

Supporting Information for

Formation of Nitrogen-Containing Organic Aerosol during Combustion of High Sulfur Content Coal

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Detailed Procedures of Operating HPLC

10 μL sample in methanol was dissolved in 90 μL H_2O and injected onto Phenomene RP C18 column (150*2.00 mm, 4 micron) manually. The sample was then eluted and separated from this column via an Agilent 1200 HPLC (Santa Clara, CA) with a gradient operated at 200 $\mu\text{L}/\text{min}$ flow rate, and injected into a Maxis (Bruker, Bremen, Germany) quadrupole time-of-flight (QTOF) mass spectrometer via ESI. The following settings was used for the ESI-UHR-TOFMS: capillary voltage was 3.8 kV; pressure of nebulizer gas was 1.0 bar; drying gas flow rate and temperature were 8.0 L/min and 200 $^{\circ}\text{C}$, respectively. The following settings were used for the HPLC: Solvent A was water containing 0.1% formic acid, and solvent B was 80% acetonitrile, 20% water containing 0.1% formic acid. The gradient settings were 2–15% solvent B in 15 min, 15–20% solvent B in 10 min, 20–25% solvent B in 10 min, 25–50% solvent B in 10 min, 50–80% solvent B in 15 min, 80–90% solvent B in 5 min, and isocratic flow at 100% solvent B for 2 min and then returned to 2% solvent B in 13 min.

Supplementary Table and Figures

Table S1. Identified Organic Compounds of the Methanol Extract from Submicrometer Particles Collected from the Combustion of PRB Coal Mixing with 4% Elemental Sulfur (by HPLC/ESI(+)/UHR-TOFMS, the total ion chromatographs for this sample and its corresponding filter blank are shown in Fig. S5)

Retention Time (min)	Major Peaks (m/z)	Calculated Ion Formula	Exact Mass of Calculated Formula	Error (ppm)
1.1	110.0089	C ₂ H ₃ N ₂ O ₂ Na	110.00922	2.927
44.8	156.1022	C ₈ H ₁₄ NO ₂	156.10245	1.625
	188.1285	C ₉ H ₁₈ NO ₃	188.12867	0.895
	210.1105	C ₉ H ₁₇ NO ₃ Na	210.11061	0.528
47.6	170.1180	C ₉ H ₁₆ NO ₂	170.11810	0.61
	202.1444	C ₁₀ H ₂₀ NO ₃	202.14432	0.403
	224.1262	C ₁₀ H ₁₉ NO ₃ Na	224.12626	0.282
49.6	184.1335	C ₁₀ H ₁₈ NO ₂	184.13375	1.378
	216.1598	C ₁₁ H ₂₂ NO ₃	216.15997	0.78
	238.1417	C ₁₁ H ₂₁ NO ₃ Na	238.14191	0.895
50.9	230.1753	C ₁₂ H ₂₄ NO ₃	230.17562	1.384
	296.2586	C ₁₈ H ₃₄ NO ₂	296.25895	1.196
51.2	296.2588	C ₁₈ H ₃₄ NO ₂	296.25895	0.521
53.8	298.2744	C ₁₈ H ₃₆ NO ₂	298.27460	0.685
	316.2852	C ₁₈ H ₃₈ NO ₃	316.28517	0.098

54.1	284.2379	C ₂₀ H ₃₀ N	284.23782	0.264
54.4	310.2385	C ₁₈ H ₃₂ NO ₃	310.23822	0.584
54.8	310.2384	C ₁₈ H ₃₂ NO ₃	310.23822	0.906
55.5	380.3321	C ₂₇ H ₄₂ N	380.33173	0.985
56.3	280.2643	C ₁₈ H ₃₄ NO	280.26404	0.929
56.9	280.2641	C ₁₈ H ₃₄ NO	280.26404	0.215
57.1	280.2641	C ₁₈ H ₃₄ NO	280.26404	0.215
57.3	280.2640	C ₁₈ H ₃₄ NO	280.26404	0.142
	296.2589	C ₁₈ H ₃₄ NO ₂	296.25895	0.183
	328.2851	C ₁₉ H ₃₈ NO ₃	328.28517	0.21
	350.2671	C ₁₉ H ₃₇ NO ₃ Na	350.26711	0.039

Figure S1. Elemental ratios for fine organic particulate matter from combustion of ILL#6 coal, a high sulfur content coal.

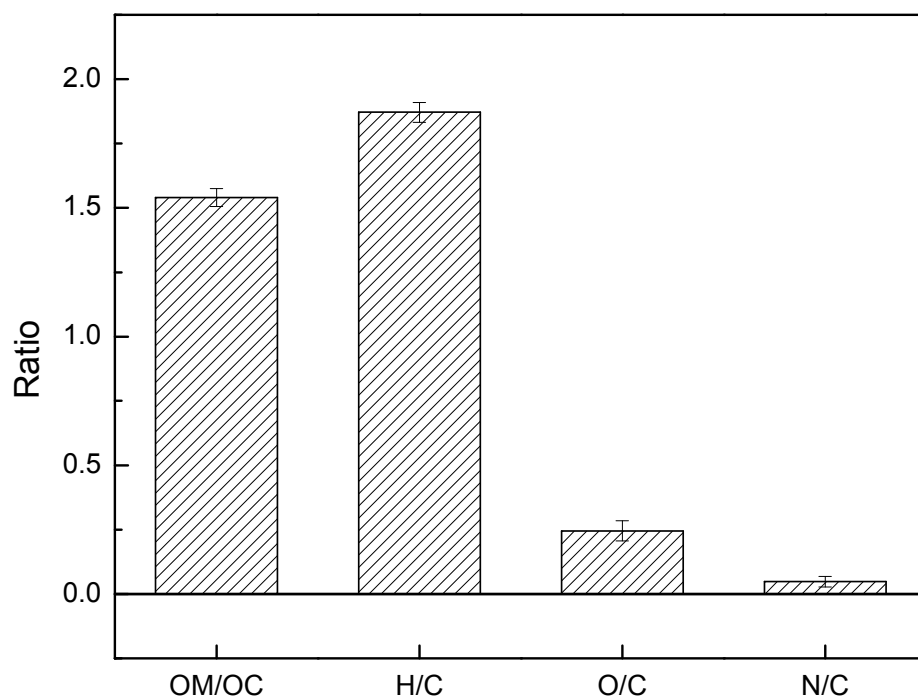


Figure S2. High resolution organic AMS spectrum of submicrometer particles from the combustion of PRB coals mixing with 4% sulfur

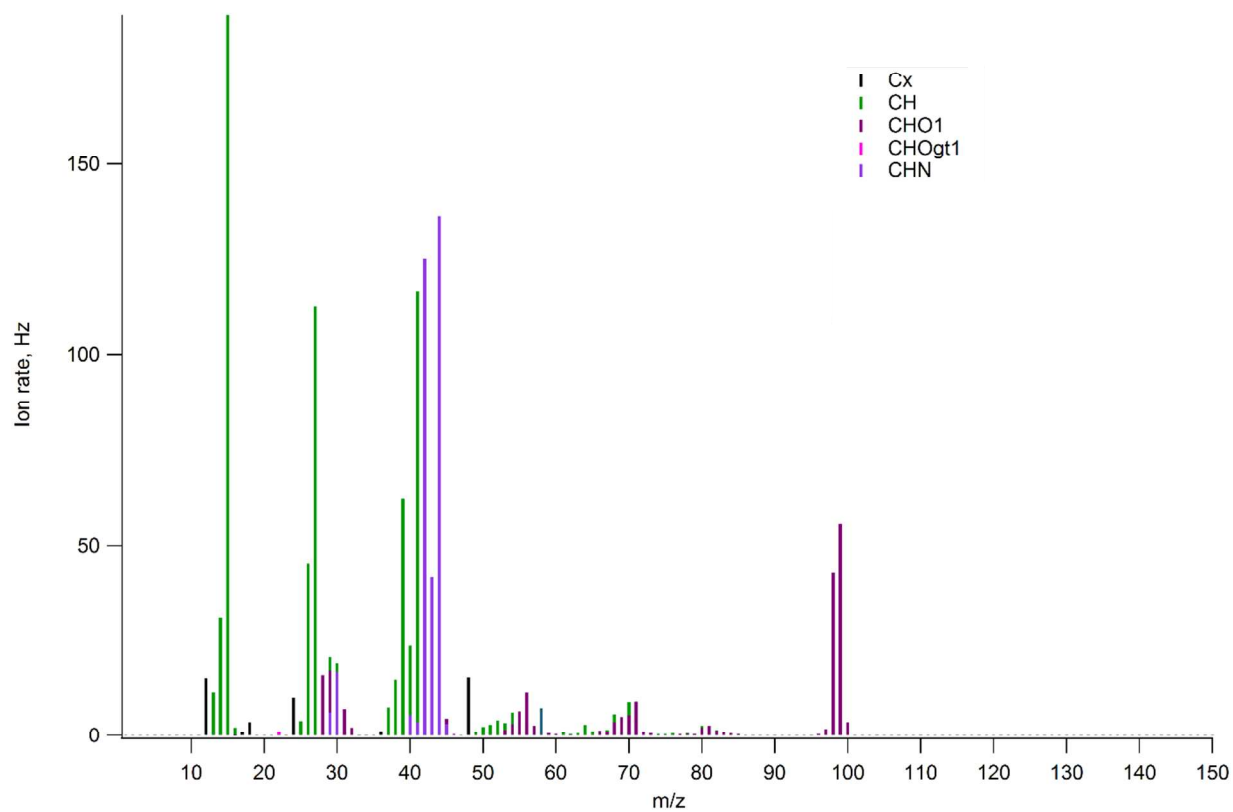
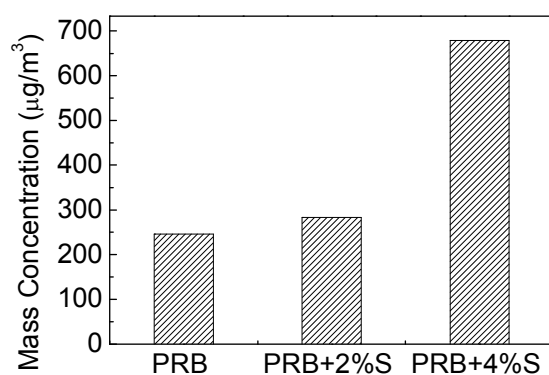
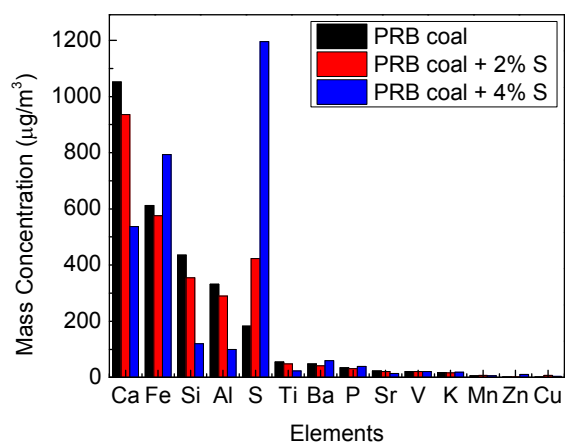


Figure S3. (A) Calculated particle mass concentrations; (B) elemental compositions; and (C) correlation of concentration between sulfur (determined by XRF) and organic matter of submicrometer particles from the combustion of PRB coals mixing with different content of sulfur (Combustion condition: temperature: 1376 K, air flow rate: 3 LPM, fuel-air equivalence ratio: 0.083)

(A)



(B)



(C)

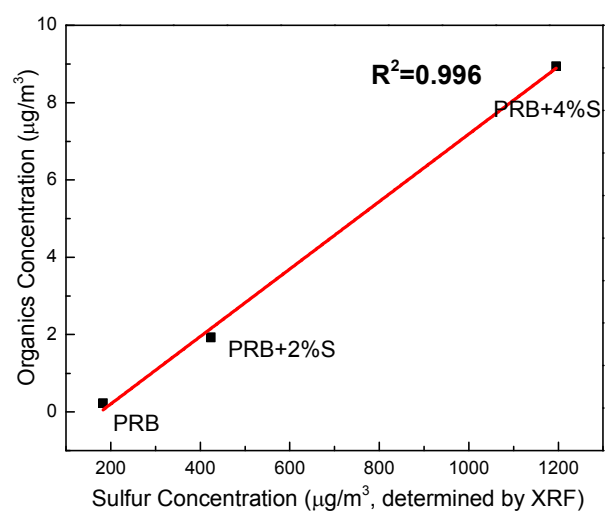


Figure S4. Total ion chromatography (LC-ESI(+)-TOFMS) of the methanol extract from (1) submicrometer particles collected from the combustion of PRB coals mixing with 4% sulfur; and (2) filter blank

