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Gasoline aromatics: a critical determinant of urban secondary organic aerosol formation

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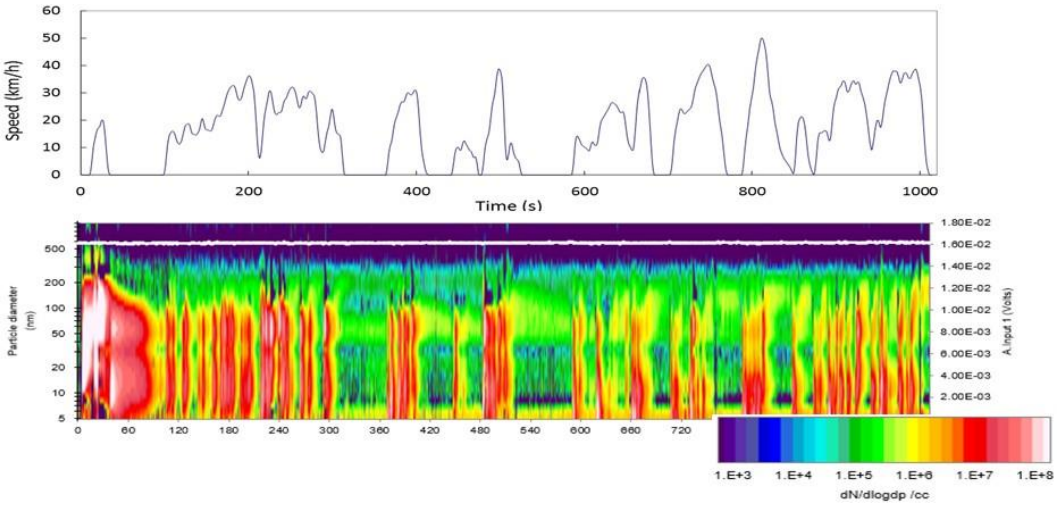

Figure S1. Time series of driving speed (a) and size distribution of primary particles (b) in a typical cold start Beijing cycle

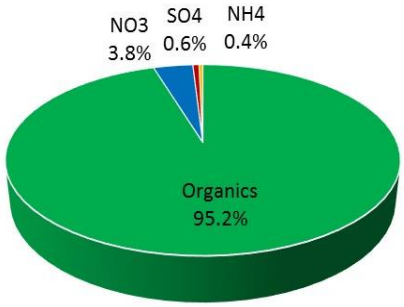

Figure S2. Chemical composition of secondary aerosols formed in a typical chamber experiment (experiment V2)

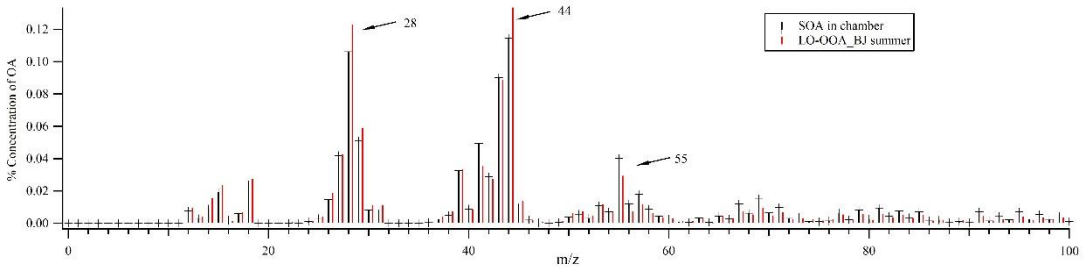

Figure S3. Spectra of secondary aerosols formed inside the chamber and the low oxidized secondary organic aerosols (LO-OOA) factor in the ambient air

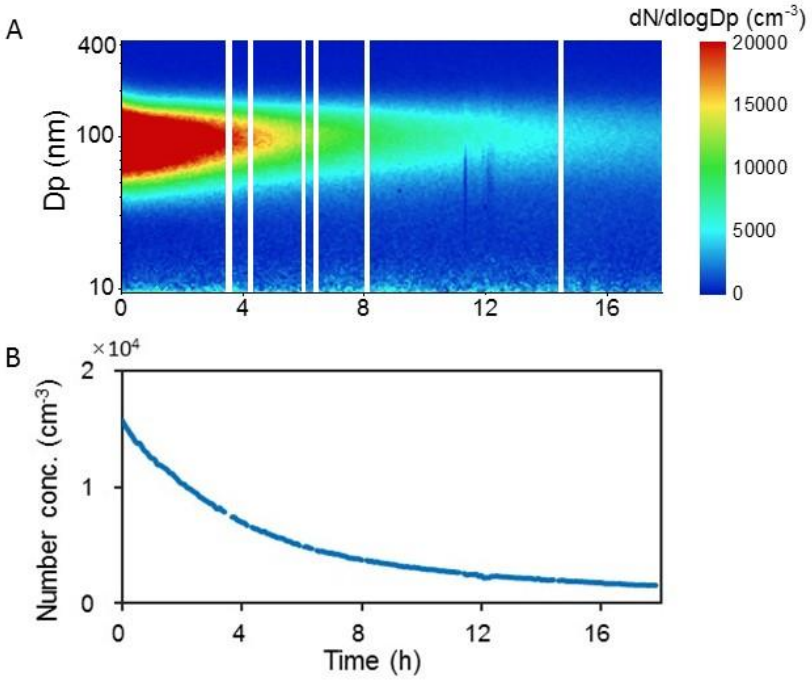

Figure S4. Wall loss of particles in the chamber. (A) size distribution of particles as a function of time; (B) decay of total particle number concentration

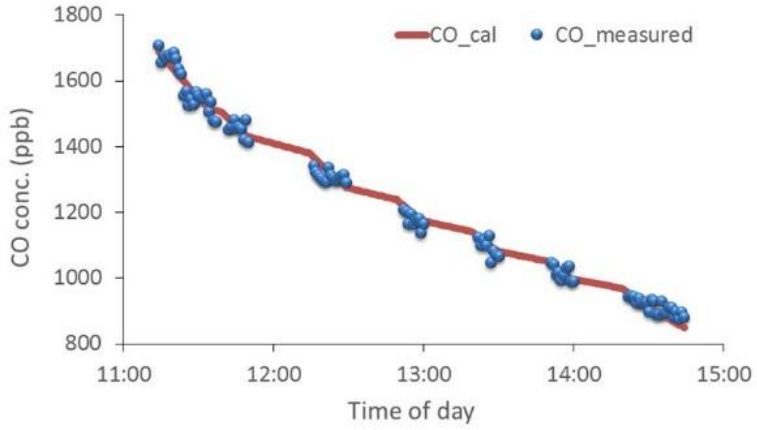

Figure S5. Comparison of calculated CO concentration based on sampling flowrate (red line) and measured CO concentration (blue dot)

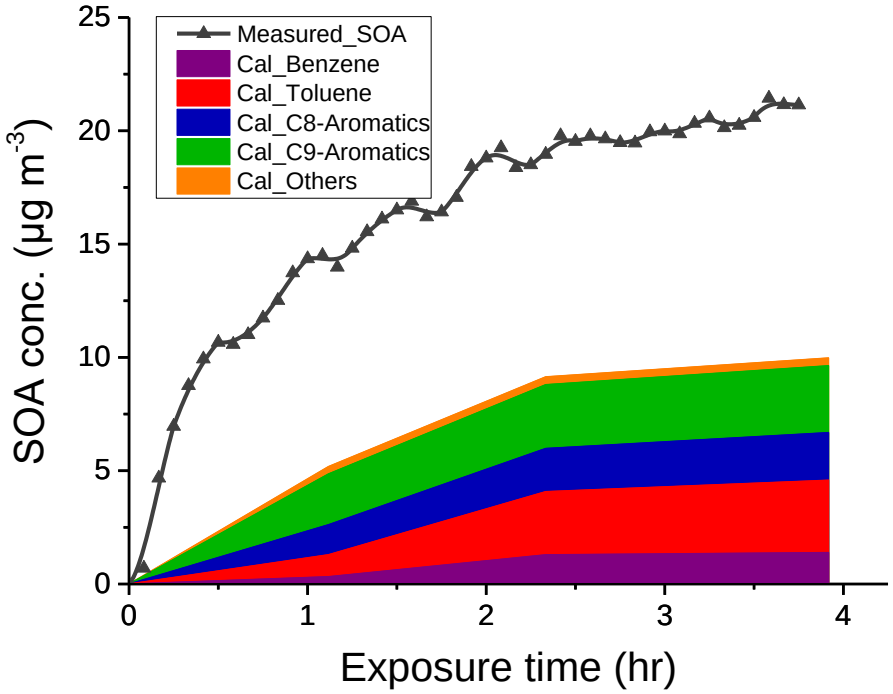

Figure S6. Observed and predicted SOA concentration, and SOA fraction from unspeciated VOCs as a function of photochemical age in typical chamber experiments using F3 fuel (experiment V2). Black line and triangles represent the corrected SOA concentrations in the chamber experiments. The purple, red, blue, green and yellow areas represent the predicted SOA from the oxidation of benzene, toluene, C8-aromatics, C9-aromatics and other VOCs, respectively. All the VOCs were measured by off-line GC-MS and only four samples were got from this experiment.

Table S1. Working parameters and emissions for the vehicle chassis dynamometer experiments

#	Fuel	Working parameters			Average concentration of gaseous pollutants in the CVS				
		Temperature in the lab / ºC	Absolute humidity in the lab / g m^{-3}	flowrate in CVS / m^3 min^{-1}	CO / ppm	CO_2 / %	THC / ppmC	NO_x / ppm	Ration of THC/NO_x
V1	F3	24.28	9.56	5.53	11.2	0.67	13.0	1.41	9.2
V2	F3	22.73	8.25	5.53	12.1	0.65	13.5	1.32	10.2
V3	F2	23.99	8.78	5.54	7.4	0.65	9.7	1.30	7.5
V4	F2	23.35	7.11	5.56	7.4	0.64	9.0	1.25	7.2
V5	F1	21.97	7.03	5.57	10.2	0.66	10.4	1.40	7.5

Table S2. Working parameters and emissions for the vehicle chassis dynamometer experiments

#	Type	Fuel	Fuel consumption ml min^{-1}	Oxidation
E1	PFI	F2	90.97	1 ml H_2O_2
E2	PFI	F1	90.97	1 ml H_2O_2
E3	PFI	F1	90.11	1 ml H_2O_2

Table S3. The mass fraction of 49 molecular species of each fuel used in the study.

Components Mass %	F1(base)	F2	F3
i-pentane	20.6703	15.7475	13.1197
Toluene	12.3573	12.5719	15.0700
2-methylpentane	9.9457	4.5159	3.7026
3-methylpentane	6.8135	3.1568	2.5876
2,2,4-trimethylpentane	5.3980	3.6992	1.8483
n-pentane	4.0422	6.2011	5.1323
1,3-methylethylbenzene	4.0266	3.9018	5.0756
ethylbenzene	3.0926	2.8490	4.7202
1,4-methylethylbenzene	2.2210	1.9301	2.6247
2,3-dimethylbutane	2.0102	0.9061	0.7431
1,3,5-trimethylbenzene	1.9125	2.0406	2.5652
1,2-methylethylbenzene	1.7616	1.5745	2.1159
3-methylhexane	1.7287	1.4560	1.2004
1,3-dimethylbenzene	1.6789	1.5825	2.5603
n-hexane	1.5839	0.8054	0.6605
2-methylhexane	1.5530	1.2492	1.0282
1,2,3,5-tetramethylbenzene	1.5087	1.5179	1.2290
2,2-dimethylbutane	1.2131	0.5288	0.4348
n-propylbenzene	1.0872	1.0073	1.3373
1,2-dimethylbenzene	0.9495	0.9217	1.3776
n-heptane	0.9440	3.6457	7.3628
1,2,4,5-tetramethylbenzene	0.7646	0.7552	0.6107
1,4-dimethylbenzene	0.7083	0.6648	1.0852
1,2-dimethyl-4-ethylbenzene	0.6906	0.7152	0.5782
1,2,3-trimethylbenzene	0.6332	2.6672	2.1563
2,3-dimethylpentane	0.6250	0.4998	0.4102
s-pentylbenzene	0.6149	0.5752	0.4654
sec-butylbenzene	0.5486	2.4360	1.9807
methylcyclopentane	0.5069	0.2969	0.2439
1,2,4-trimethylbenzene	0.4700	0.2334	0.3929
cyclopentane	0.3969	0.1990	0.1641
2,4-dimethylpentane	0.3944	0.2750	0.2237
i-propylbenzene	0.3683	0.2851	0.4040
2,2-dimethylpentane	0.3524	0.2415	0.1972
naphthalene	0.2850	0.2188	0.1770
3,3-dimethylpentane	0.2635	0.1965	0.1608
1,2-dimethyl-3-ethylbenzene	0.2540	0.2479	0.1996
1,3-di-i-propylbenzene	0.2319	0.2187	0.1766
4-methylindan	0.2145	0.2007	0.1635
3-ethylpentane	0.1528	0.1342	0.1104
1,3-dimethyl-5-ethylbenzene	0.1387	0.1332	0.1073
2,2-dimethylhexane	0.1144	0.0840	0.0489

dodecene-1	0.1051	0.0866	0.0705
1,3-octadiene	0.0955	0.3452	0.2803
1,2-methyl-n-propylbenzene	0.0691	0.3165	0.2547
1c,2t,4t-trimethylcyclohexane	0.0473	0.1606	0.1312
1c,4-dimethylcyclohexane	0.0280	0.1010	0.0813
octene-1	0.0074	3.5699	2.8977
i-butane	0.0025	1.5681	1.4817

Table S4. Parameters of instruments used in the chamber experiments

Name of the Instruments	Manufacturer	Species/Parameters	Time resolution
HR-TOF-AMS	Aerodyne Research inc.	NR-PM1 (NO_3^-, SO_4^{2-}, Cl^-, NH_4^+ and OA)	5 min
SMPS (DMA and CPC)	TSI	Particle number size distribution	5 min
CCN counter	DMT	CCN concentration	5 min
CPMA	Cambustion	Density of aerosol	10 min
LOPAP	Custom-built	HONO, HNO_3	10 min
PTR-MS	Ionicon Analytik GmbH	VOCs	1 min
Off line GC-Ms/FID	Thermo Inc.	VOCs	Sampled with VOC containers
CO_2 analyzer	Thermo Inc.	CO_2	1 min
Trace level gas analyzer	Thermo Inc.	CO, O_3, NOx, SO_2	1 min

Table S5. Emission factor of gas and particle phase pollutants from gasoline vehicle and engine exhausts using F2 and F3 fuels.

			PFI vehicle		PFI engine		GDI engine	
			F2	F3	F2	F3	F2	F3
Particle phase	PM, mg/kg	after-TWC			4.12	4.75	37.31	39.36
	PN, N/kg	after-TWC			9.6E+11	1.1E+12	9.1E+13	9.5E+13
	PAHs, mg/kg	pre-TWC					1.8	3.2
		after-TWC					0.04	0.29
Gas phase	THC, mg/kg	after-TWC	1589.37	2170.07				
	NMHC, mg/kg	pre-TWC					40069.4	52004.3
		after-TWC	695.8	1374.1				
	Aromatic, mg/kg	pre-TWC					7076.7	18333.1
		after-TWC	257.8	826.9				
SOA	mg/kg		29.2	80.5	565.0	3317.4		

Table S6. Gasoline fuel standard in different countries and regions*

Fuel Property	China				India		European Union			US EPA	Worldwide Fuel Charter Category	Australia	Brazil	California	Indonesia	Japan	Mexica	South Korea
	China III	China IV	China V (proposed)	Beijing V	Bharat III	Bharat IV	Euro III	Euro IV	Euro V									
Aromatics, vol%	40	40	40	Olefin+ Aromatics ≤ 60	42	35	42	35	35	25	35	42	35	25	40/50		35	24
Olefin, vol%	30	28	25	25	21	21	18	18	18		10	18	25				15	18
Benzene, vol%	1	1	1	1	1	1	1	1	1		1	1	1		5	1	2	0.7
Gum Content	5	5	5	5	-	-	-	-	5		5		5			5		
Lead, mg/l	5	5	5	5	5	5	5	5	5		-	5			13			13

* Table source: http://transportpolicy.net/index.php?title=Global_Comparison:_Fuels#cite_ref-2