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Elemental analysis of oxygenated organic coating on black carbon particles using a soot-particle aerosol mass spectrometer

Mutian Ma et al.

Correspondence to: Alex K. Y. Lee (alex.lee@canada.ca)

Table S1. Summary of elemental ratios and time series correlation of PMF factors based on co-located measurements in Beijing summer (Wang et al., 2020; Xie et al., 2019a), Beijing winter (Wang et al., 2019; Xie et al., 2019b), California Research at the Nexus of Air Quality and Climate Change (CalNex) 2010 campaign (Massoli et al., 2015), Fontana, CA (Chen et al., 2018; Lee et al., 2017), and Tibet (Wang et al., 2017; Xu et al., 2018).

Location / Campaign	HR-ToF-AMS				SP-AMS LV scheme[#]				R
	Study	PMF factor	H:C	O:C	Study	PMF factor	H:C	O:C	
Beijing summer	Wang et al. (2019a)	LO-OOA	1.34	0.49	Wang et al. (2020)	OOA-1	1.6	0.28	0.88
Beijing winter	Xie et al. (2019b)	LO-OOA	1.61	0.6	Wang et al. (2019)	OOA-1	1.55	0.37	0.92
Beijing winter	Xie et al. (2019b)	MO-OOA	1.36	0.97	Wang et al. (2019)	OOA-2	1.57	1.23	0.97
CalNex	Massoli et al. (2015)	SV-OOA	1.58	0.54	Massoli et al. (2015)	SV-OOA	1.83	0.45	0.92
CalNex	Massoli et al. (2015)	LV-OOA	1.2	1.4	Massoli et al. (2015)	LV-OOA	1.4	1.16	0.84
Fontana, CA	Chen et al. (2018)	VOOA	0.78	1.4	Lee et al. (2017)	OOA-2	1.63	0.63	0.76
Tibet	Xu et al. (2018)	MO-OOA	1.04	0.96	Wang et al. (2017)	BBOA	1.48	0.51	0.96

[#] The inter-conversion factors that were determined in this work, were applied for calculating H:C and O:C ratios.

Table S2. Summary of H:C, O:C and. OS_c determined by the SP-AMS 1

			True value			Tungsten vaporizer			Laser vaporizer		
Class	**Species**	**Formula**	**H:C**	**O:C**	**OSc**	**H:C**	**O:C**	**OSc**	**H:C**	**O:C**	**OSc**
Multifunctional	Citric acid	$C_6H_8O_7$	1.33	1.17	1.00	1.42	0.93	0.43	1.66	0.72	-0.21
Multifunctional	Glycolic acid	$C_2H_4O_3$	2.00	1.50	1.00	1.86	0.78	-0.31	1.71	0.53	-0.64
Multifunctional	Malic Acid	$C_4H_6O_5$	1.50	1.25	1.00	1.55	1.00	0.44	1.63	1.00	0.37
Multifunctional	Tartaric acid	$C_4H_6O_6$	1.50	1.50	1.50	1.48	1.34	1.20	1.63	1.52	1.40
Diacids	Adipic Acid	$C_6H_{10}O_4$	1.67	0.67	-0.33	1.71	0.60	-0.51	1.71	0.46	-0.79
Diacids	Azelaic Acid	$C_9H_{16}O_4$	1.78	0.44	-0.89	1.65	0.29	-1.07	1.90	0.35	-1.19
Diacids	Glutaric acid	$C_5H_8O_4$	1.60	0.80	0	1.64	0.44	-0.76	1.66	0.47	-0.71
Diacids	Malonic acid	$C_3H_4O_4$	1.33	1.33	1.33	1.36	1.12	0.87	1.61	1.10	0.59
Diacids	Oxalic acid	$C_2H_2O_4$	1.00	2.00	3.00	1.13	1.91	2.68	1.36	1.72	2.09
Diacids	Phthalic acid	$C_8H_6O_4$	0.75	0.50	0.25	0.84	0.26	-0.32	0.95	0.25	-0.46
Diacids	Pimelic acid	$C_7H_{12}O_4$	1.71	0.57	-0.57	1.66	0.42	-0.82	1.83	0.41	-1.02
Diacids	Suberic acid	$C_8H_{14}O_4$	1.75	0.50	-0.75	1.58	0.33	-0.93	1.85	0.40	-1.06
Diacids	Succinic acid	$C_4H_6O_4$	1.50	1.00	0.50	1.72	0.77	-0.18	1.48	0.83	0.17
Alcohols	Arabitol	$C_5H_{12}O_5$	2.4	1.00	-0.4	1.59	0.83	0.06	2.13	0.81	-0.51
Alcohols	Glucose	$C_6H_{12}O_6$	2.00	1.00	0	2.01	1.01	0.02	2.09	1.00	-0.10
Alcohols	Levoglucosan	$C_6H_{10}O_5$	1.67	0.83	0	1.85	0.77	-0.31	2.06	0.86	-0.33
Alcohols	Sucrose	$C_{12}H_{22}O_{11}$	1.83	0.92	0	1.90	0.900	-0.10	1.99	0.83	-0.32
Alcohols	Xylitol	$C_5H_{12}O_5$	2.40	1.00	-0.4	1.92	0.78	-0.37	2.21	0.90	-0.41

Table S3. Summary of H:C, O:C and. OS_c determined by the SP-AMS 2

			True value			Tungsten vaporizer			Laser vaporizer		
Species	**Class**	**Formula**	**H:C**	**O:C**	**OSc**	**H:C**	**O:C**	**OSc**	**H:C**	**O:C**	**OSc**
Cis-Pinonic acid	Multifunctional	$C_{10}H_{16}O_3$	1.60	0.30	-1.00	1.69	0.25	-1.19	0.48	1.30	-0.34
Citric acid	Multifunctional	$C_6H_8O_7$	1.33	1.17	1.00	1.40	1.00	0.59	0.94	1.39	0.49
Glutamic acid	Multifunctional	$C_5H_9NO_4$	1.80	0.80	-0.2		NA		0.29	2.03	-1.45
Glycolic acid	Multifunctional	$C_2H_4O_3$	2.00	1.50	1.00	1.45	1.24	1.04	0.65	1.56	-0.26
Levulinic acid	Multifunctional	$C_5H_8O_3$	1.60	0.60	-0.4		NA		1.00	1.81	0.19
Malic acid	Multifunctional	$C_4H_6O_5$	1.50	1.25	1.00	1.56	1.10	0.64	0.60	1.55	-0.35
Pyruvic acid	Multifunctional	$C_3H_4O_3$	1.33	1.00	0.67	1.32	0.74	0.15	1.52	1.94	1.10
Tartaric acid	Multifunctional	$C_4H_6O_6$	1.50	1.50	1.5	1.60	1.74	1.88	0.09	2.30	-2.12
Adipic acid	Diacids	$C_6H_{10}O_4$	1.67	0.67	-0.33	1.60	0.43	-0.74	0.46	1.87	-0.95
Azelaic acid	Diacids	$C_9H_{16}O_4$	1.78	0.44	-0.89	1.62	0.32	-0.99	0.32	1.94	-1.30
Glutaric acid	Diacids	$C_5H_8O_4$	1.6	0.80	0	1.46	0.57	-0.33	0.56	1.80	-0.68
Maleic acid	Diacids	$C_4H_4O_4$	1.00	1.00	1.00	1.56	1.10	0.64	0.65	1.34	-0.04
Malonic acid	Diacids	$C_3H_4O_4$	1.33	1.33	1.33	1.58	1.09	0.59	1.13	1.83	0.43
Oxalic acid	Diacids	$C_2H_2O_4$	1.00	2.00	3.00	0.92	2.42	3.92	1.68	1.34	2.02
Succinic acid	Diacids	$C_4H_6O_4$	1.50	1.00	0.50	1.64	0.50	-0.64	0.55	1.89	-0.79
Tricarballylic acid	Polyacids	$C_6H_8O_6$	1.33	1.00	0.67	1.30	0.65	-0.01	0.56	1.57	-0.45
1,5-Pentanediol	Alcohols	$C_5H_{12}O_2$	2.4	0.40	-1.6		NA		0.44	1.70	-0.82
Dextrose	Alcohols	$C_6H_{12}O_6$	2.00	1.00	0		NA		0.87	1.87	-0.13
Phenol	Alcohols	C_6H_6O	1.00	0.17	-0.67		NA		0.62	1.81	-0.57
Bis(2-ethylhexyl) Sebacate	Esters	$C_{26}H_{50}O_4$	1.92	0.15	-1.62		NA		0.1	2.23	-2.03

Table S4. Summary of H:C, O:C and. OS_c determined by the SP-AMS 3

			True value			Tungsten vaporizer			Laser vaporizer		
Species	**Class**	**Formula**	**H:C**	**O:C**	**OSc**	**H:C**	**O:C**	**OSc**	**H:C**	**O:C**	**OSc**
Cis-Pinonic Acid	Multifunctional	$C_{10}H_{16}O_3$	1.60	0.30	-1.00	1.43	0.22	-0.99	1.53	0.19	-1.15
Citric acid	Multifunctional	$C_6H_8O_7$	1.33	1.17	1.00	1.18	1.03	0.88	1.19	0.86	0.52
Ketoglutaric Acid	Multifunctional	$C_5H_6O_5$	1.20	1.00	0.80	1.20	0.84	0.48	1.44	0.54	-0.36
Ketopimelic acid	Multifunctional	$C_7H_{10}O_5$	1.43	0.71	0	1.10	0.57	0.04	1.39	0.42	-0.55
Tartaric acid	Multifunctional	$C_4H_6O_6$	1.50	1.50	1.50	1.40	1.51	1.62	1.66	1.55	1.43
Azelaic Acid	Diacids	$C_9H_{16}O_4$	1.78	0.44	-0.89	1.34	0.28	-0.78	1.59	0.23	-1.13
Glutaric acid	Diacids	$C_5H_8O_4$	1.60	0.80	0	1.34	0.46	-0.42	1.47	0.46	-0.54
Malonic acid	Diacids	$C_3H_4O_4$	1.33	1.33	1.33	1.24	1.12	1	1.39	0.91	0.43
Pimelic acid	Diacids	$C_7H_{12}O_4$	1.71	0.57	-0.57	1.30	0.34	-0.62	1.56	0.31	-0.94
Succinic acid	Diacids	$C_4H_6O_4$	1.50	1.00	0.50	1.57	0.51	-0.55	1.56	0.46	-0.65
Sucrose	Alcohols	$C_{12}H_{22}O_{11}$	1.83	0.92	0	1.86	0.6	-0.66	1.60	0.55	-0.50
Xylitol	Alcohols	$C_5H_{12}O_5$	2.40	1.00	-0.40	1.74	0.68	-0.38	1.87	0.63	-0.60

Table S5. Root mean squared error (RMSE) and mean absolute error (MAE) of I-A and I-Asp method

	I-A H:C	**I-A O:C**	**I-A_{sp} H:C**	**I-A_{sp} O:C**
RMSE	0.45	0.3	0.37	0.21
MAE	0.38	0.23	0.31	0.14

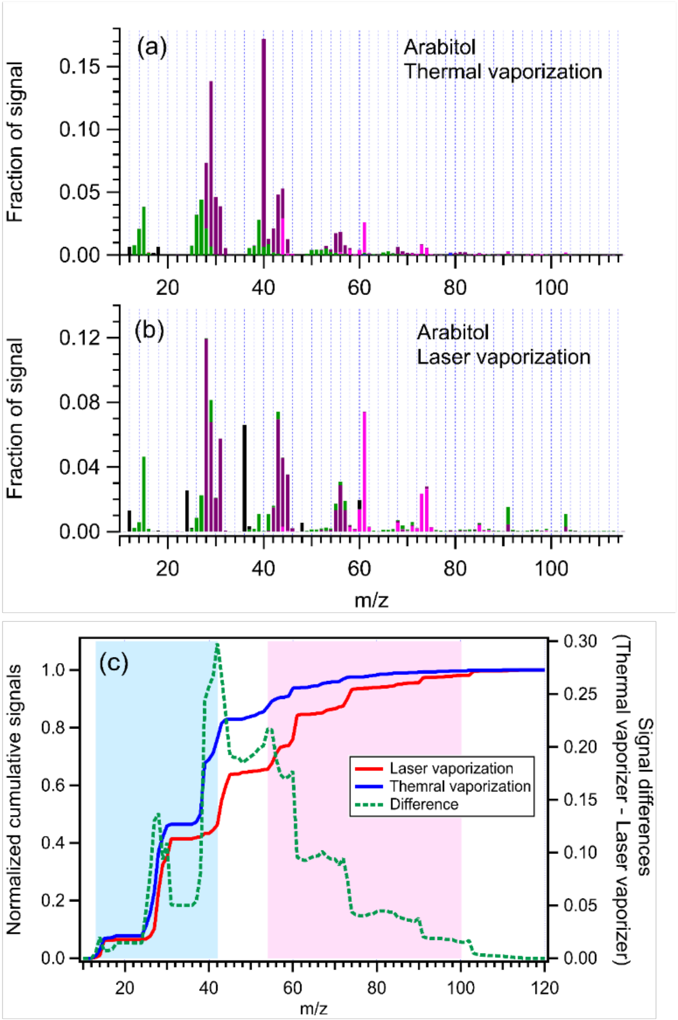

Fig. S1. Mass spectra of arabitol, measured by the SP-AMS 1 using the tungsten (a) and laser (b) vaporization schemes. (c) Normalized cumulative histogram of mass-to-charge ratios for the oxygenated organic compounds measured by the SP-AMS 1. The blue area indicates that the thermal vaporization scheme tends to provide organic fragments with smaller m/z, whereas the red area indicates that the laser vaporization scheme tends to give organic fragments with larger m/z.

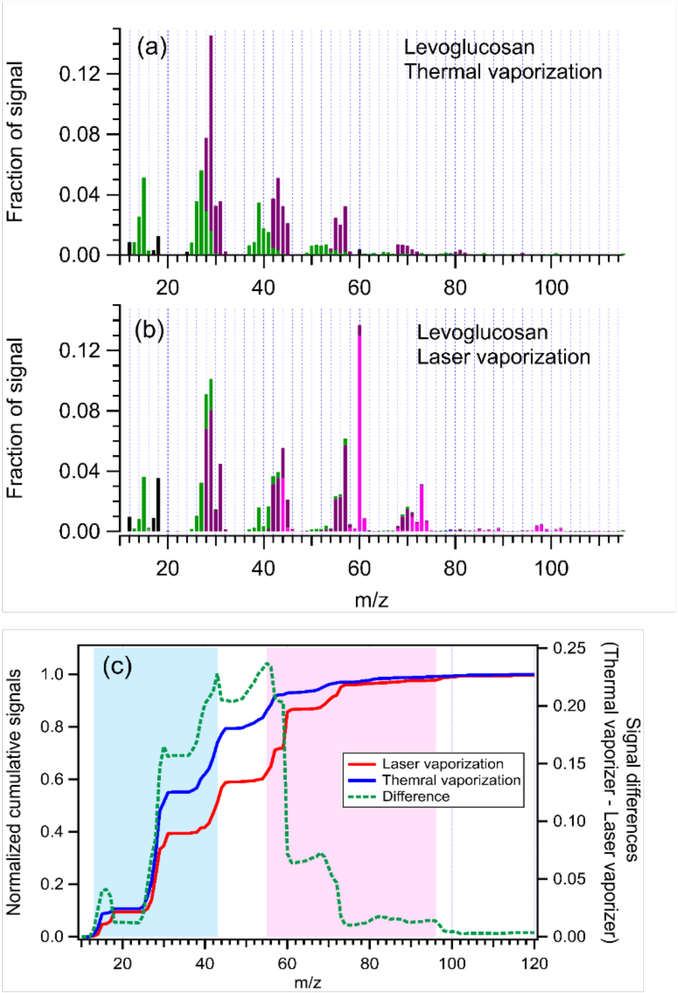

Fig. S2. Mass spectra of levoglucosan, measured by the SP-AMS 1 using the tungsten (a) and laser (b) vaporization schemes. (c) Normalized cumulative histogram of mass-to-charge ratios for the oxygenated organic compounds measured by the SP-AMS 1. The blue area indicates that the thermal vaporization scheme tends to provide organic fragments with smaller m/z, whereas the red area indicates that the laser vaporization scheme tends to give organic fragments with larger m/z.

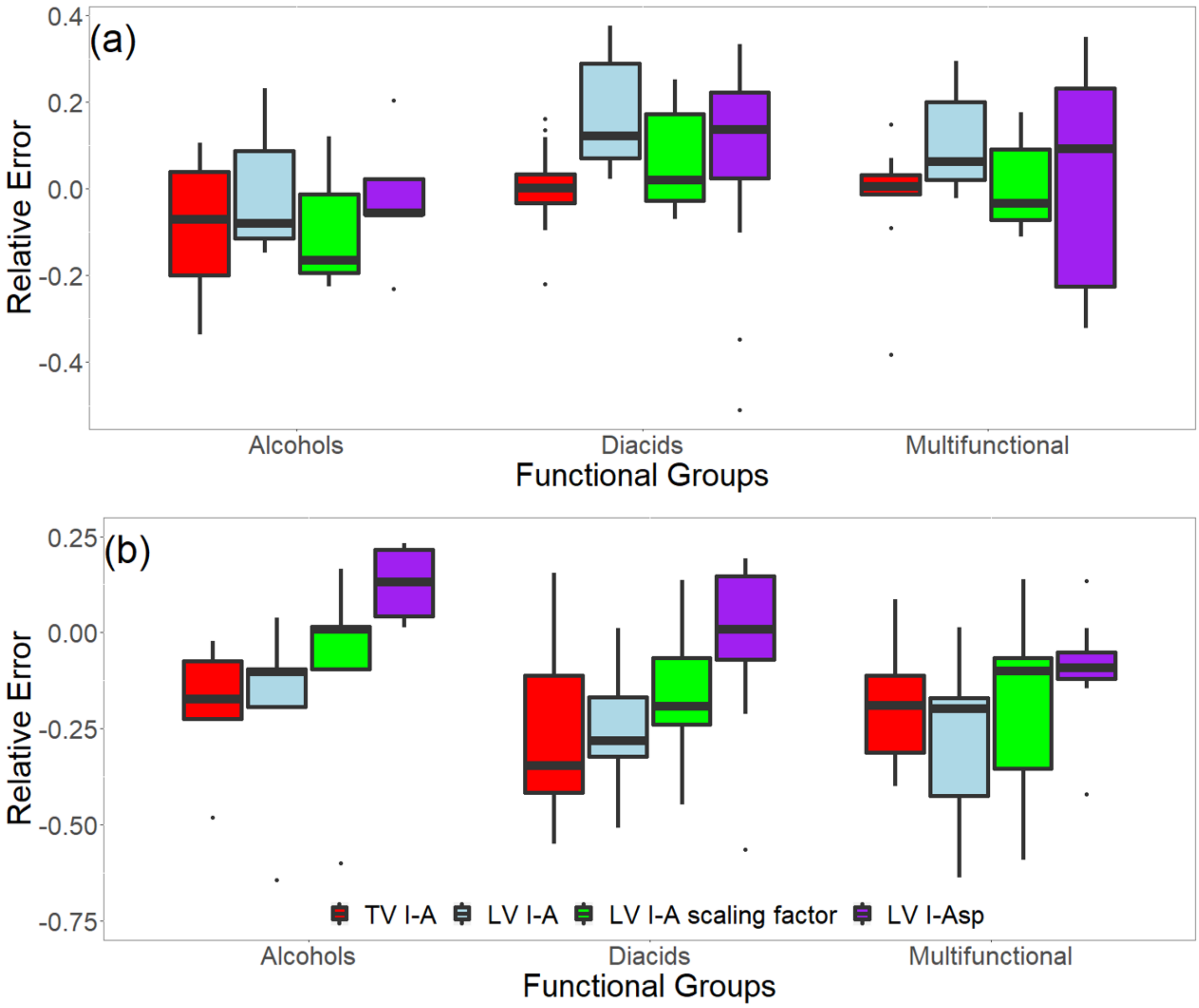

Fig. S3. Relative error of H:C (a) and O:C (b) ratios from SP-AMS 1 and 2 calculated with LV and TV methods. TV I-A (red), LV I-A(blue), LV I-A_{sp} (green) and LV I-A scaling factor (purple) are included in the comparison.

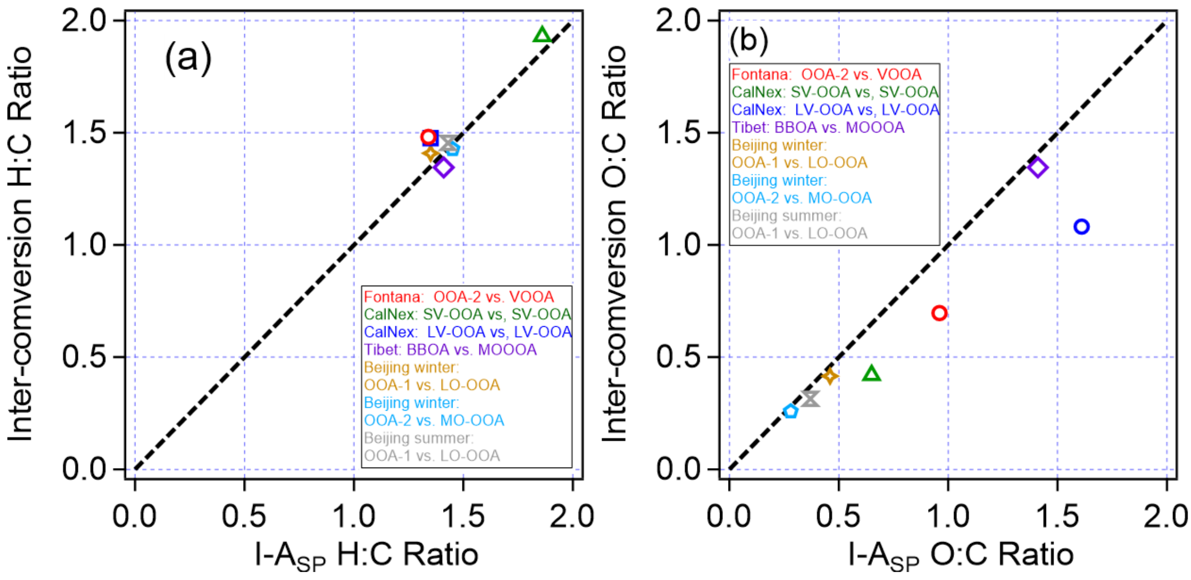

Fig. S4. Comparison of elemental ratios determined by the I-A$_{sp}$ method and the I-A method with the inter-conversion factors applied.

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