Supplement of Atmos. Chem. Phys., 20, 515–537, 2020
https://doi.org/10.5194/acp-20-515-2020-supplement

Atmospheric Chemistry and Physics
Open Access
EGU

Supplement of

Multi-generation OH oxidation as a source for highly oxygenated organic molecules from aromatics

Olga Garmash et al.

Correspondence to: Olga Garmash (olga.garmash@helsinki.fi) and Mikael Ehn (mikael.ehn@helsinki.fi)

Tables in Supplement present the spectra shown in Fig. 3 and 5 and lists the molecular composition as well as exact mass of the individual oxidation products as identified in CI-APi-TOF spectra. If two compounds overlapped on the same integer mass, the value was assigned to the dominant peak, while the value for the other one was set to "n/a".

Table S1. Products of benzene oxidation as identified in CI-APi-TOF spectra from the flow reactor. Data corresponds to Fig. 3a in the main text. All ions are negatively charged and include the reagent ion, NO_3^-. m/z is mass-to-charge ratio and f_{total} is fraction of total signal.

C	H	O	N	m/z, Th	$f_{total}x10^{-4}$	C	H	O	N	m/z, Th	$f_{total}x10^{-4}$
6	6	7	1	204.0150	9.4	6	6	13	1	299.9845	8.9
6	7	7	1	205.0228	3.1	6	7	13	1	300.9923	2.7
6	8	7	1	206.0306	22.5	6	8	13	1	302.0001	15.6
5	6	8	1	208.0099	3.1	12	12	9	1	314.0518	3.2
6	6	8	1	220.0099	6.3	6	6	14	1	315.9794	n/a
6	7	8	1	221.0177	0.8	12	14	9	1	316.0674	2.5
6	8	8	1	222.0255	55.9	6	7	14	1	316.9872	47.8
5	5	9	1	222.9970	5.5	6	8	14	1	317.9950	28.5
5	6	9	1	224.0048	9.2	12	12	10	1	330.0467	1.1
5	7	9	1	225.0126	1.6	6	6	15	1	331.9743	3.2
6	6	9	1	236.0048	5.4	12	14	10	1	332.0623	n/a
6	7	9	1	237.0126	1.2	6	7	15	1	332.9821	0.8
6	8	9	1	238.0205	10.2	6	8	15	1	333.9899	2.9
5	6	10	1	239.9997	38.3	12	14	11	1	348.0572	89.1
5	7	10	1	241.0075	4.9	6	8	16	1	349.9849	5.6
5	8	10	1	242.0154	7.9	11	14	12	1	352.0522	6.9
6	6	10	1	251.9997	1.4	10	12	13	1	354.0314	4.6
6	7	10	1	253.0075	2.6	12	12	12	1	362.0365	1.0
6	8	10	1	254.0154	17.8	12	14	12	1	364.0522	5.5
5	6	11	1	255.9946	91.1	11	14	13	1	368.0471	4.0
5	7	11	1	257.0025	7.5	12	12	13	1	378.0314	4.6
6	6	11	1	267.9946	4.7	12	14	13	1	380.0471	24.6
6	7	11	1	269.0025	0.7	11	14	14	1	384.0420	2.5
6	8	11	1	270.0103	68.4	12	14	14	1	396.0420	2.0
5	6	12	1	271.9896	7.4	11	12	15	1	398.0212	0.8
5	7	12	1	272.9974	3.4	11	14	15	1	400.0369	0.9
5	8	12	1	274.0052	2.8	12	12	15	1	410.0212	0.7
6	6	12	1	283.9896	2.9	12	14	15	1	412.0369	65.4
6	7	12	1	284.9974	51.4	11	14	16	1	416.0318	2.3
6	8	12	1	286.0052	87.5	12	14	16	1	428.0318	2.0
5	8	13	1	290.0001	3.2	12	14	17	1	444.0267	16.5

Table S2. Products of toluene oxidation as identified in CI-APi-TOF spectra from the flow reactor. Data corresponds to Fig. 3b in the main text. All ions are negatively charged and include the reagent ion, NO_3^-. m/z is mass-to-charge ratio and f_{total} is fraction of total signal.

C	H	O	N	m/z, Th	$f_{total}x10^{-4}$	C	H	O	N	m/z, Th	$f_{total}x10^{-4}$
7	8	5	1	186.0408	5.1	11	14	10	1	320.0623	9.3
7	8	6	1	202.0357	212.2	13	14	9	1	328.0674	45.2
6	6	7	1	204.0150	25.2	13	16	9	1	330.0831	10.1
7	10	6	1	204.0514	n/a	12	14	10	1	332.0623	73.0
6	8	7	1	206.0306	19.2	12	16	10	1	334.0780	3.2
5	8	8	1	210.0255	5.7	11	14	11	1	336.0572	4.4
7	8	7	1	218.0306	80.4	14	16	9	1	342.0831	49.7
7	9	7	1	219.0385	18.8	14	18	9	1	344.0987	29.5
6	6	8	1	220.0099	n/a	14	20	9	1	346.1144	77.9
7	10	7	1	220.0463	139.3	12	14	11	1	348.0572	39.9
6	8	8	1	222.0255	14.8	11	14	12	1	352.0522	3.5
7	12	7	1	222.0619	n/a	14	14	10	1	356.0623	19.6
5	6	9	1	224.0048	10.9	14	16	10	1	358.0780	45.8
6	10	8	1	224.0412	n/a	14	18	10	1	360.0936	29.4
7	8	8	1	234.0255	171.5	13	16	11	1	362.0729	11.5
6	6	9	1	236.0048	n/a	13	18	11	1	364.0885	13.9
7	10	8	1	236.0412	741.2	11	14	13	1	368.0471	15.0
6	8	9	1	238.0205	42.6	14	16	11	1	374.0729	276.7
7	12	8	1	238.0568	n/a	14	18	11	1	376.0885	349.0
5	6	10	1	239.9997	n/a	13	16	12	1	378.0678	36.7
6	10	9	1	240.0361	17.7	13	18	12	1	380.0834	12.8
5	7	10	1	241.0075	10.5	14	14	12	1	388.0522	6.2
7	8	9	1	250.0205	52.2	14	16	12	1	390.0678	66.5
6	6	10	1	251.9997	n/a	14	18	12	1	392.0834	80.2
7	10	9	1	252.0361	161.1	13	16	13	1	394.0627	12.9
6	8	10	1	254.0154	43.4	14	20	12	1	394.0991	n/a
7	12	9	1	254.0518	n/a	13	18	13	1	396.0784	7.7
5	6	11	1	255.9946	n/a	14	14	13	1	404.0471	0.8
6	10	10	1	256.0310	19.1	14	16	13	1	406.0627	61.6
7	8	10	1	266.0154	66.5	14	18	13	1	408.0784	42.7
6	6	11	1	267.9946	n/a	14	20	13	1	410.0940	17.8
7	10	10	1	268.0310	129.9	14	16	14	1	422.0576	21.6
6	8	11	1	270.0103	41.8	14	18	14	1	424.0733	29.5
7	12	10	1	270.0467	n/a	14	20	14	1	426.0889	1.4
7	8	11	1	282.0103	52.9	14	16	15	1	438.0526	8.2
6	6	12	1	283.9896	n/a	14	18	15	1	440.0682	62.0
7	10	11	1	284.0259	140.4	14	20	15	1	442.0838	4.6
6	8	12	1	286.0052	24.1	14	16	16	1	454.0475	5.4
7	12	11	1	286.0416	n/a	14	18	16	1	456.0631	4.4
7	8	12	1	298.0052	26.2	14	16	17	1	470.0424	3.1
7	9	12	1	299.0130	35.6	14	18	17	1	472.0580	3.1
7	10	12	1	300.0208	87.5	14	16	18	1	486.0373	0.9
7	8	13	1	314.0001	26.6						

Table S3. Products of naphthalene oxidation as identified in CI-APi-TOF spectra from the flow reactor. Data corresponds to Fig. 3c in the main text. All ions are negatively charged and include the reagent ion, NO_3^-. m/z is mass-to-charge ratio and f_{total} is fraction of total signal.

C	H	O	N	m/z, Th	$f_{total}x10^{-4}$	C	H	O	N	m/z, Th	$f_{total}x10^{-4}$
10	10	7	1	256.0463	80.7	20	18	8	1	400.1038	14.9
10	8	8	1	270.0255	4.7	20	16	9	1	414.0831	3.7
10	10	8	1	272.0412	39.5	20	18	9	1	416.0987	70.7
10	12	8	1	274.0569	22.3	20	20	9	1	418.1144	41.1
10	8	9	1	286.0205	6.3	20	16	10	1	430.0780	5.6
10	10	9	1	288.0361	64.9	20	18	10	1	432.0936	23.2
10	11	9	1	289.0439	26.4	20	20	10	1	434.1093	133.5
10	12	9	1	290.0518	182.8	20	16	11	1	446.0729	4.0
10	8	10	1	302.0154	4.1	20	17	11	1	447.0807	4.1
10	9	10	1	303.0232	0.9	20	18	11	1	448.0885	23.2
10	10	10	1	304.0310	46.2	20	20	11	1	450.1042	93.7
10	11	10	1	305.0389	10.9	20	21	11	1	451.1120	85.4
10	12	10	1	306.0467	143.1	20	22	11	1	452.1198	28.3
10	14	10	1	308.0623	18.8	20	16	12	1	462.0678	3.7
10	8	11	1	318.0103	3.1	20	18	12	1	464.0834	14.8
10	9	11	1	319.0181	1.6	20	20	12	1	466.0991	76.2
10	10	11	1	320.0259	28.7	20	22	12	1	468.1148	31.5
10	12	11	1	322.0416	93.5	20	16	13	1	478.0627	1.5
10	14	11	1	324.0572	47.5	20	18	13	1	480.0784	10.6
10	15	11	1	325.0651	17.0	20	20	13	1	482.0940	47.5
10	8	12	1	334.0052	3.2	20	21	13	1	483.1018	30.6
10	9	12	1	335.0130	2.5	20	22	13	1	484.1097	39.9
10	10	12	1	336.0208	16.2	20	23	13	1	485.1175	21.8
10	11	12	1	337.0287	7.1	20	24	13	1	486.1253	8.1
10	12	12	1	338.0365	50.7	20	16	14	1	494.0576	0.6
10	13	12	1	339.0443	21.0	20	18	14	1	496.0733	7.4
10	14	12	1	340.0522	42.0	20	20	14	1	498.0889	20.9
10	15	12	1	341.0600	10.7	20	21	14	1	499.0967	10.3
10	10	13	1	352.0158	11.9	20	22	14	1	500.1046	28.0
10	12	13	1	354.0314	24.4	20	23	14	1	501.1124	36.5
10	13	13	1	355.0393	7.1	20	24	14	1	502.1202	11.5
10	14	13	1	356.0471	20.8	20	18	15	1	512.0682	4.6
10	15	13	1	357.0549	8.2	20	20	15	1	514.0839	16.1
10	10	14	1	368.0107	5.7	20	22	15	1	516.0995	17.1
20	18	6	1	368.1140	n/a	20	23	15	1	517.1073	15.8
10	12	14	1	370.0263	13.0	20	24	15	1	518.1151	12.8
10	13	14	1	371.0342	4.0	20	20	16	1	530.0787	7.1
10	14	14	1	372.0420	9.4	20	22	16	1	532.0944	9.4
10	15	14	1	373.0498	4.0	20	20	17	1	546.0737	4.6
20	18	7	1	384.1089	102.1	20	22	17	1	548.0893	4.7

Table S4. Peaks identified in JPAC. Non-nitrogen containing HOM were included in HOM yield calculation and kinetic model for seeded experiment, with exception of those marked with * in m/z column. All ions are negatively charged and include the reagent ion. In non-nitrogen containing HOM, N content of 1 indicates that the HOM is likely charged by NO_3^-, while if N=0, the HOM are detected as de-protonated species. Among nitrogen-containing molecules, N=1 likely refers to deprotonated species, while N=2 likely means that the molecule is charged by NO_3^-. When N=3, it is possible that the molecule is charged by nitric acid dimer, $HNO_3{\cdot}NO_3^-$, or has two nitrogens within a molecule and is charged by NO_3^-. m/z is mass-to-charge ratio and f_{total} is fraction of total signal.

Non-nitrogen containing HOM								
C	**H**	**O**	**N**	**m/z, Th**	**f_{total}x10^{-6} panel a**	**f_{total}x10^{-6} panel b**	**f_{total}x10^{-6} panel c**	**f_{total}x10^{-6} panel d**
5	7	6	0	163.0248	8	61	13	29
6	5	6	0	173.0092	37	167	41	74
6	5	8	0	204.9990*	17	87	33	n/a
6	7	8	0	207.0146	11	55	43	25
6	5	9	0	220.9939*	14	39	44	n/a
5	4	9	1	221.9892	74	328	104	59
5	6	9	1	224.0048	47	230	43	46
6	4	9	1	233.9892	20	189	53	27
6	6	9	1	236.0048	103	429	360	142
6	7	9	1	237.0126	30	58	88	41
5	6	10	1	239.9997	177	449	122	167
5	7	10	1	241.0075	35	81	56	109
6	4	10	1	249.9841	19	302	41	51
6	6	10	1	251.9997	68	852	284	102
6	8	10	1	254.0154	130	857	236	98
5	5	11	1	254.9868	20	306	41	64
5	6	11	1	255.9946	1135	585	93	403
6	4	11	1	265.9790	22	175	45	62
6	5	11	1	266.9868*	51	44	68	n/a
6	6	11	1	267.9946	107	901	144	154
6	7	11	1	269.0025	42	271	80	67
6	8	11	1	270.0103	363	984	285	201
6	6	12	1	283.9895	124	577	220	607
6	7	12	1	284.9974*	153	215	66	132
6	8	12	1	286.0052	265	749	442	171
6	9	12	1	287.0130*	58	187	67	n/a
6	10	12	1	288.0208	55	297	69	n/a
5	8	13	1	290.0001	39	107	25	31
6	6	13	1	299.9845	277	342	140	123
6	8	13	1	302.0001	718	474	393	190
5	7	14	1	304.9872	31	85	45	41
5	8	14	1	305.9950	28	65	28	19
6	8	14	1	317.9950	374	251	83	111
6	9	14	1	319.0029*	292	210	36	n/a
6	10	14	1	320.0107	78	73	241	62
10	8	12	1	334.0052	110	180	81	55

Table S4. Continued.

C	H	O	N	m/z, Th	$f_{total}x10^{-6}$ panel a	$f_{total}x10^{-6}$ panel b	$f_{total}x10^{-6}$ panel c	$f_{total}x10^{-6}$ panel d
10	9	12	1	335.0130	61	206	31	50
10	10	12	1	336.0208	62	141	107	35
12	12	11	1	346.0416*	58	40	144	n/a
12	14	11	1	348.0572	309	62	78	58
11	14	12	1	352.0521	103	61	119	22
10	12	13	1	354.0314	47	45	93	18
12	12	12	1	362.0365*	120	60	264	n/a
12	14	12	1	364.0521	147	70	170	64
12	16	12	1	366.0678	53	53	48	23
11	14	13	1	368.0471	44	63	68	18
10	12	14	1	370.0263	27	50	42	18
12	12	13	1	378.0314	90	95	316	53
12	14	13	1	380.0471	143	119	178	33
12	16	13	1	382.0627	58	68	49	22
11	14	14	1	384.0420	52	62	53	19
10	12	15	1	386.0212	34	50	30	24
12	10	14	1	392.0107	15	25	33	14
12	12	14	1	394.0263*	71	90	269	n/a
12	14	14	1	396.0420	115	134	132	34
12	16	14	1	398.0576	97	124	62	23
11	14	15	1	400.0369	40	50	20	16
12	10	15	1	408.0056	8	29	23	13
12	12	15	1	410.0212	149	95	297	34
12	14	15	1	412.0369	166	123	78	27
11	12	16	1	414.0162	51	81	29	17
11	14	16	1	416.0318	34	46	6	14
12	10	16	1	424.0005	11	28	25	12
12	12	16	1	426.0162*	95	70	90	n/a
12	14	16	1	428.0318	126	108	102	29
12	16	16	1	430.0475	36	66	18	15
11	14	17	1	432.0267	32	38	13	7
12	12	17	1	442.0111	36	54	42	15
12	14	17	1	444.0267	338	81	51	20
12	16	17	1	446.0424	34	46	16	16
12	12	18	1	458.0060	21	38	24	8
12	14	18	1	460.0216	44	48	23	13
12	16	18	1	462.0373	24	30	28	7
12	12	19	1	474.0009	10	20	4	3
12	14	19	1	476.0166	31	27	21	9
12	16	19	1	478.0322	16	18	25	7
12	16	20	1	494.0271	11	14	13	2
12	14	21	1	508.0064	9	8	10	3
12	16	21	1	510.0220	4	9	7	4

Table S4. Continued.

Nitrogen-containing molecules						
C	**H**	**O**	**N**	**m/z, Th**	**$f_{total}x10^{-6}$ panel d**	**Likely compound**
6	4	3	1	138.0196666	101.6	deprotonated nitrophenol
6	4	4	1	154.0145812	352.7	depritonated nitrocatechol
6	5	6	2	201.0153095	673.1	nitrophenol with NO_3^-
5	5	7	2	205.0102241	50.1	
6	5	7	2	217.0102241	307.1	nitrocatechol with NO_3^-
5	5	8	2	221.0051387	49.2	
3	5	10	2	228.9949679	22.9	
6	7	8	2	235.0207888	326.3	
6	5	9	2	249.0000533	178.4	
6	6	9	3	264.0109524	1217.1	likely nitrophenol with $HNO_3^-NO_3^-$
6	7	10	2	267.010618	82.3	
5	7	11	2	271.0055326	55.8	
4	5	12	2	272.9847972	62.7	
4	7	12	2	275.0004472	31.5	
6	6	10	3	280.005867	140.3	nitrocatechol with $HNO_3^-NO_3^-$
6	5	11	2	280.9898826	71.3	
6	7	11	2	283.0055326	133.3	
5	7	12	2	287.0004472	74.0	
4	6	12	3	287.9956962	49.2	
6	5	12	2	296.9847972	50.3	
6	7	12	2	299.0004472	154.2	
5	5	13	2	300.9797118	n/a	
6	9	12	2	301.0160973	136.1	
5	7	13	2	302.9953619	100.2	
4	6	13	3	303.9906108	74.3	
6	8	12	3	314.0113463	67.8	
6	7	13	2	314.9953619	148.9	
5	7	14	2	318.9902765	117.8	
6	6	13	3	327.9906108	60.3	
6	5	14	2	328.9746264	40.4	
6	8	13	3	330.0062609	77.6	
6	7	14	2	330.9902765	195.2	
6	9	14	2	333.0059266	90.1	
6	4	14	3	341.9698754	36.8	
6	8	14	3	346.0011755	98.7	
6	7	15	2	346.9851911	171.0	
6	9	15	2	349.0008412	51.0	
6	8	15	3	361.9960901	85.0	
6	7	16	2	362.9801057	75.1	
6	8	17	3	393.9859194	71.5	
6	8	19	3	425.9757486	24.8	