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Characterization of the light-absorbing properties, chromophore composition and sources of brown carbon aerosol in Xi'an, northwestern China

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Table S1. List of target compounds and their abbreviations measured in this study.

Compounds	Abbreviation
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
9,10-Anthracenequinone	9,10AQ
Benzanthrone	BEN
Benzo[b]fluoren-11-One	BbF11O
Picene	PI
MOPs	
Syringyl Acetone	SyA
Vanillin	VAN
Vanillic Acid	VaA
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
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. *F* matrix elements constrained in the ME-2/chemical species 4 factors solution. The profiles are normalized to the $Abs_{365,MSOC}$. The 0 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
$Abs_{365,MSOC}$	-	-	-	-
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	-	-	-
9,10AQ	-	-	-	-
BEN	-	-	-	-
BbF11O	-	-	-	-
LEV	0	-	0	0
VaA	0	-	0	0
VAN	0	-	0	0
SyA	0	-	0	0

Table S3. Seasonal mean and standard deviation (value in bracket) of measured parameters in this study.

	OC (μgC m^{-3})	WSOC (μgC m^{-3})	$Abs_{365,MSOC}$ (Mm^{-1})	$Abs_{365,WSOC}$ (Mm^{-1})	$MAE_{365,WSOC}$ (m^2 gC^{-1})	$MAE_{365,MSOC}$ (m^2 gC^{-1})	AAE_{MSOC}	AAE_{WSOC}	WSOC/ OC	$Abs_{365,WSOC}$/ $Abs_{365,MSOC}$
Spring	6.48(3.35)	2.78(0.81)	4.73(1.63)	2.75(1.03)	1.01(0.31)	0.79(0.22)	4.75(0.39)	5.74(0.39)	0.47(0.15)	0.60(0.18)
Summer	3.36(1.08)	2.22(0.81)	4.05(2.08)	1.89(0.68)	0.91(0.30)	1.21(0.46)	4.59(0.62)	6.15(0.49)	0.66(0.16)	0.52(0.16)
Fall	11.10(6.58)	5.69(2.53)	15.41(7.47)	6.75(3.28)	1.18(0.16)	1.52(0.40)	4.45(0.42)	5.70(0.21)	0.57(0.14)	0.45(0.09)
Winter	22.63(10.60)	10.49(5.65)	34.42(18.39)	17.83(8.02)	1.85(0.48)	1.50(0.29)	5.18(0.23)	5.32(0.18)	0.45(0.10)	0.54(0.08)

Table S4. Seasonal light absorption of methanol-soluble BrC at wavelength of 365 nm and the sources contributions.

	Spring	Summer	Fall	Winter
$Abs_{365,MSOC}$ (M m^{-1})	4.73	4.05	15.41	34.42
Sources contribution to $Abs_{365,MSOC}$ (%)				
Secondary formation	37	63	11	18
Vehicle emission	34	16	38	2
Coal burning	29	9	29	44
Biomass burning	0	12	22	36
Sources contribution to $Abs_{365,MSOC}$ (M m^{-1})				
Secondary formation	1.75	2.55	1.70	6.20
Vehicle emission	1.61	0.65	5.86	0.69
Coal burning	1.37	0.36	4.47	15.41
Biomass burning	0	0.49	3.39	12.39

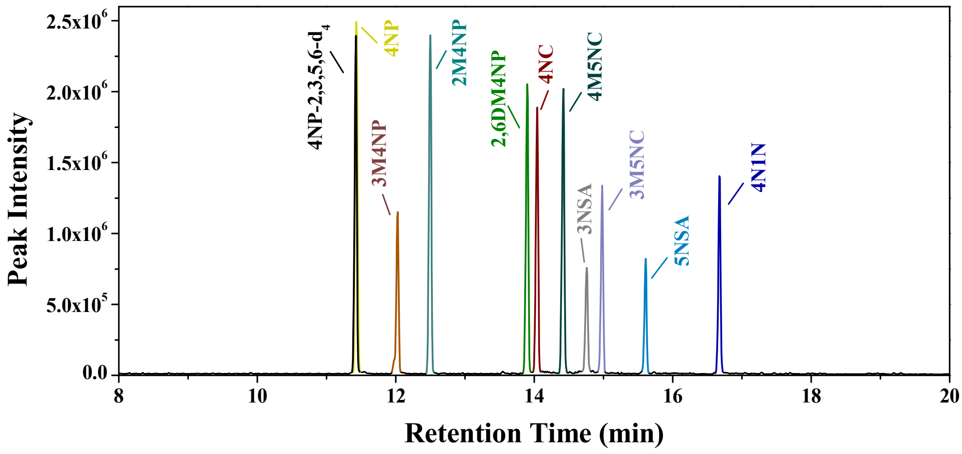

Figure S1. Selected ion monitoring chromatograms (GC-MS) for nitrated aromatic compound (NAC) standards (2 ug mL^{-1}) measured in our study.

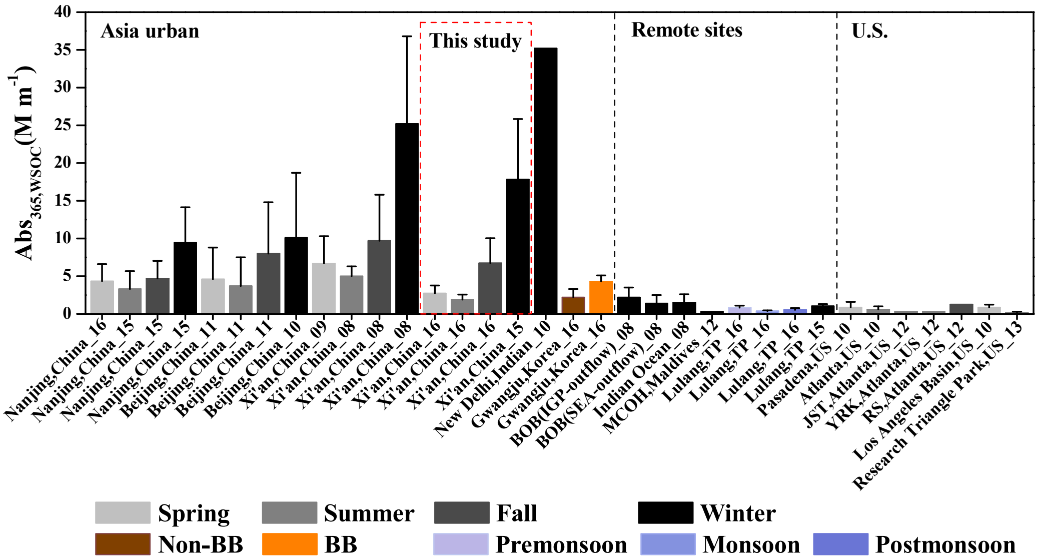

Figure S2. Comparison of Abs$_{365,WSOC}$ in Asia urban (Du et al., 2014; Kirillova et al., 2014; Chen et al., 2018; Huang et al., 2018; Park et al., 2018) , remote sites (Srinivas and Sarin, 2013; Bosch et al., 2014; Zhu et al., 2018) and the United States (Zhang et al., 2011; Liu et al., 2013; Zhang et al., 2013; Xie et al., 2019).

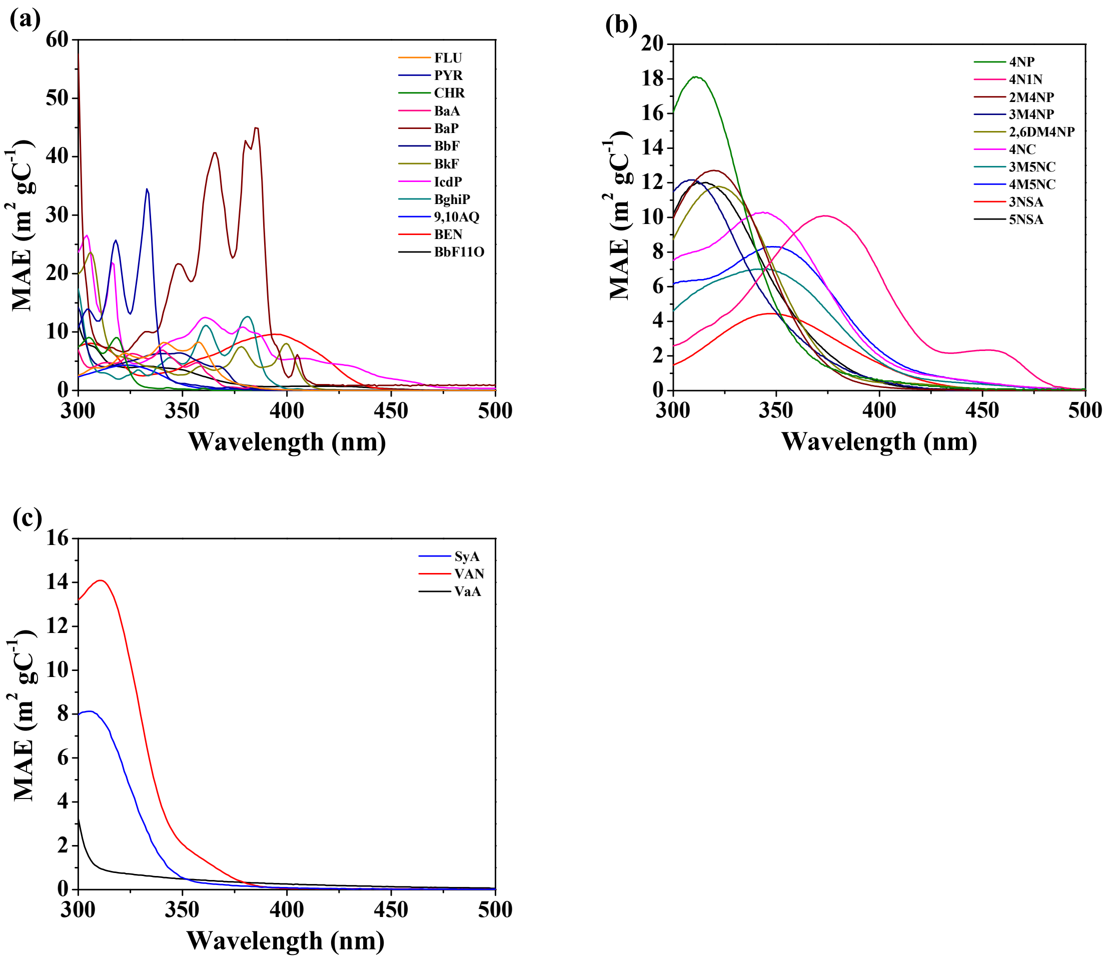

Figure S3. MAE spectra of measured (a) PAHs, (b) NACs, and (c) MOPs at wavelength of 300-500 nm.

Calculation of light absorption contribution

Light absorption contribution of individual chromophore to methanol-soluble BrC at wavelength of λ ($Cont_{chr/BrC,\lambda}$) is calculation as following equation:

$$Cont_{chr/BrC,\lambda} = \frac{Conc_{chr} \times MAE_{chr,\lambda}}{Abs_{BrC,\lambda}} \quad \text{(S1)}$$

where $Conc_{chr}$ is the concentration of individual chromophore, $MAE_{chr,\lambda}$ represents the mass absorption efficiency (MAE) of individual chromophore at wavelength of λ nm and $Abs_{BrC,\lambda}$ is the light absorption coefficient of BrC at wavelength of λ nm.

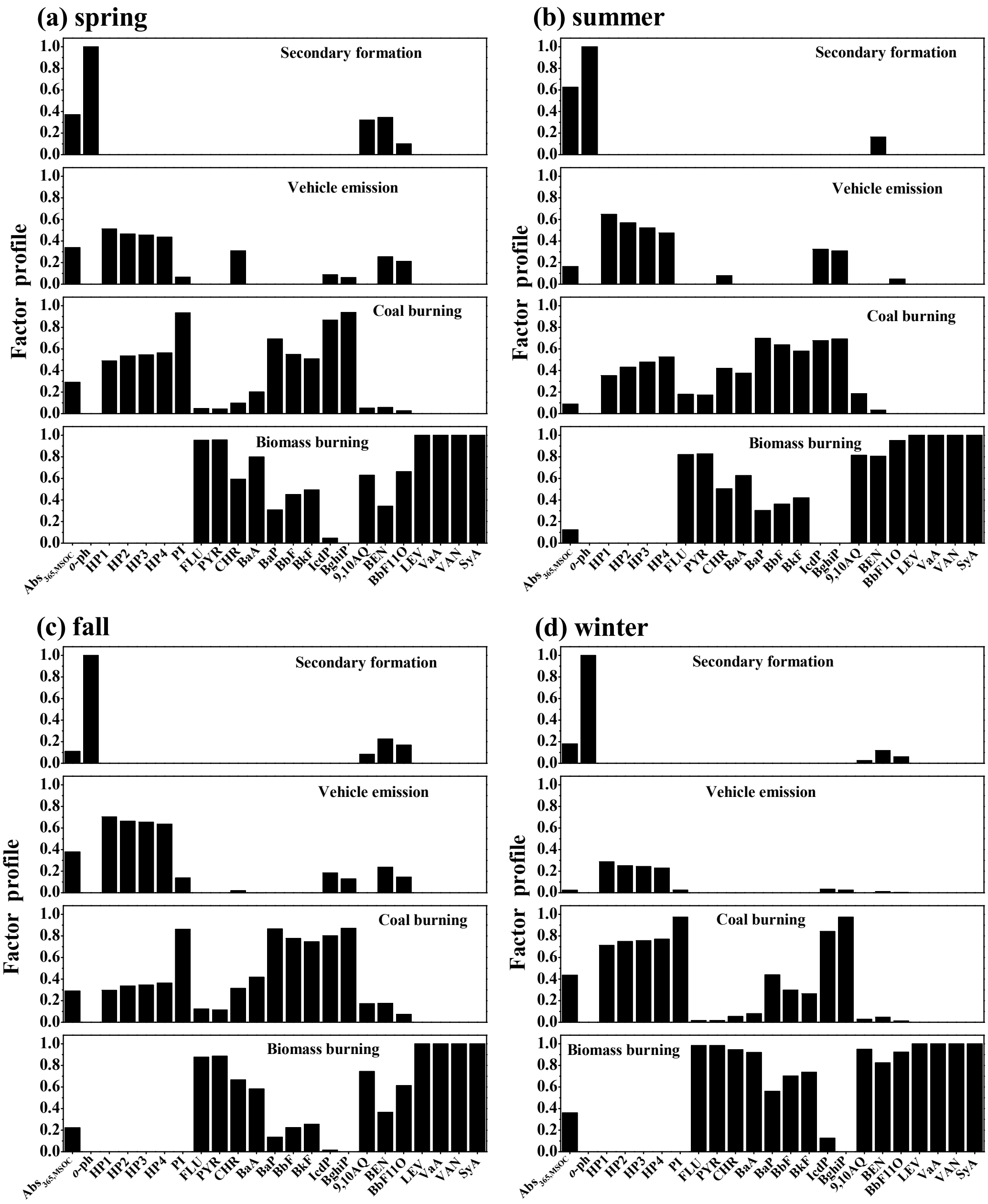

Figure S4. Factor profiles for the 4-factor solution in (a) spring, (b) summer, (c) fall, and (d) winter.

References

Bosch, C., Andersson, A., Kirillova, E. N., Budhavant, K., Tiwari, S., Praveen, P. S., Russell, L. M., Beres, N. D., Ramanathan, V., and Gustafsson, Ö.: Source-diagnostic dual-isotope composition and optical properties of water-soluble organic carbon and elemental carbon in the South Asian outflow intercepted over the Indian Ocean, J. Geophys. Res. Atmos., 119, 11743-11759. doi:10.1002/2014JD022127, 2014.

Chen, Y., Ge, X., Chen, H., Xie, X., Chen, Y., Wang, J., Ye, Z., Bao, M., Zhang, Y., and Chen, M.: Seasonal light absorption properties of water-soluble brown carbon in atmospheric fine particles in Nanjing, China, Atmos. Environ., 187, 230-240, doi:10.1016/j.atmosenv.2018.06.002, 2018.

Du, Z., He, K., Cheng, Y., Duan, F., Ma, Y., Liu, J., Zhang, X., Zheng, M., and Weber, R.: A yearlong study of water-soluble organic carbon in Beijing II: Light absorption properties, Atmos. Environ., 89, 235–241, doi:10.1016/j.atmosenv.2014.02.022, 2014.

Huang, R. J., Yang, L., Cao, J., Chen, Y., Chen, Q., Li, Y., Duan, J., Zhu, C., Dai, W., Wang, K., Lin, C., Ni, H., Corbin, J. C., Wu, Y., Zhang, R., Tie, X., Hoffmann, T., O'Dowd, C., and Dusek, U.: Brown carbon aerosol in urban Xi'an, Northwest China: the composition and light absorption properties, Environ. Sci. Technol., 52, 6825-6833, doi:10.1021/acs.est.8b02386, 2018.

Kirillova, E. N., Andersson, A., Tiwari, S., Srivastava, A. K., Bisht, S. D., and Gustafsson, Ö.: Water-soluble organic carbon aerosols during a full New Delhi winter: Isotope-based source apportionment and optical properties, J. Geophys. Res. Atmos., 119, 3476−3485, 2014.

Liu, J., Bergin, M., Guo, H., King, L., Kotra, N., Edgerton, E., and Weber, R. J.: Size-resolved measurements of brown carbon in water and methanol extracts and estimates of their contribution to ambient fine-particle light absorption, Atmos. Chem. Phys., 13, 12389–12404, doi:10.5194/acp-13-12389-2013, 2013.

Park, S., Yu, G. H., and Lee, S.: Optical absorption characteristics of brown carbon aerosols during the KORUS-AQ campaign at an urban site, Atmos. Res., 203, 16-27, doi:10.1016/j.atmosres.2017.12.002, 2018.

Srinivas, B., and Sarin, M. M.: Light-absorbing organic aerosols (brown carbon) over the tropical Indian Ocean: impact of biomass burning emissions, Environ. Res. Lett., 8, 044042, doi:10.1088/1748-9326/8/4/044042, 2013.

Xie, M. J., Chen, X., Holder, A. L., Hays, M. D., Lewandowski, M., Offenberg, J. H., Kleindienst, T. E., Jaoui, M., and Hannigan, M. P.: Light absorption of organic carbon and its sources at a southeastern U.S. location in summer, Environ. Pollut., 244, 38-46, doi:10.1016/j.envpol.2018.09.125, 2019.

Zhang, X., Lin, Y.-H., Surratt, J. D., Zotter, P., Prévôt, A. S. H., and Weber, R. J.: Light absorbing-soluble organic aerosol in Los Angeles and Atlanta: a contrast in secondary organic aerosol, Geophys. Res. Lett., 38, L21810, doi:10.1029/2011GL049385, 2011.

Zhang, X., Lin, Y.-H., Surratt, J. D., and Weber, R.: Sources, composition and absorption Ångström exponent of light-absorbing organic components in aerosol extracts from the Los Angeles Basin, Environ. Sci. Technol., 47, 3685-3693, doi:10.1021/es305047b, 2013.

Zhu, C. S., Cao, J. J., Huang, R. J., Shen, Z. X., Wang, Q. Y., and Zhang, N. N.: Light absorption properties of brown carbon over the southeastern Tibetan Plateau, Sci. Total Environ., 625, 246-251, doi:10.1016/j.scitotenv.2017.12.183, 2018.