28(0.18)	0.16(0.11)	3.9(4.0)	15.5(7.4)	4.9(7.5)
3M5NC	-	-	1.23(1.34)	6.4(3.7)	3.8(3.8)
4M5NC	-	-	1.35(1.24)	6.2(2.9)	3.8(3.3)
3NSA	-	-	-	0.84(0.56)	0.84(0.56)
5NSA	0.15(0.15)	0.29(0.41)	1.72(2.3)	2.3(2.4)	1.12(1.92)
4N1N	-	-	-	1.16(0.53)	1.16(0.53)
Total NPs	1.61(0.46)	0.61(0.41)	4.7(3.5)	24(10.0)	7.7(10.9)
Total NCs	0.28(0.18)	0.16(0.11)	6.5(6.5)	28(13.8)	8.7(13.7)
Total NACs	2.1(0.58)	1.06(0.82)	12.9(11.6)	56(23)	18.1(26)
NACs/OC(%)	0.02(0.01)	0.01(0.01)	0.05(0.02)	0.14(0.05)	0.11(0.11)
$Abs_{NACs,365}/Abs_{BrC,365}$(%)	0.14(0.04)	0.09(0.06)	0.36(0.22)	0.91(0.30)	0.38(0.38)

Table S5. Correlations between individual nitroaromatic compounds measured in this study.

R	4NP	4N1N	2M4NP	3M4NP	2,6DM4NP	4NC	3M5NC	4M5NC	3NSA	5NSA
4NP	1									
4N1N	0.78	1								
2M4NP	0.98	0.75	1							
3M4NP	0.98	0.72	0.99	1						
2,6DM4NP	0.87	0.81	0.93	0.90	1					
4NC	0.95	0.80	0.92	0.92	0.77	1				
3M5NC	0.90	0.80	0.87	0.88	0.79	0.98	1			
4M5NC	0.90	0.76	0.89	0.90	0.78	0.97	0.97	1		
3NSA	0.35	0.51	0.15	0.12	0.21	0.50	0.49	0.38	1	
5NSA	0.36	0.08	0.32	0.29	0.34	0.45	0.20	0.20	0.54	1

Table S6. Seasonal average concentrations of NACs and the source contributions.

	Spring	Summer	Fall	Winter
NACs (μg m^{-3})	2.1	1.06	12.9	56
Source contribution to NACs (%)				
Vehicle emission	41	34	23	12
Coal burning	13	14	2	39
Secondary formation	26	45	30	13
Biomass burning	20	7	45	36
Source contribution to NACs (μg m^{-3})				
Vehicle emission	0.84	0.36	3.0	6.8
Coal burning	0.27	0.15	0.26	22
Secondary formation	0.53	0.48	3.9	7.3
Biomass burning	0.41	0.07	5.8	20

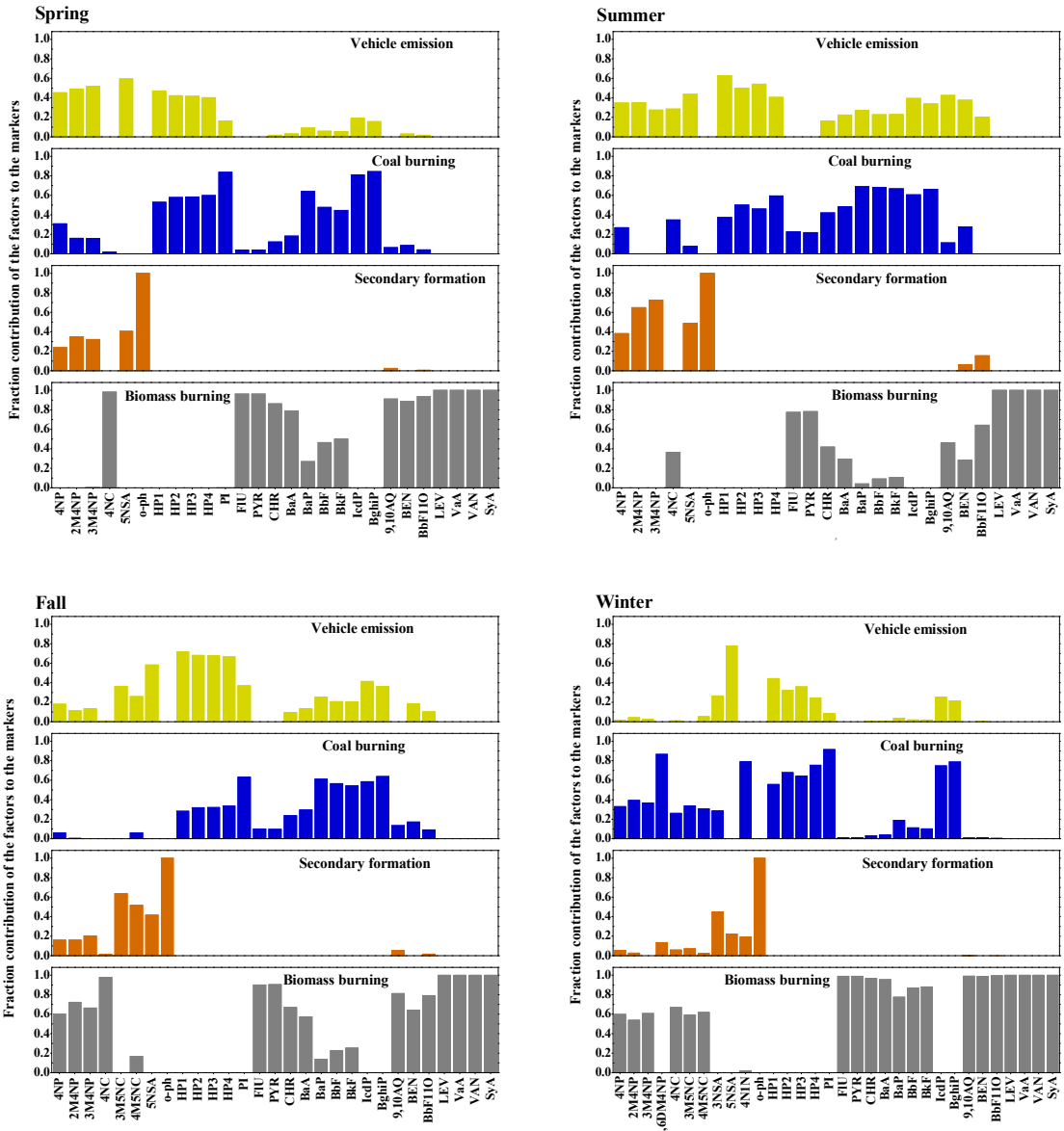
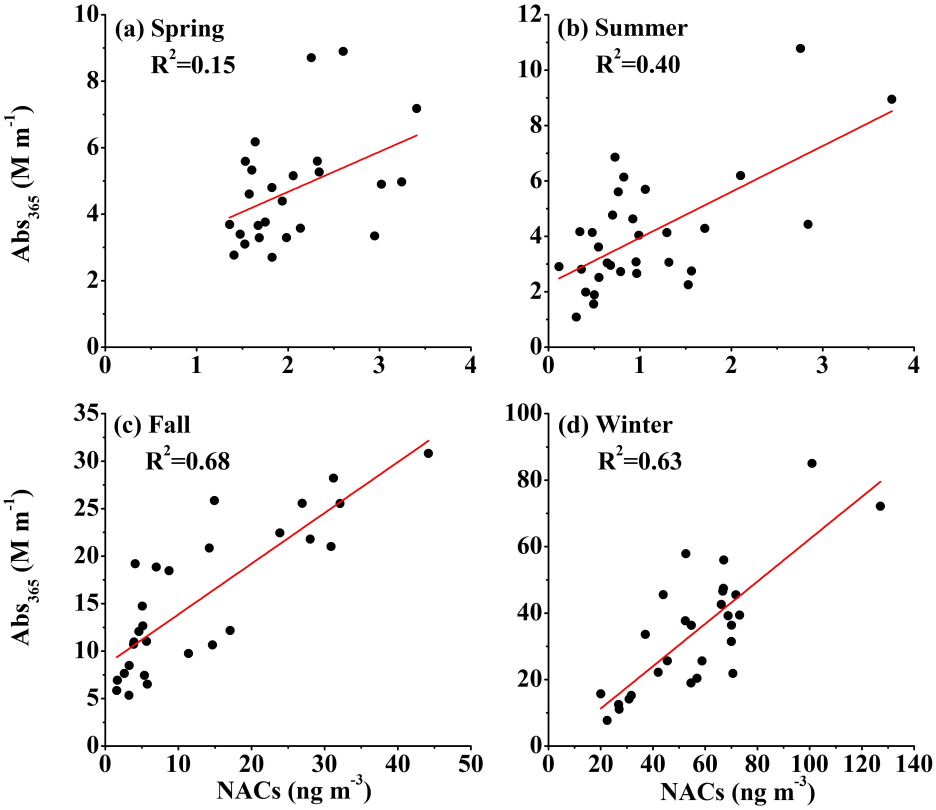


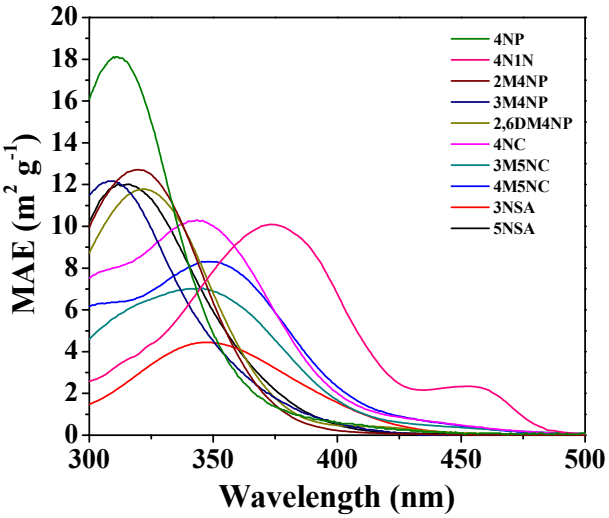
Figure S1. Factor profiles for the 4-factor solution in spring, summer, fall, and winter.



43

44 **Figure S2.** Correlations between NAC concentrations and Abs_{365} of brown carbon in four

45 seasons.



46

47 **Figure S3.** UV-Vis Spectra of individual NAC standards in methanol solution.