Supporting Information to "Mechanistic Study of Formation of Ring-retaining and Ring-opening Products from Oxidation of Aromatic Compounds under Urban Atmospheric Conditions"

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1 Additional Tables and Figures

Table S1: Description of experiments.

VOC	Initial VOC concentration, ppbv	Initial HONO injection, ppbv	Additional HONO injections[a], ppbv	Particle loading after seed injection, cm^{-3}	Temp., K	RH, %
toluene	89	28	16 (124); 28 (220)	$2.6 \cdot 10^4$	292	2%
toluene	89	30	17 (140); 6 (180); 12 (290)	$4.2 \cdot 10^4$	292	2%
toluene	89	31	21 (125); 18 (290)	$3.2 \cdot 10^4$	292	2%
toluene	89	28	23 (180)	100[b]	292	3%
124-TMB	69	30	5 (155); 10 (300)	$3.6 \cdot 10^4$	292	2%
124-TMB	69	31	13 (145); 10 (245); 5 (345)	$3.8 \cdot 10^4$	292	2%
124-TMB	69	34	18 (150); 6 (265); 13 (390)	$5.7 \cdot 10^4$	292	2%
124-TMB	69	60	-	100[b]	292	2%

[a] The following format is used: HONO injection in ppbv (time since the beginning of the experiment in min).

[b] No seed was injected in the two experiments.

Table S2: Estimated NH_4^+ CIMS sensitivity factors for species detected in toluene experiments.

Compound	*m/z*	$KE_{cm\ 50}$, eV	Sensitivity factor
$C_7H_7NO_3$	171.077	0.166	0.69
$C_7H_8O_4$	174.077	0.185	0.89
$C_7H_5NO_4$	185.056	0.166	0.69
$C_7H_7NO_4$	187.072	0.293	1
$C_7H_6O_5$	188.056	0.192	0.97
$C_7H_8O_5$	190.072	0.208	1
$C_7H_{10}O_5$	192.087	0.192	0.97
$C_7H_5NO_5$	201.051	0.175	0.79
$C_7H_6O_6$	204.051	0.198	1
$C_7H_9NO_5$	205.083	0.183	0.87
$C_7H_8O_6$	206.067	0.197	1
$C_7H_{10}O_6$	208.082	0.193	0.98
$C_7H_7NO_6$	219.062	0.188	0.93
$C_7H_9NO_6$	221.077	0.187	0.92
$C_7H_7NO_7$	235.057	0.185	0.89

$C_7H_9NO_7$	237.072	0.195	1

Table S3: Estimated NH_4^+ CIMS sensitivity factors for species detected in 1,2,4-trimethylbenzene experiments.

Compound	*m/z*	$KE_{cm\ 50}$, eV	Sensitivity factor
$C_9H_{10}O_4$	200.092	0.236	1
$C_9H_{12}O_4$	202.108	0.204	1
$C_9H_{14}O_4$	204.124	0.184	0.89
$C_9H_{11}NO_4$	215.103	0.217	1
$C_9H_{10}O_5$	216.087	0.222	1
$C_9H_{12}O_5$	218.103	0.225	1
$C_9H_{14}O_5$	220.119	0.195	1
$C_9H_9NO_5$	229.083	0.134	0.36
$C_9H_{11}NO_5$	231.098	0.199	1
$C_9H_{12}O_6$	234.098	0.207	1
$C_9H_{14}O_6$	236.114	0.225	1
$C_9H_{13}NO_6$	249.109	0.153	0.56
$C_9H_{11}NO_7$	263.088	0.207	1
$C_9H_{13}NO_8$	281.099	0.207	1

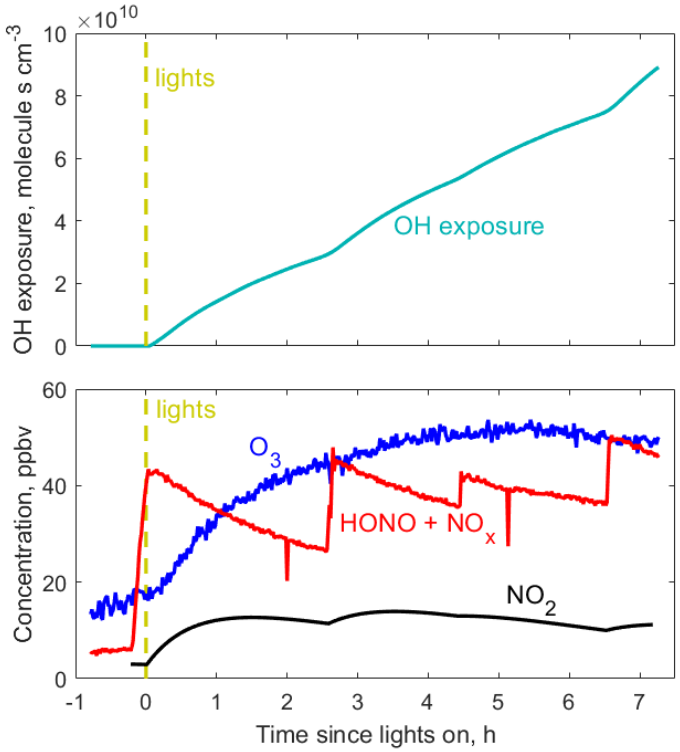

Figure S1: (a) OH exposure and (b) concentrations of O_3, NO_2, HONO+NO_x for a typical photooxidation experiment.

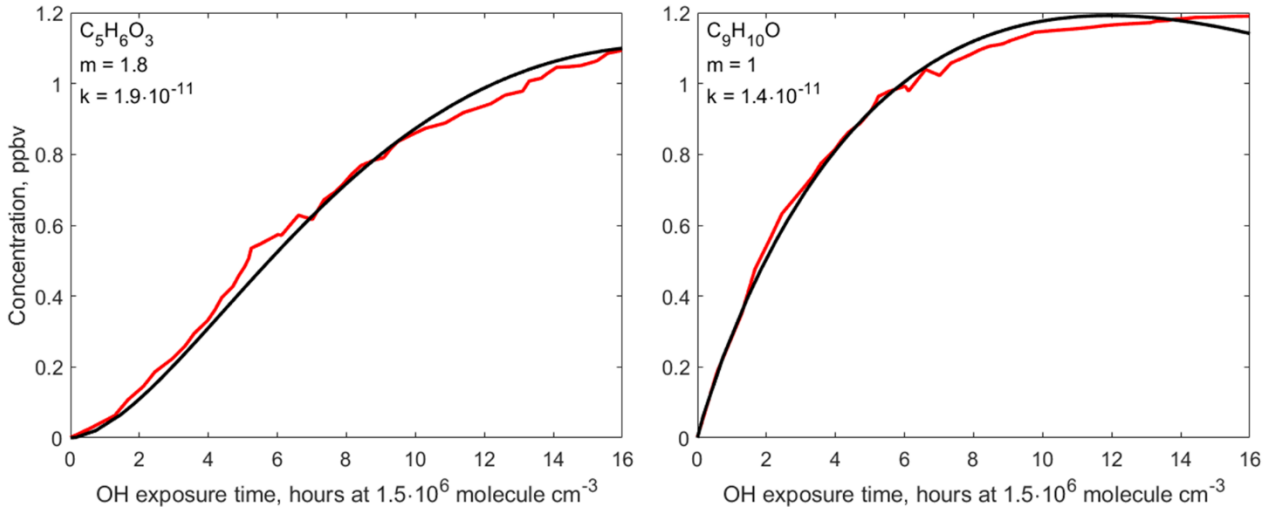

Figure S2: Species measured by NH_4^+ CIMS in 124-TMB photooxidation experiment (red) and kinetic best fit (black).

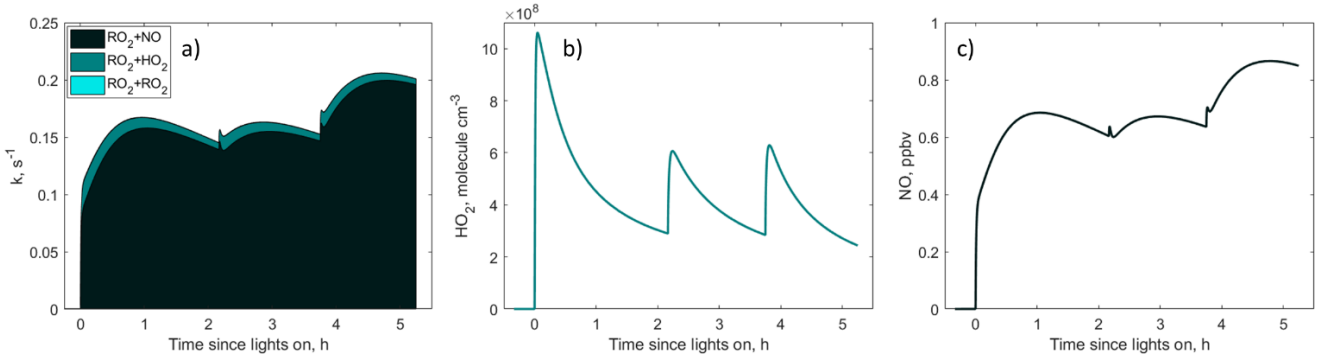

Figure S3: (a) Loss of bicyclic peroxy radicals calculated from the modelled concentrations of NO, HO_2, and RO_2; (b) and (c) modelled concentrations of NO and HO_2 during photooxidation of toluene.

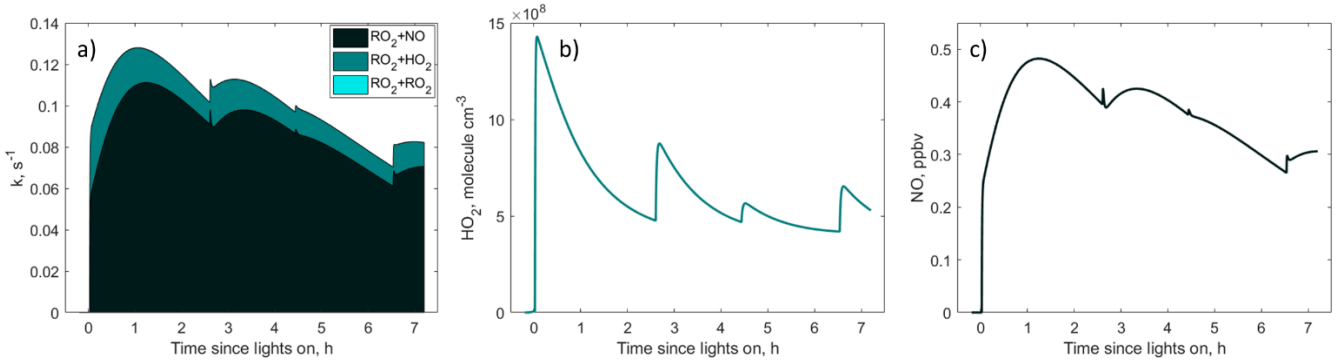

Figure S4: (a) Loss of bicyclic peroxy radicals calculated from the modelled concentrations of NO, HO_2, and RO_2; (b) and (c) modelled concentrations of HO_2 and NO during photooxidation of 124-TMB.

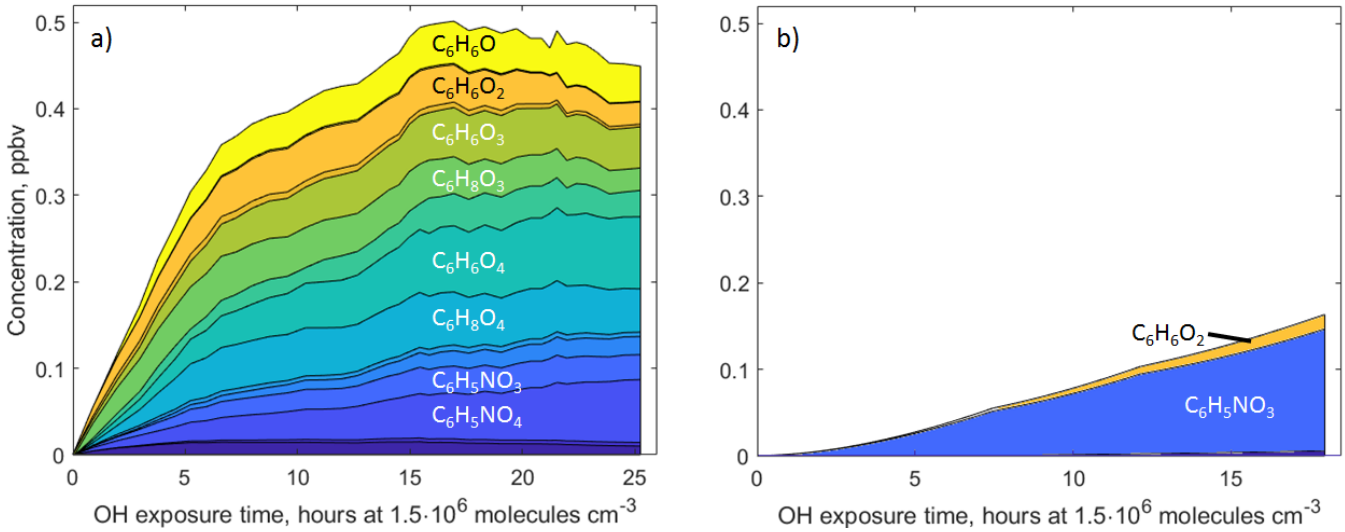

Figure S5: C_6 gas-phase products (a) detected by PTR-MS and NH_4^+ CIMS and (b) predicted by MCM v3.3.1 during oxidation of toluene.