Supplement for
The formation of nitro-aromatic compounds under high NO_x-anthropogenic VOCs dominated atmosphere in summer in Beijing, China

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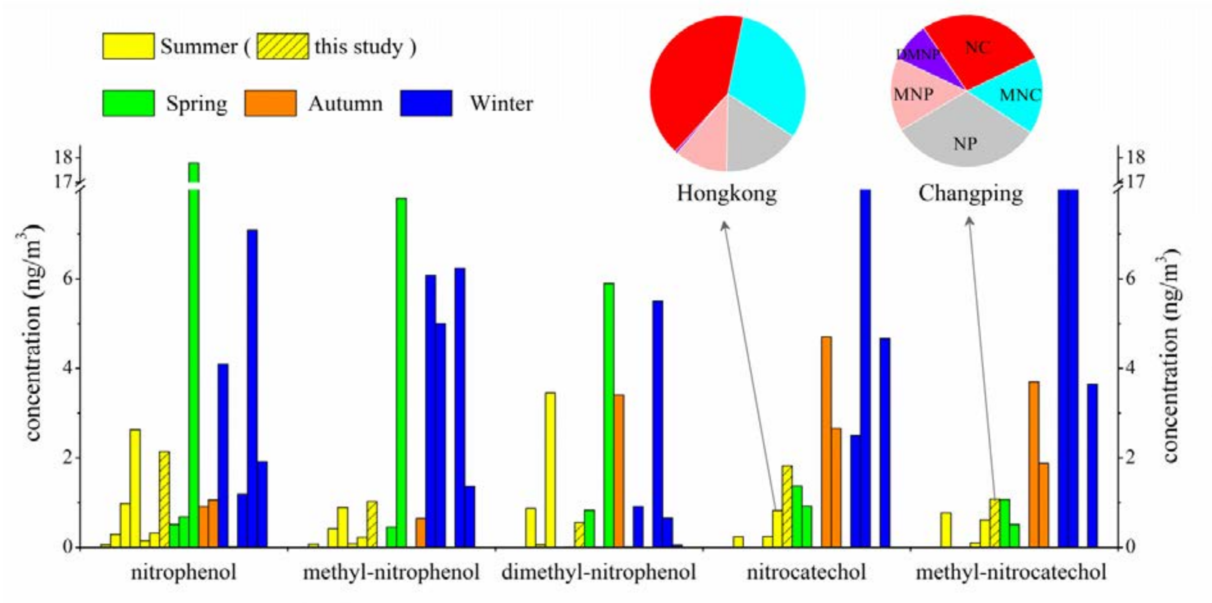

Figure S1 Comparison of individual NAC species across this and previous studies. For each species, the concentrations are respectively reported in summer (yellow) in Melptitz, Germany (Teich et al., 2017), Flanders, Belgium (Kahnt et al., 2013), Xianghe, China (Teich et al., 2017), Wangdu, China (Teich et al., 2017), Ljubljana, Slovenia (Kitanovski et al., 2012), Hong Kong, China (Chow et al., 2016), Beijing, China (this study); in spring (green) in Flanders, Belgium (Kahnt et al., 2013), Hong Kong, China (Chow et al., 2016), Rome, Italy (Cecinato et al., 2005); in autumn (orange) in Flanders, Belgium (Kahnt et al., 2013), Hong Kong, China (Chow et al., 2016); and in winter (blue) in Melptitz, Germany (Teich et al., 2017), Detling, UK (Mohr et al., 2013), Flanders, Belgium (Kahnt et al., 2013), TROPOS, Germany (Teich et al., 2017) and Hong Kong, China (Chow et al., 2016) from left side to right side. The inserted pie charts represent the NAC compositions in summer in Hong Kong (Chow et al., 2016) and Changping, respectively.

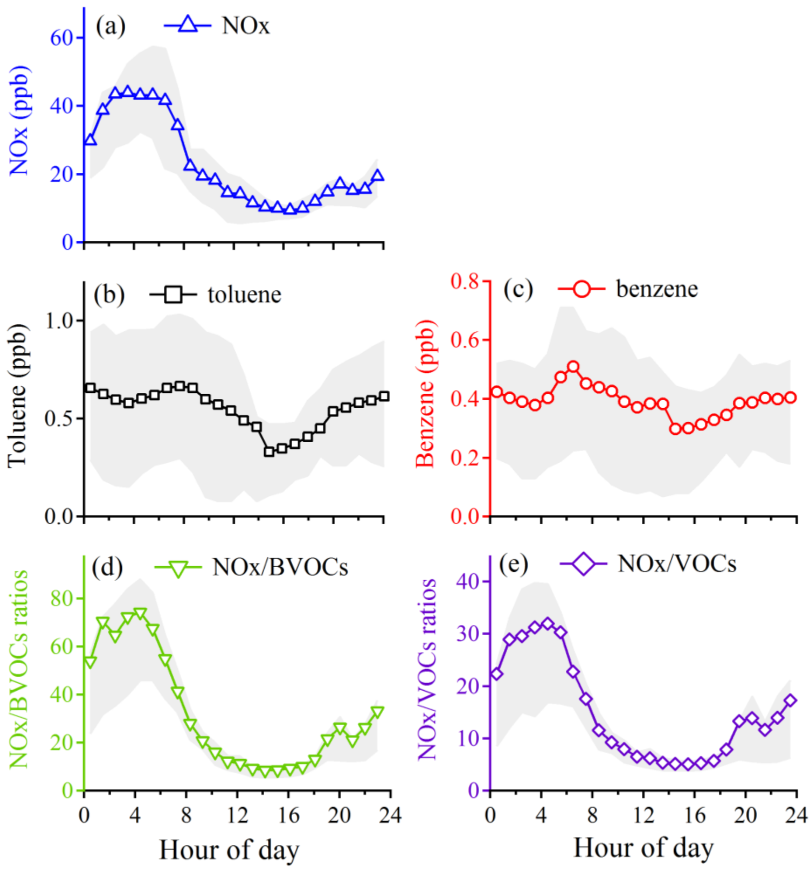

Figure S2 Diurnal variations of (a) NO_x, (b) toluene, (c) benzene, (d) NO_x/BVOCs ratios and (e) NO_x/VOCs ratios.

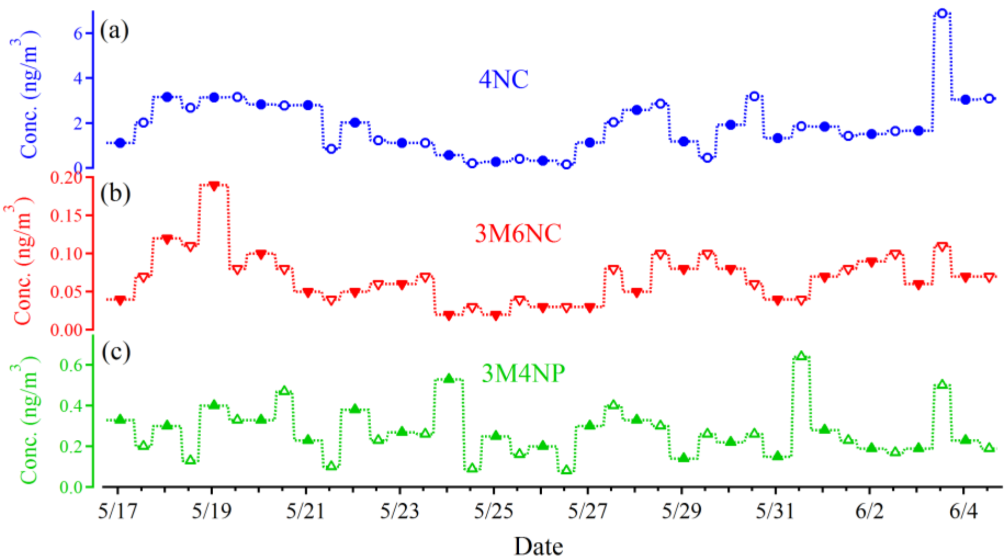

Figure S3 Time series of (a) 4-nitrocatechol (4NC), (b) 4-methyl-6-nitrocatechol (4M6NC), and (c) 3-methyl-4-nitrophenol (3M4NP).

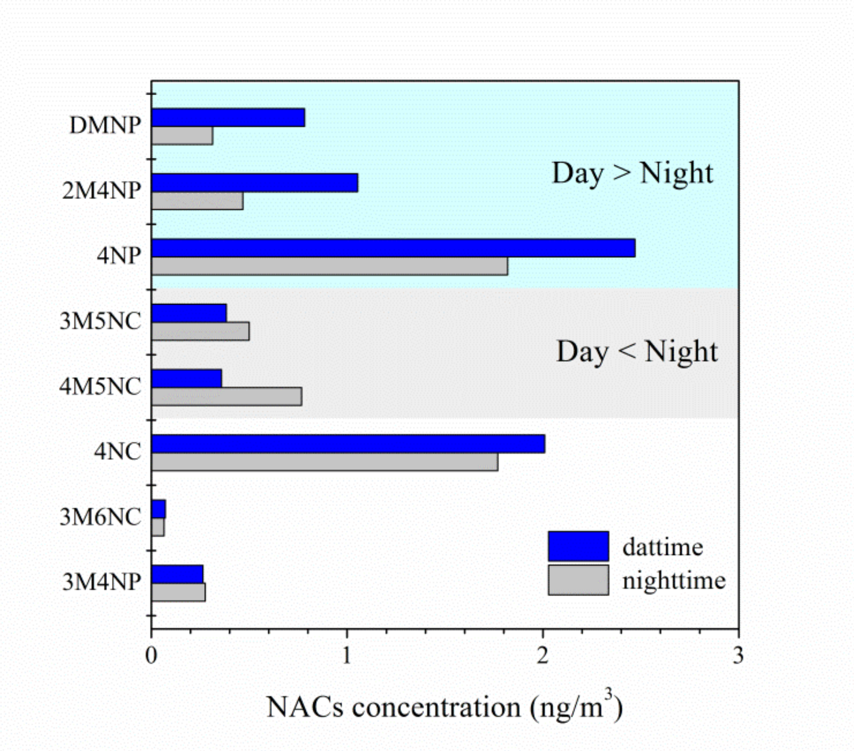

Figure S4 Day-night variations of NACs.

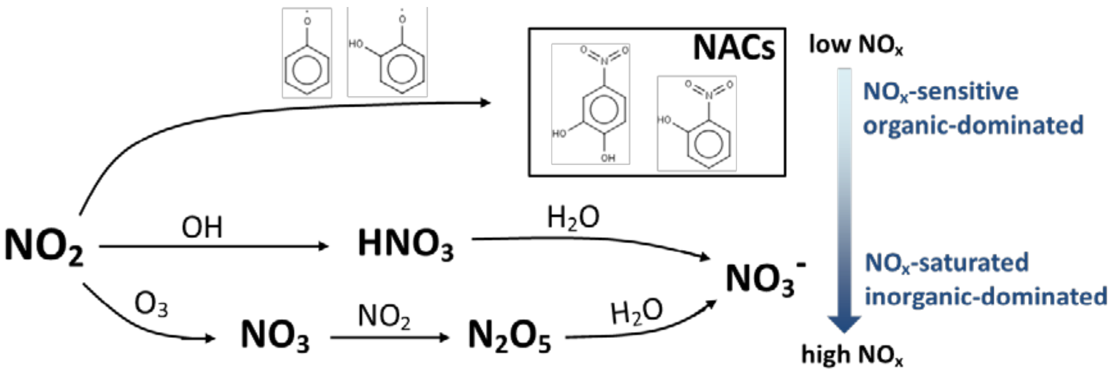

Figure S5 The schematic diagram and simplified mechanisms of the competing formation of inorganic nitrates and NACs (Logan, 1983 and MCM v3.3).

Table S1 Concentrations of nitroaromatic compounds in this and previous studies

sites	sampling period	concentrations (ng/m^3)									references
		4NP (NP)	3M4NP	2M4NP	2,6D4NP (DMNP)	4NC (NC)	4M5NC	3M6NC	3M5NC	Total	
TROPOS, Germany	Jan-Feb, 2014	7.09	2.6	3.64	0.65					13.98	(Teich et al., 2017)
Melptitz, Germany	Jan-Feb, 2014	4.09	2.44	3.64	0.91					11.08	(Teich et al., 2017)
Maniz, Germany	May, 2006-June, 2007	2.48				6.4				8.88	(Zhang et al., 2010)
Melptitz, Germany	Jul, 2014	0.06	0.03	0.04	n.d.					0.13	(Teich et al., 2017)
Seiffen, Saxony, Germany	Oct, 2007-Mar, 2008						2	2.9	0.37	5.27	(Iinuma et al., 2010)
Detling, UK	Jan-Feb, 2012	0.02	5			2.5	8.2				(Mohr et al., 2013)
Ljubljana, Slovenia	Dec, 2010-Jan, 2011	1.8	0.61	0.75		75	29	6.2	34	147.36	(Kitanovski et al., 2012)
Ljubljana, Slovenia	Aug, 2010	0.15	<0.03	0.05		0.24	0.06	<0.03	0.01	0.57	(Kitanovski et al., 2012)
Rome, Italy	Feb- Apr, 2003	17.8	7.8		5.9					31.50	(Cecinato et al., 2005)
Hamme, Flanders, Belgium	Spring , 2010	0.51			0.83	1.37	1.07			3.78	(Kahnt et al., 2013)
	Summer, 2010	0.29			0.87	0.23	0.77			2.16	
	Autumn, 2010	0.91			3.4	4.7	3.7			12.71	
	Winter, 2010	1.19			5.5	11.6	13.9			32.19	
Los Angeles	May-June, 2010		1.24		0.92	1.67	0.36			4.19	(Zhang et al., 2013)
Hong Kong	Winter, 2009-2012	1.92	0.17	1.20	0.05	4.67	1.28	0.27	2.10	11.63	(Chow et al., 2016)
	Spring, 2009-2012	0.68	0.06	0.39	0.01	0.92	0.17	0.10	0.24	2.57	
	Summer, 2009-2012	0.32	0.02	0.20	0.01	0.82	0.17	0.07	0.37	1.99	
	Antumn, 2009-2012	1.06	0.06	0.58	0.01	2.66	0.58	0.15	1.15	6.26	
Xianghe, China	Jul-Aug, 2013	0.98	0.09	0.32	0.06					1.45	(Teich et al., 2017)
Wangdu, China	Jun, 2014	2.63	0.21	0.68	3.45					6.97	(Teich et al., 2017)
		5.9 [a]								5.90	(Wang et al., 2018)
Jinan, China	Nov. 2013- Jan, 2014	48.4 [a]								48.40	(Wang et al., 2018)
Jinan, China	Sep, 2014	9.8 [a]								9.80	(Wang et al., 2018)
Yucheng, China	June, 2014	5.7 [a]								5.70	(Wang et al., 2018)
Mt. Tai, China	July-Aug, 2014	2.5 [a]								2.50	(Wang et al., 2018)
Beijing, China	May-Jun, 2016	2.15	0.27	0.76	0.55	1.89	0.56	0.07	0.44	6.62	This study

Note: a: The identified NACs included 4-nitrophenol (4NP), 2-methyl-4-nitrophenol (2M4NP), 3-methyl-4-nitrophenol (3M4NP), 4-nitrocatechol (4NC), 4-methyl-5-nitrocatechol (4M5NC), 3-methyl-5-nitrocatechol (3M5NC), 3-methyl-6- nitrocatechol (3M6NC), 3-nitro-salicylic acid (3NSA), and5-nitro-salicylic acid (5NSA).

Table S2 Pearson correlations between individual NAC species as well as their correlations with aerosol components, aerosol surface area, VOC precursors, oxidants, RH and temperature (n=38)

	total NACs	4NP	DMNP	2M4NP	3M4NP	4NC	3M6NC	3M5NC	4M5NC
total NACs	1.00								
4NP	0.88	1.00							
DMNP	0.68	**0.72**	1.00						
2M4NP	**0.85**	**0.80**	**0.88**	1.00					
3M4NP	0.63	0.56	**0.70**	0.59	1.00				
4NC	**0.92**	0.69	0.42	**0.71**	0.41	1.00			
3M6NC	0.58	0.53	0.13	0.34	0.14	0.58	1.00		
3M5NC	**0.76**	0.54	0.23	0.37	0.45	**0.80**	0.59	1.00	
4M5NC	0.52	0.24	(0.08)	0.05	0.34	0.60	0.49	**0.84**	1.00
OM	0.62	0.62	0.11	0.38	0.17	0.65	0.49	0.57	0.46
K^+	**0.49**	0.39	0.12	0.24	0.25	**0.50**	**0.43**	**0.64**	**0.53**
SO_4^{2-}	**0.45**	0.36	0.02	0.18	0.04	**0.52**	**0.51**	**0.59**	**0.47**
benzene	**0.64**	**0.57**	0.23	0.39	0.23	**0.68**	0.34	**0.67**	**0.48**
toluene	**0.70**	**0.58**	0.18	0.39	0.23	**0.76**	**0.46**	**0.74**	**0.63**
NO_2	0.33	0.16	(0.17)	(0.02)	0.21	**0.42**	0.26	**0.55**	**0.75**
O_3	0.34	**0.43**	0.37	**0.49**	(0.19)	0.32	0.17	0.11	(0.31)
aerosol surface area	**0.60**	**0.49**	0.11	0.33	0.05	**0.69**	**0.50**	**0.70**	**0.53**
RH	0.13	(0.06)	(0.21)	(0.15)	0.27	0.20	0.16	**0.39**	**0.59**
Temperature	0.21	0.38	0.30	**0.40**	(0.32)	0.17	0.16	(0.12)	(0.45)

Table S3 Pearson correlations between individual NAC species as well as their correlations with aerosol components, aerosol surface area, VOC precursors, oxidants, RH and temperature during daytime and nighttime, respectively (n=19)

Daytime

	total NACs	4NP	DMNP	2M4NP	3M4NP	4NC	3M6NC	3M5NC	4M5NC
total NACs	1.00								
4NP	0.90	1.00							
DMNP	0.79	0.84	1.00						
2M4NP	0.96	0.84	0.86	1.00					
3M4NP	0.80	0.87	0.94	0.82	1.00				
4NC	0.92	0.68	0.51	0.84	0.54	1.00			
3M6NC	0.58	0.48	0.26	0.50	0.25	0.60	1.00		
3M5NC	0.83	0.72	0.49	0.67	0.54	0.85	0.63	1.00	
4M5NC	0.85	0.64	0.41	0.75	0.49	0.92	0.68	0.85	1.00
OM	0.69	0.63	0.32	0.57	0.35	0.69	0.55	0.73	0.80
K^+	0.47	0.46	0.21	0.34	0.35	0.44	0.41	0.61	0.62
SO_4^{2-}	0.40	0.32	0.07	0.23	0.09	0.49	0.25	0.64	0.51
benzene	0.75	0.68	0.50	0.62	0.51	0.72	0.46	0.89	0.75
toluene	0.81	0.71	0.51	0.71	0.52	0.80	0.55	0.89	0.82
NO_2	0.77	0.63	0.48	0.74	0.47	0.75	0.57	0.73	0.85
O_3	0.38	0.35	0.03	0.21	(0.01)	0.47	0.39	0.62	0.43
aerosol surface area	0.57	0.46	0.19	0.42	0.20	0.65	0.50	0.79	0.73
RH	0.30	0.15	0.10	0.24	0.11	0.36	0.21	**0.47**	**0.55**
J (O^1D)	(0.72)	(0.56)	(0.63)	(0.76)	(0.67)	(0.68)	(0.14)	(0.49)	(0.60)
Temperature	0.10	0.17	(0.11)	0.01	(0.16)	0.17	0.25	0.10	0.01

Nighttime

	total NACs	4NP	DMNP	2M4NP	3M4NP	4NC	3M6NC	3M5NC	4M5NC
total NACs	1.00								
4NP	0.83	1.00							
DMNP	0.23	(0.12)	1.00						
2M4NP	0.75	0.65	0.58	1.00					
3M4NP	0.27	0.01	0.60	0.46	1.00				
4NC	0.97	0.79	0.12	0.65	0.11	1.00			
3M6NC	0.70	0.70	(0.15)	0.40	0.07	0.68	1.00		

3M5NC	0.91	0.59	0.24	0.53	0.34	0.88	0.63	1.00	
4M5NC	0.92	0.59	0.34	0.58	0.37	0.88	0.62	0.98	1.00
OM	0.64	0.79	(0.31)	0.50	(0.09)	0.67	0.48	0.43	0.41
K^+	0.66	0.46	0.12	0.57	0.18	0.67	0.44	0.68	0.61
SO_4^{2-}	0.66	0.58	0.05	0.60	(0.02)	0.68	0.65	0.56	0.53
benzene	0.64	0.65	(0.04)	0.57	(0.20)	0.72	0.29	0.46	0.42
toluene	0.79	0.76	(0.01)	0.65	(0.16)	0.86	0.45	0.60	0.58
NO_2	0.60	0.56	(0.00)	0.44	(0.05)	0.61	0.37	0.52	0.55
O_3	0.03	0.11	(0.19)	0.11	(0.65)	0.14	(0.04)	(0.05)	(0.11)
aerosol surface area	0.76	0.68	0.02	0.63	(0.17)	0.82	0.52	0.62	0.59
RH	0.46	0.37	0.59	0.77	0.62	0.33	0.34	0.31	0.34
Temperature	0.02	0.23	(0.61)	(0.17)	(0.84)	0.17	0.09	(0.06)	(0.12)

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