Supporting Information for:

New Insights into Low-Temperature Oxidation of Propane from Synchrotron Photoionization Mass Spectrometry and Multi-Scale Informatics Modeling

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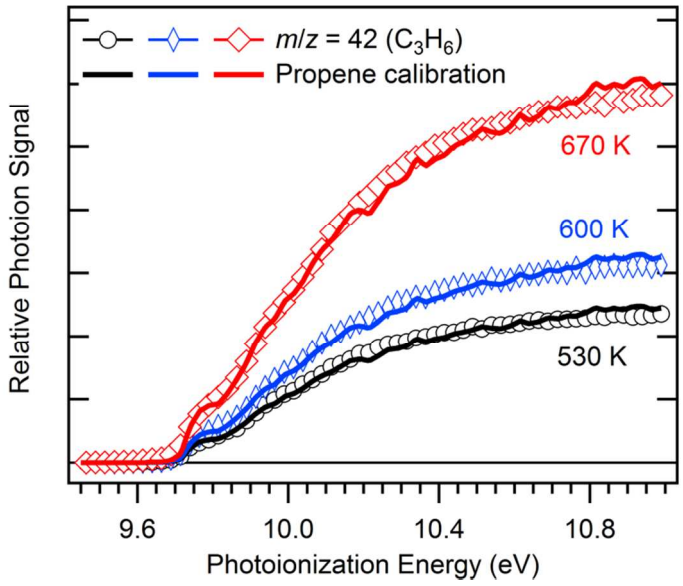

Figure S1: Photoionization product spectra of the m/z = 42 (C_3H_6) signal at 530, 600, and 670 K with a propene calibration spectrum taken from Ref. [1]. The product spectra were obtained by integration over kinetic times from 0 ms until 30 ms (530 K)/20 ms (600 and 670 K) relative to photolysis. At all three temperatures, the C_3H_6 product spectra are well-represented by the propene calibration spectrum.

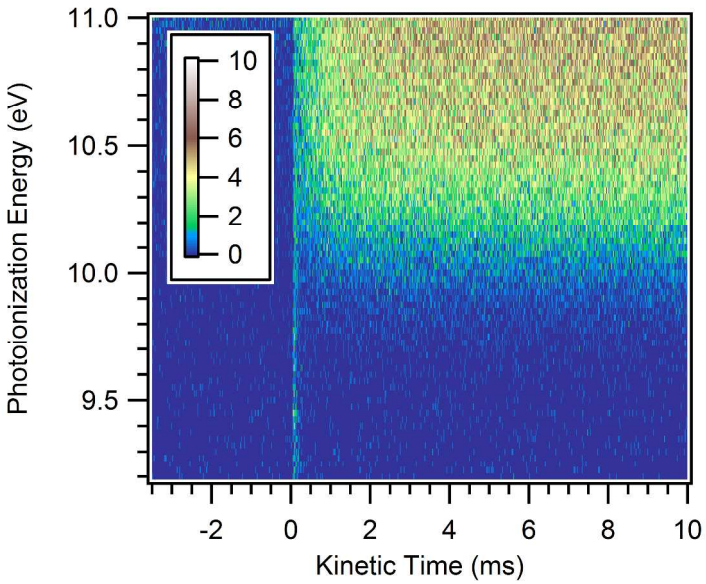

Figure S2: Time behavior of the m/z = 43 ($C_3H_7^+$) ion signal (in arbitrary units) at 530 K and 4 Torr as a function of photoionization energy. The ^{13}C contribution from C_3H_6 has been subtracted. Transient signal shortly after t = 0 at photon energies below ~ 9.8 eV arises from direct ionization of *n*- and *i*-propyl radicals. At higher energies, the ion signal is due to dissociative ionization of propyl peroxy radicals, which are stable on the experimental timescale at 530 K.

Table S1: Absolute partial photoionization cross sections of propane (C_3H_8, m/z = 44) measured at 600 K. The noise at m/z = 28 and 43 is caused by subtraction of ethene and the C13 contribution of propene, respectively. The latter were flowed through the tube together with propane to determine the absolute cross section of propane (see Ref. [1] for details on the procedure for determining absolute cross sections).

E (eV)	σ (Mb), m/z =		
	44	43	28
10.670	0.00	-0.05	-0.03
10.695	0.00	-0.01	0.01
10.720	0.01	0.00	-0.03
10.745	0.01	0.00	0.02
10.770	0.01	0.01	0.00
10.795	0.03	0.02	0.03
10.820	0.01	-0.01	0.06
10.845	0.03	-0.08	0.01
10.870	0.07	-0.03	0.03
10.895	0.11	0.01	0.00
10.920	0.13	-0.07	-0.07
10.945	0.19	0.10	0.02
10.970	0.34	0.03	0.00
10.995	0.40	-0.06	-0.03
11.020	0.72	0.11	-0.01
11.045	0.80	-0.05	-0.05
11.070	1.00	-0.06	0.00
11.095	1.23	0.09	0.01
11.120	1.73	0.05	0.05
11.145	2.44	-0.01	0.12
11.170	2.53	0.08	0.06
11.195	2.73	0.09	0.04
11.220	3.69	0.21	-0.02
11.245	4.32	0.11	0.05
11.270	5.16	0.10	-0.02
11.295	5.40	0.24	0.02
11.320	6.05	0.33	0.05
11.345	7.03	0.42	0.02
11.370	7.66	0.48	0.02
11.395	8.81	0.50	0.03
11.420	9.98	0.57	0.09
11.445	10.28	0.70	0.04
11.470	11.88	0.88	0.05
11.495	12.33	1.12	0.06
11.520	12.93	1.65	0.11

Table S2: Absolute partial photoionization cross sections of acetone (C_3H_6O, m/z = 58) measured at 298 K.

E (eV)	σ (Mb), m/z =		E (eV)	σ (Mb), m/z =	
	58	43		58	43
9.500	0.00	0.00	10.275	11.06	0.03
9.525	0.00	0.00	10.300	11.27	0.04
9.550	0.01	0.00	10.325	11.36	0.03
9.575	0.01	0.00	10.350	11.59	0.02
9.600	0.03	0.00	10.375	11.77	0.06
9.625	0.06	0.00	10.400	11.81	0.06
9.650	0.16	0.00	10.425	11.97	0.10
9.675	0.50	0.00	10.450	12.01	0.13
9.700	1.95	0.00	10.475	12.13	0.13
9.725	2.96	0.00	10.500	12.17	0.21
9.750	3.72	-0.01	10.525	12.31	0.29
9.775	4.03	0.00	10.550	12.24	0.33
9.800	4.38	0.00	10.575	12.36	0.40
9.825	4.79	0.00	10.600	12.21	0.45
9.850	5.48	0.00	10.625	12.24	0.48
9.875	6.06	0.00	10.650	12.25	0.56
9.900	6.63	0.00	10.675	12.20	0.64
9.925	6.94	0.01	10.700	12.23	0.63
9.950	7.29	0.01	10.725	12.19	0.68
9.975	7.64	0.01	10.750	12.09	0.77
10.000	7.95	0.00	10.775	12.05	0.79
10.025	8.29	0.02	10.800	11.87	0.81
10.050	8.65	0.01	10.825	11.83	0.95
10.075	8.94	0.00	10.850	11.86	0.99
10.100	9.26	0.01	10.875	11.80	1.01
10.125	9.56	0.02	10.900	11.77	1.08
10.150	9.61	0.01	10.925	11.63	1.11
10.175	10.14	0.00	10.950	11.54	1.15
10.200	10.51	0.02	10.975	11.48	1.17
10.225	10.71	0.01	11.000	11.40	1.26
10.250	10.83	-0.01			

Table S3: Absolute partial photoionization cross sections of oxetane (C_3H_6O, m/z = 58) measured at 298 K.

E (eV)	σ (Mb), m/z =				
	58	57	30	29	28
9.519	0.00	0.00	0.00	0.00	0.01
9.544	0.00	0.00	0.00	0.00	0.00
9.569	0.01	0.00	0.00	0.00	0.00
9.594	0.01	0.00	0.00	0.00	0.01
9.619	0.09	0.00	0.00	0.00	0.00
9.644	0.22	0.00	0.00	0.00	0.00
9.669	0.91	0.00	0.00	0.00	0.00
9.694	1.79	0.00	0.00	0.00	0.00
9.719	2.17	0.01	0.00	0.00	0.00
9.744	2.36	0.00	0.00	0.00	0.00
9.769	2.48	0.00	0.00	0.00	0.00
9.794	2.81	0.01	0.01	0.00	0.00
9.819	3.31	0.01	0.00	0.00	0.00
9.844	4.09	0.00	0.00	0.00	0.00
9.869	4.32	0.01	0.00	0.00	0.00
9.894	4.48	0.01	0.00	0.00	0.00
9.919	4.77	0.02	0.00	0.00	0.01
9.944	4.72	0.01	0.00	0.00	0.01
9.969	5.23	0.02	0.00	0.00	0.00
9.994	5.65	0.03	0.01	0.00	0.01
10.019	5.87	0.03	0.00	0.01	0.01
10.044	6.30	0.04	0.01	0.00	0.01
10.069	6.45	0.04	0.00	0.00	0.00
10.094	6.77	0.06	0.01	0.00	0.00
10.119	7.14	0.11	0.00	0.01	0.00
10.144	6.93	0.17	0.00	0.00	0.00
10.169	7.34	0.23	0.00	0.00	0.00
10.194	7.29	0.28	0.03	0.00	0.00
10.219	7.79	0.29	0.01	0.00	0.00
10.244	8.24	0.35	0.01	0.00	0.00
10.269	8.10	0.53	0.04	0.00	0.01
10.294	8.21	0.57	0.03	0.00	0.00
10.319	8.28	0.61	0.07	0.00	0.01
10.344	8.41	0.67	0.04	0.00	0.00
10.369	8.46	0.69	0.07	0.01	0.00
10.394	8.88	0.84	0.10	0.00	0.00
10.419	8.89	0.90	0.10	0.01	0.01
10.444	8.87	0.95	0.10	0.00	0.00

10.469	9.27	1.04	0.22	0.01	0.00
10.494	9.37	1.07	0.17	0.00	0.01
10.519	9.19	1.13	0.27	0.00	0.00
10.544	9.63	1.10	0.25	0.00	0.00
10.569	9.38	0.99	0.27	0.01	0.01
10.594	9.71	1.15	0.34	0.01	0.01
10.619	9.37	1.20	0.32	0.02	0.01
10.644	9.50	1.06	0.32	0.00	0.01
10.669	9.72	1.14	0.38	0.03	0.03
10.694	9.95	1.23	0.43	0.04	0.04
10.719	10.01	1.28	0.49	0.02	0.08
10.744	10.11	1.35	0.47	0.04	0.04
10.769	9.96	1.25	0.47	0.04	0.06
10.794	10.28	1.53	0.66	0.04	0.11
10.819	10.36	1.40	0.61	0.07	0.11
10.844	10.77	1.41	0.64	0.09	0.17
10.869	10.31	1.47	0.64	0.06	0.27
10.894	10.77	1.64	0.75	0.09	0.32
10.919	10.49	1.75	0.66	0.08	0.48
10.944	11.33	1.87	0.83	0.15	0.49
10.969	10.90	1.92	0.91	0.18	0.55
10.994	10.97	1.71	1.04	0.15	0.70
11.019	11.29	2.05	0.99	0.19	0.82
11.044	11.43	1.73	0.89	0.19	1.04
11.069	11.30	1.89	1.07	0.33	1.20
11.094	11.43	2.14	1.02	0.25	1.49
11.119	11.42	2.23	1.06	0.34	1.59
11.144	11.85	2.19	1.15	0.35	1.90
11.169	11.89	2.21	1.29	0.40	2.11
11.194	11.46	2.33	1.25	0.44	2.50
11.219	11.70	2.17	1.29	0.55	2.52

Table S4: Absolute partial photoionization cross sections of methyloxirane (C_3H_6O, m/z = 58) measured at 298 K.

E (eV)	σ (Mb), m/z =				
	58	57	43	30	28
9.519	0.00	0.00	0.00	0.00	0.00
9.544	0.00	0.00	0.00	0.00	0.00
9.569	0.00	0.00	0.00	0.00	0.00
9.594	0.00	0.00	0.00	0.00	0.00
9.619	0.00	0.00	0.00	0.00	0.00
9.644	0.00	0.00	0.00	0.00	0.00
9.669	0.00	0.00	0.00	0.00	0.00
9.694	0.01	0.00	0.00	0.00	0.00
9.719	0.00	0.00	0.00	0.00	0.00
9.744	0.00	0.00	0.00	0.00	0.00
9.769	0.00	0.00	-0.01	0.00	0.00
9.794	0.01	0.00	0.00	0.00	0.00
9.819	0.01	0.00	-0.02	0.00	0.00
9.844	0.01	0.00	0.00	0.00	0.00
9.869	0.01	0.00	-0.01	0.00	0.00
9.894	0.01	0.00	0.02	0.00	0.00
9.919	0.00	0.00	-0.01	0.00	0.00
9.944	0.02	0.00	0.00	0.00	0.00
9.969	0.02	0.00	-0.01	0.00	0.00
9.994	0.02	0.00	0.01	0.00	0.00
10.019	0.05	0.00	0.04	0.00	0.00
10.044	0.04	0.00	-0.02	0.00	0.00
10.069	0.06	0.00	0.00	0.00	0.00
10.094	0.15	0.00	-0.04	0.00	0.00
10.119	0.22	0.00	0.07	0.00	0.00
10.144	0.26	0.00	0.00	0.00	0.00
10.169	0.51	0.00	-0.03	0.00	0.00
10.194	0.69	0.00	0.14	0.00	0.00
10.219	1.21	0.00	0.06	0.00	0.00
10.244	2.09	0.00	0.03	0.00	0.00
10.269	2.70	0.00	0.02	0.00	0.00
10.294	3.23	0.00	-0.01	0.00	0.00
10.319	3.48	0.00	0.03	0.00	0.00
10.344	4.02	0.01	0.00	0.00	0.00
10.369	4.60	0.00	-0.05	0.00	0.00
10.394	5.36	0.00	0.05	0.00	0.00
10.419	5.76	0.00	0.07	0.00	0.00
10.444	6.28	0.01	0.02	0.00	0.00

10.469	6.70	0.00	0.07	0.00	0.00
10.494	7.03	0.02	0.01	0.00	0.00
10.519	7.27	0.01	0.06	0.00	0.00
10.544	7.82	0.02	0.04	0.00	0.00
10.569	8.11	0.01	0.04	0.00	0.00
10.594	8.24	0.02	0.11	0.01	0.00
10.619	8.67	0.01	0.08	0.01	0.00
10.644	8.87	0.02	0.08	0.00	0.00
10.669	9.55	0.02	0.10	0.02	0.00
10.694	9.51	0.02	0.13	0.01	0.00
10.719	9.45	0.03	0.15	0.03	0.01
10.744	9.85	0.07	0.22	0.01	0.01
10.769	9.65	0.08	0.32	0.04	0.01
10.794	10.00	0.09	0.32	0.04	0.01
10.819	9.91	0.12	0.42	0.07	0.01
10.844	9.65	0.17	0.38	0.09	0.01
10.869	9.74	0.17	0.63	0.11	0.02
10.894	9.79	0.20	0.58	0.17	0.02
10.919	10.09	0.19	0.76	0.16	0.02
10.944	9.97	0.32	0.73	0.16	0.02
10.969	10.01	0.36	0.93	0.21	0.06
10.994	10.29	0.37	0.99	0.26	0.06
11.019	10.25	0.41	0.93	0.27	0.09
11.044	10.04	0.41	1.09	0.34	0.15
11.069	9.94	0.46	1.29	0.32	0.22
11.094	10.12	0.55	1.42	0.36	0.22
11.119	10.76	0.51	1.47	0.35	0.28
11.144	10.53	0.65	1.58	0.38	0.36
11.169	10.34	0.62	1.75	0.35	0.43
11.194	10.76	0.79	1.99	0.40	0.45
11.219	11.25	0.80	2.02	0.43	0.50

Table S5: Experimental concentration-time profiles (normalized to $[Cl]_0$) for the species quantified at 530 K.

t (ms)	methyl	ethene	CH_2O	propene	CH_3CHO	acetone	propanal	methyl-oxirane
-2.0	-8.61E-5	-2.64E-3	1.74E-3	-5.84E-4	-3.31E-4	-1.72E-4	9.31E-3	-1.05E-3
-1.8	-3.45E-4	2.08E-3	1.95E-3	1.28E-4	-5.61E-4	1.61E-3	4.44E-3	9.33E-4
-1.6	2.42E-4	-3.45E-4	2.28E-3	3.24E-4	1.16E-3	8.23E-5	-4.61E-3	3.04E-4
-1.4	-2.25E-4	1.91E-4	-7.64E-4	-8.36E-4	5.37E-4	3.37E-4	-1.83E-3	-8.58E-4
-1.2	-5.09E-6	2.77E-3	-1.70E-3	-8.43E-4	6.74E-4	-1.19E-3	-3.92E-3	-6.64E-4
-1.0	3.31E-4	-3.57E-3	-1.51E-3	-1.10E-3	-3.84E-3	8.47E-4	-2.52E-3	-6.16E-4
-0.8	-1.17E-5	7.18E-3	-3.97E-6	-5.54E-4	-7.12E-4	5.92E-4	-6.70E-3	-8.36E-5
-0.6	3.32E-4	-2.91E-4	-7.88E-4	-6.33E-4	1.48E-4	2.63E-3	-2.52E-3	-1.54E-3
-0.4	1.08E-4	5.28E-4	4.55E-4	-4.78E-4	6.10E-5	-9.37E-4	1.65E-3	3.04E-4
-0.2	4.45E-4	2.39E-3	-2.27E-3	-2.25E-5	-4.67E-4	-9.37E-4	-4.61E-3	-1.78E-3
0.0	1.25E-6	-4.14E-3	1.16E-3	1.99E-2	4.71E-3	8.47E-4	-7.64E-4	-1.89E-4
0.2	1.46E-4	2.64E-3	8.20E-3	7.65E-2	3.30E-3	8.23E-5	-6.77E-4	1.23E-3
0.4	7.21E-4	8.84E-4	7.36E-3	1.05E-1	4.10E-3	1.87E-3	1.67E-4	8.65E-4
0.6	8.59E-4	7.92E-3	3.04E-3	1.24E-1	2.64E-3	-9.37E-4	5.94E-3	1.02E-3
0.8	1.65E-3	4.92E-4	5.53E-3	1.35E-1	6.45E-3	-1.45E-3	-7.04E-3	1.94E-3
1.0	4.96E-4	3.80E-3	4.88E-3	1.42E-1	4.98E-3	8.47E-4	3.69E-3	4.70E-4
1.2	2.55E-4	1.02E-2	7.39E-3	1.52E-1	5.43E-3	1.61E-3	2.63E-3	3.24E-3
1.4	1.21E-3	-2.54E-3	6.97E-3	1.56E-1	7.09E-3	3.37E-4	-4.78E-4	7.17E-4
1.6	7.80E-4	-3.88E-3	8.73E-3	1.55E-1	6.97E-3	8.47E-4	1.31E-3	1.56E-3
1.8	1.89E-3	-1.64E-4	8.46E-3	1.55E-1	7.25E-3	4.41E-3	-3.13E-3	3.05E-3
2.0	6.20E-4	3.79E-3	9.23E-3	1.58E-1	7.29E-3	4.16E-3	2.89E-3	1.61E-3
2.2	3.60E-4	-2.75E-3	8.16E-3	1.59E-1	6.47E-3	5.92E-4	3.37E-3	3.23E-3
2.4	5.84E-4	5.36E-3	8.25E-3	1.61E-1	8.25E-3	1.36E-3	8.75E-3	1.53E-3
2.6	7.15E-4	-3.88E-4	9.67E-3	1.62E-1	7.74E-3	5.92E-4	-3.27E-3	1.69E-3
2.8	1.53E-3	9.12E-3	1.43E-2	1.64E-1	7.92E-3	2.63E-3	4.93E-3	3.07E-3
3.0	1.12E-3	4.89E-4	1.32E-2	1.62E-1	8.35E-3	2.12E-3	-2.87E-3	2.47E-3
3.2	1.75E-3	2.16E-3	1.10E-2	1.67E-1	9.37E-3	5.92E-4	6.05E-3	3.29E-3
3.4	5.19E-4	8.45E-3	1.06E-2	1.66E-1	7.24E-3	1.61E-3	-1.03E-3	2.14E-3
3.6	8.00E-4	-7.00E-4	6.59E-3	1.63E-1	8.06E-3	1.61E-3	7.22E-3	1.24E-3
3.8	1.05E-3	4.40E-3	1.29E-2	1.65E-1	8.40E-3	2.37E-3	-2.63E-3	2.04E-3
4.0	2.49E-4	1.40E-4	1.29E-2	1.66E-1	1.02E-2	-4.27E-4	4.25E-3	2.36E-3
4.2	1.30E-3	4.04E-4	1.19E-2	1.65E-1	7.86E-3	8.23E-5	2.78E-3	2.54E-3
4.4	1.05E-3	6.88E-4	1.05E-2	1.68E-1	9.77E-3	2.12E-3	-2.86E-3	2.87E-3
4.6	1.04E-3	6.02E-3	1.24E-2	1.69E-1	1.06E-2	1.36E-3	5.57E-4	2.29E-3
4.8	8.37E-4	-7.67E-3	1.21E-2	1.73E-1	9.21E-3	-1.72E-4	6.07E-3	6.05E-4
5.0	9.35E-4	1.32E-3	6.67E-3	1.70E-1	9.23E-3	4.41E-3	-2.48E-4	1.53E-3
5.2	3.51E-4	6.37E-3	1.52E-2	1.69E-1	9.01E-3	8.23E-5	1.10E-3	2.71E-3
5.4	9.64E-4	-4.31E-5	1.82E-2	1.68E-1	1.05E-2	-4.27E-4	1.57E-2	2.14E-3
5.6	-1.07E-4	3.59E-4	9.99E-3	1.71E-1	9.32E-3	2.88E-3	1.01E-2	2.65E-3

5.8	1.06E-3	-4.62E-4	1.52E-2	1.75E-1	9.43E-3	1.36E-3	1.68E-3	2.77E-3
6.0	9.37E-4	-7.36E-3	8.89E-3	1.74E-1	7.35E-3	8.23E-5	1.65E-3	1.73E-3
6.2	4.75E-4	5.82E-3	1.35E-2	1.71E-1	9.89E-3	4.92E-3	2.32E-3	2.05E-3
6.4	1.08E-3	6.39E-3	1.06E-2	1.75E-1	9.28E-3	5.18E-3	5.08E-3	2.03E-3
6.6	-1.17E-6	2.51E-3	2.11E-2	1.70E-1	1.18E-2	2.88E-3	-1.91E-3	1.04E-3
6.8	5.95E-4	-5.03E-3	1.06E-2	1.69E-1	9.60E-3	1.61E-3	-1.23E-3	2.19E-3
7.0	4.69E-4	4.19E-4	1.39E-2	1.75E-1	1.09E-2	2.63E-3	5.02E-3	3.09E-3
7.2	9.40E-4	1.92E-3	1.49E-2	1.74E-1	1.00E-2	2.12E-3	2.91E-3	2.16E-3
7.4	3.85E-4	2.68E-3	1.88E-2	1.73E-1	9.69E-3	2.37E-3	1.68E-2	2.05E-3
7.6	9.66E-4	4.19E-3	1.02E-2	1.71E-1	8.79E-3	8.47E-4	-6.17E-3	1.95E-3
7.8	6.11E-4	7.64E-4	1.61E-2	1.75E-1	8.37E-3	3.90E-3	1.05E-2	3.00E-3
8.0	2.66E-4	2.05E-3	2.02E-2	1.73E-1	9.76E-3	-1.72E-4	-2.01E-3	1.98E-3
8.2	1.55E-5	5.99E-3	1.43E-2	1.75E-1	9.93E-3	2.12E-3	4.24E-3	2.45E-3
8.4	7.11E-4	1.32E-3	1.58E-2	1.80E-1	1.13E-2	8.23E-5	6.32E-3	2.20E-3
8.6	2.60E-4	8.77E-3	2.08E-2	1.76E-1	1.07E-2	-6.82E-4	4.22E-3	2.58E-3
8.8	9.47E-4	-4.54E-3	1.70E-2	1.78E-1	1.08E-2	8.23E-5	-7.62E-3	2.72E-3
9.0	3.42E-4	-1.02E-3	8.82E-3	1.74E-1	9.33E-3	3.14E-3	1.53E-2	3.20E-3
9.2	1.34E-4	2.10E-3	1.69E-2	1.77E-1	7.33E-3	2.37E-3	5.60E-3	2.23E-3
9.4	1.40E-3	4.96E-3	1.24E-2	1.80E-1	1.06E-2	2.12E-3	4.90E-3	2.52E-3
9.6	3.97E-4	5.20E-3	1.71E-2	1.79E-1	7.70E-3	3.65E-3	5.59E-3	6.75E-4
9.8	1.38E-3	1.91E-3	1.12E-2	1.78E-1	1.14E-2	1.36E-3	1.27E-5	2.66E-3
10.0	1.31E-3	-1.87E-3	1.46E-2	1.85E-1	9.57E-3	2.37E-3	9.76E-3	3.18E-3
10.2	1.13E-4	7.58E-3	1.25E-2	1.80E-1	1.18E-2	2.63E-3	9.06E-3	2.60E-3
10.4	8.60E-4	-4.54E-4	1.95E-2	1.77E-1	1.41E-2	4.16E-3	2.09E-3	2.02E-3
10.6	6.03E-4	-1.86E-3	1.08E-2	1.80E-1	1.03E-2	3.39E-3	2.09E-3	2.84E-3
10.8	8.40E-4	9.77E-3	1.82E-2	1.76E-1	9.37E-3	4.67E-3	-2.79E-3	3.90E-3
11.0	8.07E-4	7.51E-3	2.05E-2	1.82E-1	1.26E-2	2.12E-3	3.48E-3	4.53E-3
11.2	6.92E-4	1.80E-3	1.48E-2	1.83E-1	1.16E-2	3.37E-4	-8.36E-3	3.61E-3
11.4	2.68E-4	4.84E-3	1.25E-2	1.86E-1	1.19E-2	-4.27E-4	-3.49E-3	2.06E-3
11.6	3.79E-4	-6.55E-3	1.88E-2	1.78E-1	9.78E-3	-4.27E-4	-1.40E-3	3.51E-3
11.8	5.66E-4	7.29E-3	1.50E-2	1.84E-1	1.00E-2	1.36E-3	6.95E-3	3.02E-3
12.0	1.34E-4	3.55E-3	1.38E-2	1.81E-1	1.04E-2	-1.70E-3	1.38E-3	3.51E-3
12.2	1.21E-3	3.89E-3	1.94E-2	1.78E-1	1.07E-2	8.47E-4	3.47E-3	4.42E-3
12.4	4.60E-4	-5.96E-3	1.52E-2	1.85E-1	9.84E-3	2.12E-3	1.32E-2	4.04E-3
12.6	7.24E-4	5.38E-3	2.45E-2	1.80E-1	1.00E-2	2.63E-3	-2.11E-3	1.57E-3
12.8	7.13E-4	7.07E-3	1.55E-2	1.85E-1	1.02E-2	4.67E-3	-7.15E-4	3.65E-3
13.0	9.22E-4	3.55E-3	2.14E-2	1.85E-1	1.14E-2	5.92E-4	-4.89E-3	2.63E-3
13.2	8.12E-4	-2.61E-3	1.37E-2	1.87E-1	1.08E-2	1.10E-3	-1.41E-3	3.16E-3
13.4	9.48E-4	3.92E-3	2.10E-2	1.83E-1	7.59E-3	8.47E-4	-7.17E-4	3.74E-3
13.6	-1.02E-4	1.99E-3	1.51E-2	1.89E-1	9.65E-3	1.87E-3	2.07E-3	4.47E-3
13.8	1.06E-3	5.08E-3	1.74E-2	1.85E-1	9.93E-3	-1.19E-3	3.46E-3	3.60E-3
14.0	1.41E-4	5.72E-3	1.42E-2	1.90E-1	1.10E-2	1.36E-3	-2.81E-3	3.45E-3
14.2	6.92E-4	9.11E-3	1.89E-2	1.92E-1	1.27E-2	1.10E-3	8.33E-3	3.89E-3

14.4	9.42E-4	2.19E-4	1.67E-2	1.86E-1	1.12E-2	1.61E-3	2.06E-3	3.60E-3
14.6	1.35E-4	9.76E-3	1.39E-2	1.96E-1	1.12E-2	1.87E-3	8.33E-3	3.60E-3
14.8	1.06E-3	6.12E-3	2.42E-2	1.87E-1	7.90E-3	5.92E-4	4.85E-3	5.29E-3
15.0	8.55E-4	-2.28E-5	1.85E-2	1.90E-1	1.34E-2	4.16E-3	4.15E-3	3.79E-3
15.2	1.40E-3	7.91E-3	1.81E-2	1.90E-1	1.13E-2	1.10E-3	-4.20E-3	3.35E-3
15.4	6.20E-4	3.96E-3	2.08E-2	1.93E-1	1.23E-2	2.12E-3	1.39E-2	4.95E-3
15.6	2.61E-5	-1.53E-4	2.03E-2	1.90E-1	1.20E-2	-4.27E-4	4.15E-3	2.68E-3
15.8	1.71E-3	8.80E-3	2.74E-2	1.94E-1	1.19E-2	1.61E-3	1.88E-2	4.66E-3
16.0	2.64E-4	6.90E-3	1.86E-2	1.92E-1	9.70E-3	3.14E-3	1.04E-2	4.85E-3
16.2	3.90E-4	7.79E-3	2.34E-2	1.97E-1	1.36E-2	8.23E-5	8.33E-3	4.80E-3
16.4	1.16E-3	2.77E-4	2.55E-2	1.87E-1	1.35E-2	-6.82E-4	9.02E-3	5.29E-3
16.6	2.57E-4	6.84E-3	1.89E-2	1.94E-1	9.92E-3	-4.27E-4	-2.64E-5	4.46E-3
16.8	3.52E-4	-3.04E-3	1.96E-2	1.96E-1	1.02E-2	3.37E-4	5.54E-3	5.48E-3
17.0	1.04E-3	-4.28E-3	1.84E-2	1.94E-1	1.20E-2	2.37E-3	1.53E-2	5.58E-3
17.2	5.08E-4	-2.10E-3	2.11E-2	1.96E-1	9.23E-3	2.37E-3	6.24E-3	2.24E-3
17.4	5.02E-4	2.78E-3	2.24E-2	1.93E-1	9.38E-3	3.14E-3	1.04E-2	3.35E-3
17.6	1.06E-3	-2.09E-3	2.04E-2	1.94E-1	1.17E-2	6.45E-3	1.37E-3	4.08E-3
17.8	-1.07E-4	1.28E-2	2.07E-2	2.00E-1	1.13E-2	8.47E-4	1.39E-2	2.58E-3
18.0	8.34E-4	2.97E-3	2.01E-2	1.96E-1	9.85E-3	1.87E-3	2.76E-3	3.88E-3
18.2	7.21E-4	1.05E-2	2.46E-2	1.95E-1	1.26E-2	2.88E-3	6.69E-4	5.29E-3
18.4	5.85E-4	-3.11E-4	2.48E-2	1.96E-1	1.07E-2	-1.19E-3	9.72E-3	3.59E-3
18.6	4.73E-4	4.79E-3	3.03E-2	1.94E-1	8.16E-3	2.12E-3	6.93E-3	6.59E-3
18.8	3.84E-4	-6.75E-3	2.07E-2	1.98E-1	1.24E-2	5.43E-3	1.37E-3	5.77E-3
19.0	8.16E-4	8.14E-3	2.59E-2	1.93E-1	9.76E-3	3.39E-3	-6.99E-3	5.14E-3
19.2	8.48E-4	-1.91E-3	2.20E-2	1.95E-1	1.24E-2	3.37E-4	6.93E-3	3.35E-3
19.4	3.55E-4	4.64E-3	1.68E-2	1.98E-1	1.15E-2	3.39E-3	1.18E-2	5.63E-3
19.6	2.36E-4	6.99E-3	3.00E-2	2.01E-1	1.27E-2	2.88E-3	1.11E-2	5.29E-3
19.8	1.40E-3	2.94E-3	2.52E-2	2.03E-1	1.31E-2	1.36E-3	8.33E-3	4.61E-3
20.0	5.93E-4	6.01E-3	2.62E-2	2.01E-1	1.04E-2	1.87E-3	4.85E-3	5.92E-3
20.2	3.86E-4	1.15E-3	2.35E-2	2.02E-1	1.38E-2	3.90E-3	5.54E-3	5.48E-3
20.4	1.05E-3	1.82E-3	2.49E-2	2.01E-1	1.19E-2	3.90E-3	4.15E-3	5.09E-3
20.6	5.93E-4	7.29E-3	3.40E-2	2.00E-1	1.11E-2	2.12E-3	6.24E-3	3.79E-3
20.8	7.16E-6	-3.56E-4	2.44E-2	1.94E-1	1.32E-2	3.37E-4	3.45E-3	3.45E-3
21.0	8.01E-4	1.04E-2	2.18E-2	2.04E-1	1.14E-2	4.16E-3	6.24E-3	4.37E-3
21.2	1.12E-3	4.37E-3	2.18E-2	2.02E-1	1.41E-2	5.18E-3	6.24E-3	5.67E-3
21.4	3.52E-4	4.83E-3	1.72E-2	2.01E-1	1.09E-2	3.14E-3	1.18E-2	3.69E-3
21.6	1.08E-3	3.14E-3	3.11E-2	2.00E-1	1.74E-2	1.87E-3	1.60E-2	4.66E-3
21.8	2.35E-4	4.16E-3	2.29E-2	2.03E-1	1.16E-2	2.12E-3	1.53E-2	3.83E-3
22.0	2.77E-5	1.55E-4	2.44E-2	2.02E-1	1.46E-2	8.47E-4	5.54E-3	4.66E-3
22.2	-1.02E-4	1.07E-2	2.40E-2	2.04E-1	1.28E-2	1.36E-3	4.85E-3	5.29E-3
22.4	1.40E-4	1.46E-2	2.19E-2	2.08E-1	1.38E-2	3.14E-3	7.63E-3	5.33E-3
22.6	2.54E-4	8.32E-3	2.40E-2	2.02E-1	1.45E-2	3.14E-3	5.54E-3	5.58E-3
22.8	4.79E-4	-3.66E-3	2.54E-2	1.98E-1	1.19E-2	8.47E-4	3.45E-3	3.64E-3

23.0	4.83E-4	4.60E-3	3.22E-2	2.01E-1	1.67E-2	2.63E-3	2.06E-3	5.92E-3
23.2	8.17E-4	7.68E-3	3.05E-2	2.03E-1	1.08E-2	8.47E-4	6.69E-4	4.13E-3
23.4	2.16E-3	4.94E-3	1.77E-2	2.05E-1	1.12E-2	-9.37E-4	1.18E-2	6.35E-3
23.6	1.63E-3	5.80E-3	2.85E-2	2.09E-1	1.23E-2	1.10E-3	1.04E-2	5.48E-3
23.8	1.38E-4	5.53E-3	2.59E-2	2.06E-1	1.21E-2	2.88E-3	6.24E-3	4.42E-3
24.0	3.75E-4	1.72E-3	3.39E-2	2.05E-1	1.41E-2	5.92E-4	-7.24E-4	4.90E-3
24.2	3.99E-4	1.81E-2	2.94E-2	2.05E-1	1.29E-2	4.41E-3	1.39E-2	4.71E-3
24.4	-1.04E-4	1.05E-2	2.32E-2	2.04E-1	1.32E-2	2.63E-3	9.02E-3	5.14E-3
24.6	3.81E-5	4.84E-3	3.05E-2	2.07E-1	1.37E-2	5.92E-4	1.46E-2	4.90E-3
24.8	9.57E-4	6.83E-5	2.93E-2	2.04E-1	1.28E-2	1.61E-3	9.02E-3	4.75E-3
25.0	1.09E-3	3.89E-3	2.52E-2	2.10E-1	1.10E-2	3.14E-3	-1.42E-3	4.13E-3
25.2	2.63E-4	2.72E-3	3.51E-2	2.07E-1	1.41E-2	6.45E-3	2.06E-3	3.16E-3
25.4	7.14E-4	6.42E-3	2.26E-2	2.04E-1	1.15E-2	1.36E-3	4.85E-3	5.87E-3
25.6	1.45E-4	6.05E-3	2.91E-2	2.08E-1	1.52E-2	3.90E-3	1.32E-2	7.32E-3
25.8	4.76E-4	8.00E-3	2.33E-2	1.99E-1	1.34E-2	3.39E-3	1.11E-2	5.00E-3
26.0	4.68E-4	8.34E-3	2.91E-2	2.07E-1	1.56E-2	1.87E-3	1.25E-2	5.77E-3
26.2	1.20E-3	1.48E-2	2.61E-2	2.08E-1	1.26E-2	2.37E-3	9.02E-3	3.01E-3
26.4	7.23E-4	1.89E-3	2.57E-2	2.06E-1	1.31E-2	1.87E-3	-3.51E-3	5.38E-3
26.6	-1.01E-4	7.39E-3	3.12E-2	2.09E-1	1.40E-2	3.65E-3	2.06E-3	5.92E-3
26.8	7.13E-4	1.55E-2	3.17E-2	2.11E-1	1.35E-2	8.23E-5	2.06E-3	6.93E-3
27.0	3.82E-4	5.36E-3	3.16E-2	2.07E-1	1.11E-2	2.12E-3	1.11E-2	6.40E-3
27.2	2.72E-4	7.23E-3	2.37E-2	2.06E-1	1.76E-2	2.63E-3	7.63E-3	7.32E-3
27.4	6.18E-4	-4.58E-4	2.45E-2	2.04E-1	1.10E-2	3.39E-3	1.25E-2	5.87E-3
27.6	3.57E-4	-3.19E-3	2.81E-2	2.03E-1	1.17E-2	1.87E-3	8.33E-3	6.88E-3
27.8	4.48E-4	6.89E-3	3.76E-2	2.07E-1	1.55E-2	5.18E-3	1.53E-2	6.11E-3
28.0	7.15E-4	8.37E-3	2.58E-2	2.09E-1	1.50E-2	1.87E-3	1.36E-3	6.01E-3
28.2	7.41E-4	5.95E-3	3.07E-2	2.10E-1	1.75E-2	3.39E-3	2.76E-3	5.96E-3
28.4	2.33E-4	1.23E-2	3.20E-2	2.05E-1	1.41E-2	3.90E-3	5.54E-3	5.14E-3
28.6	1.35E-4	1.51E-2	2.68E-2	2.01E-1	1.50E-2	1.10E-3	6.93E-3	6.50E-3
28.8	4.75E-4	6.20E-3	2.87E-2	2.04E-1	1.44E-2	-6.82E-4	1.11E-2	6.11E-3
29.0	5.91E-4	5.62E-3	2.73E-2	2.00E-1	1.21E-2	4.41E-3	4.85E-3	6.21E-3
29.2	6.39E-4	1.34E-2	3.21E-2	2.09E-1	1.14E-2	3.37E-4	1.11E-2	5.29E-3
29.4	7.33E-4	3.01E-3	3.27E-2	2.06E-1	1.51E-2	1.36E-3	8.33E-3	6.54E-3
29.6	7.78E-6	9.34E-3	2.93E-2	2.10E-1	1.37E-2	4.67E-3	6.93E-3	6.45E-3
29.8	1.17E-3	1.97E-3	2.69E-2	2.06E-1	1.77E-2	3.39E-3	1.60E-2	7.37E-3
30.0	2.53E-4	3.14E-3	2.65E-2	2.04E-1	1.24E-2	2.12E-3	5.54E-3	6.25E-3

Table S6: Experimental concentration-time profiles (normalized to $[Cl]_0$) for the species quantified at 600 K.

t (ms)	methyl	ethene	CH_2O	propene	CH_3CHO	acetone	propanal	oxetane	methyl-oxirane
-2.0	-4.38E-5	9.23E-3	-2.64E-3	-8.08E-4	1.55E-3	8.00E-4	-2.40E-3	3.26E-4	-2.46E-3
-1.8	-2.57E-4	-7.25E-4	1.96E-3	-1.09E-3	-6.50E-4	-1.59E-4	1.40E-3	-6.48E-5	-2.46E-3
-1.6	-4.21E-4	-8.63E-3	-2.93E-3	-1.13E-3	-1.24E-4	5.26E-4	1.78E-3	2.14E-4	2.13E-3
-1.4	-1.52E-4	1.52E-3	3.02E-4	-2.51E-4	-8.49E-4	3.89E-4	2.54E-3	1.58E-4	-1.14E-3
-1.2	-4.21E-4	6.66E-3	-1.71E-3	-1.52E-3	-2.36E-3	1.15E-4	2.16E-3	4.68E-5	-1.80E-3
-1.0	-1.55E-4	-7.19E-3	-3.10E-3	-9.39E-4	5.20E-4	-4.33E-4	-1.64E-3	-1.76E-4	3.31E-6
-0.8	-4.21E-4	-1.42E-2	-2.05E-3	-1.02E-3	-1.97E-4	2.52E-4	-4.99E-4	1.03E-4	1.67E-4
-0.6	-2.93E-4	2.22E-3	-3.35E-4	-1.20E-3	1.31E-3	-2.96E-4	-2.40E-3	-1.21E-4	-9.80E-4
-0.4	2.11E-4	-6.16E-4	-6.30E-4	-5.98E-4	-1.21E-3	1.15E-4	-2.02E-3	4.68E-5	-1.80E-3
-0.2	-2.90E-4	-3.91E-4	-1.64E-3	1.30E-3	-1.54E-3	-2.96E-4	-5.44E-3	-1.21E-4	-1.61E-4
0.0	-1.73E-5	1.07E-2	2.74E-3	1.91E-2	8.74E-3	1.48E-3	-3.46E-3	6.05E-4	-2.91E-3
0.2	5.01E-4	1.30E-2	-1.36E-3	1.01E-1	7.75E-3	-5.70E-4	-1.01E-3	-2.32E-4	-3.45E-3
0.4	1.19E-3	1.30E-2	3.57E-3	1.54E-1	4.33E-3	-5.70E-4	-5.09E-5	-2.32E-4	-3.40E-4
0.6	9.27E-4	1.64E-2	4.89E-3	1.83E-1	5.64E-3	-2.21E-5	-3.99E-3	-9.02E-6	8.55E-4
0.8	1.21E-3	-2.69E-3	1.62E-2	2.05E-1	5.18E-3	1.76E-3	3.86E-3	7.16E-4	3.24E-3
1.0	2.23E-3	4.18E-3	1.24E-2	2.16E-1	4.79E-3	8.00E-4	2.64E-3	3.26E-4	2.56E-3
1.2	2.62E-3	1.08E-2	8.60E-3	2.32E-1	5.80E-3	1.21E-3	3.33E-3	4.93E-4	2.08E-3
1.4	9.32E-4	-7.28E-3	6.06E-3	2.40E-1	4.93E-3	1.35E-3	7.85E-3	5.49E-4	2.95E-3
1.6	1.18E-3	4.81E-3	1.44E-2	2.48E-1	6.55E-3	8.00E-4	6.19E-4	3.26E-4	7.46E-4
1.8	1.70E-3	1.64E-2	1.90E-2	2.47E-1	4.34E-3	3.40E-3	1.05E-2	1.39E-3	1.69E-3
2.0	1.32E-3	2.56E-3	9.65E-3	2.54E-1	5.52E-3	1.48E-3	6.35E-3	6.05E-4	3.31E-3
2.2	1.27E-3	4.42E-4	1.54E-2	2.60E-1	6.10E-3	-2.21E-5	1.02E-2	-9.02E-6	3.50E-3
2.4	7.88E-4	3.02E-3	1.84E-2	2.68E-1	7.54E-3	1.90E-3	1.25E-2	7.72E-4	1.58E-3
2.6	2.35E-3	-1.34E-3	1.29E-2	2.69E-1	8.40E-3	2.44E-3	9.58E-3	9.95E-4	6.89E-3
2.8	2.56E-3	1.56E-2	1.33E-2	2.63E-1	5.06E-3	2.85E-3	5.50E-3	1.16E-3	3.71E-3
3.0	1.33E-3	1.47E-2	1.67E-2	2.77E-1	8.29E-3	1.90E-3	9.41E-3	7.72E-4	7.44E-3
3.2	1.70E-3	6.63E-3	1.60E-2	2.80E-1	6.63E-3	3.13E-3	1.52E-2	1.27E-3	4.63E-3
3.4	1.03E-3	6.29E-4	1.38E-2	2.80E-1	6.68E-3	1.62E-3	3.60E-3	6.61E-4	3.97E-3
3.6	2.21E-3	-8.46E-5	1.32E-2	2.84E-1	8.41E-3	2.72E-3	3.76E-3	1.11E-3	2.19E-3
3.8	2.36E-3	-9.51E-4	1.05E-2	2.87E-1	1.03E-2	3.68E-3	5.83E-3	1.50E-3	5.01E-3
4.0	1.57E-3	-5.25E-3	2.08E-2	2.93E-1	6.26E-3	2.17E-3	7.91E-3	8.84E-4	8.67E-3
4.2	1.45E-3	-5.10E-4	1.79E-2	2.97E-1	8.64E-3	1.76E-3	5.82E-3	7.16E-4	7.92E-3
4.4	3.15E-3	-1.30E-3	1.40E-2	2.97E-1	5.69E-3	1.62E-3	1.02E-2	6.61E-4	5.71E-3
4.6	2.24E-3	2.02E-2	1.81E-2	3.05E-1	7.37E-3	2.03E-3	8.89E-3	8.28E-4	2.37E-3
4.8	1.42E-3	1.81E-2	1.44E-2	3.04E-1	1.01E-2	2.03E-3	9.49E-3	8.28E-4	2.65E-3
5.0	1.29E-3	1.21E-2	1.37E-2	3.14E-1	9.94E-3	2.58E-3	8.96E-3	1.05E-3	7.20E-3
5.2	1.43E-3	-7.40E-3	1.31E-2	3.12E-1	4.20E-3	5.59E-3	8.43E-3	2.28E-3	6.03E-3
5.4	1.05E-3	7.10E-3	1.71E-2	3.08E-1	5.15E-3	9.37E-4	1.02E-2	3.82E-4	6.50E-3
5.6	1.69E-3	1.14E-2	2.08E-2	3.20E-1	5.01E-3	2.72E-3	6.65E-3	1.11E-3	5.35E-3

5.8	1.19E-3	-4.36E-4	2.23E-2	3.28E-1	7.32E-3	1.21E-3	1.15E-2	4.93E-4	1.75E-3
6.0	1.76E-3	1.48E-2	2.08E-2	3.27E-1	1.25E-2	2.99E-3	1.48E-2	1.22E-3	8.32E-3
6.2	1.68E-3	9.62E-4	1.98E-2	3.36E-1	9.79E-3	2.58E-3	7.07E-3	1.05E-3	7.04E-3
6.4	2.11E-3	8.13E-3	1.89E-2	3.36E-1	9.60E-3	1.90E-3	6.59E-3	7.72E-4	7.23E-3
6.6	1.83E-3	1.44E-2	2.11E-2	3.43E-1	9.15E-3	2.58E-3	4.97E-3	1.05E-3	1.86E-3
6.8	1.67E-3	-2.89E-3	1.91E-2	3.36E-1	8.32E-3	2.03E-3	4.12E-3	8.28E-4	6.66E-3
7.0	1.20E-3	-4.54E-3	1.83E-2	3.48E-1	1.29E-2	2.99E-3	1.01E-2	1.22E-3	1.47E-3
7.2	3.02E-3	1.30E-2	2.31E-2	3.43E-1	1.29E-2	2.85E-3	1.12E-2	1.16E-3	4.97E-3
7.4	1.21E-3	5.02E-3	2.95E-2	3.47E-1	8.27E-3	4.09E-3	8.06E-3	1.67E-3	7.50E-3
7.6	1.17E-3	3.11E-3	1.51E-2	3.55E-1	1.04E-2	3.68E-3	5.33E-3	1.50E-3	7.90E-3
7.8	1.96E-3	1.47E-2	2.31E-2	3.58E-1	1.15E-2	3.95E-3	8.68E-3	1.61E-3	7.16E-3
8.0	2.48E-3	7.87E-3	2.68E-2	3.64E-1	5.63E-3	3.27E-3	4.81E-3	1.33E-3	6.09E-3
8.2	9.14E-4	1.52E-2	3.02E-2	3.67E-1	1.04E-2	2.85E-3	1.05E-2	1.16E-3	7.49E-3
8.4	1.05E-3	8.66E-3	3.18E-2	3.64E-1	9.70E-3	3.13E-3	6.97E-3	1.27E-3	7.26E-3
8.6	9.52E-4	-5.48E-3	2.05E-2	3.67E-1	1.20E-2	2.72E-3	1.26E-2	1.11E-3	8.83E-3
8.8	2.20E-3	9.14E-3	2.33E-2	3.75E-1	9.78E-3	2.31E-3	1.22E-2	9.40E-4	1.06E-2
9.0	1.94E-3	7.70E-3	2.35E-2	3.77E-1	9.46E-3	2.31E-3	1.10E-2	9.40E-4	7.39E-3
9.2	1.34E-3	3.09E-3	2.66E-2	3.85E-1	1.21E-2	1.76E-3	1.32E-2	7.16E-4	7.01E-3
9.4	1.55E-3	1.58E-2	3.19E-2	3.79E-1	1.48E-2	3.27E-3	2.93E-3	1.33E-3	5.81E-3
9.6	2.47E-3	5.28E-3	3.00E-2	3.95E-1	1.27E-2	3.95E-3	8.21E-3	1.61E-3	9.85E-3
9.8	1.82E-3	7.08E-4	3.30E-2	3.96E-1	1.25E-2	3.81E-3	1.01E-2	1.55E-3	6.04E-3
10.0	1.17E-3	3.42E-2	2.74E-2	4.01E-1	1.38E-2	3.27E-3	9.27E-3	1.33E-3	6.16E-3
10.2	9.04E-4	2.18E-2	3.02E-2	4.07E-1	9.21E-3	3.13E-3	1.53E-2	1.27E-3	4.31E-3
10.4	1.32E-3	6.62E-3	3.88E-2	4.09E-1	1.30E-2	4.22E-3	1.03E-2	1.72E-3	9.35E-3
10.6	1.56E-3	1.32E-2	2.91E-2	4.11E-1	1.02E-2	2.03E-3	7.66E-3	8.28E-4	1.19E-2
10.8	3.05E-3	1.37E-2	2.90E-2	4.14E-1	1.38E-2	4.09E-3	8.01E-3	1.67E-3	1.21E-2
11.0	1.57E-3	-5.29E-3	2.62E-2	4.26E-1	1.06E-2	4.77E-3	1.25E-2	1.94E-3	7.94E-3
11.2	1.17E-3	9.39E-3	3.60E-2	4.16E-1	1.36E-2	3.68E-3	1.97E-2	1.50E-3	6.43E-3
11.4	1.57E-3	1.29E-2	3.23E-2	4.16E-1	1.08E-2	1.90E-3	1.17E-2	7.72E-4	5.75E-3
11.6	1.54E-3	1.28E-2	4.28E-2	4.26E-1	1.11E-2	6.00E-3	1.25E-2	2.45E-3	9.66E-3
11.8	8.04E-4	1.76E-2	3.08E-2	4.32E-1	1.01E-2	4.63E-3	7.50E-3	1.89E-3	9.14E-3
12.0	1.69E-3	1.64E-2	3.01E-2	4.26E-1	1.05E-2	3.81E-3	1.36E-2	1.55E-3	1.04E-2
12.2	1.39E-3	1.55E-2	4.37E-2	4.42E-1	1.23E-2	3.27E-3	1.58E-2	1.33E-3	1.19E-2
12.4	1.28E-3	-9.26E-3	3.37E-2	4.32E-1	6.66E-3	3.54E-3	1.50E-2	1.44E-3	9.23E-3
12.6	1.94E-3	5.73E-3	4.15E-2	4.41E-1	1.07E-2	5.59E-3	1.16E-2	2.28E-3	9.38E-3
12.8	1.83E-3	3.59E-2	3.15E-2	4.36E-1	1.54E-2	2.85E-3	9.69E-3	1.16E-3	6.74E-3
13.0	1.73E-3	1.64E-2	4.16E-2	4.51E-1	1.44E-2	3.27E-3	1.46E-2	1.33E-3	1.11E-2
13.2	1.30E-3	8.17E-3	4.69E-2	4.57E-1	1.05E-2	2.72E-3	1.27E-2	1.11E-3	8.67E-3
13.4	2.42E-3	6.09E-3	3.82E-2	4.67E-1	1.16E-2	3.81E-3	1.57E-2	1.55E-3	9.64E-3
13.6	2.72E-3	1.00E-2	4.03E-2	4.58E-1	1.10E-2	2.72E-3	1.53E-2	1.11E-3	1.09E-2
13.8	1.21E-3	2.57E-2	3.83E-2	4.64E-1	1.20E-2	2.85E-3	5.06E-3	1.16E-3	7.64E-3
14.0	7.96E-4	1.92E-2	3.54E-2	4.63E-1	1.44E-2	5.32E-3	1.38E-2	2.17E-3	1.47E-2
14.2	1.06E-3	9.82E-3	4.03E-2	4.75E-1	1.10E-2	4.36E-3	1.34E-2	1.78E-3	9.25E-3

14.4	1.22E-3	2.05E-2	3.72E-2	4.71E-1	1.15E-2	3.40E-3	1.03E-2	1.39E-3	1.10E-2
14.6	1.84E-3	1.28E-2	3.91E-2	4.73E-1	9.26E-3	3.27E-3	6.54E-3	1.33E-3	1.48E-2
14.8	6.85E-4	1.15E-2	4.30E-2	4.71E-1	1.46E-2	1.35E-3	1.72E-2	5.49E-4	9.38E-3
15.0	1.30E-3	1.27E-2	4.02E-2	4.84E-1	9.12E-3	4.91E-3	1.56E-2	2.00E-3	1.45E-2
15.2	1.56E-3	2.49E-2	4.99E-2	4.89E-1	1.26E-2	3.68E-3	9.17E-3	1.50E-3	8.87E-3
15.4	4.95E-4	1.87E-2	4.90E-2	4.78E-1	1.18E-2	4.77E-3	1.11E-2	1.94E-3	1.56E-2
15.6	1.43E-3	1.34E-2	4.51E-2	4.92E-1	1.35E-2	2.31E-3	1.18E-2	9.40E-4	1.46E-2
15.8	1.21E-3	2.22E-2	3.84E-2	4.97E-1	1.14E-2	4.50E-3	6.49E-3	1.83E-3	1.43E-2
16.0	1.30E-3	6.93E-3	4.67E-2	5.01E-1	1.25E-2	4.63E-3	1.10E-2	1.89E-3	1.43E-2
16.2	1.59E-3	3.42E-3	3.44E-2	4.99E-1	1.25E-2	4.36E-3	1.63E-2	1.78E-3	1.41E-2
16.4	2.20E-3	9.48E-3	4.74E-2	5.09E-1	1.32E-2	3.27E-3	1.44E-2	1.33E-3	1.49E-2
16.6	3.91E-4	2.06E-2	3.61E-2	5.04E-1	1.10E-2	2.17E-3	9.50E-3	8.84E-4	9.48E-3
16.8	1.39E-3	3.19E-3	5.58E-2	5.11E-1	8.76E-3	2.58E-3	7.98E-3	1.05E-3	1.54E-2
17.0	3.62E-4	1.74E-2	4.44E-2	5.16E-1	1.17E-2	3.95E-3	1.40E-2	1.61E-3	1.67E-2
17.2	1.07E-3	1.74E-2	4.01E-2	5.13E-1	1.07E-2	2.85E-3	7.21E-3	1.16E-3	1.32E-2
17.4	1.17E-3	1.64E-2	3.63E-2	5.16E-1	1.22E-2	3.27E-3	1.06E-2	1.33E-3	7.82E-3
17.6	5.09E-4	2.36E-2	4.73E-2	5.22E-1	1.42E-2	2.72E-3	1.25E-2	1.11E-3	1.22E-2
17.8	2.20E-3	3.44E-2	4.37E-2	5.29E-1	1.52E-2	4.22E-3	1.25E-2	1.72E-3	1.55E-2
18.0	1.21E-3	9.40E-3	4.44E-2	5.33E-1	1.05E-2	2.17E-3	5.29E-3	8.84E-4	1.90E-2
18.2	1.03E-3	1.58E-2	4.48E-2	5.42E-1	1.21E-2	3.27E-3	1.25E-2	1.33E-3	1.34E-2
18.4	1.68E-3	2.86E-2	4.47E-2	5.31E-1	1.30E-2	6.00E-3	1.25E-2	2.45E-3	1.29E-2
18.6	4.84E-4	1.47E-2	5.09E-2	5.32E-1	9.50E-3	3.13E-3	1.02E-2	1.27E-3	1.96E-2
18.8	1.70E-3	5.34E-3	4.89E-2	5.48E-1	1.43E-2	2.85E-3	6.42E-3	1.16E-3	1.62E-2
19.0	1.27E-3	2.37E-2	4.94E-2	5.46E-1	1.24E-2	2.58E-3	1.40E-2	1.05E-3	7.95E-3
19.2	1.30E-3	1.67E-2	5.19E-2	5.47E-1	1.57E-2	3.54E-3	3.37E-3	1.44E-3	8.28E-3
19.4	5.15E-4	1.74E-2	4.81E-2	5.52E-1	1.57E-2	3.27E-3	1.70E-2	1.33E-3	1.32E-2
19.6	1.85E-3	1.78E-2	4.97E-2	5.49E-1	1.14E-2	2.03E-3	1.63E-2	8.28E-4	1.66E-2
19.8	5.14E-4	2.62E-2	5.58E-2	5.48E-1	1.33E-2	3.81E-3	1.10E-2	1.55E-3	1.22E-2
20.0	9.14E-4	1.16E-2	4.03E-2	5.58E-1	1.45E-2	3.27E-3	9.06E-3	1.33E-3	1.45E-2
20.2	1.59E-3	1.52E-2	5.45E-2	5.55E-1	1.39E-2	4.09E-3	1.63E-2	1.67E-3	1.15E-2
20.4	1.20E-3	1.87E-2	5.40E-2	5.62E-1	1.37E-2	3.81E-3	1.32E-2	1.55E-3	1.58E-2
20.6	5.28E-4	2.16E-2	4.91E-2	5.52E-1	1.51E-2	1.62E-3	1.13E-2	6.61E-4	1.37E-2
20.8	2.00E-3	9.58E-3	5.69E-2	5.70E-1	1.29E-2	2.99E-3	1.13E-2	1.22E-3	1.30E-2
21.0	5.13E-4	1.28E-3	5.61E-2	5.70E-1	1.07E-2	2.85E-3	1.36E-2	1.16E-3	1.56E-2
21.2	1.32E-3	1.08E-2	5.19E-2	5.78E-1	1.34E-2	1.48E-3	1.59E-2	6.05E-4	1.25E-2
21.4	3.85E-4	1.50E-2	4.58E-2	5.69E-1	1.49E-2	4.77E-3	1.28E-2	1.94E-3	1.45E-2
21.6	1.04E-3	2.14E-2	5.64E-2	5.70E-1	1.37E-2	3.95E-3	1.13E-2	1.61E-3	8.91E-3
21.8	1.53E-3	9.78E-3	5.40E-2	5.69E-1	1.11E-2	4.36E-3	1.66E-2	1.78E-3	1.37E-2
22.0	1.03E-3	2.22E-2	5.52E-2	5.83E-1	1.49E-2	3.54E-3	1.55E-2	1.44E-3	1.60E-2
22.2	7.66E-4	1.31E-2	5.43E-2	5.87E-1	1.17E-2	4.77E-3	1.21E-2	1.94E-3	1.02E-2
22.4	3.96E-4	2.64E-2	4.94E-2	5.82E-1	1.07E-2	2.58E-3	7.90E-3	1.05E-3	1.10E-2
22.6	4.15E-4	1.04E-2	6.03E-2	5.87E-1	1.52E-2	3.54E-3	1.44E-2	1.44E-3	1.35E-2
22.8	7.56E-4	1.24E-2	5.84E-2	5.86E-1	1.09E-2	5.87E-3	1.44E-2	2.39E-3	1.35E-2

23.0	9.04E-4	2.29E-2	5.70E-2	5.88E-1	1.44E-2	3.13E-3	1.59E-2	1.27E-3	1.27E-2
23.2	1.29E-3	2.26E-2	4.93E-2	6.00E-1	1.25E-2	3.13E-3	1.36E-2	1.27E-3	1.96E-2
23.4	8.94E-4	1.58E-2	5.07E-2	5.98E-1	1.85E-2	4.91E-3	1.55E-2	2.00E-3	1.50E-2
23.6	1.39E-3	2.56E-2	4.56E-2	5.99E-1	1.05E-2	4.77E-3	1.28E-2	1.94E-3	1.74E-2
23.8	1.04E-3	1.50E-2	5.06E-2	5.99E-1	1.24E-2	2.44E-3	1.25E-2	9.95E-4	1.10E-2
24.0	7.40E-4	2.33E-2	6.08E-2	5.99E-1	1.47E-2	4.50E-3	1.51E-2	1.83E-3	1.73E-2
24.2	4.87E-4	3.06E-2	5.94E-2	6.11E-1	1.50E-2	2.99E-3	7.14E-3	1.22E-3	1.53E-2
24.4	5.20E-4	2.42E-2	5.82E-2	6.06E-1	1.10E-2	4.63E-3	1.44E-2	1.89E-3	1.15E-2
24.6	1.42E-3	1.33E-2	5.41E-2	6.08E-1	1.20E-2	3.95E-3	1.63E-2	1.61E-3	1.64E-2
24.8	1.01E-3	1.52E-2	4.99E-2	6.09E-1	1.42E-2	3.27E-3	1.25E-2	1.33E-3	1.64E-2
25.0	2.83E-3	2.22E-2	5.45E-2	6.07E-1	1.23E-2	2.17E-3	8.65E-3	8.84E-4	1.91E-2
25.2	7.72E-4	1.79E-2	6.62E-2	6.12E-1	1.29E-2	2.85E-3	1.13E-2	1.16E-3	1.58E-2
25.4	6.62E-4	2.36E-2	5.20E-2	6.08E-1	1.11E-2	4.09E-3	9.41E-3	1.67E-3	1.69E-2
25.6	8.06E-4	3.24E-2	5.93E-2	6.23E-1	1.35E-2	4.50E-3	1.70E-2	1.83E-3	2.07E-2
25.8	1.00E-3	2.35E-3	5.65E-2	6.04E-1	1.13E-2	3.27E-3	6.37E-3	1.33E-3	1.91E-2
26.0	2.45E-3	2.17E-2	5.51E-2	6.18E-1	9.12E-3	4.63E-3	1.09E-2	1.89E-3	1.81E-2
26.2	9.97E-4	2.42E-2	5.60E-2	6.14E-1	1.42E-2	3.40E-3	1.24E-2	1.39E-3	1.45E-2
26.4	4.95E-4	2.99E-2	6.28E-2	6.26E-1	1.62E-2	3.27E-3	1.02E-2	1.33E-3	1.38E-2
26.6	1.27E-3	2.13E-2	5.24E-2	6.26E-1	1.27E-2	5.46E-3	1.17E-2	2.22E-3	1.79E-2
26.8	9.45E-4	2.68E-2	7.20E-2	6.26E-1	1.19E-2	2.99E-3	1.32E-2	1.22E-3	1.89E-2
27.0	6.37E-4	1.53E-2	5.24E-2	6.27E-1	1.23E-2	3.13E-3	1.24E-2	1.27E-3	1.76E-2
27.2	7.46E-4	2.52E-2	6.10E-2	6.28E-1	1.48E-2	2.99E-3	1.93E-2	1.22E-3	1.71E-2
27.4	1.06E-3	2.32E-3	5.62E-2	6.28E-1	1.63E-2	2.85E-3	8.27E-3	1.16E-3	2.22E-2
27.6	1.02E-3	1.85E-2	5.72E-2	6.30E-1	1.31E-2	2.99E-3	1.62E-2	1.22E-3	1.61E-2
27.8	2.47E-4	9.20E-3	5.86E-2	6.30E-1	1.11E-2	2.58E-3	5.23E-3	1.05E-3	1.45E-2
28.0	1.87E-3	2.64E-2	6.09E-2	6.35E-1	1.07E-2	4.09E-3	1.66E-2	1.67E-3	1.28E-2
28.2	1.27E-3	2.84E-2	5.06E-2	6.36E-1	1.68E-2	2.72E-3	9.41E-3	1.11E-3	1.77E-2
28.4	7.76E-4	2.78E-2	6.65E-2	6.35E-1	1.88E-2	4.77E-3	2.19E-3	1.94E-3	2.13E-2
28.6	3.75E-4	2.57E-2	6.46E-2	6.38E-1	1.61E-2	2.58E-3	1.05E-2	1.05E-3	1.35E-2
28.8	5.20E-4	4.84E-2	5.99E-2	6.23E-1	1.61E-2	1.76E-3	7.89E-3	7.16E-4	1.64E-2
29.0	1.31E-3	1.71E-2	6.50E-2	6.22E-1	1.49E-2	3.40E-3	1.05E-3	1.39E-3	1.32E-2
29.2	1.34E-3	1.71E-2	6.63E-2	6.22E-1	1.48E-2	2.58E-3	1.13E-2	1.05E-3	1.64E-2
29.4	6.34E-4	1.45E-2	6.80E-2	6.36E-1	1.29E-2	4.50E-3	2.08E-2	1.83E-3	2.22E-2
29.6	5.36E-4	8.90E-3	5.96E-2	6.33E-1	1.65E-2	2.85E-3	8.27E-3	1.16E-3	1.59E-2
29.8	9.02E-4	3.44E-2	4.85E-2	6.35E-1	1.65E-2	1.76E-3	1.59E-2	7.16E-4	1.58E-2
30.0	7.83E-4	2.19E-2	6.75E-2	6.36E-1	1.62E-2	1.90E-3	1.17E-2	7.72E-4	1.58E-2

Table S7: Experimental concentration-time profiles (normalized to $[Cl]_0$) for the species quantified at 670 K.

t (ms)	methyl	ethene	CH_2O	propene	CH_3CHO	acetone	propanal	oxetane	methyl-oxirane
-2.0	-4.53E-4	2.38E-2	8.60E-4	-2.75E-4	-1.30E-3	-3.91E-4	1.05E-4	-1.37E-3	-1.36E-3
-1.8	-6.74E-5	9.85E-4	-1.72E-3	-3.31E-4	-4.04E-4	5.13E-4	2.78E-3	1.80E-3	-2.80E-4
-1.6	2.69E-5	2.10E-2	8.05E-4	-1.27E-5	-1.82E-3	1.43E-4	-3.24E-3	5.03E-4	4.42E-5
-1.4	3.31E-5	1.12E-2	4.45E-3	-1.39E-3	1.11E-3	-2.68E-4	3.28E-4	-9.39E-4	-1.79E-3
-1.2	-3.27E-4	1.12E-2	5.07E-4	-1.67E-3	1.13E-3	1.43E-4	-1.23E-3	5.03E-4	-1.15E-3
-1.0	1.46E-4	-1.28E-3	-3.85E-3	-1.13E-3	3.84E-3	-3.09E-4	-7.88E-4	-1.08E-3	1.99E-3
-0.8	1.60E-4	8.04E-4	1.34E-3	-5.66E-4	-9.01E-4	2.01E-5	-1.23E-3	7.07E-5	-9.29E-4
-0.6	-4.53E-4	-1.90E-3	4.20E-3	-8.52E-4	1.16E-3	-2.26E-4	-1.01E-3	-7.95E-4	-9.29E-4
-0.4	-2.62E-4	4.15E-3	-1.83E-4	-5.62E-4	-9.47E-4	-6.21E-5	-1.18E-4	-2.18E-4	4.42E-5
-0.2	2.77E-4	-9.64E-3	-2.94E-3	-2.34E-3	-1.29E-3	-2.68E-4	-3.02E-3	-9.39E-4	-6.05E-4
0.0	8.85E-4	2.39E-3	2.64E-3	1.39E-2	5.24E-3	1.02E-4	3.17E-3	3.59E-4	-2.04E-3
0.2	3.21E-3	2.73E-2	2.53E-3	1.09E-1	3.83E-3	-1.85E-4	5.38E-3	-6.51E-4	1.35E-3
0.4	6.58E-3	-1.55E-2	6.94E-3	1.85E-1	2.30E-3	-2.10E-5	-2.32E-3	-7.36E-5	3.12E-3
0.6	6.65E-3	2.20E-2	1.65E-2	2.51E-1	6.15E-3	2.67E-4	2.36E-3	9.36E-4	4.88E-3
0.8	9.13E-3	-1.16E-2	1.15E-2	2.90E-1	4.37E-3	4.72E-4	2.45E-3	1.66E-3	9.53E-3
1.0	6.95E-3	2.23E-2	1.83E-2	3.29E-1	7.04E-3	7.60E-4	5.75E-3	2.67E-3	9.07E-3
1.2	1.01E-2	7.39E-3	1.63E-2	3.62E-1	3.21E-3	1.21E-3	1.31E-3	4.25E-3	7.60E-3
1.4	6.59E-3	-1.65E-3	2.17E-2	3.83E-1	9.77E-3	1.05E-3	4.96E-3	3.68E-3	8.68E-3
1.6	9.15E-3	6.65E-3	2.48E-2	4.20E-1	7.04E-3	3.90E-4	-7.12E-4	1.37E-3	9.05E-3
1.8	1.07E-2	1.08E-2	2.47E-2	4.29E-1	1.08E-2	1.38E-3	7.06E-3	4.83E-3	1.12E-2
2.0	1.20E-2	4.11E-2	2.71E-2	4.50E-1	5.36E-3	9.65E-4	5.48E-3	3.39E-3	8.32E-3
2.2	1.09E-2	2.68E-2	3.91E-2	4.67E-1	1.04E-2	1.13E-3	8.20E-4	3.97E-3	1.09E-2
2.4	1.01E-2	3.36E-2	3.65E-2	4.82E-1	9.18E-3	1.29E-3	4.89E-3	4.54E-3	1.30E-2
2.6	1.38E-2	3.14E-2	2.87E-2	5.01E-1	8.35E-3	3.49E-4	6.75E-3	1.22E-3	1.39E-2
2.8	1.06E-2	4.27E-2	3.45E-2	5.20E-1	7.90E-3	1.34E-3	6.85E-3	4.69E-3	9.01E-3
3.0	9.77E-3	5.43E-2	3.47E-2	5.37E-1	1.11E-2	1.17E-3	6.74E-3	4.11E-3	1.47E-2
3.2	9.30E-3	2.71E-2	4.74E-2	5.38E-1	1.17E-2	5.13E-4	4.42E-3	1.80E-3	1.62E-2
3.4	1.29E-2	4.98E-2	3.74E-2	5.57E-1	8.29E-3	1.09E-3	7.69E-3	3.82E-3	1.71E-2
3.6	1.03E-2	4.80E-2	4.80E-2	5.62E-1	5.58E-3	1.05E-3	1.81E-3	3.68E-3	1.46E-2
3.8	1.14E-2	6.06E-2	3.50E-2	5.93E-1	1.12E-2	5.13E-4	1.31E-3	1.80E-3	1.37E-2
4.0	1.04E-2	4.25E-2	4.66E-2	5.82E-1	9.00E-3	1.17E-3	6.84E-3	4.11E-3	1.54E-2
4.2	1.24E-2	5.08E-2	4.33E-2	5.91E-1	5.81E-3	1.29E-3	5.01E-3	4.54E-3	1.69E-2
4.4	1.02E-2	6.82E-2	3.79E-2	6.06E-1	1.21E-2	1.09E-3	5.42E-3	3.82E-3	1.57E-2
4.6	1.13E-2	5.99E-2	4.16E-2	6.18E-1	1.17E-2	1.46E-3	4.49E-3	5.12E-3	1.74E-2
4.8	1.05E-2	5.35E-2	4.98E-2	6.35E-1	1.26E-2	1.01E-3	7.81E-3	3.53E-3	1.52E-2
5.0	1.16E-2	5.63E-2	5.87E-2	6.43E-1	8.01E-3	8.42E-4	8.24E-3	2.96E-3	1.55E-2
5.2	1.15E-2	5.75E-2	5.56E-2	6.34E-1	8.35E-3	1.09E-3	8.44E-3	3.82E-3	1.80E-2
5.4	1.17E-2	5.93E-2	4.97E-2	6.61E-1	5.72E-3	8.83E-4	8.65E-3	3.10E-3	1.66E-2
5.6	1.07E-2	7.63E-2	4.85E-2	6.65E-1	1.03E-2	1.09E-3	6.85E-3	3.82E-3	1.77E-2

5.8	1.14E-2	6.17E-2	4.45E-2	6.78E-1	9.82E-3	1.21E-3	6.61E-3	4.25E-3	2.10E-2
6.0	1.13E-2	5.91E-2	5.02E-2	6.83E-1	8.08E-3	1.34E-3	6.60E-3	4.69E-3	1.69E-2
6.2	1.20E-2	5.99E-2	5.59E-2	6.88E-1	9.82E-3	8.01E-4	1.04E-2	2.81E-3	2.04E-2
6.4	1.24E-2	6.31E-2	5.29E-2	6.92E-1	8.75E-3	1.58E-3	6.36E-3	5.55E-3	1.52E-2
6.6	1.12E-2	5.71E-2	5.55E-2	6.95E-1	1.22E-2	3.90E-4	6.13E-3	1.37E-3	1.55E-2
6.8	9.50E-3	6.74E-2	6.06E-2	6.99E-1	9.14E-3	1.42E-3	2.99E-3	4.98E-3	2.04E-2
7.0	1.09E-2	4.05E-2	5.89E-2	7.10E-1	6.60E-3	1.25E-3	7.46E-3	4.40E-3	2.11E-2
7.2	9.85E-3	6.43E-2	5.91E-2	7.18E-1	9.09E-3	1.46E-3	1.08E-2	5.12E-3	1.83E-2
7.4	9.62E-3	9.27E-2	5.81E-2	7.14E-1	6.69E-3	1.01E-3	1.28E-2	3.53E-3	1.99E-2
7.6	1.03E-2	7.29E-2	6.39E-2	7.24E-1	1.03E-2	1.58E-3	6.55E-3	5.55E-3	1.96E-2
7.8	1.04E-2	8.38E-2	5.95E-2	7.41E-1	9.45E-3	9.24E-4	6.32E-3	3.24E-3	1.83E-2
8.0	1.08E-2	7.86E-2	7.08E-2	7.40E-1	9.74E-3	8.42E-4	6.77E-3	2.96E-3	2.00E-2
8.2	9.11E-3	6.55E-2	6.91E-2	7.40E-1	6.09E-3	1.01E-3	7.21E-3	3.53E-3	2.07E-2
8.4	8.37E-3	8.17E-2	7.43E-2	7.47E-1	9.97E-3	1.38E-3	7.21E-3	4.83E-3	1.79E-2
8.6	9.55E-3	5.45E-2	6.95E-2	7.49E-1	7.98E-3	1.21E-3	4.75E-3	4.25E-3	1.86E-2
8.8	9.26E-3	8.09E-2	7.55E-2	7.58E-1	1.43E-2	1.66E-3	7.21E-3	5.84E-3	2.07E-2
9.0	7.08E-3	7.49E-2	7.32E-2	7.62E-1	7.37E-3	2.26E-4	1.06E-2	7.92E-4	2.08E-2
9.2	1.15E-2	8.98E-2	7.53E-2	7.57E-1	1.48E-2	7.60E-4	7.21E-3	2.67E-3	1.97E-2
9.4	8.02E-3	9.84E-2	8.15E-2	7.56E-1	7.44E-3	8.83E-4	7.65E-3	3.10E-3	1.90E-2
9.6	7.80E-3	8.61E-2	7.15E-2	7.68E-1	1.29E-2	1.09E-3	8.99E-3	3.82E-3	2.33E-2
9.8	8.12E-3	8.45E-2	7.41E-2	7.68E-1	1.13E-2	1.54E-3	8.32E-3	5.41E-3	2.27E-2
10.0	9.58E-3	9.73E-2	8.23E-2	7.70E-1	1.33E-2	9.24E-4	1.17E-2	3.24E-3	2.24E-2
10.2	1.04E-2	9.86E-2	8.59E-2	7.69E-1	1.29E-2	5.96E-4	2.29E-3	2.09E-3	2.12E-2
10.4	6.34E-3	8.36E-2	7.88E-2	7.81E-1	9.40E-3	1.21E-3	1.03E-2	4.25E-3	2.28E-2
10.6	8.06E-3	9.81E-2	7.46E-2	7.75E-1	9.04E-3	1.46E-3	1.01E-2	5.12E-3	2.49E-2
10.8	9.47E-3	6.77E-2	8.15E-2	7.89E-1	1.15E-2	5.96E-4	1.01E-2	2.09E-3	2.11E-2
11.0	7.45E-3	9.27E-2	7.21E-2	7.89E-1	8.56E-3	1.25E-3	1.17E-2	4.40E-3	2.41E-2
11.2	7.88E-3	5.17E-2	7.95E-2	7.90E-1	9.79E-3	1.17E-3	4.08E-3	4.11E-3	1.78E-2
11.4	7.37E-3	9.52E-2	1.02E-1	7.93E-1	6.89E-3	9.65E-4	6.98E-3	3.39E-3	1.95E-2
11.6	9.07E-3	9.95E-2	9.67E-2	7.87E-1	8.90E-3	1.34E-3	6.53E-3	4.69E-3	2.42E-2
11.8	6.42E-3	1.10E-1	8.01E-2	7.96E-1	1.09E-2	1.13E-3	5.64E-3	3.97E-3	2.18E-2
12.0	8.82E-3	9.69E-2	7.90E-2	8.02E-1	9.92E-3	8.42E-4	2.07E-3	2.96E-3	1.98E-2
12.2	6.89E-3	1.01E-1	7.48E-2	8.03E-1	8.29E-3	1.13E-3	4.75E-3	3.97E-3	2.02E-2
12.4	8.26E-3	1.19E-1	9.37E-2	8.12E-1	1.36E-2	1.79E-3	8.99E-3	6.27E-3	2.20E-2
12.6	8.17E-3	9.51E-2	8.87E-2	8.04E-1	8.13E-3	7.60E-4	6.98E-3	2.67E-3	2.11E-2
12.8	8.59E-3	9.41E-2	9.20E-2	8.07E-1	1.32E-2	8.42E-4	6.08E-3	2.96E-3	2.16E-2
13.0	7.07E-3	7.53E-2	8.86E-2	8.12E-1	9.33E-3	1.01E-3	5.19E-3	3.53E-3	2.60E-2
13.2	6.01E-3	9.86E-2	8.70E-2	8.14E-1	9.95E-3	1.17E-3	7.20E-3	4.11E-3	2.31E-2
13.4	5.78E-3	1.10E-1	9.64E-2	8.18E-1	1.28E-2	1.38E-3	6.31E-3	4.83E-3	2.36E-2
13.6	6.68E-3	1.21E-1	1.00E-1	8.10E-1	9.68E-3	1.42E-3	7.20E-3	4.98E-3	1.99E-2
13.8	6.24E-3	1.02E-1	9.09E-2	8.12E-1	1.11E-2	1.62E-3	3.85E-3	5.70E-3	2.19E-2
14.0	5.08E-3	9.27E-2	8.37E-2	8.23E-1	1.48E-2	1.62E-3	6.75E-3	5.70E-3	1.62E-2
14.2	5.56E-3	1.05E-1	8.78E-2	8.28E-1	1.35E-2	2.49E-3	5.41E-3	8.73E-3	1.74E-2

14.4	4.99E-3	1.16E-1	8.74E-2	8.22E-1	1.03E-2	1.54E-3	5.64E-3	5.41E-3	1.69E-2
14.6	4.95E-3	9.77E-2	1.11E-1	8.39E-1	1.00E-2	2.08E-3	4.30E-3	7.28E-3	1.93E-2
14.8	6.39E-3	1.27E-1	9.68E-2	8.25E-1	9.32E-3	1.13E-3	7.65E-3	3.97E-3	2.10E-2
15.0	5.23E-3	1.14E-1	8.69E-2	8.41E-1	9.54E-3	3.90E-4	9.43E-3	1.37E-3	1.73E-2
15.2	5.31E-3	9.30E-2	1.04E-1	8.23E-1	9.39E-3	9.65E-4	6.98E-3	3.39E-3	1.87E-2
15.4	4.82E-3	1.01E-1	1.09E-1	8.29E-1	1.10E-2	1.13E-3	1.08E-2	3.97E-3	1.73E-2
15.6	5.25E-3	1.42E-1	1.24E-1	8.30E-1	1.12E-2	5.96E-4	6.31E-3	2.09E-3	1.76E-2
15.8	5.90E-3	1.11E-1	1.02E-1	8.36E-1	8.98E-3	1.66E-3	1.17E-2	5.84E-3	2.03E-2
16.0	5.28E-3	1.19E-1	1.01E-1	8.42E-1	1.46E-2	1.09E-3	2.96E-3	3.82E-3	1.72E-2
16.2	4.80E-3	1.36E-1	1.17E-1	8.38E-1	1.47E-2	1.13E-3	1.21E-2	3.97E-3	1.50E-2
16.4	5.31E-3	9.63E-2	9.70E-2	8.37E-1	9.98E-3	1.02E-4	1.17E-2	3.59E-4	1.59E-2
16.6	3.96E-3	1.32E-1	9.05E-2	8.37E-1	9.86E-3	1.42E-3	9.43E-3	4.98E-3	1.37E-2
16.8	5.02E-3	1.53E-1	9.76E-2	8.42E-1	9.90E-3	1.54E-3	5.41E-3	5.41E-3	1.71E-2
17.0	4.78E-3	1.01E-1	8.73E-2	8.40E-1	7.77E-3	1.50E-3	4.97E-3	5.26E-3	1.39E-2
17.2	3.73E-3	9.16E-2	1.13E-1	8.39E-1	1.20E-2	1.17E-3	6.53E-3	4.11E-3	1.78E-2
17.4	4.99E-3	9.53E-2	1.07E-1	8.49E-1	1.12E-2	1.79E-3	7.65E-3	6.27E-3	1.31E-2
17.6	2.97E-3	1.01E-1	9.49E-2	8.46E-1	5.65E-3	9.65E-4	1.08E-2	3.39E-3	1.48E-2
17.8	2.84E-3	1.27E-1	1.11E-1	8.56E-1	1.21E-2	5.13E-4	9.43E-3	1.80E-3	1.58E-2
18.0	4.90E-3	1.15E-1	1.13E-1	8.43E-1	1.38E-2	9.65E-4	5.19E-3	3.39E-3	1.54E-2
18.2	4.48E-3	1.35E-1	9.92E-2	8.53E-1	1.03E-2	1.09E-3	8.09E-3	3.82E-3	1.99E-2
18.4	4.06E-3	1.26E-1	1.01E-1	8.51E-1	1.20E-2	1.42E-3	3.63E-3	4.98E-3	1.64E-2
18.6	4.75E-3	1.32E-1	1.11E-1	8.41E-1	1.24E-2	1.05E-3	1.35E-2	3.68E-3	1.87E-2
18.8	2.56E-3	1.23E-1	9.45E-2	8.61E-1	1.11E-2	1.09E-3	2.29E-3	3.82E-3	2.10E-2
19.0	3.04E-3	1.20E-1	9.65E-2	8.62E-1	1.26E-2	8.42E-4	8.76E-3	2.96E-3	1.69E-2
19.2	4.84E-3	1.31E-1	9.40E-2	8.57E-1	9.67E-3	1.34E-3	7.87E-3	4.69E-3	1.62E-2
19.4	3.48E-3	1.11E-1	1.09E-1	8.56E-1	1.11E-2	1.50E-3	4.30E-3	5.26E-3	1.35E-2
19.6	3.32E-3	1.22E-1	1.12E-1	8.69E-1	1.08E-2	1.42E-3	1.08E-2	4.98E-3	1.64E-2
19.8	3.84E-3	1.29E-1	1.02E-1	8.68E-1	6.89E-3	1.62E-3	1.50E-2	5.70E-3	1.79E-2
20.0	5.14E-3	1.26E-1	9.87E-2	8.71E-1	9.92E-3	1.25E-3	1.28E-2	4.40E-3	1.37E-2

Table S8: Experimental intensity-time profiles for the species identified but not quantified at 530 K. The intensities are given in arbitrary units.

t (ms)	C_2H_5 + C_2H_5OO	C_3H_7OO (sum of n- and iso)	CH_3OO	C_3H_7OOH (sum of n- and iso)	hexane isomers	*t* (ms)	C_3H_7
-2.0	-0.091	-0.005	-0.022	0.004	-0.110	-0.20	-0.023
-1.8	-0.106	0.011	-0.022	-0.016	0.194	-0.18	0.001
-1.6	0.333	0.010	-0.022	0.009	0.079	-0.16	-0.023
-1.4	0.251	-0.011	-0.022	-0.011	0.060	-0.14	0.001
-1.2	-0.136	0.022	-0.022	0.010	-0.013	-0.12	0.049
-1.0	0.235	-0.004	0.007	-0.009	0.032	-0.10	-0.023
-0.8	0.140	0.007	-0.022	-0.011	-0.259	-0.08	0.044
-0.6	0.012	-0.001	0.036	0.010	-0.237	-0.06	0.023
-0.4	-0.177	-0.001	-0.022	0.014	-0.028	-0.04	-0.023
-0.2	0.245	-0.003	0.067	-0.029	-0.047	-0.02	0.022
0.0	0.134	0.287	-0.022	0.006	0.453	0.00	-0.023
0.2	-0.083	0.378	0.384	0.021	0.138	0.02	0.002
0.4	0.036	0.456	0.325	0.014	0.008	0.04	-0.003
0.6	0.083	0.496	0.326	0.029	0.073	0.06	0.648
0.8	0.290	0.598	0.306	0.049	0.286	0.08	1.000
1.0	0.226	0.668	0.456	0.069	0.233	0.10	0.841
1.2	0.393	0.713	0.472	0.067	0.095	0.12	0.477
1.4	0.426	0.713	0.616	0.097	0.296	0.14	0.621
1.6	0.397	0.737	0.625	0.087	0.699	0.16	0.280
1.8	0.204	0.770	0.500	0.135	-0.068	0.18	0.174
2.0	0.129	0.812	0.915	0.122	0.117	0.20	0.313
2.2	0.341	0.782	0.620	0.101	0.768	0.22	0.111
2.4	0.326	0.817	0.534	0.122	0.115	0.24	0.118
2.6	0.471	0.825	0.650	0.108	0.429	0.26	0.228
2.8	0.301	0.856	0.504	0.164	0.274	0.28	0.049
3.0	0.342	0.818	0.594	0.188	0.312	0.30	0.090
3.2	0.287	0.821	0.531	0.194	0.343	0.32	0.044
3.4	0.217	0.853	0.646	0.169	0.654	0.34	0.045
3.6	0.375	0.873	0.472	0.174	0.438	0.36	0.041
3.8	0.185	0.830	0.644	0.189	0.093	0.38	-0.003
4.0	0.310	0.824	0.621	0.193	0.809	0.40	0.004
4.2	0.289	0.872	0.589	0.217	0.751	0.42	0.020
4.4	0.585	0.880	0.444	0.255	0.220	0.44	0.096
4.6	0.275	0.872	0.819	0.222	0.351	0.46	-0.023
4.8	0.398	0.890	0.737	0.248	0.263	0.48	0.018
5.0	0.302	0.892	0.761	0.244	0.239	0.50	0.026
5.2	0.338	0.893	0.614	0.199	0.478	0.52	0.042
5.4	0.565	0.869	0.674	0.219	0.363	0.54	-0.023

5.6	0.502	0.903	0.529	0.252	0.630	0.56	-0.023
5.8	0.649	0.899	0.556	0.265	0.231	0.58	0.021
6.0	0.482	0.851	0.673	0.248	0.623	0.60	0.020
6.2	0.589	0.897	0.712	0.252	0.303	0.62	0.094
6.4	0.607	0.905	0.300	0.266	0.695	0.64	0.019
6.6	0.144	0.910	0.528	0.249	0.676	0.66	0.025
6.8	0.299	0.851	0.624	0.265	0.409	0.68	-0.023
7.0	0.399	0.896	0.591	0.267	0.314	0.70	0.000
7.2	0.313	0.924	0.617	0.276	0.055	0.72	-0.023
7.4	0.380	0.885	0.586	0.303	0.406	0.74	-0.023
7.6	0.348	0.903	0.819	0.310	0.505	0.76	0.025
7.8	0.210	0.889	0.588	0.309	0.362	0.78	0.004
8.0	0.349	0.910	0.673	0.312	0.115	0.80	0.026
8.2	0.567	0.885	0.600	0.328	0.481	0.82	-0.023
8.4	0.185	0.908	0.737	0.340	0.508	0.84	-0.002
8.6	0.520	0.875	0.618	0.356	0.387	0.86	-0.023
8.8	0.457	0.922	0.676	0.310	0.612	0.88	-0.002
9.0	0.141	0.896	0.850	0.338	0.433	0.90	0.021
9.2	0.266	0.884	0.793	0.364	0.121	0.92	0.019
9.4	0.655	0.894	0.705	0.429	0.587	0.94	-0.002
9.6	0.169	0.881	0.704	0.400	0.379	0.96	-0.001
9.8	0.264	0.875	0.825	0.426	0.439	0.98	0.048
10.0	0.342	0.886	0.585	0.359	0.385	1.00	0.046
10.2	0.252	0.883	0.560	0.371	0.785	1.02	-0.023
10.4	0.651	0.889	0.531	0.407	0.430	1.04	-0.023
10.6	0.469	0.922	0.648	0.361	0.473	1.06	0.001
10.8	0.303	0.913	0.657	0.382	0.533	1.08	0.003
11.0	0.376	0.957	0.586	0.472	0.178	1.10	0.023
11.2	0.466	0.916	0.739	0.462	0.432	1.12	0.023
11.4	0.547	0.898	0.787	0.427	0.534	1.14	0.023
11.6	0.564	0.919	0.300	0.428	0.470	1.16	-0.003
11.8	0.539	0.905	0.730	0.405	0.411	1.18	0.002
12.0	0.290	0.872	0.732	0.427	0.183	1.20	0.048
12.2	0.310	0.894	0.679	0.428	0.432	1.22	0.049
12.4	0.673	0.908	0.504	0.442	0.328	1.24	-0.023
12.6	0.731	0.931	0.705	0.424	0.503	1.26	-0.023
12.8	0.224	0.905	0.678	0.461	0.443	1.28	-0.002
13.0	0.648	0.926	0.590	0.385	0.296	1.30	-0.023
13.2	0.494	0.938	0.621	0.493	-0.076	1.32	0.026
13.4	0.212	0.956	0.474	0.511	0.279	1.34	0.017
13.6	0.408	0.882	0.645	0.451	0.685	1.36	-0.023
13.8	0.786	0.933	0.849	0.540	-0.150	1.38	-0.023
14.0	0.476	0.911	0.880	0.484	0.145	1.40	-0.023

14.2	0.630	0.911	0.764	0.484	0.207	1.42	-0.023
14.4	0.587	0.926	0.705	0.544	0.402	1.44	-0.023
14.6	0.392	0.933	0.528	0.519	0.745	1.46	0.017
14.8	0.270	0.930	0.618	0.560	0.875	1.48	-0.001
15.0	0.066	0.938	0.827	0.528	0.567	1.50	0.039
15.2	0.551	0.921	0.737	0.502	0.567	1.52	0.041
15.4	0.402	0.912	0.533	0.549	0.310	1.54	0.067
15.6	0.334	0.899	0.943	0.541	0.593	1.56	-0.003
15.8	0.725	0.944	0.701	0.476	0.278	1.58	-0.023
16.0	0.395	0.910	0.760	0.599	0.374	1.60	-0.002
16.2	0.610	0.897	0.760	0.519	0.449	1.62	-0.002
16.4	0.592	0.901	0.763	0.605	0.736	1.64	-0.003
16.6	0.462	0.968	0.938	0.593	0.376	1.66	-0.003
16.8	0.482	0.944	1.000	0.628	0.616	1.68	0.003
17.0	0.301	0.902	0.794	0.591	0.312	1.70	0.025
17.2	0.404	0.935	0.706	0.596	0.511	1.72	0.003
17.4	0.606	0.940	0.678	0.590	0.417	1.74	0.089
17.6	0.356	0.936	0.827	0.616	0.311	1.76	0.097
17.8	0.300	0.927	0.847	0.599	0.517	1.78	0.037
18.0	0.725	0.955	0.706	0.619	0.713	1.80	0.001
18.2	0.580	0.939	0.586	0.670	0.823	1.82	-0.023
18.4	0.544	0.951	0.644	0.605	0.651	1.84	0.003
18.6	1.000	0.942	0.703	0.589	0.424	1.86	-0.002
18.8	0.110	0.929	0.296	0.614	0.596	1.88	-0.023
19.0	0.607	0.931	0.798	0.652	0.298	1.90	-0.003
19.2	0.606	0.940	0.851	0.701	0.525	1.92	0.089
19.4	0.383	0.922	0.851	0.648	0.923	1.94	0.021
19.6	0.107	0.918	0.845	0.640	0.266	1.96	0.042
19.8	0.494	0.893	0.587	0.644	0.539	1.98	0.051
20.0	0.449	0.951	0.730	0.684	0.457	2.00	0.045
20.2	0.590	0.954	0.708	0.660	0.560	2.02	0.029
20.4	0.388	0.973	0.590	0.750	0.463	2.04	0.018
20.6	0.645	0.962	0.703	0.654	0.611	2.06	0.001
20.8	0.721	1.000	0.738	0.713	0.355	2.08	0.002
21.0	0.451	0.942	0.532	0.653	0.313	2.10	-0.023
21.2	0.790	0.917	0.622	0.698	0.548	2.12	-0.023
21.4	0.571	0.952	0.808	0.728	0.777	2.14	0.024
21.6	0.313	0.950	0.655	0.641	0.423	2.16	0.001
21.8	0.606	0.978	0.503	0.732	-0.076	2.18	0.003
22.0	0.599	0.930	0.561	0.701	0.551	2.20	0.064
22.2	0.275	0.941	0.383	0.755	0.429	2.22	0.002
22.4	0.490	0.933	0.732	0.737	0.858	2.24	-0.023
22.6	0.470	0.978	0.910	0.828	0.463	2.26	0.000

22.8	0.574	0.980	0.674	0.683	0.701	2.28	-0.003
23.0	0.391	0.948	0.677	0.754	0.972	2.30	0.004
23.2	0.407	0.983	0.759	0.733	0.626	2.32	0.037
23.4	0.334	0.928	0.821	0.699	0.347	2.34	0.020
23.6	0.496	0.935	0.904	0.770	0.839	2.36	0.000
23.8	0.835	0.949	0.912	0.740	0.341	2.38	0.069
24.0	0.679	0.959	0.558	0.749	0.509	2.40	-0.001
24.2	0.281	0.970	0.708	0.851	0.500	2.42	0.000
24.4	0.584	0.938	0.796	0.785	0.673	2.44	0.023
24.6	0.403	0.919	0.621	0.773	0.615	2.46	-0.003
24.8	0.657	0.978	0.767	0.776	0.667	2.48	0.002
25.0	0.710	0.952	0.919	0.860	0.298	2.50	0.004
25.2	0.352	0.924	0.421	0.851	0.865	2.52	0.018
25.4	0.316	0.932	0.446	0.811	0.794	2.54	0.045
25.6	0.859	0.945	0.620	0.870	0.485	2.56	-0.023
25.8	0.218	0.939	0.942	0.817	0.308	2.58	0.039
26.0	0.456	0.942	0.673	0.832	0.484	2.60	-0.023
26.2	0.715	0.931	0.930	0.852	0.791	2.62	0.023
26.4	0.259	0.995	0.470	0.787	0.774	2.64	-0.023
26.6	0.637	0.972	0.530	0.764	0.319	2.66	-0.002
26.8	0.319	0.975	0.386	0.821	0.669	2.68	0.003
27.0	0.449	0.926	0.740	0.822	0.161	2.70	0.027
27.2	0.574	0.955	0.821	0.854	0.259	2.72	-0.001
27.4	0.721	0.936	0.559	0.855	0.339	2.74	-0.023
27.6	0.766	0.918	0.650	0.806	0.130	2.76	0.028
27.8	0.495	0.943	0.558	0.895	0.619	2.78	0.049
28.0	0.585	0.936	0.646	0.895	0.684	2.80	-0.023
28.2	0.728	0.940	0.769	0.870	0.627	2.82	0.022
28.4	0.773	0.985	0.555	0.817	0.460	2.84	-0.003
28.6	0.872	0.976	0.789	0.840	0.343	2.86	0.044
28.8	0.763	0.933	0.764	0.897	0.194	2.88	0.022
29.0	0.907	0.945	0.679	0.929	0.262	2.90	0.020
29.2	0.586	0.960	0.615	1.000	0.473	2.92	0.066
29.4	0.711	0.961	0.530	0.895	0.474	2.94	-0.023
29.6	0.674	0.946	0.885	0.900	1.000	2.96	-0.003
29.8	0.637	0.939	0.737	0.832	0.839	2.98	-0.003
30.0	0.648	0.965	0.877	0.853	0.481	3.00	0.019

Table S9: Experimental intensity-time profiles for the species identified but not quantified at 600 K. The intensities are given in arbitrary units.

t (ms)	C_2H_5 + C_2H_5OO	C_3H_7OO (sum of n- and iso-)	CH_3OO	$C3H_7OOH$ (sum of n- and iso-)	hexane isomers	*t* (ms)	C_3H_7
-2.0	0.060	-0.074	-0.018	0.000	0.073	-0.20	0.010
-1.8	-0.061	0.045	-0.018	-0.023	-0.081	-0.18	-0.021
-1.6	0.152	0.029	-0.018	-0.001	-0.046	-0.16	0.006
-1.4	0.042	0.019	-0.018	-0.029	0.018	-0.14	0.008
-1.2	-0.139	-0.004	-0.018	0.014	-0.063	-0.12	-0.021
-1.0	-0.204	-0.004	0.025	-0.002	-0.002	-0.10	0.035
-0.8	-0.064	-0.026	-0.018	0.002	-0.049	-0.08	0.004
-0.6	0.174	0.043	-0.018	-0.010	0.046	-0.06	-0.021
-0.4	0.152	0.000	0.026	0.017	-0.029	-0.04	-0.021
-0.2	-0.322	0.004	-0.018	0.001	-0.001	-0.02	0.005
0.0	0.241	0.551	0.025	-0.023	0.005	0.00	0.032
0.2	0.304	0.600	0.383	0.009	0.065	0.02	-0.021
0.4	0.405	0.588	0.464	0.020	0.049	0.04	-0.021
0.6	0.310	0.625	0.682	0.070	0.166	0.06	0.342
0.8	0.295	0.721	0.620	0.096	0.329	0.08	0.867
1.0	0.153	0.753	0.246	0.098	0.496	0.10	0.919
1.2	0.327	0.811	0.203	0.119	0.306	0.12	0.831
1.4	0.189	0.853	0.506	0.157	0.264	0.14	0.806
1.6	0.210	0.903	0.954	0.203	0.454	0.16	1.000
1.8	0.223	0.919	0.685	0.186	0.274	0.18	0.745
2.0	0.317	0.913	0.466	0.258	0.780	0.20	0.536
2.2	0.135	0.912	0.732	0.224	0.429	0.22	0.378
2.4	0.148	0.962	0.552	0.249	0.663	0.24	0.271
2.6	0.502	0.886	0.782	0.261	0.626	0.26	0.296
2.8	0.322	0.936	0.857	0.293	0.696	0.28	0.242
3.0	0.337	0.957	0.467	0.314	0.554	0.30	0.162
3.2	0.393	0.954	0.331	0.316	0.393	0.32	0.289
3.4	0.297	0.918	0.386	0.343	0.462	0.34	0.117
3.6	0.414	0.951	0.901	0.281	0.488	0.36	0.244
3.8	0.629	0.943	0.952	0.347	0.608	0.38	0.136
4.0	0.387	0.936	0.734	0.342	0.420	0.40	0.144
4.2	0.475	0.922	0.511	0.321	0.624	0.42	-0.021
4.4	0.274	0.958	0.686	0.356	0.445	0.44	0.098
4.6	0.182	0.938	0.604	0.343	0.298	0.46	0.112
4.8	0.177	0.999	0.644	0.364	0.587	0.48	0.033
5.0	-0.018	0.908	0.287	0.400	0.249	0.50	-0.021
5.2	0.234	0.971	0.603	0.384	0.764	0.52	0.028
5.4	0.066	0.985	0.508	0.391	0.286	0.54	0.172

5.6	0.386	0.947	0.725	0.405	0.435	0.56	0.026
5.8	0.375	0.884	0.685	0.384	0.361	0.58	0.028
6.0	0.273	0.956	0.768	0.460	0.607	0.60	0.092
6.2	0.383	0.944	0.726	0.443	0.097	0.62	0.059
6.4	0.098	0.928	0.775	0.436	0.190	0.64	0.002
6.6	0.363	0.967	0.648	0.428	0.651	0.66	0.075
6.8	0.538	0.903	0.815	0.424	0.435	0.68	0.081
7.0	0.224	0.977	0.950	0.445	0.618	0.70	0.055
7.2	0.447	0.960	0.556	0.518	0.376	0.72	0.011
7.4	0.280	1.000	0.600	0.480	0.520	0.74	0.009
7.6	0.236	0.882	0.379	0.497	0.246	0.76	0.064
7.8	-0.039	0.923	0.863	0.488	0.462	0.78	0.010
8.0	0.174	0.884	0.464	0.506	0.400	0.80	0.054
8.2	0.546	0.943	0.506	0.490	0.527	0.82	0.113
8.4	0.348	0.901	0.794	0.502	0.649	0.84	-0.021
8.6	0.399	0.947	0.732	0.494	0.678	0.86	0.032
8.8	0.475	0.959	1.000	0.478	0.346	0.88	0.062
9.0	0.127	0.947	0.510	0.472	0.534	0.90	-0.021
9.2	1.000	0.933	0.561	0.526	0.684	0.92	0.082
9.4	0.457	0.889	0.420	0.473	0.265	0.94	0.028
9.6	0.253	0.854	0.801	0.552	0.743	0.96	-0.021
9.8	0.373	0.920	0.748	0.574	0.317	0.98	0.061
10.0	0.608	0.863	0.506	0.643	0.581	1.00	0.002
10.2	0.470	0.830	0.605	0.585	0.572	1.02	0.010
10.4	0.281	0.897	0.466	0.602	0.686	1.04	0.062
10.6	0.534	0.934	0.644	0.606	0.655	1.06	-0.021
10.8	0.563	0.920	0.378	0.570	0.507	1.08	0.033
11.0	0.417	0.854	0.552	0.551	0.978	1.10	0.055
11.2	0.344	0.889	0.523	0.618	0.227	1.12	0.086
11.4	0.164	0.892	0.512	0.582	0.415	1.14	0.057
11.6	0.343	0.883	0.866	0.581	0.335	1.16	-0.021
11.8	0.159	0.857	0.727	0.576	0.459	1.18	0.003
12.0	0.377	0.808	0.467	0.557	0.444	1.20	0.011
12.2	0.685	0.907	0.421	0.624	0.768	1.22	0.061
12.4	0.608	0.962	0.335	0.687	0.361	1.24	0.002
12.6	0.521	0.842	0.650	0.650	0.435	1.26	0.003
12.8	0.429	0.866	0.739	0.672	0.673	1.28	0.036
13.0	0.237	0.810	0.728	0.655	0.642	1.30	0.057
13.2	0.563	0.835	0.651	0.618	0.791	1.32	0.088
13.4	0.422	0.811	0.858	0.627	0.432	1.34	-0.021
13.6	0.346	0.886	0.993	0.684	0.934	1.36	0.004
13.8	0.523	0.815	0.552	0.642	0.476	1.38	0.057
14.0	0.280	0.840	0.338	0.677	0.380	1.40	0.026

14.2	0.672	0.764	0.685	0.683	0.713	1.42	0.026
14.4	0.297	0.865	0.430	0.644	0.330	1.44	0.037
14.6	0.461	0.832	0.725	0.624	0.635	1.46	0.027
14.8	0.356	0.811	0.551	0.680	0.532	1.48	0.011
15.0	0.576	0.805	0.729	0.703	0.596	1.50	0.004
15.2	0.124	0.856	0.815	0.702	0.530	1.52	0.005
15.4	0.316	0.779	0.814	0.620	0.689	1.54	0.058
15.6	0.069	0.868	0.653	0.668	0.821	1.56	0.005
15.8	0.692	0.832	0.685	0.743	0.739	1.58	0.054
16.0	-0.095	0.873	0.551	0.768	0.778	1.60	0.036
16.2	0.370	0.825	0.420	0.764	0.583	1.62	0.026
16.4	0.352	0.766	0.641	0.734	0.368	1.64	0.030
16.6	0.768	0.790	0.735	0.805	0.686	1.66	0.088
16.8	0.440	0.855	0.289	0.690	0.461	1.68	0.006
17.0	0.597	0.857	0.508	0.717	0.491	1.70	0.010
17.2	0.097	0.759	0.554	0.803	0.793	1.72	0.055
17.4	0.316	0.725	0.595	0.649	0.394	1.74	0.035
17.6	0.373	0.785	0.549	0.766	0.656	1.76	0.028
17.8	0.411	0.825	0.553	0.751	0.791	1.78	0.038
18.0	0.782	0.754	0.511	0.767	0.440	1.80	0.032
18.2	0.479	0.738	0.562	0.725	0.639	1.82	0.034
18.4	0.719	0.696	0.287	0.765	0.694	1.84	0.007
18.6	0.393	0.825	0.552	0.781	0.667	1.86	0.004
18.8	0.565	0.750	0.420	0.765	0.457	1.88	0.004
19.0	0.284	0.771	0.377	0.761	0.612	1.90	0.010
19.2	0.256	0.777	0.114	0.772	0.569	1.92	0.009
19.4	0.252	0.804	0.651	0.821	0.420	1.94	0.107
19.6	0.321	0.747	0.291	0.831	0.508	1.96	0.008
19.8	0.600	0.809	0.554	0.802	0.715	1.98	0.129
20.0	0.570	0.787	0.417	0.812	0.893	2.00	0.011
20.2	0.802	0.693	0.420	0.806	0.644	2.02	0.006
20.4	0.530	0.713	0.464	0.810	0.582	2.04	-0.021
20.6	0.411	0.818	0.507	0.840	0.714	2.06	0.065
20.8	0.591	0.683	0.732	0.851	0.338	2.08	0.123
21.0	0.825	0.702	0.421	0.794	0.520	2.10	0.053
21.2	0.585	0.721	0.422	0.800	0.582	2.12	-0.021
21.4	0.190	0.692	0.248	0.858	0.737	2.14	0.003
21.6	0.482	0.818	0.381	0.774	0.414	2.16	-0.021
21.8	0.064	0.717	0.377	0.810	0.841	2.18	0.109
22.0	0.571	0.792	0.380	0.780	0.821	2.20	-0.021
22.2	0.298	0.741	0.596	0.825	0.831	2.22	0.009
22.4	0.537	0.744	0.337	0.831	0.657	2.24	0.059
22.6	0.357	0.727	0.419	0.851	0.471	2.26	0.063

22.8	0.720	0.725	0.686	0.862	0.648	2.28	-0.021
23.0	0.260	0.666	0.686	0.802	0.661	2.30	0.009
23.2	0.465	0.671	0.333	0.864	0.731	2.32	-0.021
23.4	0.437	0.709	0.378	0.851	0.667	2.34	0.063
23.6	0.055	0.740	0.743	0.889	0.807	2.36	0.032
23.8	0.364	0.675	0.331	0.851	0.608	2.38	-0.021
24.0	0.497	0.769	0.555	0.796	0.275	2.40	-0.021
24.2	0.332	0.731	0.640	0.853	0.509	2.42	-0.021
24.4	0.445	0.737	0.465	0.844	0.628	2.44	0.054
24.6	0.462	0.727	0.376	0.873	0.570	2.46	0.056
24.8	0.303	0.713	0.375	0.875	0.466	2.48	0.086
25.0	0.507	0.681	0.383	0.880	0.531	2.50	-0.021
25.2	0.667	0.668	0.156	0.911	0.785	2.52	0.029
25.4	0.228	0.668	0.429	0.883	1.000	2.54	0.004
25.6	0.362	0.680	0.424	0.931	0.504	2.56	0.009
25.8	0.360	0.674	0.294	0.944	0.409	2.58	0.002
26.0	0.457	0.704	0.381	0.921	0.394	2.60	0.033
26.2	0.213	0.620	0.463	0.887	0.889	2.62	0.033
26.4	0.133	0.672	0.395	0.890	0.845	2.64	0.087
26.6	0.499	0.638	0.515	0.966	0.699	2.66	-0.021
26.8	0.543	0.701	0.292	0.890	0.496	2.68	0.066
27.0	0.530	0.695	0.335	0.882	0.695	2.70	0.006
27.2	0.378	0.687	0.470	0.913	0.552	2.72	0.005
27.4	0.296	0.703	0.488	0.899	0.481	2.74	-0.021
27.6	0.525	0.735	0.245	0.919	0.730	2.76	0.004
27.8	0.494	0.648	0.294	1.000	0.418	2.78	0.029
28.0	0.576	0.636	0.518	0.915	0.523	2.80	0.005
28.2	0.787	0.614	0.506	0.924	0.396	2.82	-0.021
28.4	0.873	0.635	0.378	0.967	0.598	2.84	-0.021
28.6	0.412	0.675	0.331	0.953	0.762	2.86	0.028
28.8	0.313	0.651	0.418	0.913	0.545	2.88	-0.021
29.0	0.261	0.660	0.508	0.942	0.705	2.90	0.005
29.2	0.525	0.696	0.505	0.947	0.432	2.92	0.010
29.4	0.480	0.716	0.463	0.951	0.753	2.94	0.008
29.6	0.538	0.607	0.464	0.978	0.540	2.96	0.129
29.8	0.459	0.634	0.207	0.903	0.711	2.98	0.064
30.0	0.745	0.672	0.200	0.970	0.394	3.00	0.034

Table S10: Experimental intensity-time profiles for the species identified but not quantified at 670 K. The intensities are given in arbitrary units.

t (ms)	C_2H_5 + C_2H_5OO	C_3H_7OO (sum of n- and iso-)	CH_3OO	C_3H_7OOH (sum of n- and iso-)	hexane isomers	*t* (ms)	C_3H_7
-2.0	0.445	-0.076	-0.012	0.015	0.059	-0.20	0.006
-1.8	0.137	-0.013	-0.012	-0.028	-0.035	-0.18	-0.014
-1.6	0.342	0.110	0.095	0.023	-0.117	-0.16	-0.014
-1.4	-0.477	0.041	0.098	0.027	0.028	-0.14	0.011
-1.2	-0.034	0.005	-0.012	-0.035	-0.049	-0.12	0.004
-1.0	0.063	-0.033	-0.012	-0.043	-0.150	-0.10	0.005
-0.8	-0.010	-0.047	-0.012	-0.011	-0.124	-0.08	-0.014
-0.6	0.051	0.017	-0.012	0.025	-0.033	-0.06	-0.014
-0.4	0.216	0.057	0.095	-0.029	-0.079	-0.04	0.029
-0.2	-0.219	0.053	-0.012	-0.004	0.116	-0.02	-0.014
0.0	-0.056	0.675	-0.012	-0.058	0.054	0.00	-0.014
0.2	0.067	1.000	0.095	0.059	0.067	0.02	0.008
0.4	0.561	0.782	0.590	0.091	0.123	0.04	-0.014
0.6	0.664	0.720	0.789	0.141	0.106	0.06	0.448
0.8	0.505	0.760	0.995	0.294	0.335	0.08	0.711
1.0	0.683	0.733	0.720	0.414	0.387	0.10	0.778
1.2	-0.033	0.836	1.000	0.498	0.458	0.12	0.721
1.4	0.652	0.749	0.789	0.607	0.484	0.14	1.000
1.6	0.526	0.677	0.390	0.646	0.536	0.16	0.744
1.8	0.163	0.668	0.890	0.581	0.380	0.18	0.437
2.0	0.086	0.561	0.589	0.770	0.509	0.20	0.816
2.2	0.066	0.582	0.789	0.815	0.609	0.22	0.922
2.4	0.396	0.629	0.192	0.708	0.646	0.24	0.677
2.6	0.484	0.570	0.487	0.852	0.466	0.26	0.568
2.8	0.074	0.454	0.686	1.000	0.542	0.28	0.673
3.0	0.074	0.560	0.188	0.799	0.729	0.30	0.397
3.2	0.184	0.385	0.696	0.676	0.607	0.32	0.410
3.4	0.388	0.484	0.390	0.926	0.541	0.34	0.437
3.6	0.550	0.496	0.397	0.856	0.594	0.36	0.320
3.8	0.626	0.417	0.088	0.899	0.521	0.38	0.045
4.0	0.181	0.498	0.499	0.906	0.699	0.40	0.218
4.2	0.380	0.332	0.711	0.964	0.526	0.42	0.312
4.4	-0.165	0.491	0.391	0.903	0.572	0.44	0.200
4.6	0.371	0.342	0.389	0.959	0.530	0.46	0.213
4.8	1.000	0.305	0.591	0.920	0.627	0.48	0.212
5.0	0.411	0.423	0.200	0.850	0.655	0.50	0.067
5.2	0.742	0.269	0.587	0.863	0.519	0.52	0.283
5.4	0.002	0.358	0.391	0.872	0.613	0.54	0.263

5.6	0.432	0.316	-0.012	0.881	0.564	0.56	0.121
5.8	0.465	0.243	-0.012	0.983	0.749	0.58	0.219
6.0	0.364	0.283	0.388	0.826	0.689	0.60	0.157
6.2	0.095	0.268	0.195	0.857	0.582	0.62	0.110
6.4	-0.028	0.213	0.394	0.793	0.610	0.64	0.109
6.6	0.080	0.202	0.290	0.887	0.723	0.66	0.148
6.8	0.262	0.186	0.110	0.870	0.482	0.68	0.129
7.0	0.453	0.305	0.596	0.795	0.698	0.70	0.199
7.2	0.275	0.122	0.189	0.676	0.681	0.72	0.169
7.4	0.324	0.199	0.491	0.663	0.788	0.74	0.079
7.6	0.101	0.153	0.187	0.666	0.652	0.76	0.287
7.8	-0.052	0.103	0.088	0.692	0.566	0.78	0.063
8.0	0.016	0.151	0.088	0.720	0.605	0.80	0.273
8.2	0.278	0.274	0.487	0.754	0.582	0.82	0.233
8.4	0.565	0.276	0.188	0.734	0.786	0.84	0.182
8.6	0.353	0.271	0.390	0.671	0.797	0.86	0.069
8.8	0.035	0.213	0.291	0.650	0.914	0.88	0.074
9.0	0.300	0.136	-0.012	0.707	0.577	0.90	0.129
9.2	0.895	0.096	0.089	0.737	0.532	0.92	0.188
9.4	0.090	0.190	0.290	0.813	0.559	0.94	0.124
9.6	0.142	0.071	0.287	0.595	0.480	0.96	0.127
9.8	0.236	0.241	0.188	0.674	0.573	0.98	0.157
10.0	-0.240	0.240	0.288	0.682	0.595	1.00	0.047
10.2	0.562	0.236	0.089	0.575	0.795	1.02	0.207
10.4	0.046	0.145	-0.012	0.614	0.806	1.04	0.139
10.6	0.143	-0.041	0.189	0.541	0.680	1.06	0.090
10.8	0.622	0.151	0.088	0.739	0.775	1.08	0.138
11.0	-0.119	0.101	-0.012	0.561	0.999	1.10	0.056
11.2	0.324	0.191	-0.012	0.732	0.718	1.12	0.052
11.4	-0.246	0.150	0.088	0.636	0.717	1.14	0.096
11.6	-0.064	0.073	0.192	0.566	0.865	1.16	0.132
11.8	0.060	0.119	0.298	0.669	0.611	1.18	0.152
12.0	0.313	0.110	0.092	0.577	0.600	1.20	0.076
12.2	0.707	0.090	-0.012	0.658	0.731	1.22	0.117
12.4	0.297	-0.031	0.088	0.617	0.592	1.24	0.094
12.6	-0.065	0.154	0.088	0.525	0.802	1.26	0.164
12.8	0.670	0.065	-0.012	0.633	0.589	1.28	0.106
13.0	0.070	0.219	-0.012	0.654	0.627	1.30	0.114
13.2	0.233	0.202	0.088	0.611	0.772	1.32	0.098
13.4	0.156	0.203	0.516	0.699	0.662	1.34	0.092
13.6	-0.081	0.055	0.088	0.569	0.771	1.36	0.116
13.8	0.530	0.080	0.088	0.583	0.676	1.38	0.041
14.0	0.368	0.081	-0.012	0.500	0.760	1.40	0.204

14.2	0.442	0.176	0.287	0.492	0.732	1.42	0.045
14.4	-0.016	0.092	0.088	0.618	0.622	1.44	0.166
14.6	0.648	0.049	-0.012	0.617	0.643	1.46	0.087
14.8	0.412	0.032	0.088	0.513	0.677	1.48	0.114
15.0	0.240	0.041	-0.012	0.454	0.715	1.50	0.108
15.2	0.268	0.147	0.092	0.474	0.722	1.52	0.129
15.4	0.499	0.036	0.089	0.604	0.551	1.54	0.068
15.6	0.222	0.171	0.088	0.482	0.779	1.56	0.051
15.8	-0.048	0.067	0.188	0.545	0.648	1.58	0.048
16.0	0.343	0.172	-0.012	0.529	0.652	1.60	0.144
16.2	0.086	0.089	0.288	0.538	0.738	1.62	0.130
16.4	0.566	0.039	0.088	0.534	0.736	1.64	0.073
16.6	0.600	-0.048	0.287	0.511	0.688	1.66	0.029
16.8	0.063	0.078	0.088	0.440	0.587	1.68	0.075
17.0	0.241	0.029	0.089	0.546	1.000	1.70	0.047
17.2	0.277	0.125	-0.012	0.508	0.745	1.72	0.024
17.4	0.440	-0.068	0.114	0.554	0.641	1.74	0.089
17.6	0.075	-0.043	-0.012	0.483	0.763	1.76	0.028
17.8	-0.166	0.075	-0.012	0.428	0.743	1.78	0.079
18.0	-0.134	0.090	0.088	0.402	0.725	1.80	0.112
18.2	0.515	0.144	-0.012	0.484	0.694	1.82	0.115
18.4	-0.251	0.041	0.088	0.452	0.685	1.84	0.043
18.6	-0.534	0.039	0.187	0.332	0.823	1.86	0.064
18.8	0.318	0.127	0.088	0.296	0.781	1.88	0.074
19.0	0.237	0.130	0.088	0.423	0.705	1.90	0.074
19.2	0.164	0.073	-0.012	0.438	0.716	1.92	0.063
19.4	0.251	0.048	0.088	0.470	0.808	1.94	0.139
19.6	0.525	0.092	0.092	0.484	0.812	1.96	0.043
19.8	0.258	-0.002	-0.012	0.417	0.610	1.98	0.114
20.0	0.301	0.095	0.088	0.453	0.746	2.00	0.032

Table S11. Selected set of reactions responsible for the production of experimentally measured secondary products.[a]

				$k(T)$[c]		
	A[b]	n	E_a	530	600	670
Selected C_3H_7 formation reactions						
$Cl + C_3H_8 = HCl + n\text{-}C_3H_7$	8.82E-11	0.00	1.02E+02	7.27E-11	7.43E-11	7.57E-11
$Cl + C_3H_8 = HCl + i\text{-}C_3H_7$	6.33E-11	0.00	-6.39E+01	7.14E-11	7.04E-11	6.96E-11
$OH + C_3H_8 = H_2O + n\text{-}C_3H_7$	1.79E-14	0.97	8.09E+02	1.73E-12	2.33E-12	2.99E-12
$OH + C_3H_8 = H_2O + i\text{-}C_3H_7$	8.00E-17	1.61	-3.52E+00	1.98E-12	2.42E-12	2.89E-12
Selected R + RO_2 reactions						
$n\text{-}C_3H_7O_2 + n\text{-}C_3H_7 = n\text{-}C_3H_7O + n\text{-}C_3H_7O$	1.25E-11	0.00	-5.03E+02	3.23E-11	2.89E-11	2.65E-11
$n\text{-}C_3H_7O_2 + i\text{-}C_3H_7 = n\text{-}C_3H_7O + i\text{-}C_3H_7O$	1.16E-11	0.00	-5.03E+02	2.99E-11	2.68E-11	2.45E-11
$i\text{-}C_3H_7O_2 + n\text{-}C_3H_7 = i\text{-}C_3H_7O + n\text{-}C_3H_7O$	1.12E-11	0.00	-5.03E+02	2.90E-11	2.59E-11	2.38E-11
$i\text{-}C_3H_7O_2 + i\text{-}C_3H_7 = i\text{-}C_3H_7O + i\text{-}C_3H_7O$	1.12E-11	0.00	-5.03E+02	2.88E-11	2.58E-11	2.37E-11
$n\text{-}C_3H_7O_2 + C_2H_5 = n\text{-}C_3H_7O + C_2H_5O$	1.16E-11	0.00	-5.03E+02	3.00E-11	2.69E-11	2.46E-11
$i\text{-}C_3H_7O_2 + C_2H_5 = i\text{-}C_3H_7O + C_2H_5O$	1.16E-11	0.00	-5.03E+02	3.00E-11	2.69E-11	2.46E-11
$n\text{-}C_3H_7O_2 + CH_3 = n\text{-}C_3H_7O + CH_3O$	1.16E-11	0.00	-5.03E+02	3.00E-11	2.68E-11	2.46E-11
$i\text{-}C_3H_7O_2 + CH_3 = i\text{-}C_3H_7O + CH_3O$	1.17E-11	0.00	-5.03E+02	3.03E-11	2.71E-11	2.48E-11
$n\text{-}C_3H_7 + HO_2 = n\text{-}C_3H_7O + OH$	6.28E-08	-1.18	5.78E+01	3.48E-11	3.04E-11	2.70E-11
$i\text{-}C_3H_7 + HO_2 = i\text{-}C_3H_7O + OH$	3.17E-07	-1.46	1.09E+02	2.79E-11	2.39E-11	2.07E-11
$C_2H_5 + HO_2 = C_2H_5O + OH$	5.48E-09	-0.85	-1.15E+01	2.80E-11	2.51E-11	2.28E-11
$CH_3 + HO_2 = CH_3O + OH$	2.62E-12	0.27	-3.46E+02	2.74E-11	2.63E-11	2.55E-11
$CH_3 + HO_2 = CH_4 + O_2$	1.98E-19	2.23	-1.52E+03	4.14E-12	3.91E-12	3.84E-12
$HO_2 + OH = H_2O + O_2$	3.20E-04	-2.49	2.94E+02			
	2.01E-15	1.24	-6.58E+02	4.72E-11	4.07E-11	3.62E-11
$HO_2 + H = OH + OH$	1.11E-11	0.29	-6.35E+01	7.93E-11	8.11E-11	8.29E-11
$HO_2 + H = H_2 + O_2$	1.86E-17	1.94	-3.24E+02	6.66E-12	7.88E-12	9.23E-12
$HO_2 + Cl = ClO + OH$	4.10E-11	0.00	4.50E+02	1.75E-11	1.94E-11	2.10E-11
Selected RO_2 + RO_2 reactions						
$n\text{-}C_3H_7O_2 + n\text{-}C_3H_7O_2 =$ propanal + n-propanol + O_2	2.36E-08	-1.61	9.36E+02	1.66E-13	1.67E-13	1.64E-13
$n\text{-}C_3H_7O_2 + i\text{-}C_3H_7O_2 =$ propanal + i-propanol + O_2	2.34E-08	-1.61	9.36E+02	1.65E-13	1.66E-13	1.63E-13
$i\text{-}C_3H_7O_2 + n\text{-}C_3H_7O_2 =$ acetone + n-propanol + O_2	2.34E-08	-1.61	9.36E+02	1.65E-13	1.66E-13	1.63E-13
$i\text{-}C_3H_7O_2 + i\text{-}C_3H_7O_2 =$ acetone + i-propanol + O_2	2.34E-08	-1.61	9.36E+02	1.65E-13	1.66E-13	1.63E-13
$n\text{-}C_3H_7O_2 + n\text{-}C_3H_7O_2 = n\text{-}C_3H_7O + n\text{-}C_3H_7O + O_2$	2.34E-08	-1.61	9.36E+02	1.65E-13	1.66E-13	1.63E-13
$n\text{-}C_3H_7O_2 + i\text{-}C_3H_7O_2 = n\text{-}C_3H_7O + i\text{-}C_3H_7O + O_2$	2.41E-08	-1.61	9.36E+02	1.69E-13	1.70E-13	1.68E-13
$i\text{-}C_3H_7O_2 + i\text{-}C_3H_7O_2 = i\text{-}C_3H_7O + i\text{-}C_3H_7O + O_2$	2.46E-08	-1.61	9.36E+02	1.73E-13	1.74E-13	1.71E-13
$n\text{-}C_3H_7O_2 + C_5H_5O_2 = n\text{-}C_3H_7O + C_2H_5O + O_2$	2.32E-08	-1.61	9.36E+02	1.63E-13	1.64E-13	1.62E-13
$i\text{-}C_3H_7O_2 + C_5H_5O_2 = i\text{-}C_3H_7O + C_2H_5O + O_2$	2.32E-08	-1.61	9.36E+02	1.63E-13	1.64E-13	1.62E-13
$n\text{-}C_3H_7O_2 + HO_2 = n\text{-}C_3H_7OOH + O_2$	1.01E-12	0.00	-7.02E+02	3.80E-12	3.26E-12	2.88E-12
$i\text{-}C_3H_7O_2 + HO_2 = i\text{-}C_3H_7OOH + O_2$	8.04E-13	0.00	-7.02E+02	3.02E-12	2.59E-12	2.29E-12
$C_2H_5O_2 + HO_2 = C_2H_5OOH + O_2$	2.91E-14	0.00	-1.65E+03	6.51E-13	4.53E-13	3.40E-13
$HO_2 + HO_2 = HOOH + O_2$	1.43E-21	2.72	-1.81E+03	1.09E-12	1.03E-12	1.01E-12

Selected peroxide decomposition reactions						
n-$C_3H_7OOH = n$-$C_3H_7O + OH$	3.80E+21	-2.00	2.24E+04	5.61E-03	6.12E-01	2.44E+01
i-$C_3H_7OOH = i$-$C_3H_7O + OH$	1.65E+22	-2.34	2.34E+04	4.73E-04	6.13E-02	2.79E+00
$OCHCH_2CH_2OOH = OCHCH_2CH_2O + OH$	3.41E+64	-15.90	2.81E+04	1.66E-02	1.12E+00	2.56E+01
$C_2H_5OOH = C_2H_5O + OH$	6.31E+14	0.00	2.13E+04	2.27E-03	2.46E-01	1.00E+01
$HOOH = OH + OH$				8.94E-10	1.48E-07	7.91E-06
Selected oxy radical consumption reactions						
n-$C_3H_7O = C_2H_5 + CH_2O$	1.22E+32	-7.45	8.56E+03	6.02E+04	1.57E+05	3.06E+05
i-$C_3H_7O = CH_3CHO + CH_3$	1.76E+31	-7.20	8.25E+03	7.37E+04	1.86E+05	3.53E+05
$OCHCH_2CH_2O = vinoxy + CH_2O$	4.94E+10	0.86	2.92E+03	4.37E+10	9.26E+10	1.69E+11
$CH_3CH_2O = CH_3 + CH_2O$	1.35E+38	-6.96	1.20E+04	2.26E+09	1.33E+10	4.98E+10
$CH_3O = CH_2O + H$				1.76E+00	1.49E+01	7.44E+01
$vinoxy + O_2 = CH_2O + CO + OH$	3.32E-11	0.00	2.11E+03	6.16E-13	9.80E-13	1.42E-12
$CH_3O + O_2 = CH_2O + HO_2$	1.05E-13	0.00	1.31E+03	8.86E-15	1.18E-14	1.48E-14
Selected R + O_2 reactions for R = H, CH_3, and C_2H_5						
$C_2H_5 + O_2 = C_2H_5O_2$				1.87E-13	9.96E-14	5.61E-14
$C_2H_5 + O_2 = C_2H_4 + HO_2$	2.34E-17	1.09	-9.94E+02	1.42E-13	1.31E-13	1.24E-13
$C_2H_5O_2 = C_2H_4 + HO_2$				1.46E-01	2.48E+00	1.99E+01
$CH_3 + O_2 = CH_3O_2$				6.65E-15	4.19E-15	2.76E-15
$H + O_2 = HO_2$				8.64E-16	6.71E-16	5.32E-16
Selected additional C_3H_7 consumption reactions						
n-$C_3H_7 = CH_3 + C_2H_4$				5.28E-01	9.20E+00	7.61E+01
$Cl + n$-$C_3H_7 = HCl + propene$	5.28E-10	0.00	2.90E+02	3.06E-10	3.26E-10	3.43E-10
$Cl + i$-$C_3H_7 = HCl + propene$	7.57E-10	0.00	2.90E+02	4.38E-10	4.67E-10	4.91E-10

[a] The selected reactions presented above constitute a small subset of the overall kinetic model. However, model predictions that include only these secondary reactions are identical to those using the full model for the measured secondary products.

[b] A, n, and E_a are Arrhenius parameters in $k = AT^n\exp(-E_a/T)$ with A in units of $cm^3\ s^{-1}$ for bimolecular reactions and s^{-1} for unimolecular reactions and E_a in units of K.

[c] $k(T)$ in units of $cm^3\ s^{-1}$ for bimolecular reactions and s^{-1} for unimolecular reactions at the temperatures listed in K. Rate constants for pressure-dependent reactions are evaluated at 4 Torr.

References

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