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Nitrogen-containing secondary organic aerosol formation by acrolein reaction with ammonia/ammonium

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Table S1: The top 30 ion peaks in the mass spectra for acrolein-ammonia and acrolein-ammonium residue samples. The peaks are sorted by their *m/z* values.

Top 30 ion peaks of the acrolein-ammonia residue sample			Top 30 ion peaks of the acrolein-ammonium sulfate residue sample			Top 30 ion peaks of the acrolein-ammonium chloride residue sample		
Measured *m/z*	Assigned formula	Mass accuracy (ppm)	Measured *m/z*	Assigned formula	Mass accuracy (ppm)	Measured *m/z*	Assigned formula	Mass accuracy (ppm)
111.0915	$C_6H_{11}N_2^+$	-1.6	148.0968	$C_6H_{14}O_3N^+$	-0.1	166.1074	$C_6H_{16}O_4N^+$	+0.1
112.0756	$C_6H_{10}ON^+$	-0.8	168.1018	$C_9H_{14}O_2N^+$	-0.6	168.102	$C_9H_{14}O_2N^+$	+0.6
129.1021	$C_6H_{13}ON_2^+$	-1.1	185.1283	$C_9H_{17}O_2N_2^+$	-0.8	186.1127	$C_9H_{16}O_3N^+$	+1.2
166.1338	$C_9H_{16}N_3^+$	-0.4	186.1125	$C_9H_{16}O_3N^+$	+0.2	204.1232	$C_9H_{18}O_4N^+$	+0.8
167.1175	$C_9H_{15}ON_2^+$	-2.3	187.1159	unassigned		206.118	$C_{12}H_{16}O_2N^+$	+2.2
168.1021	$C_9H_{14}O_2N^+$	+1.2	204.123	$C_9H_{18}O_4N^+$	-0.2	222.1335	$C_9H_{20}O_5N^+$	-0.4
183.1604	$C_9H_{19}N_4^+$	-0.1	206.1178	$C_{12}H_{16}O_2N^+$	+1.2	224.1286	$C_{12}H_{18}O_3N^+$	+2.1
184.1444	$C_9H_{18}ON_3^+$	-0.2	222.1334	$C_9H_{20}O_5N^+$	-0.9	241.1544	$C_{12}H_{21}O_3N_2^+$	-1.1
185.1279	$C_9H_{17}O_2N_2^+$	-3.0	224.1283	$C_{12}H_{18}O_3N^+$	+0.8	242.1394	$C_{12}H_{20}O_4N^+$	+3.0
186.1125	$C_9H_{16}O_3N^+$	+0.2	241.1545	$C_{12}H_{21}O_3N_2^+$	-0.7	243.1436	unassigned	
204.1232	$C_9H_{18}O_4N^+$	+0.8	242.1390	$C_{12}H_{20}O_4N^+$	+1.3	260.1500	$C_{12}H_{22}O_5N^+$	+2.9
210.1602	$C_{11}H_{20}ON_3^+$	+0.5	243.1428	unassigned		261.1591	$C_{15}H_{21}O_2N_2^+$	-2.5
221.1760	$C_{12}H_{21}N_4^+$	-0.3	244.1334	$C_{15}H_{18}O_2N^+$	+0.8	262.1445	$C_{15}H_{20}O_3N^+$	+2.8
222.1599	$C_{12}H_{20}ON_3^+$	-0.8	260.1496	$C_{12}H_{22}O_5N^+$	+1.3	278.1596	$C_{12}H_{24}O_6N^+$	-0.8
223.1446	$C_{12}H_{19}O_2N_2^+$	+2.2	278.1599	$C_{12}H_{24}O_6N^+$	+0.3	279.1708	$C_{15}H_{23}O_3N_2^+$	+1.7
224.1287	$C_{12}H_{18}O_3N^+$	+2.6	279.169	unassigned		280.1570	unassigned	
239.1868	$C_{12}H_{23}ON_4^+$	+0.7	280.1575	unassigned		281.1583	unassigned	
240.1724	unassigned		297.1812	$C_{15}H_{25}O_4N_2^+$	+1.1	297.1813	$C_{15}H_{25}O_4N_2^+$	+1.4

241.1551	$C_{12}H_{21}O_3N_2^+$	+1.8	298.1675	unassigned		298.1671	unassigned	
242.1390	$C_{12}H_{20}O_4N^+$	+1.3	315.192	$C_{15}H_{27}O_5N_2^+$	+1.8	315.1919	$C_{15}H_{27}O_5N_2^+$	+1.4
260.1500	$C_{12}H_{22}O_5N^+$	+2.9	316.1834	unassigned		316.1787	unassigned	
278.1865	$C_{15}H_{24}O_2N_3^+$	+0.7	333.2029	$C_{15}H_{29}O_6N_2^+$	+2.7	317.1867	$C_{18}H_{25}O_3N_2^+$	+2.3
295.2136	$C_{15}H_{27}O_2N_4^+$	+2.5	334.1903	unassigned		335.1975	$C_{18}H_{27}O_4N_2^+$	+2.9
296.1993	unassigned		335.1975	$C_{18}H_{27}O_4N_2^+$	+2.9	336.187	unassigned	
297.1862	unassigned		353.2072	$C_{18}H_{29}O_5N_2^+$	+0.3	353.2076	$C_{18}H_{29}O_5N_2^+$	+1.4
315.1922	$C_{15}H_{27}O_5N_2^+$	+2.4	354.1958	unassigned		354.1993	unassigned	
316.1999	$C_{14}H_{22}N_9^+$	+2.0	371.2182	$C_{18}H_{31}O_6N_2^+$	+1.4	371.2181	$C_{18}H_{31}O_6N_2^+$	+1.2
334.2135	$C_{18}H_{28}O_3N_3^+$	+2.9	389.2325	$C_{23}H_{33}O_5^+$	+0.6	391.2236	$C_{21}H_{31}O_5N_2^+$	+2.2
351.2396	$C_{18}H_{31}O_3N_4^+$	+1.5	409.2344	$C_{21}H_{33}O_6N_2^+$	+2.7	409.2345	$C_{21}H_{33}O_6N_2^+$	+2.9
401.2905	$C_{23}H_{37}O_2N_4^+$	-1.5	427.245	$C_{21}H_{35}O_7N_2^+$	+2.6	427.2449	$C_{21}H_{35}O_7N_2^+$	+2.4

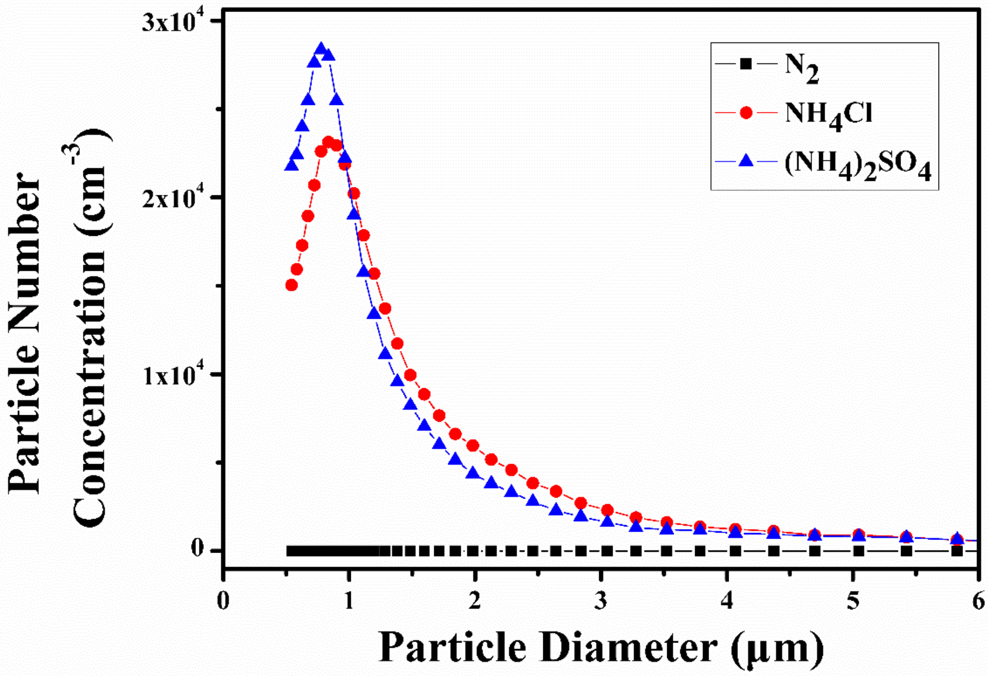

Figure S1: Size distributions of the ammonium sulfate (blue triangles) and ammonium chloride (red circles) particles we made in this work. Soon after a bag was filled with ~100L N_2 and ammonium aerosol particles (generated by the atomizer), the aerosols in the bag were directly detected by an Aerodynamic Particle Sizer (APS). The N_2 control (black squares) shows that no particles were present in the nitrogen flow used in the experiments.

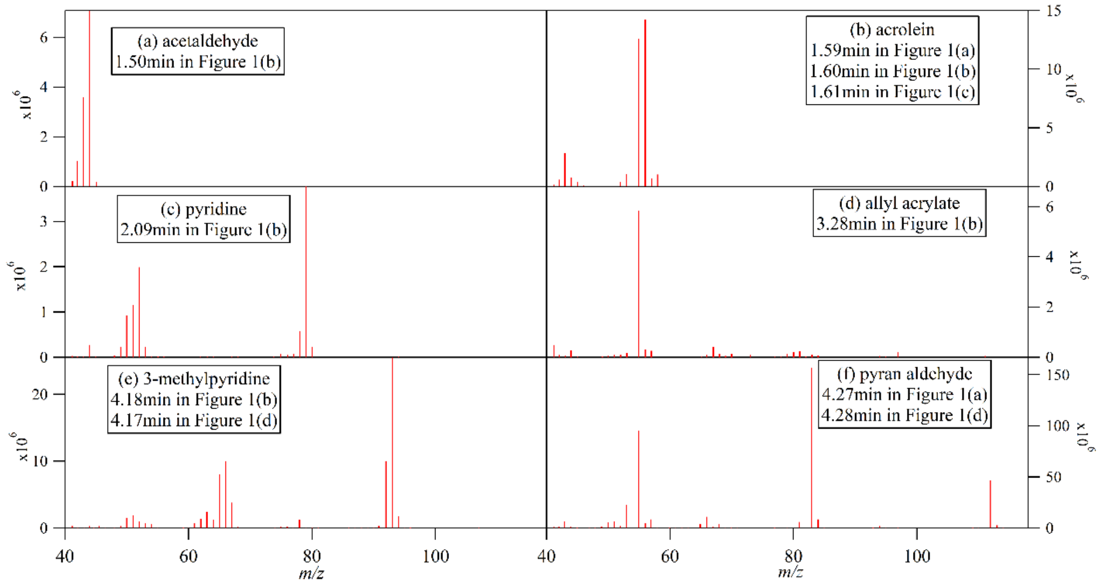

Figure S2: The observed electron impact mass spectra for the main chromatographic peaks in GC traces in Figure 1.

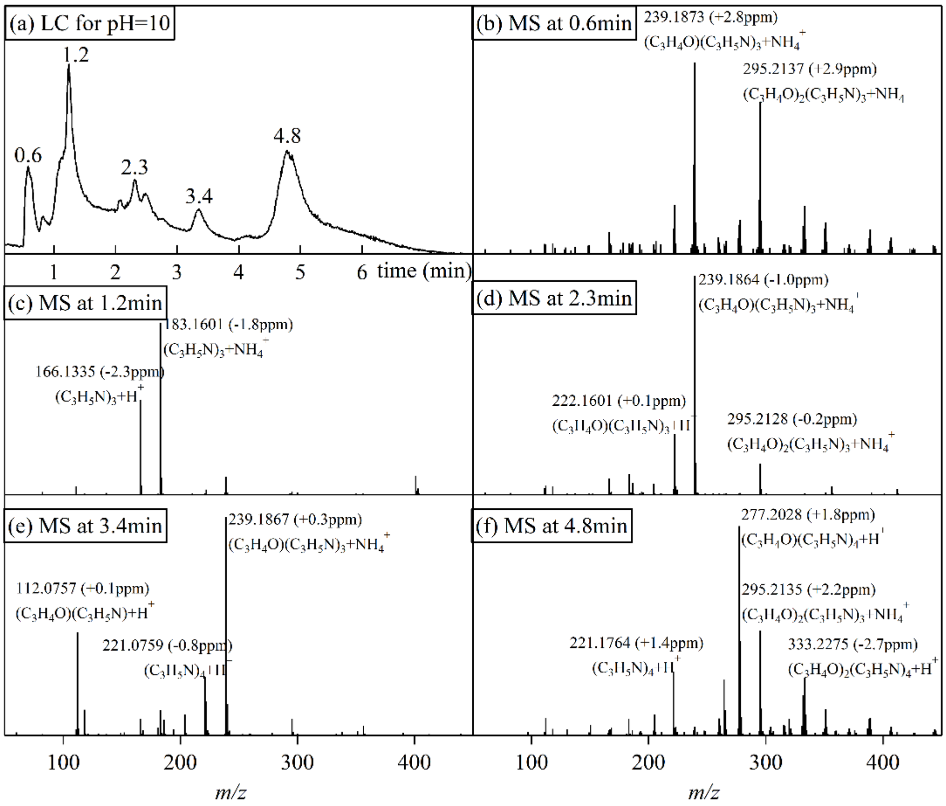

Figure S3: The UPLC HRMS results for the acrolein reaction with ammonium in the alkaline bulk solutions. (a) The UPLC traces for samples in bulk solutions with pH=10. (b-f) the mass spectra for the peaks around 0.6 min, 1.2 min, 2.3 min, 3.4 min and 4.8 min. The *m/z* values and the corresponding assigned formulae for main ions are marked. The figures in the parentheses are the fractional deviations between the detected and theoretical *m/z* of the assigned ionic formulas.

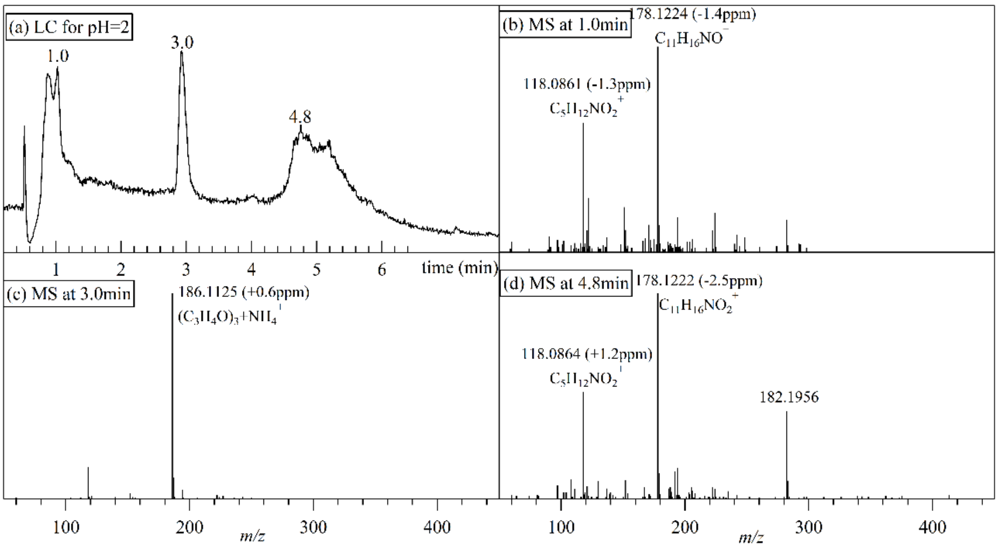

Figure S4: The UPLC ESI HR-MS results for the acrolein reaction with ammonium in the highly acidic bulk solutions. (a) the LC traces for samples in bulk solutions with pH=2. (b-d) the mass spectra for the peaks around 1.0 min, 3.0 min and 4.8 min. The *m/z* values and the corresponding assigned formulae for main ions are marked. The figures in the parentheses are the fractional deviations between the detected and theoretical *m/z* of the assigned ionic formulas.

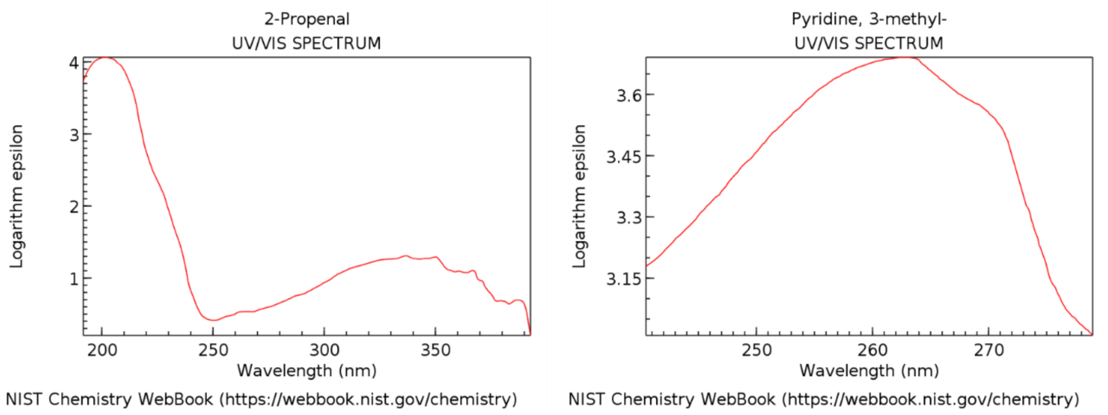

Figure S5: The reference UV/vis spectra for acrolein and 3-methylpyridine, adopted from NIST chemistry webbook (http://webbook.nist.gov/chemistry)