

Analysis of Sugars and Polyols in Atmospheric Aerosols by Chloride Attachment in Liquid Chromatography / Negative Ion Electrospray Mass Spectrometry

Eric C. H. Wan and Jian Zhen Yu *

Department of Chemistry, Hong Kong University of Science & Technology

Clear Water Bay, Kowloon, Hong Kong, China

*Corresponding author phone: 852-2358-7389; fax: 852-2358-1594; email: chjianyu@ust.hk

Supplementary Materials

Table S1. Concentrations (ng m⁻³) of sugar and polyol compounds in the ambient aerosol samples.

Sampling date	Glycerol	Erythritol	methyltetros	Xylitol	Mannitol	Xylose	Fructose	Glucose	Levoglucosan	Sucrose	Trehalose	Melezitose	Raffinose	sum	%OC ^a
2-Aug-2004	1.38	3.89	2.06	3.15	2.45	52.48	6.07	0.76	4.14	5.18	nd ^b	1.02	nd	82.6	1.4%
9-Aug-2004	8.92	5.31	6.81	7.18	1.65	10.24	19.84	3.02	61.44	15.92	nd	nd	nd	140.3	0.5%
16-Aug-2004	8.81	4.11	3.89	6.23	6.29	87.13	11.06	4.21	40.12	3.51	nd	nd	nd	175.4	1.4%
28-Sep-2004	3.66	5.12	20.30	7.44	7.59	24.39	35.31	10.73	127.2	21.10	0.27	5.95	0.13	269.2	1.2%
5-Oct-2004	0.72	1.94	13.89	0.90	3.62	12.22	5.60	0.89	14.30	11.23	nd	4.39	nd	69.7	0.3%
12-Oct-2004	5.13	7.86	20.36	10.77	17.28	309.0	24.83	5.04	116.4	47.69	nd	16.27	3.41	584.0	2.9%
19-Oct-2004	48.94	28.94	172.1	29.09	16.23	417.4	65.75	8.88	300.3	128.2	15.86	67.98	16.16	1316	3.6%
20-Oct-2004	13.31	6.98	50.11	17.58	14.02	109.7	34.96	10.77	219.8	22.35	2.53	11.63	2.78	516.5	1.8%
21-Oct-2004	18.19	9.28	33.95	15.80	7.84	26.06	13.84	1.73	66.46	12.82	0.24	5.03	1.37	212.6	1.0%
22-Oct-2004	13.70	7.12	15.26	10.86	13.40	127.2	18.30	5.10	102.0	13.14	2.67	4.47	0.23	333.4	1.5%
23-Oct-2004	6.10	4.93	6.80	7.31	7.87	78.85	12.89	2.06	49.33	18.84	nd	6.09	0.61	201.7	1.5%
24-Oct-2004	8.21	5.82	10.64	13.61	4.53	66.87	19.56	8.14	99.53	34.72	1.82	26.21	3.83	303.5	1.4%
25-Oct-2004	5.03	3.43	2.13	0.95	4.22	25.25	15.60	6.83	89.94	35.21	0.25	19.50	2.16	210.5	0.7%
26-Oct-2004	3.57	3.14	12.14	5.14	4.54	5.00	12.56	3.82	36.87	12.95	nd	5.14	0.56	105.4	0.4%
5-Jan-2005	12.45	4.56	8.41	15.09	21.03	86.13	26.09	4.12	488.7	11.28	nd	4.97	0.08	682.9	1.4%
6-Jan-2005	10.60	4.21	10.75	4.97	2.65	75.96	15.76	7.97	185.5	3.98	1.83	nd	nd	324.2	1.1%
10-Jan-2005	16.90	5.26	17.18	10.91	2.40	30.74	12.10	4.09	272.7	0.17	nd	nd	nd	372.5	1.1%
11-Jan-2005	9.62	3.75	9.64	5.50	10.47	68.89	17.57	3.60	409.4	3.55	nd	nd	nd	542.0	1.5%
18-Jan-2005	6.09	3.19	4.56	7.42	9.12	27.18	19.24	6.04	146.2	3.16	nd	nd	nd	232.2	1.1%
19-Jan-2005	3.85	1.31	11.22	2.51	4.64	22.79	12.22	4.15	80.90	nd	nd	nd	nd	143.6	0.6%
24-Jan-2005	20.91	2.85	5.28	1.09	0.84	13.02	5.63	0.79	47.30	1.17	nd	nd	nd	98.9	0.8%
25-Jan-2005	3.79	1.01	2.39	1.95	0.83	75.74	18.79	4.68	34.91	nd	nd	nd	nd	144.1	1.4%
26-Jan-2005	13.77	5.09	1.59	6.36	1.59	6.94	4.15	0.92	46.00	1.55	nd	nd	nd	88.0	1.3%
15-Mar-2005	8.13	2.76	6.04	10.65	3.25	7.86	9.23	3.01	78.02	nd	nd	nd	nd	128.9	1.3%
16-Mar-2005	1.48	3.71	1.33	0.75	nd	38.35	5.51	0.45	19.16	0.08	nd	nd	nd	70.8	0.8%
29-Mar-2005	18.45	4.51	2.90	7.53	4.27	24.82	8.89	1.94	18.44	6.33	nd	nd	nd	98.1	1.6%
7-Apr-2005	2.76	3.62	4.27	3.73	nd	15.59	2.45	0.65	4.44	nd	nd	nd	nd	37.5	0.6%
8-Apr-2005	3.23	1.00	4.13	nd	nd	88.78	2.39	0.38	22.49	nd	nd	nd	nd	122.4	2.2%
21-Apr-2005	0.28	1.00	1.19	nd	1.78	36.31	6.99	3.09	5.03	6.90	nd	nd	nd	62.6	0.8%
22-Apr-2005	0.28	1.00	1.19	nd	nd	50.22	1.79	0.58	4.32	6.52	nd	nd	nd	65.9	1.8%
mean	9.27	4.89	15.42	7.94	6.71	67.37	15.50	3.95	106	17.10	3.18	13.74	2.85	258	1.3%
range	0.3-48.9	1.0-28.9	1.2-172.1	nd-29.1	nd-21.0	5.0-417.4	1.8-65.7	0.4-10.8	4.1-488.7	nd-128.2	nd-15.9	nd-68.0	nd-16.2	38-1316	0.3%-3.6%

^a on a carbon mass basis. ^b nd refers to not detected.

Table S2. Concentrations ($\mu\text{g m}^{-3}$) of major constituents in the ambient aerosol samples.

Sampling date	OC	EC	SO_4^{2-}	NO_3^-	Cl^-	F^-	oxalate	Na^+	NH_4^+	K^+	Mg^{2+}	Ca^{2+}
2-Aug-04	2.31	1.85	2.46	0.10	0.029	0.000	0.103	0.115	5.22	0.08	0.014	0.075
9-Aug-04	11.27	3.23	19.82	1.35	0.075	0.035	0.825	0.153	24.00	0.44	0.022	0.143
16-Aug-04	5.06	1.05	5.87	0.27	0.040	0.022	0.240	0.221	10.10	0.12	0.024	0.186
28-Sep-04	9.67	1.97	15.24	5.03	0.244	0.048	1.259	0.573	20.28	1.45	0.085	0.256
5-Oct-04	8.66	2.48	8.51	0.51	0.078	0.060	0.700	0.211	12.61	1.36	0.035	0.156
12-Oct-04	8.20	2.59	17.96	0.66	0.113	0.053	0.699	0.422	20.88	1.39	0.046	0.224
19-Oct-04	15.12	3.31	19.08	0.95	0.232	0.076	0.684	0.334	20.89	2.28	0.069	1.226
20-Oct-04	12.22	1.29	18.43	1.18	0.101	0.085	0.877	0.225	21.76	2.28	0.043	0.145
21-Oct-04	9.08	2.17	13.16	0.87	0.132	0.055	0.771	0.483	16.95	1.17	0.037	0.144
22-Oct-04	9.13	1.73	16.17	0.47	0.070	0.079	0.646	0.342	19.37	1.27	0.053	0.120
23-Oct-04	5.44	0.79	11.34	0.55	0.063	0.029	0.369	0.566	14.74	0.74	0.076	0.160
24-Oct-04	9.09	2.52	15.26	0.85	0.176	0.036	0.538	0.487	18.08	1.54	0.075	0.402
25-Oct-04	12.38	3.12	15.39	0.76	0.274	0.058	0.536	0.331	17.99	2.14	0.068	1.084
26-Oct-04	11.52	2.55	15.67	0.74	0.119	0.085	0.609	0.236	18.53	2.07	0.006	0.558
5-Jan-05	21.20	5.20	10.88	4.11	0.716	0.158	0.845	0.882	15.13	2.68	0.113	0.407
6-Jan-05	12.78	2.54	10.46	1.80	0.151	0.111	0.773	0.269	15.24	1.52	0.032	0.074
10-Jan-05	14.12	2.43	13.68	3.18	0.345	0.129	0.578	0.307	18.63	1.52	0.026	0.000
11-Jan-05	15.93	3.45	11.55	3.58	0.193	0.140	0.534	0.313	16.65	1.99	0.040	0.000
18-Jan-05	8.93	2.09	12.52	2.50	0.336	0.075	0.600	0.705	16.97	0.96	0.114	0.223
19-Jan-05	10.18	1.80	12.91	2.78	0.286	0.081	0.660	0.356	18.29	0.99	0.032	0.067
24-Jan-05	5.30	0.78	8.41	0.51	0.051	0.046	0.487	0.419	12.42	0.24	0.034	0.061
25-Jan-05	4.10	0.90	4.83	2.26	0.277	0.023	0.281	0.116	11.46	0.18	0.011	0.020
26-Jan-05	2.92	0.53	6.04	0.55	0.154	0.025	0.213	0.199	11.08	0.16	0.023	0.009
15-Mar-05	4.17	0.92	6.94	1.97	0.755	0.048	0.431	0.170	13.75	0.25	0.016	0.040
16-Mar-05	3.63	0.60	5.93	0.16	0.145	0.034	0.426	0.175	10.69	0.19	0.027	0.022
29-Mar-05	2.49	0.93	10.39	1.91	1.568	0.029	0.583	0.667	16.57	0.33	0.096	0.249
7-Apr-05	2.46	0.37	6.33	0.64	0.172	0.016	0.237	0.221	11.64	0.15	0.024	0.071
8-Apr-05	2.31	1.08	7.22	0.86	0.097	0.013	0.202	0.149	12.73	0.23	0.027	0.167
21-Apr-05	3.08	0.88	9.35	0.24	0.031	0.024	0.412	0.159	14.39	0.15	0.030	0.107
22-Apr-05	1.53	0.54	7.08	0.11	0.014	0.013	0.215	0.134	11.04	0.17	0.020	0.081
mean	8.14	1.86	11.3	1.38	0.23	0.06	0.54	0.33	15.60	1.00	0.04	0.22
Range	1.5-21.2	0.4-5.2	2.5-19.8	0.1-5.0	0.0-1.6	0.0-0.2	0.1-1.3	0.1-0.9	5.2-24.0	0.1-2.7	0.0-0.1	0.0-1.2

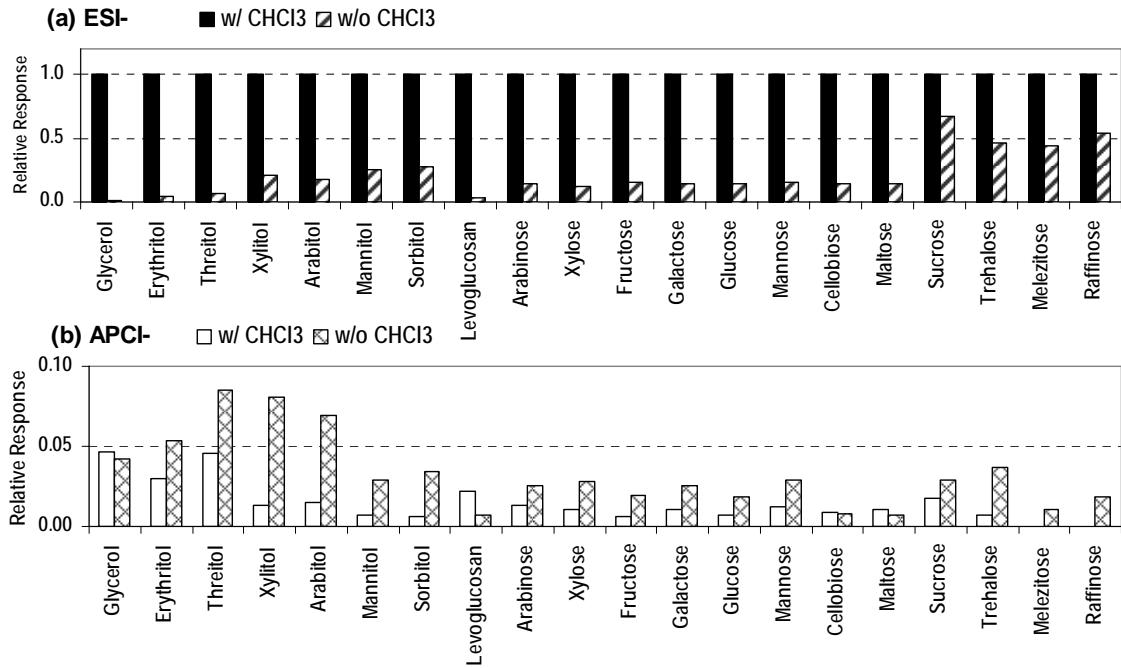


Figure S1. Comparison of detection sensitivity with and without addition of CHCl₃ under two ionization modes, (a) ESI- and (b) APCI-.

(Peak areas are normalized against those obtained with ESI-/presence of CHCl₃ for individual analytes. Fig. 2a and Fig. 2b are plotted on different scales to show the smaller responses with APCI. LC-MS conditions: direct fusion of 10 ppm individual standards at 20 μ L/min, mobile phase: 10% H₂O: 90% acetonitrile; ESI parameters: capillary voltage, 3.5 kV, extractor, 2 V, RF lens voltage, 0.3 V, desolvation flow, 800 L/hr, cone flow, 20 L/hr, desolvation temperature, 300 °C, cone temperature: 120 °C; APCI parameters: Corona current, 0.5 μ A, extractor, 2 V, RF lens voltage, 0.3 V, desolvation flow, 900 L/hr, cone flow, 20 L/hr, desolvation temperature, 350 °C, cone temperature: 120 °C.)