Supplement of Atmos. Chem. Phys., 23, 14561–14576, 2023
https://doi.org/10.5194/acp-23-14561-2023-supplement

Atmospheric Chemistry and Physics
Open Access

Supplement of

Bulk and molecular-level composition of primary organic aerosol from wood, straw, cow dung, and plastic burning

Jun Zhang et al.

Correspondence to: Andre S. H. Prevot (andre.prevot@psi.ch) and David M. Bell (david.bell@psi.ch)

Plastic bags burning emission correction. In three out of four plastic bags burning experiments, the mass spectrum at the middle to end burning stages had considerable $C_xH_yO_z$ family contribution (~23%). It is unlikely from the plastic bags, given the fact that polyethylene is the main component of plastic bags, but from the emission of other fuels remaining in the chimney. As the combustion progressed, the chimney was heated, and the volatile substances remaining on the chimney evaporated and were then partitioned to the particles for detection. However, at the early stage, before the chimney got hot, the mass spectra consisted mainly of hydrocarbons (see Figure S2a). Therefore, we take only the early burning stage of these three burning experiments into account for the average mass spectrum in Figure 1(f). The absolute concentration of the three AMS mass spectra derived from the early-stage burning is scaled to the uncontaminated burning experiment ions based on *m/z* 81 and *m/z* 83, which are stable and characteristic for hydrocarbons. The difference on average is 0.4% ± 1.0% which is very minor as shown in Figure S2 b. The mass spectra of three contaminated burning over the whole burning stages indicate that the measured organics was 14.6% ± 8.7% overestimated. Correspondingly, the emission factors for PM and OM are corrected for each plastic bags burning.

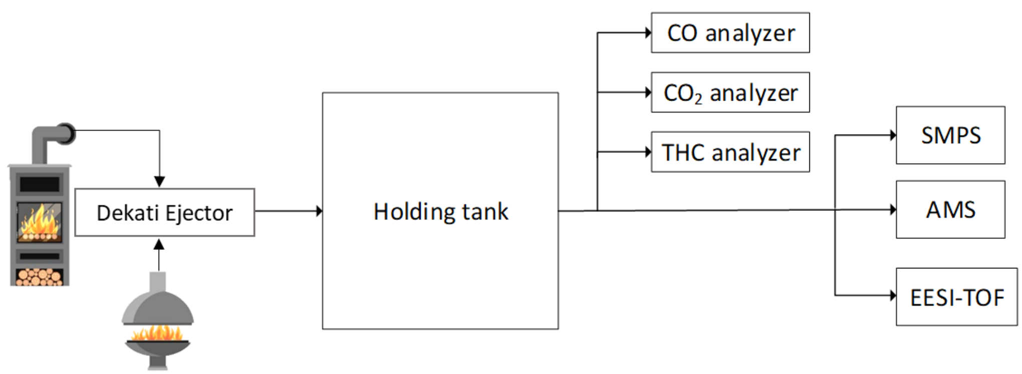

Figure S1. Schematic diagram of experimental setup.

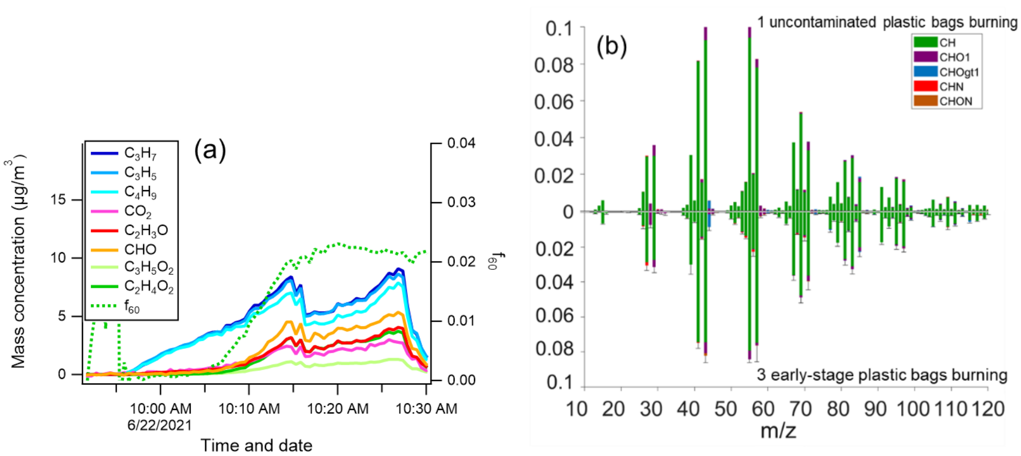

Figure S2 (a) The time series of some ions measured by the AMS during the plastic bags burning for the contaminated case; (b) the mass spectrum comparison of uncontaminated plastic bags burning experiment at the top v.s. the average of 3 early-stage burning at the bottom.

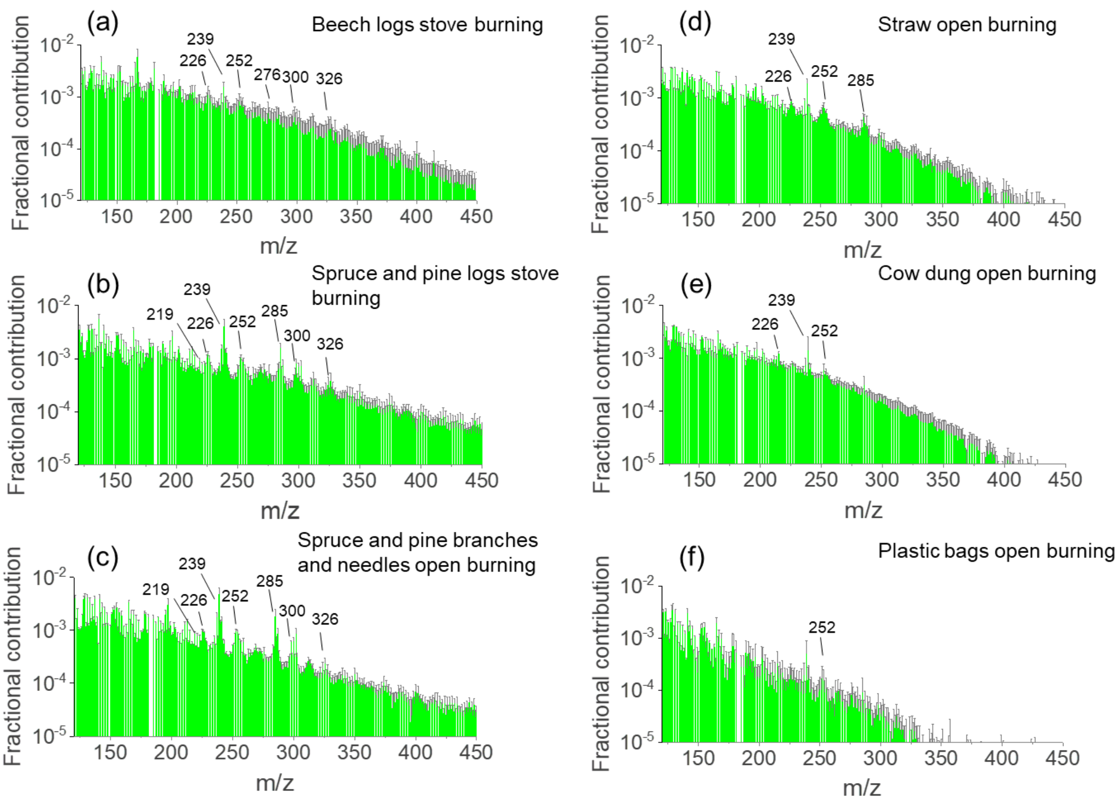

Figure S3. Average AMS POA mass spectral profiles in the range from m/z 120 to 450 of (a) beech logs stove burning (n=6; n is the number of experiments), (b) spruce and pine logs stove burning (n=9), (c) spruce and pine branches and needles open burning (n=4), (d) straw open burning (n=6), (e) cow dung open burning (n=5), and (f) plastic bags open burning (n=4). The m/z for some ions are marked in the figure. The error bar denotes half standard deviation in grey.

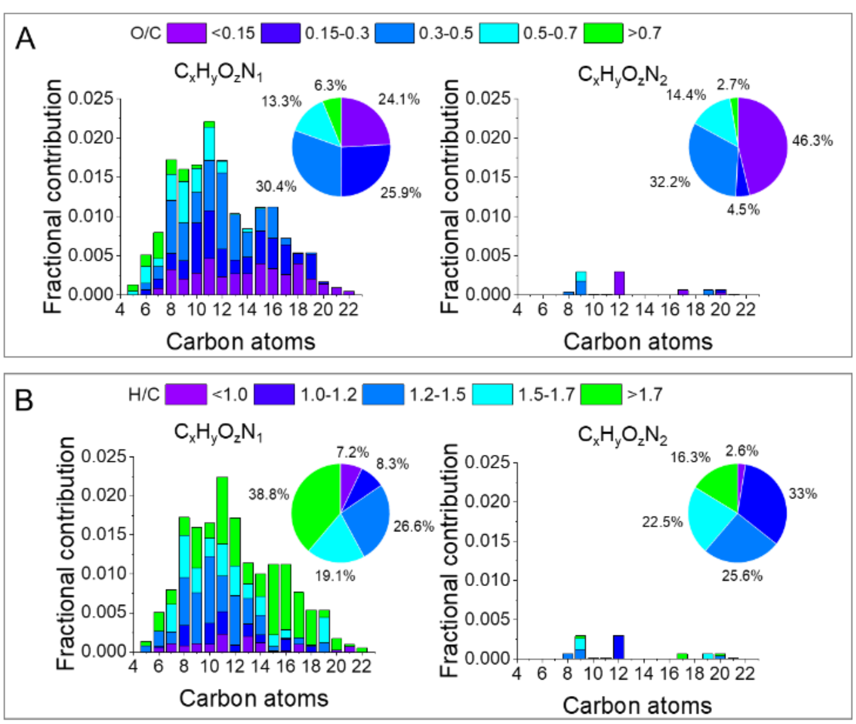

Figure S4. The average carbon and oxygen distribution of cow dung open burning.

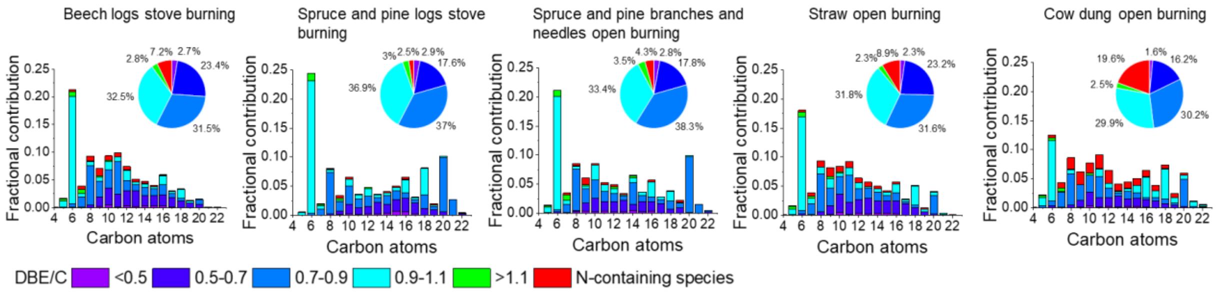

Figure S5. The average carbon and oxygen distribution colored by the DBE/C for non-nitrogen-containing species with the EESI-TOF. The nitrogen-containing species are colored in red. The pie charts are the corresponding contribution of DBE/C.

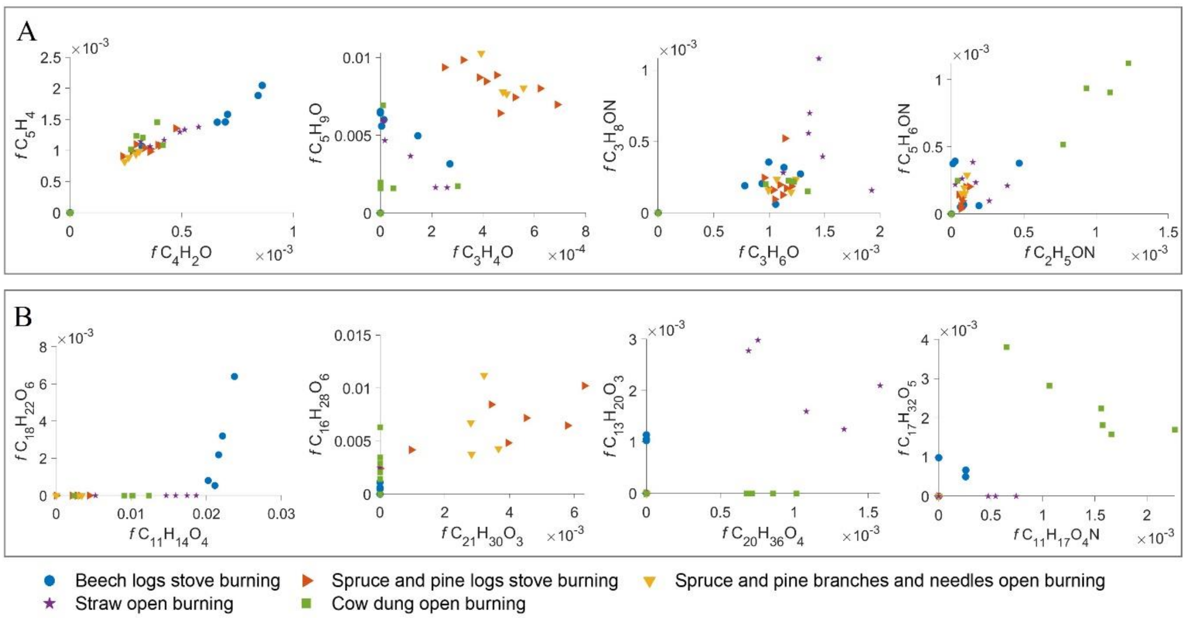

Figure S6. The scatter plots of marker ions from (A) AMS and (B) EESI-TOF.

Table S1. The emission factors of CO, CO_2, THC, PM, and BC as well as MCE values from each burns. It is noted as n.a. where the data is not available. The short dash line denotes the corresponding value is not calculated under the category due to a lack of required data. BS, SPS, SPO, SO, CDO, PBO indicate beech wood stove burning, spruce and pine logs stove burning, spruce and pine branches and needles open burning, straw open burning, and cow dung open burning, respectively.

Exp. No.	Burning type	MCE	Emission factors								
			CO	CO_2	THC	BC data is not available			BC data is available		
						PM	OM	BC	PM	OM	BC
BS1	beech stove	0.94	65.6	1525.1	14.9	5.4	3.1	n.a.	-	-	-
BS2	beech stove	0.94	58.5	1541.5	13.2	5.3	3.5	n.a.	-	-	-
BS3	beech stove	0.91	89.0	1459.4	20.7	14.0	5.3	-	9.6	8.3	3.28
BS4	beech stove	0.88	124.3	1388.4	27.3	12.0	4.6	-	8.2	7.1	2.57
BS5	beech stove	0.91	91.8	1420.3	20.4	-	-	-	9.7	9.3	1.44
SPS1	spruce stove	0.90	56.7	1698.3	10.3	6.3	2.3	n.a.	-	-	-
SPS2	spruce stove	0.92	71.9	1661.1	15.9	4.3	1.6	n.a.	-	-	-

SPS3	spruce stove	0.90	98.3	1618.4	17.5	2.6	1.1	n.a.	-	-	-
SPS4	spruce stove	0.92	72.8	1650.8	19.3	3.6	2.2	n.a.	-	-	-
SPS5	spruce stove	0.87	142.2	1509.2	25.8	9.2	4.8	n.a.	-	-	-
SPS6	spruce stove	0.93	76.1	1658.6	13.9	5.9	1.1	n.a.	-	-	-
SPS7	spruce stove	0.94	66.5	1680.3	12.7	4.0	1.8	n.a.	-	-	-
SPS8	spruce stove	0.91	85.9	1649.1	13.5	3.2	0.9	n.a.	-	-	-
SPO1	spruce + pine open	0.95	54.2	1707.9	9.1	5.4	2.3	n.a.	-	-	-
SPO2	spruce + pine open	0.91	64.6	1658.6	16.2	10.4	4.3	n.a.	-	-	-
SPO3	spruce + pine open	0.91	70.5	1647.6	15.9	11.6	3.6	n.a.	-	-	-
SPO4	spruce + pine open	0.93	64.6	1661.5	15.3	10.4	4.9	n.a.	-	-	-
SO1	straw open	0.92	40.6	1554.5	8.3	2.8	0.9	n.a.	-	-	-
SO2	straw open	0.94	61.7	1433.0	36.6	-	-	-	2.2	1.9	0.62
SO3	straw open	0.94	48.9	1481.8	26.0	-	-	-	4.0	3.6	0.93
SO4	straw open	1.00	0.2	1636.4	0.7	1.6	1.7	n.a.	-	-	-
SO5	straw open	0.98	17.8	1598.6	3.9	1.7	1.6	n.a.	-	-	-
SO6	straw open	0.89	97.4	1366.1	39.3	-	-	-	4.6	4.3	0.54
CDO1	cow dung open	0.81	79.0	1414.7	29.4	8.0	7.6	n.a.	-	-	-
CDO2	cow dung open	0.89	53.0	1448.9	24.9	14.3	16.2	-	14.9	14.2	0.56
CDO3	cow dung open	0.88	81.8	1436.9	22.6	4.9	5.9	-	5.1	4.8	0.81
CDO4	cow dung open	0.90	99.1	1377.4	26.5	-	-	-	12.6	12.5	0.5
CDO5	cow dung open	0.89	107.6	1292.2	32.6	-	-	-	33.0	32.5	1.3
CDO6	cow dung open	0.85	133.0	1227.2	46.1	-	-	-	26.2	25.9	0.76
PBO1	plastic bag open	0.99	6.2	3022.2	2.9	3.09	n.a	-	3.85	n.a.	0.89
PBO2	plastic bag open	0.99	13.1	3028.9	5.6	1.22	1.44	-	1.20	0.92	0.88
PBO3	plastic bag open	0.99	10.0	3026.9	3.2	-	-	-	2.54	1.34	0.72
PBO4	plastic bag open	0.95	88.0	2748.4	61.1	-	-	-	3.40	n.a.	1.43

Table S2. The compounds from EESI-TOF with p-value smaller than 0.1 during pairwise comparisons and their fold changes measured by EESI-TOF. The average p-value (p_mean), the standard deviation of p-values (p_std), the average base-2 logarithmic fold change (log2FC_mean), and the standard deviation of log2FC (log2FC_std) are listed.

Burning types	Monoisotopic mass	Formula	p_mean	p_std	log_2FC_mean	log_2FC_std
Beech logs stove burning	181.1103	$C_{10}H_{15}O_2N$	0.06	0.05	-1.06	1.12
	210.0893	$C_{11}H_{14}O_4$	0.01	0.00	1.48	0.41
	252.1727	$C_{15}H_{24}O_3$	0.04	0.01	3.10	1.89
	261.1213	$C_{11}H_{19}O_6N$	0.03	0.03	-0.54	1.28
	300.2666	$C_{18}H_{36}O_3$	0.05	0.06	-1.82	1.49
	306.2560	$C_{20}H_{34}O_2$	0.03	0.03	-3.28	1.79
	310.2145	$C_{18}H_{30}O_4$	0.07	0.03	-1.13	1.46
	324.2666	$C_{20}H_{36}O_3$	0.02	0.01	-3.19	0.00
	334.1417	$C_{18}H_{22}O_6$	0.04	0.01	3.38	2.33
Spruce and pine burning	116.1202	$C_7H_{16}O$	0.02	0.02	-2.81	0.00
	124.0889	$C_8H_{12}O$	0.05	0.04	-2.30	0.75
	127.0634	$C_6H_9O_2N$	0.03	0.01	-1.37	0.00
	132.0423	$C_5H_8O_4$	0.00	0.00	-1.27	0.68
	133.0528	C_8H_7ON	0.02	0.02	-2.19	0.40
	134.0579	$C_5H_{10}O_4$	0.02	0.03	-1.53	1.66

137.0841	$C_8H_{11}ON$	0.01	0.02	-2.78	0.27
139.0998	$C_8H_{13}ON$	0.04	0.05	-2.17	0.57
140.0474	$C_7H_8O_3$	0.04	0.03	-1.82	1.11
141.0790	$C_7H_{11}O_2N$	0.02	0.02	-1.86	0.33
141.1154	$C_8H_{15}ON$	0.02	0.02	-1.94	0.00
148.0525	$C_9H_8O_2$	0.03	0.00	-2.44	1.54
151.0634	$C_8H_9O_2N$	0.02	0.02	-1.99	0.00
152.0474	$C_8H_8O_3$	0.03	0.02	-2.58	1.81
153.0790	$C_8H_{11}O_2N$	0.01	0.02	-2.83	0.00
154.0630	$C_8H_{10}O_3$	0.02	0.03	-3.09	1.39
155.0583	$C_7H_9O_3N$	0.02	0.02	-2.53	0.00
157.0892	$C_{11}H_{11}N$	0.02	0.03	-2.29	0.00
164.0474	$C_9H_8O_3$	0.02	0.01	-1.24	0.78
167.0947	$C_9H_{13}O_2N$	0.02	0.02	-2.69	0.00
168.0423	$C_8H_8O_4$	0.00	0.01	-1.88	1.57
168.0787	$C_9H_{12}O_3$	0.03	0.02	-3.09	2.13
169.0739	$C_8H_{11}O_3N$	0.02	0.02	-3.15	0.68
173.0688	$C_7H_{11}O_4N$	0.03	0.01	-2.10	0.00
174.0529	$C_7H_{10}O_5$	0.01	0.01	-1.96	0.92
175.0481	$C_6H_9O_5N$	0.04	0.01	-2.77	0.00
176.0838	$C_{11}H_{12}O_2$	0.04	0.05	-2.69	2.19
178.0266	$C_9H_6O_4$	0.01	0.01	1.04	1.08
180.0787	$C_{10}H_{12}O_3$	0.04	0.02	-2.50	2.73
181.1103	$C_{10}H_{15}O_2N$	0.01	0.02	-2.79	0.00
182.0944	$C_{10}H_{14}O_3$	0.03	0.01	-2.09	2.31
183.0532	$C_8H_9O_4N$	0.03	0.01	-2.50	0.00
183.1049	$C_{13}H_{13}N$	0.02	0.02	-3.38	0.00
185.0688	$C_8H_{11}O_4N$	0.01	0.02	-3.46	0.54
188.0321	$C_7H_8O_6$	0.04	0.05	0.09	0.46
188.0838	$C_{12}H_{12}O_2$	0.04	0.01	-2.54	2.12
189.0790	$C_{11}H_{11}O_2N$	0.01	0.02	-2.83	0.00
190.0842	$C_8H_{14}O_5$	0.04	0.04	-2.39	2.16
191.0794	$C_7H_{13}O_5N$	0.04	0.01	-2.13	0.00
191.0947	$C_{11}H_{13}O_2N$	0.02	0.02	-2.56	0.00
192.0423	$C_{10}H_8O_4$	0.06	0.04	-0.77	1.06
192.0787	$C_{11}H_{12}O_3$	0.02	0.03	-1.14	0.77
194.0944	$C_{11}H_{14}O_3$	0.00	0.00	-4.96	2.40
195.0896	$C_{10}H_{13}O_3N$	0.02	0.02	-3.40	0.00
195.1049	$C_{14}H_{13}N$	0.02	0.02	-3.21	0.00
196.0736	$C_{10}H_{12}O_4$	0.01	0.01	-1.15	0.75
196.1100	$C_{11}H_{16}O_3$	0.03	0.02	-2.93	2.31
197.0688	$C_9H_{11}O_4N$	0.02	0.02	-2.73	0.00
197.1205	$C_{14}H_{15}N$	0.03	0.01	-2.26	0.00

199.0998	$C_{13}H_{13}ON$	0.03	0.05	-2.53	0.90
207.0896	$C_{11}H_{13}O_3N$	0.02	0.02	-2.92	0.00
208.0736	$C_{11}H_{12}O_4$	0.01	0.00	-1.38	1.53
208.1100	$C_{12}H_{16}O_3$	0.05	0.03	-2.26	2.15
209.1053	$C_{11}H_{15}O_3N$	0.01	0.02	-2.85	0.00
210.0893	$C_{11}H_{14}O_4$	0.00	0.00	-3.99	2.52
211.0957	$C_9H_{13}O_3N_3$	0.03	0.01	-3.48	0.00
212.0685	$C_{10}H_{12}O_5$	0.00	0.00	-2.97	1.77
213.1366	$C_{11}H_{19}O_3N$	0.02	0.02	-2.72	0.00
216.1151	$C_{14}H_{16}O_2$	0.04	0.03	-3.58	1.15
217.0951	$C_9H_{15}O_5N$	0.04	0.01	-2.59	0.00
217.1216	$C_{12}H_{15}ON_3$	0.02	0.02	-3.12	0.00
219.0743	$C_8H_{13}O_6N$	0.03	0.01	-2.71	0.89
220.1100	$C_{13}H_{16}O_3$	0.03	0.03	-3.26	2.37
221.1012	$C_7H_{15}O_5N_3$	0.02	0.02	-3.21	0.00
225.1002	$C_{11}H_{15}O_4N$	0.03	0.01	-2.60	0.00
225.1366	$C_{12}H_{19}O_3N$	0.03	0.01	-2.27	0.55
227.0794	$C_{10}H_{13}O_5N$	0.02	0.02	-2.50	0.00
228.1151	$C_{15}H_{16}O_2$	0.05	0.03	-2.71	1.89
228.2091	$C_{14}H_{28}O_2$	0.03	0.01	-3.47	0.00
232.1464	$C_{15}H_{20}O_2$	0.02	0.02	-3.48	0.00
233.1264	$C_{10}H_{19}O_5N$	0.02	0.02	-2.88	0.00
234.1104	$C_{10}H_{18}O_6$	0.01	0.01	2.20	1.79
235.1056	$C_9H_{17}O_6N$	0.02	0.02	-2.89	0.00
235.1362	$C_{17}H_{17}N$	0.04	0.01	-2.16	0.00
239.1370	$C_9H_{21}O_6N$	0.02	0.02	-3.31	0.00
241.1315	$C_{12}H_{19}O_4N$	0.02	0.02	-2.91	0.00
242.2247	$C_{15}H_{30}O_2$	0.02	0.02	-3.78	0.00
243.1471	$C_{12}H_{21}O_4N$	0.02	0.02	-3.24	0.00
253.2043	$C_{15}H_{27}O_2N$	0.02	0.02	-2.34	0.00
254.1155	$C_{13}H_{18}O_5$	0.00	0.00	-2.48	1.99
254.1366	$C_{10}H_{22}O_7$	0.05	0.02	-2.54	0.77
256.0583	$C_{11}H_{12}O_7$	0.01	0.00	2.61	1.79
256.2404	$C_{16}H_{32}O_2$	0.02	0.04	-5.60	1.18
258.1621	$C_{17}H_{22}O_2$	0.03	0.02	2.29	2.10
259.1421	$C_{12}H_{21}O_5N$	0.02	0.02	-2.56	0.00
261.1213	$C_{11}H_{19}O_6N$	0.03	0.05	-2.40	1.38
268.1676	$C_{15}H_{24}O_4$	0.01	0.00	1.86	1.51
269.1628	$C_{14}H_{23}O_4N$	0.02	0.02	-2.85	0.00
270.0740	$C_{12}H_{14}O_7$	0.05	0.01	2.13	1.87
272.2353	$C_{16}H_{32}O_3$	0.01	0.02	-3.50	0.00
284.0897	$C_{13}H_{16}O_7$	0.05	0.03	1.49	1.63
284.1777	$C_{19}H_{24}O_2$	0.03	0.03	1.45	1.73

	286.1934	$C_{19}H_{26}O_2$	0.03	0.02	2.70	2.45
	288.1727	$C_{18}H_{24}O_3$	0.06	0.04	1.40	1.84
	298.1053	$C_{14}H_{18}O_7$	0.04	0.04	1.62	1.69
	299.2462	$C_{17}H_{33}O_3N$	0.04	0.01	-2.66	0.00
	299.2826	$C_{18}H_{37}O_2N$	0.03	0.01	-1.77	0.00
	300.2666	$C_{18}H_{36}O_3$	0.03	0.06	-3.48	1.00
	303.2047	$C_{15}H_{29}O_5N$	0.03	0.01	-3.20	0.00
	303.2411	$C_{16}H_{33}O_4N$	0.04	0.01	-3.51	0.00
	306.2560	$C_{20}H_{34}O_2$	0.02	0.02	1.11	1.86
	310.2145	$C_{18}H_{30}O_4$	0.01	0.02	-3.24	0.00
	312.2091	$C_{21}H_{28}O_2$	0.00	0.00	2.90	1.67
	314.2247	$C_{21}H_{30}O_2$	0.03	0.01	2.41	2.65
	314.2459	$C_{18}H_{34}O_4$	0.05	0.05	-3.17	1.04
	316.1887	$C_{16}H_{28}O_6$	0.00	0.00	2.07	0.66
	318.2196	$C_{20}H_{30}O_3$	0.03	0.03	1.56	0.77
	320.2353	$C_{20}H_{32}O_3$	0.03	0.05	1.65	2.16
	328.2251	$C_{18}H_{32}O_5$	0.04	0.01	-2.85	0.00
	330.2196	$C_{21}H_{30}O_3$	0.00	0.00	4.67	1.69
	332.2353	$C_{21}H_{32}O_3$	0.01	0.00	2.65	2.72
	333.2153	$C_{16}H_{31}O_6N$	0.00	0.00	2.74	0.57
	356.1836	$C_{18}H_{28}O_7$	0.01	0.00	3.44	1.81
	362.2459	$C_{22}H_{34}O_4$	0.02	0.01	2.37	2.13
Straw open burning	178.0266	$C_9H_6O_4$	0.02	0.01	-0.03	0.24
	181.1103	$C_{10}H_{15}O_2N$	0.05	0.04	-0.09	1.17
	190.1206	$C_9H_{18}O_4$	0.07	0.03	1.12	2.48
	224.1413	$C_{13}H_{20}O_3$	0.01	0.00	2.80	0.50
	232.1100	$C_{14}H_{16}O_3$	0.02	0.01	0.65	0.22
	238.1206	$C_{13}H_{18}O_4$	0.01	0.01	1.87	0.40
	272.1625	$C_{14}H_{24}O_5$	0.04	0.05	2.60	1.82
	283.1056	$C_{13}H_{17}O_6N$	0.03	0.02	1.82	1.09
	340.2615	$C_{20}H_{36}O_4$	0.03	0.04	2.20	0.47
Cow dung open burning	114.1045	$C_7H_{14}O$	0.04	0.04	1.47	1.16
	116.1202	$C_7H_{16}O$	0.00	0.00	2.59	0.73
	137.0841	$C_8H_{11}ON$	0.02	0.02	2.16	0.96
	139.0634	$C_7H_9O_2N$	0.03	0.02	1.46	0.94
	139.0998	$C_8H_{13}ON$	0.02	0.02	1.93	0.91
	141.0790	$C_7H_{11}O_2N$	0.02	0.02	1.62	0.60
	141.1154	$C_8H_{15}ON$	0.04	0.04	1.55	1.23
	143.1311	$C_8H_{17}ON$	0.06	0.05	1.58	1.37
	149.0841	$C_9H_{11}ON$	0.02	0.01	2.77	1.62
	153.0790	$C_8H_{11}O_2N$	0.04	0.04	1.94	1.04
	153.1154	$C_9H_{15}ON$	0.03	0.04	1.80	0.95
	158.1672	$C_{10}H_{22}O$	0.02	0.02	2.70	1.74

165.0790	$C_9H_{11}O_2N$	0.00	0.00	3.06	0.87
165.1154	$C_{10}H_{15}ON$	0.00	0.00	3.27	0.89
167.0947	$C_9H_{13}O_2N$	0.02	0.02	1.92	0.82
167.1311	$C_{10}H_{17}ON$	0.02	0.01	2.70	1.45
175.0634	$C_{10}H_9O_2N$	0.06	0.05	2.16	1.71
175.0998	$C_{11}H_{13}ON$	0.06	0.05	2.49	2.08
176.0685	$C_7H_{12}O_5$	0.02	0.01	-4.33	1.96
177.0790	$C_{10}H_{11}O_2N$	0.02	0.01	2.87	1.60
177.1154	$C_{11}H_{15}ON$	0.02	0.01	3.22	2.02
179.0947	$C_{10}H_{13}O_2N$	0.02	0.01	3.03	1.74
179.1311	$C_{11}H_{17}ON$	0.01	0.01	2.42	0.90
181.0852	$C_8H_{11}O_2N_3$	0.02	0.01	2.90	1.50
181.1103	$C_{10}H_{15}O_2N$	0.03	0.03	2.08	0.95
182.0427	$C_5H_{10}O_7$	0.07	0.04	2.37	2.22
185.0688	$C_8H_{11}O_4N$	0.04	0.04	2.28	1.15
185.1053	$C_9H_{15}O_3N$	0.01	0.02	2.53	0.93
189.0790	$C_{11}H_{11}O_2N$	0.04	0.03	1.34	1.47
189.1154	$C_{12}H_{15}ON$	0.02	0.01	3.18	1.80
193.1103	$C_{11}H_{15}O_2N$	0.04	0.04	1.65	0.89
194.0579	$C_{10}H_{10}O_4$	0.02	0.01	-4.79	0.00
194.1672	$C_{13}H_{22}O$	0.06	0.05	2.53	2.05
195.1624	$C_{12}H_{21}ON$	0.02	0.01	2.21	1.18
197.1781	$C_{12}H_{23}ON$	0.02	0.02	2.11	1.34
199.0845	$C_9H_{13}O_4N$	0.00	0.00	2.17	0.71
199.0998	$C_{13}H_{13}ON$	0.05	0.04	1.21	1.48
201.0638	$C_8H_{11}O_5N$	0.06	0.05	1.65	1.63
201.1154	$C_{13}H_{15}ON$	0.06	0.05	2.33	1.97
207.0896	$C_{11}H_{13}O_3N$	0.02	0.02	1.89	0.57
207.1260	$C_{12}H_{17}O_2N$	0.00	0.00	3.74	0.93
208.1676	$C_{10}H_{24}O_4$	0.06	0.05	2.87	2.27
209.1053	$C_{11}H_{15}O_3N$	0.03	0.03	1.64	0.70
209.1264	$C_8H_{19}O_5N$	0.03	0.03	1.88	1.46
210.0893	$C_{11}H_{14}O_4$	0.03	0.04	-0.13	0.88
213.1366	$C_{11}H_{19}O_3N$	0.03	0.02	2.08	1.02
223.1421	$C_9H_{21}O_5N$	0.00	0.00	2.71	0.70
225.1114	$C_{10}H_{15}O_3N_3$	0.06	0.05	1.98	1.59
225.2094	$C_{14}H_{27}ON$	0.06	0.05	2.01	1.60
227.0794	$C_{10}H_{13}O_5N$	0.02	0.03	1.80	0.37
227.1158	$C_{11}H_{17}O_4N$	0.00	0.00	2.82	0.57
233.1053	$C_{13}H_{15}O_3N$	0.02	0.01	2.86	1.43
236.0897	$C_9H_{16}O_7$	0.02	0.02	-3.31	0.00
237.1002	$C_{12}H_{15}O_4N$	0.02	0.02	0.90	0.55
238.1206	$C_{13}H_{18}O_4$	0.02	0.02	-4.82	0.00

241.0699	$C_9H_{11}O_5N_3$	0.06	0.05	1.68	1.48
241.2407	$C_{15}H_{31}ON$	0.02	0.01	2.69	1.48
243.1471	$C_{12}H_{21}O_4N$	0.02	0.02	2.23	0.78
245.0900	$C_{10}H_{15}O_6N$	0.00	0.00	1.57	0.51
245.1264	$C_{11}H_{19}O_5N$	0.02	0.03	2.04	0.58
246.1104	$C_{11}H_{18}O_6$	0.01	0.02	3.12	0.76
246.1216	$C_{10}H_{18}O_5N_2$	0.01	0.01	-4.77	0.00
246.1468	$C_{12}H_{22}O_5$	0.01	0.01	1.87	0.73
247.1421	$C_{11}H_{21}O_5N$	0.04	0.04	0.87	0.57
253.0951	$C_{12}H_{15}O_5N$	0.02	0.02	1.77	1.12
255.1260	$C_{16}H_{17}O_2N$	0.02	0.01	2.93	1.54
259.1421	$C_{12}H_{21}O_5N$	0.02	0.03	2.13	0.57
266.2247	$C_{17}H_{30}O_2$	0.02	0.01	2.01	1.53
267.2200	$C_{16}H_{29}O_2N$	0.06	0.05	1.73	1.39
268.0947	$C_{13}H_{16}O_6$	0.05	0.03	-2.41	1.14
268.2404	$C_{17}H_{32}O_2$	0.02	0.03	2.10	0.66
269.1628	$C_{14}H_{23}O_4N$	0.01	0.02	2.34	0.80
269.2356	$C_{16}H_{31}O_2N$	0.04	0.04	1.75	1.31
269.2720	$C_{17}H_{35}ON$	0.02	0.01	2.60	1.50
273.1213	$C_{12}H_{19}O_6N$	0.00	0.00	2.50	0.64
280.1887	$C_{13}H_{28}O_6$	0.06	0.05	2.38	2.04
283.1632	$C_{11}H_{25}O_7N$	0.02	0.02	2.38	1.34
284.2717	$C_{18}H_{36}O_2$	0.01	0.01	2.42	0.96
285.1213	$C_{13}H_{19}O_6N$	0.02	0.01	2.45	1.31
285.1577	$C_{14}H_{23}O_5N$	0.00	0.00	3.05	0.70
285.2669	$C_{17}H_{35}O_2N$	0.06	0.05	1.99	1.60
286.2510	$C_{17}H_{34}O_3$	0.03	0.02	1.71	1.68
287.1734	$C_{14}H_{25}O_5N$	0.01	0.02	2.36	0.59
289.1526	$C_{13}H_{23}O_6N$	0.02	0.01	2.39	1.27
293.2469	$C_{17}H_{31}ON_3$	0.06	0.05	1.55	1.31
295.2149	$C_{17}H_{29}O_3N$	0.03	0.03	1.85	1.25
295.2877	$C_{19}H_{37}ON$	0.02	0.01	2.15	1.16
296.2717	$C_{19}H_{36}O_2$	0.01	0.02	1.65	0.38
297.1577	$C_{15}H_{23}O_5N$	0.02	0.01	2.74	1.51
299.2098	$C_{16}H_{29}O_4N$	0.06	0.05	1.78	1.52
300.2666	$C_{18}H_{36}O_3$	0.00	0.00	2.39	0.66
301.1468	$C_{21}H_{19}ON$	0.00	0.00	2.94	0.53
301.2254	$C_{16}H_{31}O_4N$	0.06	0.05	2.60	2.18
302.2823	$C_{18}H_{38}O_3$	0.06	0.05	2.45	1.91
303.1431	$C_{12}H_{21}O_6N_3$	0.06	0.05	1.87	1.48
304.2278	$C_{19}H_{30}O_2N$	0.06	0.05	2.67	2.08
307.2625	$C_{18}H_{33}ON_3$	0.02	0.01	2.36	1.19
310.2145	$C_{18}H_{30}O_4$	0.04	0.03	1.42	1.65

311.2938	$C_{18}H_{37}ON_3$	0.02	0.01	2.04	1.08
312.2666	$C_{19}H_{36}O_3$	0.01	0.01	1.88	0.39
312.3394	$C_{21}H_{44}O$	0.02	0.01	2.45	1.23
316.1887	$C_{16}H_{28}O_6$	0.04	0.03	-1.11	2.11
316.2251	$C_{17}H_{32}O_5$	0.00	0.00	3.52	0.47
322.2874	$C_{21}H_{38}O_2$	0.03	0.03	1.80	1.25
325.2983	$C_{20}H_{39}O_2N$	0.02	0.01	2.13	1.19
336.1574	$C_{18}H_{24}O_6$	0.06	0.05	1.87	1.59
336.1938	$C_{19}H_{28}O_5$	0.02	0.01	2.81	1.48
337.2254	$C_{19}H_{31}O_4N$	0.06	0.05	1.87	1.46
338.2823	$C_{21}H_{38}O_3$	0.03	0.02	2.22	1.36
338.3187	$C_{22}H_{42}O_2$	0.03	0.02	2.50	1.48
339.2676	$C_{22}H_{33}N_3$	0.06	0.05	1.61	1.38
340.2615	$C_{20}H_{36}O_4$	0.06	0.04	0.28	1.65
340.2979	$C_{21}H_{40}O_3$	0.02	0.01	2.79	1.56
340.3343	$C_{22}H_{44}O_2$	0.01	0.01	2.57	0.21
341.2469	$C_{21}H_{31}ON_3$	0.06	0.05	1.72	1.36
341.2932	$C_{20}H_{39}O_3N$	0.02	0.01	2.24	1.16
347.2309	$C_{17}H_{33}O_6N$	0.06	0.05	1.66	1.31
352.3343	$C_{23}H_{44}O_2$	0.05	0.04	1.25	1.34
354.2772	$C_{21}H_{38}O_4$	0.04	0.05	2.09	1.31
354.3136	$C_{22}H_{42}O_3$	0.06	0.05	1.62	1.45
354.3500	$C_{23}H_{46}O_2$	0.06	0.05	1.72	1.68
366.3500	$C_{24}H_{46}O_2$	0.06	0.05	1.95	1.55
368.3293	$C_{23}H_{44}O_3$	0.03	0.02	2.15	1.24
376.2463	$C_{19}H_{36}O_7$	0.02	0.01	2.55	1.42
382.3813	$C_{25}H_{50}O_2$	0.06	0.05	1.61	1.30
384.2262	$C_{19}H_{32}O_6N_2$	0.05	0.02	1.20	1.30
386.3034	$C_{22}H_{42}O_5$	0.06	0.05	1.84	1.47
394.3449	$C_{25}H_{46}O_3$	0.04	0.03	1.21	1.16
396.3242	$C_{24}H_{44}O_4$	0.03	0.03	1.98	1.20

Table S3. The fragment ions from AMS with p-value smaller than 0.1 during pairwise comparisons and their fold changes in 5 types of burning.

Burning types	*m/z*	Formula	p_mean	p_std	log_2FC_mean	log_2FC_std
Beech logs stove burning	16.0313	C	0.05	0.04	0.70	0.42
	24.0000	C_2	0.04	0.05	-0.11	0.23
	30.0106	CH_2O	0.03	0.03	-0.03	0.34
	30.0344	CH_4ON	0.03	0.02	-1.83	0.72
	42.0344	C_2H_4ON	0.02	0.02	-0.42	0.68
	43.0422	C_2H_5ON	0.04	0.03	-0.11	0.99
	51.0235	C_4H_3	0.03	0.03	0.35	0.21
	52.0313	C_4H_4	0.03	0.03	0.38	0.24

	53.0027	C_3HO	0.05	0.03	0.45	0.46
	54.0344	C_3H_4ON	0.04	0.05	-0.60	0.74
	55.0422	C_3H_5ON	0.01	0.00	-0.42	0.92
	55.9898	C_2O_2	0.06	0.05	-0.28	0.37
	56.0501	C_3H_6ON	0.05	0.04	-0.78	0.87
	57.0579	C_3H_7ON	0.01	0.01	-0.03	0.49
	59.0497	C_3H_7O	0.01	0.01	-0.46	0.19
	63.9949	C_4O	0.01	0.01	0.24	0.14
	64.0313	C_5H_4	0.03	0.03	0.45	0.31
	66.0106	C_4H_2O	0.02	0.02	0.72	0.43
	67.0184	C_4H_3O	0.03	0.01	0.69	0.48
	68.0501	C_4H_6ON	0.08	0.02	-1.58	0.71
	70.0055	$C_3H_2O_2$	0.05	0.04	-0.30	0.28
	71.0735	C_4H_9ON	0.03	0.03	-0.01	0.51
	77.0027	C_5HO	0.05	0.05	0.67	0.36
	79.0184	C_5H_3O	0.04	0.02	0.69	0.71
	89.0392	C_7H_5	0.04	0.03	0.32	0.28
	91.0031	$C_2H_3O_4$	0.05	0.04	0.55	0.39
	92.9977	C_5HO_2	0.01	0.00	0.24	0.19
	93.0341	C_6H_5O	0.06	0.03	0.74	1.11
	97.0654	C_6H_9O	0.01	0.01	-1.15	0.78
	99.0685	C_5H_9ON	0.04	0.04	-0.14	0.32
	101.0239	$C_4H_5O_3$	0.04	0.04	-0.21	0.44
	102.0106	C_7H_2O	0.02	0.04	0.69	0.08
	102.0470	C_8H_6	0.01	0.02	0.45	0.23
	106.0419	C_7H_6O	0.06	0.01	0.44	0.80
	108.0211	$C_6H_4O_2$	0.06	0.03	0.51	0.68
	111.0810	$C_7H_{11}O$	0.03	0.03	-1.16	0.67
	111.1175	C_8H_{15}	0.06	0.04	-0.40	0.71
Spruce and pine burning	15.9949	O	0.01	0.01	0.71	0.15
	24.0000	C_2	0.00	0.00	0.74	0.18
	25.0078	C_2H	0.02	0.02	-0.13	0.03
	26.0031	CN	0.00	0.00	-1.28	0.47
	26.0157	C_2H_2	0.00	0.00	0.41	0.14
	27.0109	CHON	0.03	0.02	-0.70	0.50
	27.9949	CO	0.01	0.01	0.64	0.18
	30.0106	CH_2O	0.00	0.00	0.95	0.22
	33.0335	CH_5O	0.00	0.00	0.87	0.12
	36.0000	C_3	0.00	0.00	1.18	0.15
	39.0109	C_2HON	0.00	0.00	-6.03	0.45
	39.9949	C_2O	0.03	0.04	1.26	0.79
	41.9980	CON	0.00	0.00	-2.49	0.12
	42.0344	C_2H_4ON	0.00	0.00	-2.38	0.69

43.0058	$CHON$	0.00	0.00	-4.00	0.37
43.0422	C_2H_5ON	0.00	0.00	-4.33	0.37
43.9898	CO_2	0.01	0.01	0.89	0.18
44.0262	C_2H_4O	0.01	0.01	0.86	0.20
44.0626	C_3H_8	0.01	0.01	-1.24	0.19
46.0055	CH_2O_2	0.00	0.01	-0.37	0.02
47.0133	CH_3O_2	0.00	0.00	0.84	0.21
48.0000	C_4	0.00	0.00	0.53	0.16
48.0211	CH_4O_2	0.00	0.00	0.26	0.06
49.0290	CH_5O_2	0.02	0.02	0.24	0.09
51.0109	C_3HON	0.00	0.00	-1.83	0.34
52.0061	C_2N_2	0.02	0.01	-0.67	0.10
52.0187	C_3H_2ON	0.02	0.00	-1.43	0.55
53.0266	C_3H_3ON	0.00	0.00	-1.57	0.52
53.0392	C_4H_5	0.01	0.01	-0.22	0.11
53.9980	C_2ON	0.00	0.00	-1.20	0.05
54.0344	C_3H_4ON	0.00	0.00	-2.39	0.61
55.0184	C_3H_3O	0.04	0.04	0.31	0.16
55.0184	C_3H_3O	0.00	0.01	-0.28	0.03
55.0422	C_3H_5ON	0.00	0.00	-3.26	0.70
55.9898	C_2O_2	0.00	0.00	0.97	0.26
56.0136	C_2H_2ON	0.00	0.00	-1.76	0.12
56.0262	C_3H_4O	0.00	0.00	0.98	0.19
56.0501	C_3H_6ON	0.00	0.01	-2.25	0.49
56.0626	C_4H_8	0.06	0.02	-0.15	0.08
56.9977	C_2HO_2	0.03	0.04	0.22	0.08
56.9977	C_2HO_2	0.00	0.00	-0.17	0.02
57.0215	C_2H_3ON	0.00	0.00	-2.85	0.43
57.0341	C_3H_5O	0.00	0.00	0.75	0.20
57.0579	C_3H_7ON	0.00	0.00	-3.39	0.66
58.0055	$C_2H_2O_2$	0.00	0.00	1.30	0.29
59.0007	CHO_2N	0.01	0.01	-0.40	0.09
60.0000	C_5	0.02	0.02	-1.09	0.01
60.0086	CH_2O_2N	0.01	0.02	-1.86	0.29
60.0211	$C_2H_4O_2$	0.01	0.01	0.82	0.22
60.0450	C_2H_6ON	0.01	0.01	1.32	0.62
60.9926	CHO_3	0.01	0.01	-0.61	0.07
61.0164	CH_3O_2N	0.00	0.00	-1.90	0.20
61.0290	$C_2H_5O_2$	0.00	0.00	0.60	0.16
62.0004	CH_2O_3	0.00	0.00	-0.44	0.01
63.0235	C_5H_3	0.00	0.00	-0.35	0.18
63.0320	CH_5O_2N	0.00	0.00	-1.46	0.42
64.0187	C_4H_2ON	0.00	0.00	-1.06	0.22

64.0313	C_5H_4	0.01	0.02	-0.38	0.16
65.0027	C_4HO	0.00	0.00	-0.68	0.10
65.0392	C_5H_5	0.00	0.00	-0.47	0.12
66.0470	C_5H_6	0.00	0.00	-0.52	0.11
67.0058	C_3HON	0.00	0.00	-1.14	0.17
67.0296	$C_3H_3N_2$	0.01	0.01	-1.88	0.07
68.0136	C_3H_2ON	0.00	0.00	-0.98	0.18
70.0055	$C_3H_2O_2$	0.00	0.00	0.90	0.23
70.0419	C_4H_6O	0.00	0.00	0.63	0.18
70.0657	C_4H_8ON	0.01	0.02	-1.72	0.50
71.0007	C_2HO_2N	0.00	0.00	-1.26	0.17
71.0133	$C_3H_3O_2$	0.00	0.00	1.01	0.21
71.0371	C_3H_5ON	0.00	0.00	-1.35	0.21
71.0497	C_4H_7O	0.02	0.04	0.59	0.12
71.0735	C_4H_9ON	0.00	0.00	-3.23	0.14
72.0211	$C_3H_4O_2$	0.00	0.00	1.33	0.25
72.0450	C_3H_6ON	0.01	0.01	-1.13	0.19
72.0814	$C_4H_{10}ON$	0.00	0.00	-0.60	0.10
73.0290	$C_3H_5O_2$	0.00	0.00	0.69	0.18
73.0892	$C_4H_{11}ON$	0.00	0.00	-0.85	0.08
74.0368	$C_3H_6O_2$	0.00	0.00	0.53	0.20
74.0606	C_3H_8ON	0.00	0.00	0.32	0.15
75.0082	$C_2H_3O_3$	0.01	0.00	-0.52	0.18
75.9949	C_5O	0.00	0.00	-0.28	0.02
77.0027	C_5HO	0.01	0.02	-0.81	0.23
77.0392	C_6H_5	0.03	0.03	-0.24	0.20
77.0603	$C_3H_9O_2$	0.00	0.00	-1.08	0.58
78.0106	C_5H_2O	0.00	0.00	-0.85	0.15
79.0422	C_5H_5ON	0.00	0.00	0.98	0.64
80.9977	C_4HO_2	0.00	0.00	-0.55	0.08
81.0453	$C_4H_5N_2$	0.00	0.01	-1.98	0.12
82.0531	$C_4H_6N_2$	0.00	0.00	-2.01	0.16
83.0133	$C_4H_3O_2$	0.00	0.00	0.86	0.24
84.0450	C_4H_6ON	0.01	0.01	-0.69	0.22
84.0814	$C_5H_{10}ON$	0.00	0.00	-1.01	0.21
85.0528	C_4H_7ON	0.00	0.00	-1.19	0.33
85.0654	C_5H_9O	0.00	0.00	1.59	0.31
85.0892	$C_5H_{11}ON$	0.01	0.01	-1.97	0.22
86.0116	$C_2H_2O_2N$	0.01	0.01	-0.96	0.44
86.0157	C_7H_2	0.00	0.00	1.76	0.29
86.0732	$C_5H_{10}O$	0.00	0.00	-2.45	0.07
87.9796	C_2O_4	0.03	0.01	-0.04	0.02
89.0027	C_6HO	0.01	0.01	-0.15	0.02

89.0113	$C_2H_3O_3N$	0.03	0.04	-0.75	0.06
89.0239	$C_3H_5O_3$	0.00	0.00	1.67	0.24
89.0392	C_7H_5	0.05	0.05	-0.25	0.16
89.0603	$C_4H_9O_2$	0.07	0.02	-0.59	0.34
90.0470	C_7H_6	0.01	0.01	-0.39	0.14
91.0395	$C_3H_7O_3$	0.00	0.00	1.87	0.52
92.0110	$C_2H_4O_4$	0.00	0.00	-0.98	0.11
92.0348	$C_2H_6O_3N$	0.01	0.01	-1.56	0.12
92.0474	$C_3H_8O_3$	0.01	0.02	0.77	0.35
93.0552	$C_3H_9O_3$	0.00	0.00	0.83	0.54
94.0055	$C_5H_2O_2$	0.01	0.01	-0.44	0.05
94.0266	$C_2H_6O_4$	0.01	0.02	0.83	0.16
95.0610	$C_5H_7N_2$	0.01	0.01	-1.36	0.15
96.0000	C_8	0.02	0.02	-0.34	0.00
96.0211	$C_5H_4O_2$	0.01	0.01	0.84	0.24
96.0324	C_4H_4ON	0.01	0.01	-1.49	0.02
97.0078	C_8H	0.00	0.00	-0.46	0.16
97.0290	$C_5H_5O_2$	0.01	0.01	0.80	0.21
97.0402	C_4H_5ON	0.00	0.00	-1.46	0.26
98.0004	$C_4H_2O_3$	0.00	0.01	-0.47	0.07
98.0368	$C_5H_6O_2$	0.00	0.00	0.73	0.21
99.0235	C_8H_3	0.02	0.02	0.42	0.20
99.0446	$C_5H_7O_2$	0.02	0.04	0.61	0.17
99.0685	C_5H_9ON	0.03	0.05	-0.60	0.24
99.0810	$C_6H_{11}O$	0.01	0.01	0.65	0.24
100.0161	$C_4H_4O_3$	0.02	0.01	0.30	0.15
100.0399	$C_4H_6O_2N$	0.01	0.01	-1.09	0.23
100.0637	C_4H_8ON	0.01	0.01	-0.59	0.21
100.1253	C_7H_{16}	0.00	0.00	-0.09	0.03
101.0239	$C_4H_5O_3$	0.00	0.00	0.96	0.22
101.0392	C_8H_5	0.00	0.01	0.78	0.19
101.0477	$C_4H_7O_2N$	0.00	0.00	-2.16	0.39
102.0106	C_7H_2O	0.00	0.00	-0.77	0.05
102.0317	$C_4H_6O_3$	0.00	0.00	1.53	0.21
102.0470	C_8H_6	0.00	0.00	-0.43	0.17
103.0184	C_7H_3O	0.01	0.01	-0.61	0.14
103.0548	C_8H_7	0.01	0.01	-0.29	0.20
104.0348	$C_3H_6O_3N$	0.02	0.01	-0.98	0.12
105.0188	$C_3H_5O_4$	0.00	0.00	-1.20	0.25
105.0552	$C_4H_9O_3$	0.00	0.00	1.16	0.62
106.0055	$C_6H_2O_2$	0.00	0.00	-0.25	0.02
108.0000	C_9	0.02	0.03	-0.22	0.08
108.0576	C_7H_8O	0.04	0.02	-0.36	0.22

	109.0078	C_9H	0.00	0.00	-0.47	0.09
	109.0528	C_6H_7ON	0.00	0.00	-1.29	0.15
	110.0606	C_6H_8ON	0.00	0.00	-1.66	0.25
	111.0685	C_6H_9ON	0.00	0.00	-1.48	0.27
	111.1175	C_8H_{15}	0.03	0.05	-1.36	0.27
	112.0161	$C_5H_4O_3$	0.00	0.00	0.81	0.25
	112.0637	C_5H_8ON	0.00	0.00	-0.95	0.05
	113.0239	$C_5H_5O_3$	0.02	0.01	0.49	0.21
	113.0967	$C_7H_{13}O$	0.01	0.01	0.41	0.19
	113.1331	C_8H_{17}	0.02	0.03	-0.90	0.48
	114.0317	$C_5H_6O_3$	0.00	0.00	0.75	0.17
	114.0470	C_9H_6	0.01	0.01	-0.45	0.20
	114.1409	C_8H_{18}	0.00	0.00	-0.13	0.03
	115.0031	$C_4H_3O_4$	0.00	0.00	-0.62	0.03
	115.0395	$C_5H_7O_3$	0.00	0.00	2.93	0.19
	115.0760	$C_6H_{11}O_2$	0.01	0.01	-1.23	0.71
	116.0110	$C_4H_4O_4$	0.00	0.00	-0.37	0.07
	116.0474	$C_5H_8O_3$	0.00	0.00	1.81	0.46
	116.0586	$C_4H_8O_2N$	0.00	0.00	2.20	0.55
	116.0626	C_9H_8	0.00	0.00	-0.85	0.40
	117.0552	$C_5H_9O_3$	0.00	0.00	1.76	0.36
	117.9902	$C_3H_2O_5$	0.00	0.00	-0.09	0.03
	118.0419	C_8H_6O	0.00	0.00	1.44	0.31
	118.0630	$C_5H_{10}O_3$	0.00	0.00	-1.79	0.19
	118.0743	$C_4H_{10}O_2N$	0.00	0.00	2.26	0.41
	118.9980	$C_3H_3O_5$	0.02	0.03	0.10	0.07
	119.0709	$C_5H_{11}O_3$	0.00	0.00	0.94	0.51
	120.0576	C_8H_8O	0.03	0.04	-0.90	0.31
Straw open burning	36.0000	C_3	0.02	0.04	-2.42	0.36
	58.0419	C_3H_6O	0.02	0.03	0.35	0.24
	58.0657	C_3H_8ON	0.05	0.04	0.84	0.78
	59.0735	C_3H_9ON	0.07	0.02	0.50	0.63
	100.0525	$C_5H_8O_2$	0.06	0.03	0.61	0.86
	120.0576	C_8H_8O	0.04	0.04	0.81	0.47
Cow dung open burning	13.0078	CH	0.01	0.02	-1.06	0.45
	15.0235	CH_3	0.02	0.03	-1.01	0.42
	15.9949	O	0.01	0.02	-0.98	0.26
	17.0027	HO	0.01	0.02	-1.28	0.39
	18.0106	H_2O	0.01	0.02	-1.35	0.41
	27.9949	CO	0.03	0.04	-1.21	0.49
	29.0392	C_2H_5	0.03	0.05	0.48	0.17
	30.0470	C_2H_6	0.03	0.04	-1.15	0.64
	41.0027	C_2HO	0.04	0.04	-1.13	0.69

41.0266	C_2H_3N	0.04	0.04	1.86	0.64
43.0184	C_2H_3O	0.03	0.02	-0.76	0.47
43.9898	CO_2	0.01	0.02	-1.36	0.42
51.9949	C_3O	0.06	0.04	-0.49	0.36
53.0027	C_3HO	0.03	0.02	-0.67	0.39
59.0371	C_2H_5ON	0.06	0.02	1.73	1.34
64.0187	C_4H_2ON	0.06	0.05	0.95	0.69
68.9977	C_3HO_2	0.04	0.01	-1.43	1.11
70.0657	C_4H_8ON	0.01	0.01	1.47	0.58
72.0450	C_3H_6ON	0.03	0.03	1.32	0.71
72.0814	$C_4H_{10}ON$	0.02	0.03	0.85	0.41
80.0501	C_5H_6ON	0.02	0.01	1.43	0.74
83.0133	$C_4H_3O_2$	0.03	0.05	-1.37	0.61
85.0290	$C_4H_5O_2$	0.03	0.03	-1.29	0.72
86.0606	C_4H_8ON	0.05	0.03	0.41	0.41
86.0970	$C_5H_{12}ON$	0.03	0.04	0.75	0.48
92.0110	$C_2H_4O_4$	0.03	0.04	-0.21	0.25
92.0626	C_7H_8	0.04	0.04	0.62	0.41
93.0705	C_7H_9	0.03	0.04	0.63	0.30
100.0889	$C_6H_{12}O$	0.03	0.00	0.36	0.27
103.9898	C_6O_2	0.04	0.04	0.13	0.08
105.0341	C_7H_5O	0.04	0.04	-1.59	0.85
105.0705	C_8H_9	0.02	0.01	0.54	0.24
106.0783	C_8H_{10}	0.03	0.04	0.72	0.38
107.0861	C_8H_{11}	0.03	0.04	0.71	0.36
108.0211	$C_6H_4O_2$	0.03	0.02	-0.79	0.42
111.0810	$C_7H_{11}O$	0.02	0.01	0.79	0.54
112.0763	$C_6H_{10}ON$	0.04	0.02	0.49	0.36
115.0031	$C_4H_3O_4$	0.02	0.02	-0.07	0.32
116.0110	$C_4H_4O_4$	0.03	0.04	0.07	0.04
119.0861	C_9H_{11}	0.01	0.01	0.61	0.20
120.0940	C_9H_{12}	0.04	0.04	0.60	0.32