Supporting information for: Characterization of gas-phase organics using proton transfer reaction time-of-flight mass spectrometry: residential coal combustion

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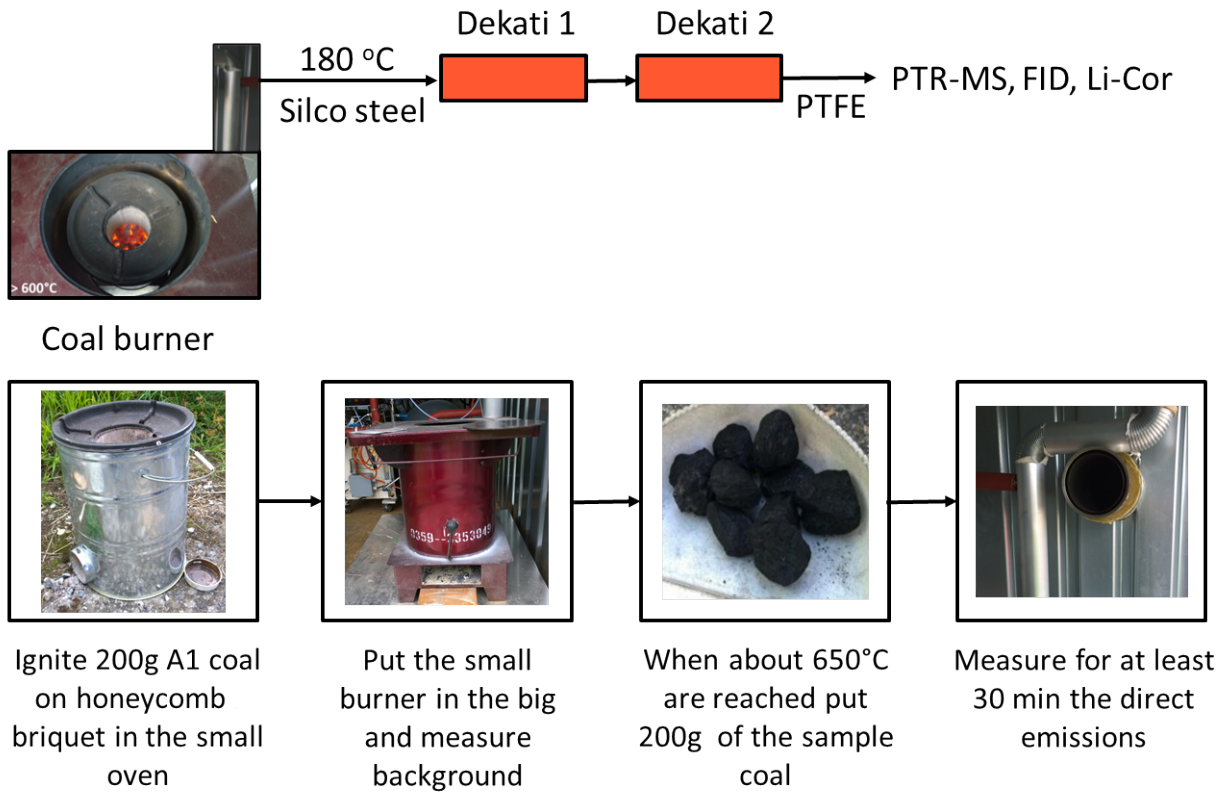

Figure S1: Experimental setup and coal burning procedure.

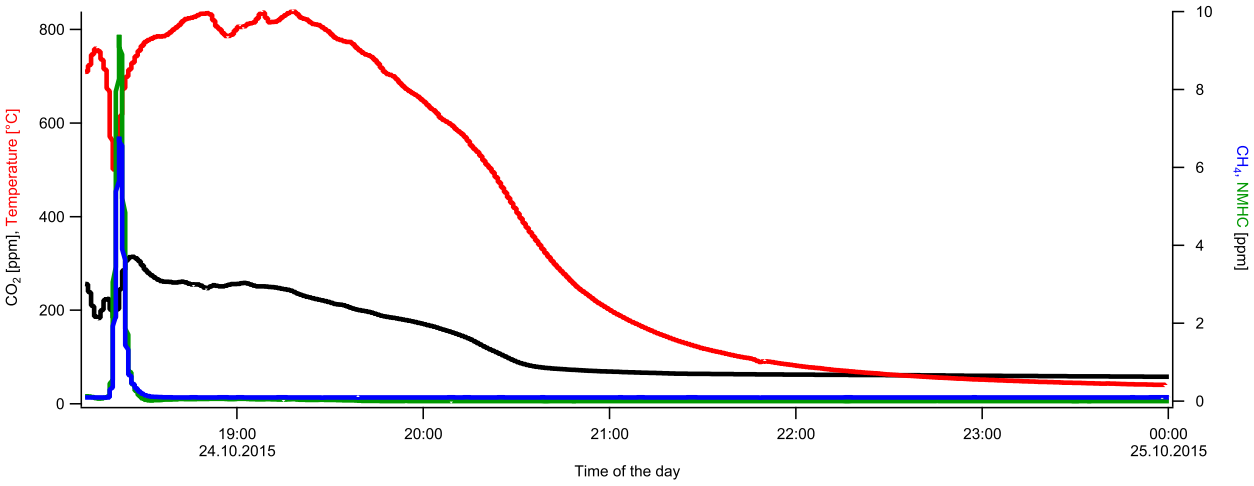

Figure S2: Time series of an overnight coal burning experiment (B2) for methane (CH_4), total non methane hydrocarbons (NMHC), carbon dioxide (CO_2) and the temperature in the combustion chamber. All concentrations after 100 times dilution.

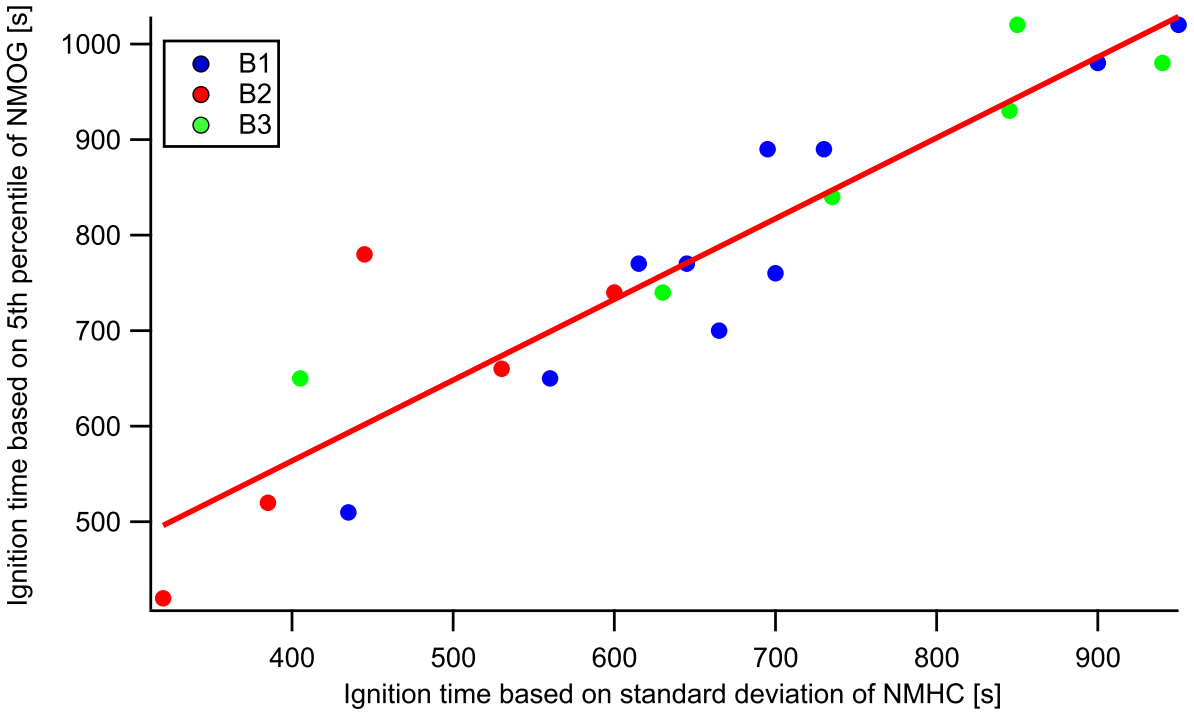

Figure S3: Correlation of two different methods to estimate the time until ignition either taking the time until the NMOG concentration reaches 5% of the peak value or taking the time until the concentration of NMHC reaches a concentration of less than ten times the standard deviation.

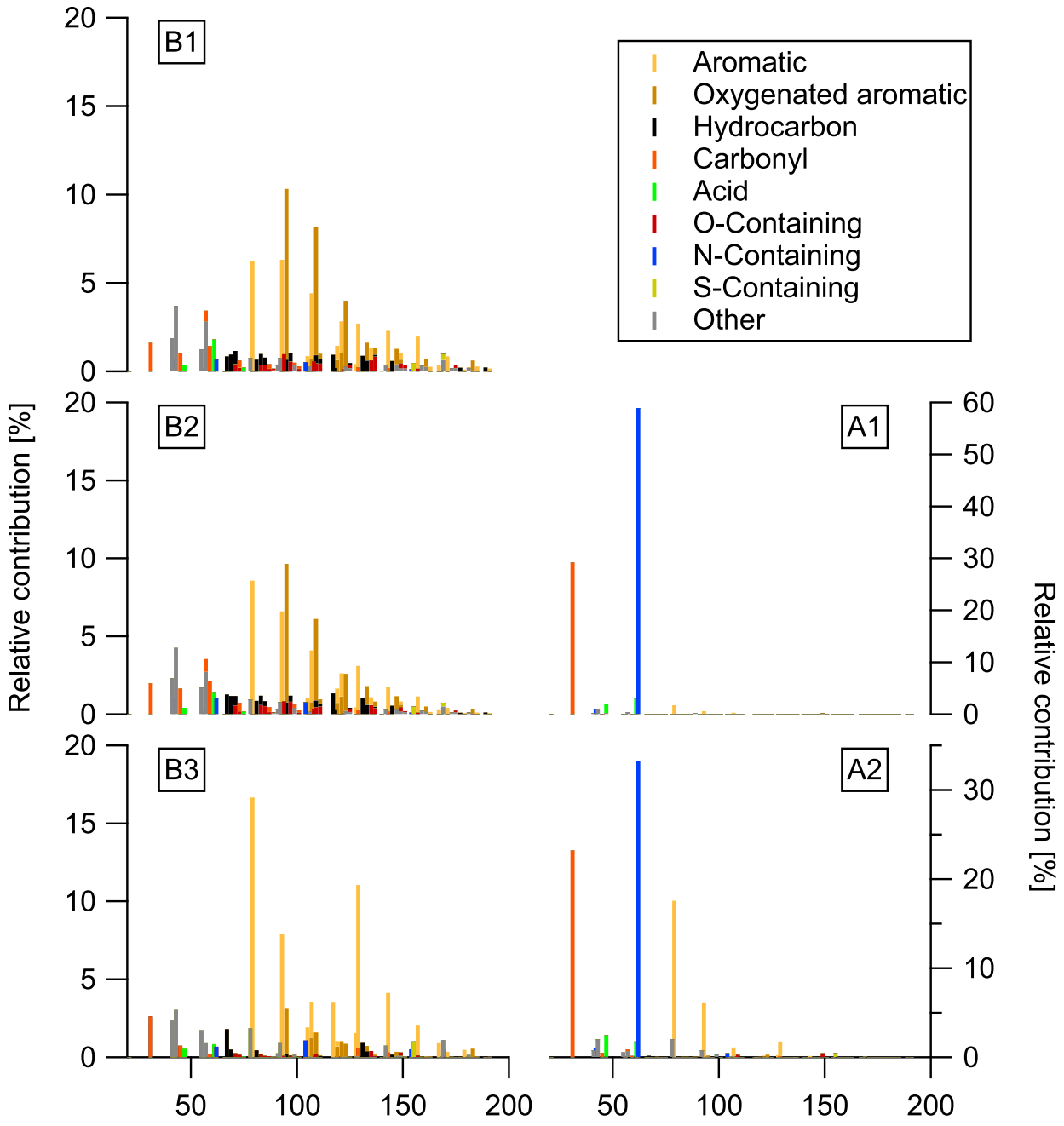

Figure S4: Transmission and reaction rate corrected, normalized raw spectra as measured with the PTR-ToF-MS from three bituminous (B) and two anthracite (A) coals. These are average spectra from all experiments listed in Table S1.

Table S1: List of experiments with estimated time till ignition and starting phase temperature.

Date	Coal	Time till ignition [s]	Starting temperature [$°C$]
14.10.2015	A2		
16.10.2015	A1		
16.10.2015	A2		
17.10.2015	A1		
01.10.2015	B1	890	540
02.10.2015	B1	770	625
04.10.2015	B1	700	740
06.10.2015	B2	520	734
07.10.2015	B2	420	675
08.10.2015	B2	780	690
09.10.2015	B3	650	720
10.10.2015	B3	930	700
12.10.2015	B3	980	740
13.10.2015	B3	1020	730
17.10.2015	B1	510	650
19.10.2015	B1	1020	400
20.10.2015	B1	650	740
21.10.2015	B1	760	680
22.10.2015	B1	1280	540
23.10.2015	B2	740	710
24.10.2015	B1	770	710
24.10.2015	B2	660	775
25.10.2015	B1	980	630
25.10.2015	B3	840	700
26.10.2015	B1	890	600
26.10.2015	B3	740	700

Table S2: Exact m/z, family, and k rates of all fitted ions.

Ion	m/z	Family	k ($10^{-9}\, cm^3 s^{-1}$)
H_3O^+	21.0218	None	2
CH_3O^+	31.0178	Carbonyl	2
$C_3H_5^+$	41.0386	Other	2
$C_2H_2O^+$	42.01	Other	2
$C_2H_4N^+$	42.0338	N-Containing	3.82

Table S2: Continued: Exact m/z, family, and k rates of all fitted ions.

Ion	m/z	Family	k ($10^{-9}\,cm^3s^{-1}$)
$C_3H_6^+$	42.0464	Other	2
$C_2H_3O^+$	43.0178	Other	2
$C_3H_7^+$	43.0542	Other	2
CH_2NO^+	44.0131	N-containing	2
$C_2H_5O^+$	45.0335	Carbonyl	3.02
CH_4NO^+	46.0287	N-Containing	2
$CH_3O_2^+$	47.0128	Acid	1.89
$H_3N_2O^+$	47.024	Other	2
$C_3H_5O^+$	57.0335	Carbonyl	3.43
$C_4H_9^+$	57.0699	Other	2
$C_3H_7O^+$	59.0491	Carbonyl	3.1
$C_2H_6NO^+$	60.0444	N-containing	2
$C_2H_5O_2^+$	61.0284	Acid	2.11
$CH_4NO_2^+$	62.0237	N-containing	2
$C_5H_7^+$	67.0542	Other	2
$C_4H_5O^+$	69.0335	O-Containing	1.69
$C_5H_9^+$	69.0699	Other	2
$C_4H_7O^+$	71.0491	O-Containing	3.16
$C_5H_{11}^+$	71.0855	Other	2
$C_3H_6NO^+$	72.0444	N-containing	2
$C_3H_5O_2^+$	73.0284	Carbonyl	2
$C_4H_9O^+$	73.0648	Carbonyl	3.09
$C_3H_7O_2^+$	75.0441	O-Containing	2.24
$C_6H_6^+$	78.0464	Other	2

Table S2: Continued: Exact m/z, family, and k rates of all fitted ions.

Ion	m/z	Family	k ($10^{-9}\,cm^3s^{-1}$)
$C_6H_7^+$	79.0542	Aromatic	1.93
$C_6H_9^+$	81.0699	Other	2
$C_5H_7O^+$	83.0491	O-Containing	2
$C_6H_{11}^+$	83.0855	Other	2
$C_4H_5O_2^+$	85.0284	O-Containing	2
$C_5H_9O^+$	85.0648	O-Containing	2
$C_6H_{13}^+$	85.1012	Other	2
$C_4H_7O_2^+$	87.0441	O-Containing	1.07
$C_5H_{11}O^+$	87.0804	O-Containing	2
$C_2H_5N_2O_2^+$	89.0346	N-containing	2
$C_4H_9O_2^+$	89.0597	O-Containing	4.15
$C_7H_7^+$	91.0542	Other	2
$C_7H_8^+$	92.0621	Other	2
$C_7H_9^+$	93.0699	Aromatic	2.08
$C_6H_6O^+$	94.0413	O-Containing	2
$C_6H_7O^+$	95.0491	Oxy Aromatic	2.13
$C_7H_{11}^+$	95.0855	Other	2
$C_5H_5O_2^+$	97.0284	O-Containing	3.88
$C_6H_9O^+$	97.0648	O-Containing	2
$C_7H_{13}^+$	97.1012	Other	2
$C_4H_3O_3^+$	99.0077	O-Containing	2
$C_5H_7O_2^+$	99.0441	O-Containing	2
$C_6H_{11}O^+$	99.0804	O-Containing	2
$C_7H_{15}^+$	99.1168	Other	2

Table S2: Continued: Exact m/z, family, and k rates of all fitted ions.

Ion	m/z	Family	k ($10^{-9}\,cm^3s^{-1}$)
$C_4H_6NO_2^+$	100.039	N-containing	2
$C_5H_{10}NO^+$	100.076	N-containing	2
$C_4H_5O_3^+$	101.023	O-Containing	2
$C_5H_9O_2^+$	101.06	O-Containing	2
$C_6H_{13}O^+$	101.096	O-Containing	2
$C_7H_5N^+$	103.042	N-Containing	2
$C_5H_{11}O_2^+$	103.075	Acid	2
$C_7H_6N^+$	104.049	N-Containing	2
$C_7H_5O^+$	105.033	O-Containing	2
$C_8H_9^+$	105.07	Aromatic	2.27
$C_8H_{10}^+$	106.078	Other	2
$C_7H_7O^+$	107.048	Oxy Aromatic	3.63
$C_8H_{11}^+$	107.086	Aromatic	2.26
$C_7H_8O^+$	108.057	Oxy Aromatic	2
$C_6H_5O_2^+$	109.028	Carbonyl	2
$C_7H_9O^+$	109.065	Oxy Aromatic	2.27
$C_6H_7O_2^+$	111.044	Oxy Aromatic	2
$C_7H_{11}O^+$	111.08	O-Containing	2
$C_8H_{15}^+$	111.117	Other	2
$C_5H_5O_3^+$	113.023	Acid	2
$C_7H_{13}O^+$	113.096	O-Containing	2
$C_8H_5N^+$	115.042	N-Containing	2
$C_6H_{11}O_2^+$	115.075	O-Containing	2
$C_7H_{15}O^+$	115.112	Carbonyl	2.74

Table S2: Continued: Exact m/z, family, and k rates of all fitted ions.

Ion	m/z	Family	k ($10^{-9}\,cm^3s^{-1}$)
$C_6H_3N_3^+$	117.032	N-Containing	2
$C_8H_7N^+$	117.057	N-Containing	2
$C_9H_9^+$	117.07	Aromatic	2.24
$C_6H_{13}O_2^+$	117.091	O-Containing	2
$C_8H_8N^+$	118.065	N-Containing	2
$C_8H_7O^+$	119.049	Oxy Aromatic	2
$C_9H_{11}^+$	119.086	Aromatic	2
$C_9H_{12}^+$	120.093	Other	2
$C_8H_9O^+$	121.065	Oxy Aromatic	3.23
$C_9H_{13}^+$	121.101	Aromatic	2.41
$C_7H_7O_2^+$	123.044	Oxy Aromatic	2
$C_8H_{11}O^+$	123.08	Oxy Aromatic	2
$C_9H_5N^+$	127.042	N-Containing	2
$C_7H_{11}O_2^+$	127.075	O-Containing	2
$C_5H_{19}OS^+$	127.115	S-Containing	2
$C_{10}H_8^+$	128.062	Aromatic	2
$C_9H_7N^+$	129.057	N-Containing	2
$C_{10}H_9^+$	129.07	Aromatic	2.45
$C_7H_{13}O_2^+$	129.091	O-Containing	2
$C_8H_{17}O^+$	129.127	Carbonyl	2
$C_9H_7O^+$	131.049	O-Containing	2
$C_{10}H_{11}^+$	131.086	Aromatic	2
$C_9H_9O^+$	133.065	Oxy Aromatic	2
$C_{10}H_{13}^+$	133.101	Aromatic	2

Table S2: Continued: Exact m/z, family, and k rates of all fitted ions.

Ion	m/z	Family	k ($10^{-9}\,cm^3s^{-1}$)
$C_8H_7S^+$	135.026	S-Containing	2
$C_{10}H_{15}{}^+$	135.117	Aromatic	2
$C_8H_{10}NO^+$	136.076	Other	2
$C_8H_9O_2{}^+$	137.06	Oxy Aromatic	2
$C_9H_{13}O^+$	137.096	O-Containing	2
$C_7H_7O_3{}^+$	139.039	O-Containing	2
$C_8H_{11}O_2{}^+$	139.075	O-Containing	2
$C_7H_9O_3{}^+$	141.055	O-Containing	2
$C_8H_{13}O_2{}^+$	141.091	O-Containing	2
$C_9H_{17}O^+$	141.127	O-Containing	2
$C_{11}H_{10}{}^+$	142.078	O-Containing	2
$C_{11}H_{11}{}^+$	143.086	Aromatic	2.71
$C_8H_{15}O_2{}^+$	143.107	O-Containing	2
$C_9H_{19}O^+$	143.143	Carbonyl	2
$C_{11}H_{13}{}^+$	145.101	Aromatic	2
$C_9H_7O_2{}^+$	147.044	Oxy Aromatic	2
$C_8H_9N_3{}^+$	147.079	N-Containing	2
$C_{11}H_{15}{}^+$	147.117	Other	2
$C_8H_5O_3{}^+$	149.023	Oxy Aromatic	2
$C_6H_{13}O_4{}^+$	149.081	O-Containing	2
$C_{11}H_{17}{}^+$	149.132	Other	2
$C_9H_{11}O_2{}^+$	151.075	O-Containing	2
$C_{10}H_{15}O^+$	151.112	O-Containing	2
$C_{12}H_9{}^+$	153.07	Aromatic	2.86

Table S2: Continued: Exact m/z, family, and k rates of all fitted ions.

Ion	m/z	Family	k ($10^{-9}\,cm^3s^{-1}$)
$C_8H_{15}N_3^+$	153.126	N-Containing	2
$C_{11}H_8N^+$	154.065	N-Containing	2
$C_{12}H_{11}^+$	155.086	Aromatic	2.81
$C_{10}H_{19}O^+$	155.143	O-Containing	2
$C_{11}H_9O^+$	157.065	O-Containing	2
$C_{12}H_{13}^+$	157.101	Aromatic	2
$C_{10}H_7O_2^+$	159.044	Oxy Aromatic	2
$C_9H_9N_3^+$	159.079	N-Containing	2
$C_{12}H_{15}^+$	159.117	Other	2
$C_6H_5N_6^+$	161.057	N-Containing	2
$C_{11}H_{13}O^+$	161.096	O-Containing	2
$C_9H_{21}S^+$	161.136	S-Containing	2
$C_{10}H_{11}S^+$	163.058	S-Containing	2
$C_9H_{11}N_2O^+$	163.087	N-containing	2
$C_{12}H_{19}^+$	163.148	Other	2
$C_{13}H_{11}^+$	167.086	Aromatic	2.88
$C_{12}H_{10}N^+$	168.081	N-Containing	2
$C_{12}H_9O^+$	169.065	Oxy Aromatic	2
$C_7H_{21}S_2^+$	169.108	S-Containing	2
$C_{13}H_{15}^+$	171.117	Aromatic	2
$C_{11}H_9O_2^+$	173.06	O-Containing	2
$C_5H_{19}NO_5^+$	173.126	N-containing	2
$C_7H_{15}N_2O_3^+$	175.108	N-containing	2
$C_{13}H_{19}^+$	175.148	Other	2

Table S2: Continued: Exact m/z, family, and k rates of all fitted ions.

Ion	m/z	Family	k ($10^{-9}\,cm^3 s^{-1}$)
$C_{13}H_7N^+$	177.057	N-Containing	2
$C_7H_{15}NO_4^+$	177.1	N-containing	2
$C_{13}H_{21}^+$	177.164	Other	2
$C_{14}H_{11}^+$	179.086	Aromatic	3.09
$C_{12}H_{21}N^+$	179.167	N-Containing	2
$C_{13}H_{10}N^+$	180.081	N-Containing	2
$C_{13}H_9O^+$	181.065	Oxy Aromatic	2
$C_{14}H_{13}^+$	181.101	Aromatic	2
$C_{13}H_{11}O^+$	183.08	Oxy Aromatic	2
$C_{12}H_9S^+$	185.042	S-Containing	2
$C_{11}H_{21}S^+$	185.136	S-Containing	2
$C_{15}H_9^+$	189.07	Other	2
$C_{14}H_{21}^+$	189.164	Other	2
$C_{15}H_{13}^+$	193.101	Other	2
$C_{10}H_{15}NO_3^+$	197.105	N-containing	2
$C_{13}H_{11}S^+$	199.058	S-Containing	2
$C_{10}H_{19}N_2O_2^+$	199.144	N-containing	2
$C_{16}H_{11}^+$	203.086	Other	3.37
$C_{15}H_{25}^+$	205.195	Other	2
$C_{14}H_9O_2^+$	209.06	O-Containing	2
$C_{18}H_{13}^+$	229.101	Other	2
$C_{17}H_{11}O^+$	231.08	O-Containing	2
$C_{20}H_{13}^+$	253.101	Other	2

Table S3: NMOG emission factors from burning different coals in $mg\,kg_{coal}^{-1}$.

Coal	Aromatics	O-Aromatics	Carbonyls	Acids	O-Cont	N-Cont	Hydrocarb	S-Cont	Other	Total
B1	2119 ± 791	2136 ± 1142	360 ± 115	138 ± 45	510 ± 364	99 ± 19	711 ± 487	57 ± 34	1079 ± 646	7209 ± 3643
B2	940 ± 360	766 ± 421	251 ± 94	60 ± 22	220 ± 104	80 ± 21	354 ± 159	26 ± 20	522 ± 212	3219 ± 1413
B3	4012 ± 821	815 ± 220	406 ± 114	112 ± 45	169 ± 61	217 ± 47	668 ± 190	115 ± 49	1086 ± 285	7600 ± 1634
A1	3 ± 2	<1	29 ± 18	5 ± 2	<1	60 ± 21	<1	<1	3 ± 0	100 ± 43
A2	65 ± 70	2 ± 1	46 ± 26	8 ± 6	2 ± 1	60 ± 24	1 ± 0	1 ± 1	16 ± 13	201 ± 142